



The Alliance of Laboratories in Europe for
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ALERT Doctoral School 2020

Point based numerical methods in geomechanics

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Preface

The ALERT Doctoral School 2020 on “Point based numerical methods in geomechanics” has been initially foreseen to take place as usual in Aussois. But due to the COVID-19 pandemic developing since early 2020, and after careful consideration, the Bureau and the BoD finally decided to cancel the ALERT workshop in 2020 but not the Doctoral School, the PhD Prize as well as the Invited Lecture.

Hopefully, the two organizers of the school, Pr. Manolo Pastor (Universidad Politécnica de Madrid) and Pr. Wei Wu (BOKU Vienna), accepted immediately to set up the first doctoral E-School of our ALERT network. I sincerely thank the organizers and all the contributors to the school for their effort! The organizers of the school decided to cover the following methods like SPH, MPM, PFEM or LBM-DEM. The underlying theory will of course be described, but the authors will also focus on the applications of these methods in geomechanics. A special emphasis is proposed on fast granular flow, fast landslides or snow avalanches. The fundamental coupling between the solid and the fluid phase will be also tackled in the frame of particle based method.

It has to be pointed out that the school will run remotely every morning over four days. In the last day, PhD students will have the possibility to present their research on particle based numerical methods. I hope that our students will take the opportunity that is offered to them, ALERT Geomaterials is definitely a forum where new ideas may appear, discussions take place between all the members of our community.

On behalf of the ALERT Board of Directors I wish all participants a successful ALERT Doctoral E-School 2020!

Frédéric Collin
Director of ALERT Geomaterials
University of Liege

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Foreword

Analysis and design in geomechanics are much dominated by the mesh-based numerical methods such as FEM. However, the mesh-based methods suffer from severe mesh distortion for problems with large deformation. Moreover, the mesh-based methods are not well suited for free surface flow and problems with discontinuities. Recently, there is increasing interest in the geomechanics community to apply the particle-based continuum methods to the problems with free surface flow, large deformation and discontinuous deformation. The last decades saw rapid development of numerous particle-based methods in computational mechanics, e.g. SPH (Smooth Particle Hydrodynamics) and MPM (Material Particle Method). Geomechanics with complex material behaviour and problem setting offers an excellent playground for meshfree methods. The lectures in this workshop offer an overview of some widely used particle-based numerical methods in geomechanics. Both mathematical fundamentals and application examples are provided.

After a first introduction of the course, the first four lectures deal with SPH methods. The material covers an introduction to SPH in geomechanics (H.Bui), constitutive modelling in SPH of fast granular flows (W.Wu), applications of SPH in geomechanics (H.Bui), and depth integrated SPH models for fast landslides (M.Pastor). MPM techniques and their application to snow will be addressed next (J.Gaume). The two last lectures will focus on PFEM, covering implicit MPM and coupled MPM-FEM approaches in geomechanics and their application to engineering (A.Larese) and Lattice Boltzmann coupled to DEM methods (S.Sun). Time has been allocated in the course for participants' own research, followed by a table ronde where we hope animated discussion will take place.

Wei Wu
Manuel Pastor

Smoothed particle hydrodynamics (SPH) and its applications in geomechanicsⁱ

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In this lecture note, we present the fundamental concepts of SPH and its applications in geomechanics and geotechnical engineering. In the first part of the lecture note, we will focus on establishing fundamental SPH equations and discussing how they are applied in solving partial differential equations in geomechanics. Through this process, we hope to provide readers with a better understanding of SPH formulations to avoid misuse or misinterpretation of its capacity and limitation. Discussions on several outstanding issues and recommendations for further developments will also be presented. The second part of the lecture will focus on demonstrating the applications of SPH in the fields of geomechanics and geotechnical engineering through various examples, ranging from the most fundamental to more complex applications involving multiphase flows. We hope this lecture note will provide readers with a better understanding of SPH and its potential in solving problems in geomechanics and geotechnical engineering.

1 Introduction

Robust numerical methods for solving complex problems involving multi-phase multi-physical processes are crucial and also an increasing trend in recent years in the

ⁱThis review is distributed as a lecture note to participants attending the ALERT GEOMATERIALS Doctoral School 2020. It should not be considered as a publication by any mean. The lecture note contains materials and ongoing work developed mainly in Ha H. Bui's group at Monash University, some of which are through collaboration with Giang D. Nguyen's group at the University of Adelaide. ¹Email address: ha.bui@monash.edu (Ha H. Bui)

field of computational geomechanics. The key reason is because most popular existing computational tools for field scale-application are still heavily relied on the traditional finite element method (FEM), which is a continuum mesh-based method and is well-known for suffering from mesh-distortion issues associated with large deformation of geomaterials. Alternative to FEM is continuum point-based methods, which offer great capacity for solving field-scale applications involving large-deformation and post-failure of geomaterials. Among several existing point-based methods, SPH is the only numerical method that is completely mesh-free and requires no background mesh. The method was originally developed for astrophysics applications [1, 2], but soon becoming a popular method for various engineering applications [3-30]. The fundamental difference between SPH and other point-based FEM methods is that SPH solve the governing PDE equations in strong form. Since there is no need to go through the weak forms, it is more straightforward to incorporate SPH approximation of a new PDE describing a new physical phenomenon in an existing SPH framework. Nevertheless, there exists common misinterpretations in the literature on the capacity and limitation of SPH, which simply refer to SPH as a numerical method that is suffered from numerical instability and inaccuracy, without acknowledging its true capacity and potential. Interestingly, most of these interpretations came from experts in mesh-based methods or from misuses of fundamental SPH kernel approximation [31]. In this note, we will attempt to provide readers with a better understanding of SPH and its true capacity and performance. To achieve this, we will present a comprehensive review of the fundamental concepts of SPH. We acknowledge that there exists many excellent SPH reviews literature [32-35], but to the best of our knowledge, there is no comprehensive SPH review dedicated to geomechanics applications.

2 The fundamentals of SPH

There are many different ways to approach the fundamental of SPH in the literature, many of which simply refer to the method as an interpolation procedure, which can be used to approximate a field quantity or its spatial derivatives. We have been working on this method for many years, with a particular focus on advancing its applications to solve challenging problems in the geomechanics field. In our view, SPH is more than a numerical method since the foundation of SPH and its governing equations can be naturally derived from considerations of several fundamental physical processes [36], which makes SPH more appealing for solving physical problems.

2.1 *Basic SPH formulations from fundamental physics*

Let us first establish the basic SPH formulation. Consider a continuum field represented by a collection of point masses (or particles), each occupies a certain volume of the continuum domain and carries the corresponding mass of the occupying volume, as shown in Figure 1.

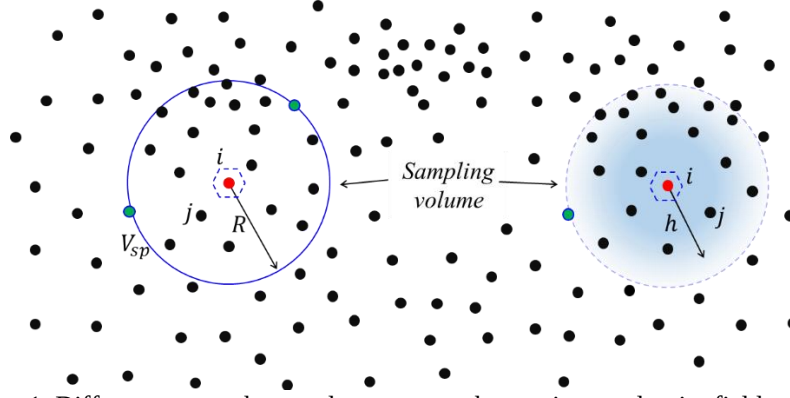


Figure 1. Different approaches used to compute the continuous density field at a particular point in a continuum field represented by a collection of points or particle masses (after [32]).

One of the most simplest, but interesting, questions would raise from this consideration is: *How do I calculate the continuous density field at a particular point from this collection of particles?* Perhaps, the most common answer to the above question is to consider a local sampling volume of mass distribution, assuming spherical volume in 3D and circular area in 2D as shown in Figure 1. The continuous density field at the central point of the sampling volume can be then computed by taking the total mass of particles located within the sampling volume and dividing by the sampling volume:

$$\rho(\mathbf{x}_i) = \frac{1}{V_{sp}} \sum_{j=1}^N m_j \quad (1)$$

where $\rho(\mathbf{x}_i)$ is the continuous density field at the central point of the sampling volume $\mathbf{x}_i$; N is the total number of “neighbouring” particles located within the sampling volume V_{sp} ; m_j is the mass of a particle j located within the sampling volume.

The immediate issue that arises from this approach is that the estimated continuous density field would be significantly affected by the distribution of particles, i.e. clustered/spare regions of particle mass distribution. Although this issue can be fixed by adjusting the sampling volume (V_{sp}) following a certain criterion, a small adjustment/variation of the sampling volume would significantly affect the calculation result (e.g. it can either include or exclude a particle mass from the calculation). Accordingly, the estimated continuous density field would be highly sensitive to the sampling volume and thus leading to a very noise density field estimation. A simple solution¹ to improve the estimated density field is to adopt a weighted average approach, in which particles close to the centre of the sampling volume participate more to the

¹ There exists alternative methods (such as mesh-based methods) which can be used to estimate the continuous density field from the collection of point masses. These are however beyond the scope of this note.

computation, while those located away from the centre have less contribution. This idea can be mathematically formulated using the following equation [32-34, 37]:

$$\rho(\mathbf{x}_i) = \sum_{j=1}^N m_j W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (2)$$

where $W(\mathbf{x}_i - \mathbf{x}_j, h)$ is a weighting function, which has a dimension of inversed volume ($\sim V_{sp}^{-1}$) and is dependent on the particle distance ($\mathbf{x}_i - \mathbf{x}_j$) and a scalar parameter h (to be defined later). The reader can see that the accuracy of the above density estimation rests on the choice of the weighting function $W(\mathbf{x}_i - \mathbf{x}_j, h)$. For instance, to fix the issue associated with the use of Equation (1), the weighting function $W(\mathbf{x}_i - \mathbf{x}_j, h)$ needs to have the following properties:

1. It should be defined in such a way that its magnitude reaches a peak value at the centre of the sampling volume and gradually reduces and asymptotically approaches zero as the distance from a particle mass to the centre of the sampling volume increases (Figure 1). This can be achieved by defining the weighting function W as a function of particle spacing ($\mathbf{x}_i - \mathbf{x}_j$) and a scalar parameter (h) defining the rate of falling-off of W .
2. It should be positive and symmetric with respect to the particle distance. This guarantees particles with the same distance from the centre of the sampling volume will have equal contributions to the density estimation.
3. The conservation of total mass $\int \rho dV = \sum_{j=1}^N m_j$ requires the following condition of the weighting function:

$$\int W(\mathbf{x}_i - \mathbf{x}_j, h) dV = 1 \quad (3)$$

There exists a number of weighting functions in the literature that satisfies the above requirements. We will come back to this topic later with an in-deep discussion on the selection of a proper weighting function. Finally, if Equation (2) is rewritten as:

$$\rho(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho(\mathbf{x}_j)} \rho(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (4)$$

one can immediately see that the above equation can be generalised in the following form for an arbitrary function $f(\mathbf{x}_i)$:

$$f(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (5)$$

Equation (5) is the basic SPH formula, which is commonly reported in the literature. It forms the basis of all existing SPH formalisms. The reader can immediately see that, by choosing $f = \rho$, Equation (5) will return to Equation (2) for the SPH density approximation. Alternatively, if we choose f to be a random field variable, such as temperature $f = T$, Equation (5) can be used to estimate the temperature at the central of the sampling volume as follows:

$$T(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} T(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (6)$$

This suggests that Equation (5) is a general SPH approximation equation, which can be used to estimate any field variable in the continuum space. Finally, to close this section, one would need to define the SPH approximation for the spatial derivative of a field function. This can be achieved by replacing the function $f(\mathbf{x})$ in Equation (5) by its spatial derivative $\partial f(\mathbf{x})/\partial \mathbf{x}$, leading to:

$$\begin{aligned} \frac{\partial f(\mathbf{x}_i)}{\partial \mathbf{x}_i} &= \sum_{j=1}^N \frac{m_j}{\rho_j} \frac{\partial f(\mathbf{x}_j)}{\partial \mathbf{x}_j} W(\mathbf{x}_i - \mathbf{x}_j, h) \\ &= \sum_{j=1}^N \frac{m_j}{\rho_j} \left[\frac{\partial [f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h)]}{\partial \mathbf{x}_j} - f(\mathbf{x}_j) \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial \mathbf{x}_j} \right] \end{aligned} \quad (7)$$

The first term on the left-hand side of Equation (7) is the summation approximation of the volume integral of the gradient of $[f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h)]$:

$$\sum_{j=1}^N \frac{m_j}{\rho_j} \frac{\partial [f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h)]}{\partial \mathbf{x}_j} = \int_V \frac{\partial [f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h)]}{\partial \mathbf{x}_j} dV \quad (8)$$

where we have replaced dV with m_j/ρ_j . By applying the Gaussian theorem to convert the volume integral to the surface integral, we have:

$$\int_V \frac{\partial f(\mathbf{x}_j)}{\partial \mathbf{x}_j} W(\mathbf{x}_i - \mathbf{x}_j, h) dV = \int_S f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \vec{n} \cdot d\mathbf{S} \quad (9)$$

where $\vec{n}$ is the unit normal vector of the surface S . For a symmetric and positive weighting function, the above surface integral vanishes and thus the SPH approximation formulation for the spatial derivative of a field function can be simplified to:

$$\frac{\partial f(\mathbf{x}_i)}{\partial \mathbf{x}_i} = \sum_{j=1}^N \frac{m_j}{\rho_j} f(\mathbf{x}_j) \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial \mathbf{x}_i} \quad (10)$$

This equation suggests that the SPH approximation of the spatial gradient of a function can be achieved without requiring to calculate the spatial derivative of the function itself, but instead through the spatial derivative of the weight function. Accordingly, an additional condition is required for choosing a suitable weighting function for SPH, that the weighting function must have smooth derivatives. A similar approach can be applied to derive the SPH approximation for higher-order derivatives of a function, but this will be further explored in the subsequent section in a more mathematical sense.

Upon this point, the reader should have seen that Equation (5) is the fundamental SPH formulation, which forms the basis of all existing SPH formalisms. It is worth to remind that this equation was derived from the fundamental question related to *how a continuous physical quantity is estimated from the continuum field consisting of a collection of particle masses*. Therefore, in this note, we argue that the fundamental

SPH formulation established in Equation (5) is not just a mathematical equation, but having more physical senses.

2.2 SPH formulations from interpolant theory

In the above section, we have taken a slightly different approach to derive the fundamental SPH formula to demonstrate that SPH is more than a numerical method. In this section, we will present the conventional way to derive the fundamental SPH formulations based on the kernel interpolation theory, which was originally developed by Gingold and Monaghan [1] and Lucy [2] for astrophysical applications. This will allow us to have a more rigorous way to evaluate the accuracy as well as numerical errors produced by SPH formula.

2.2.1 Basics SPH formulation and its derivatives

The heart of SPH is based on the interpolation theory, which consists of two key steps: integral representation and particle approximation. The integral representation step involves the expression of a scalar function $f(\mathbf{x})$ using the following identity:

$$f(\mathbf{x}) = \int f(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x}' \quad (11)$$

where $\delta(\mathbf{x} - \mathbf{x}')$ is the Dirac delta function, which is zero everywhere but infinite at $\mathbf{x} = \mathbf{x}'$. To make effective use of Equation (11), one needs to replace the Dirac delta function δ by a finite function, which is computable. For instance, if we replace the Dirac delta function δ by a weighting function $W(\mathbf{x} - \mathbf{x}', h)$, which is a function of the distance $(\mathbf{x} - \mathbf{x}')$ and a characteristic length h such that:

$$\lim_{h \rightarrow 0} W(\mathbf{x} - \mathbf{x}', h) = \delta(\mathbf{x} - \mathbf{x}') \quad (12)$$

Equation (11) can be rewritten as follows:

$$f(\mathbf{x}) \approx \int f(\mathbf{x}') W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}' \quad (13)$$

The choice of the weighting function (hereafter called kernel function) decides the accuracy of the above integral approximation. The reader can see from Equation (13) that, for $\mathbf{x} \equiv \mathbf{x}'$, the following condition of the kernel function is required $\int W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}' = 1$, which is similar to the condition expressed in Equation (3) as discussed in Section 2.1. Several other key requirements for the selection of suitable kernel function are discussed in Section 2.1, and thus will not be repeated here. To obtain the final form of SPH formulation, one needs to discretise Equation (13) onto a set of point masses (or particles) representing a continuum field, as shown in Figure 1 (i.e. particle approximation step). This can be achieved by replacing the integral in Equation (13) with the summation over a set of particles, each of which has a volume of $d\mathbf{x}' = m/\rho$:

$$f(\mathbf{x}_i) \approx \sum_{j=1}^N \frac{m_j}{\rho_j} f(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (14)$$

Equation (14) is commonly known as the SPH summation equation, and together with Equation (13), form the basic of all existing SPH formalisms. It states that the value of a scalar function at particle i can be approximated using the weighting average of its values at “neighbouring” particles located within the influence domain of the kernel function characterised by the characteristic length h . It is noted that Equation (14) is exactly similar to Equation (5), which was derived in Section 2.1, although the approaches taken to derive these equations are different. The interpolant approach offers a more rigorous way (in the mathematical sense) to derive SPH approximation equations for higher-order gradient terms. For instance, the gradient of function $f(\mathbf{x})$ can be straightforwardly derived by taking derivative of Equation (13) and subsequently discretising the resulting equation onto particles, gives:

$$\nabla f(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} f(\mathbf{x}_j) \nabla_i W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (15)$$

Similarly, the SPH approximation of a vector quantity $\mathbf{f}(\mathbf{x})$ and its divergence can be straightforwardly obtained using the same approach, which can be immediately written as follows, respectively:

$$\mathbf{f}(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} \mathbf{f}(\mathbf{x}_j) W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (16)$$

$$\nabla \cdot \mathbf{f}(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} \mathbf{f}(\mathbf{x}_j) \cdot \nabla_i W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (17)$$

Unfortunately, these SPH approximations do not always achieve satisfaction results and often results in very poor gradient estimations. For instance, the use of Equation (15) does not ensure the gradient of a constant field variable vanishes, which is troublesome when being used to estimate the strain rate or the gradient of the velocity field for computational fluid or solid mechanics. These issues have led to several alternative SPH formulations in the literature, which will be discussed in the subsequent section.

2.2.2 Alternative SPH formulations for its first derivatives

As discussed in the above section, the use of SPH formulations presented in Section 2.2.1 often results in poor results. To have a better understanding of issues caused by these formulations, let's consider the source of errors associated with these formulations. For instance, the errors introduced by the SPH approximation for the gradient of a scalar function in Equation (15) can be obtained by applying Taylor-series to expand $f(\mathbf{x}_j)$ around $\mathbf{x}_i$, leading to:

$$\begin{aligned}
\nabla f_i &= \sum_{j=1}^N \frac{m_j}{\rho_j} f_j \nabla_i W_{ij} = \sum_{j=1}^N \frac{m_j}{\rho_j} \left[f_i + \frac{\partial f_i}{\partial \mathbf{x}^\alpha} (\mathbf{x}_j - \mathbf{x}_i) + O(h^2) \right] \nabla_i W_{ij} \\
&= f_i \sum_{j=1}^N \frac{m_j}{\rho_j} \nabla_i W_{ij} + \frac{\partial f_i}{\partial \mathbf{x}^\alpha} \sum_{j=1}^N \frac{m_j}{\rho_j} (\mathbf{x}_j - \mathbf{x}_i) \nabla_i W_{ij} + O(h^2)
\end{aligned} \tag{18}$$

where to simplify our expression, we have replaced $f(\mathbf{x}_j) \equiv f_j$, $\nabla W(\mathbf{x}_i - \mathbf{x}_j, h) \equiv \nabla W_{ij}$, and α is the index denoting coordinate direction with repeated indices implying summation.

Equation (18) indicates that the errors introduced by Equation (15) is controlled by the first and second terms in the second line of Equation (18), that is how well the SPH approximations for these terms hold:

$$\sum_{j=1}^N \frac{m_j}{\rho_j} \nabla_i W_{ij} \approx 0 \quad \text{and} \quad \sum_{j=1}^N \frac{m_j}{\rho_j} (\mathbf{x}_j - \mathbf{x}_i) \nabla_i W_{ij} \approx \delta^{\alpha\beta} \tag{19}$$

A straightforward way to mitigate these errors is to subtract the first term in the second line of Equation (18) from Equation (15), which results in the following alternative SPH approximation for the gradient of function $f(\mathbf{x}_i)$:

$$\nabla f(\mathbf{x}_i) = \sum_{j=1}^N \frac{m_j}{\rho_j} [f(\mathbf{x}_j) - f(\mathbf{x}_i)] \nabla_i W(\mathbf{x}_i - \mathbf{x}_j, h) \tag{20}$$

It is noted that Equation (20) can also be derived from the following consideration: $\nabla f = \nabla f - f(\nabla 1)$ and is commonly used in the literature. Although this alternative formulation exactly guarantees the vanishing of SPH approximation of the gradient of a constant function, its numerical errors is still controlled by the errors associated with the second term in the second line of Equation (18). To completely eliminate these errors (i.e. up to second-order accuracy), one can divide Equation (20) by the second term in the second line of Equation (18), leading to the following normalised SPH formulation for the kernel derivative:

$$\nabla f(\mathbf{x}_i) = \frac{\sum_{j=1}^N \frac{m_j}{\rho_j} [f(\mathbf{x}_j) - f(\mathbf{x}_i)] \nabla_i W(\mathbf{x}_i - \mathbf{x}_j, h)}{\sum_{j=1}^N \frac{m_j}{\rho_j} (\mathbf{x}_j - \mathbf{x}_i) \nabla_i W_{ij}} \tag{21}$$

Figure 2 illustrates the accuracy of Equation (21) when being applied to evaluate the gradient of a linear function for a random particle distribution. It can see that the equation exactly reproduces the gradient of the linear field function and is completely free from the kernel truncation errors at the boundary.

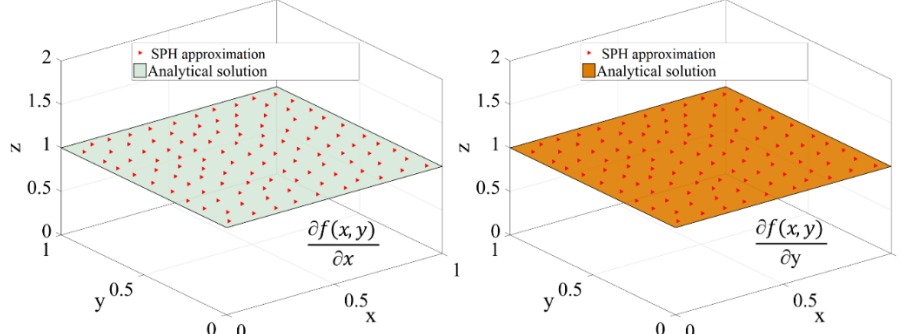


Figure 2. SPH approximations for the gradient of a linear function $f(x, y) = x + y$

An alternative SPH approximation formulation for the gradient of a function at particle i can also be derived by considering the following arrangement:

$$\nabla f|_i = \frac{[\nabla(\rho f) - f \nabla \rho]}{\rho} \Big|_i = \frac{1}{\rho_i} \sum_{j=1}^N m_j [f_j - f_i] \nabla_i W_{ij} \quad (22)$$

which again guarantees the vanishing of SPH approximation of the gradient of a constant function and can be equally used as an alternative to Equation (20). The reader can apply the same Taylor series expansion approach to evaluate the errors associated with this equation as well as to improve the accuracy of this equation as done for Equation (20). We will not repeat this process here.

Finally, it is worth to mention the following well-known SPH gradient operators, which are commonly used to evaluate the gradient of the pressure or stress in the momentum equation (to be discussed later). These SPH gradient operators can be derived from the following considerations:

$$\nabla f|_i = \rho \left[\frac{f}{\rho^2} \nabla \rho + \nabla \left(\frac{f}{\rho} \right) \right]_i = \rho_i \sum_{j=1}^N m_j \left[\frac{f_i}{\rho_i^2} + \frac{f_j}{\rho_j^2} \right] \nabla_i W_{ij} \quad (23)$$

And

$$\nabla f|_i = \nabla f + f(\nabla 1)|_i = \sum_{j=1}^N m_j \left[\frac{f_i + f_j}{\rho_j} \right] \nabla_i W_{ij} \quad (24)$$

The reader can see that the above SPH operators do not guarantee the gradient approximation of a constant field function vanished, but instead they result in an operator that produces a sort of pair-wise contribution from both particles i and j for a given pair of interaction. This SPH approximation property is particularly useful when being applied to discretise the momentum equation of a continuum system, which strictly requires the conservations of both linear and angular momenta. Although we can eliminate numerical errors associated with the above SPH operators (i.e. using the Taylor series), we prefer not to do so because the exact conservation of momentum equation requires these errors and these are one of several interesting features of the SPH method. We will go back to this issue later. Finally, the same methodology discussed

above can be applied to obtain the SPH approximation of the gradient of a vector field, and thus will not be repeated.

2.2.3 SPH formulation for second derivatives

The SPH approximation for the second derivatives of a scalar function or vector quantities can be obtained in a way similar to the approximation of the first derivatives. By taking derivatives of Equation (14) and applying Taylor series expansion, one could derive the following SPH operator²:

$$\nabla^2 f \approx \sum_{j=1}^N \frac{m_j}{\rho_j} (f_j - f_i) \nabla_i^2 W_{ij} \quad (25)$$

which guarantees the vanishing of gradients of both constant and linear field functions. The remaining errors associated with this SPH operator (up to the third order of accuracy) are:

$$\begin{aligned} \frac{\partial f_i}{\partial \mathbf{x}^\alpha} \sum_{j=1}^N \frac{m_j}{\rho_j} \mathbf{x}_{ji}^\alpha \nabla_i^2 W_{ij} + \frac{1}{2} \frac{\partial}{\partial \mathbf{x}^\alpha} \left(\frac{\partial f_i}{\partial \mathbf{x}^\beta} \right) \sum_{j=1}^N \frac{m_j}{\rho_j} \mathbf{x}_{ji}^\alpha \mathbf{x}_{ji}^\beta \nabla_i^2 W_{ij} \\ + O(h^3) \end{aligned} \quad (26)$$

which again relies on how well the SPH approximations for these terms hold:

$$\sum_{j=1}^N \frac{m_j}{\rho_j} \nabla_i^2 W_{ij} \approx 0 \quad \text{and} \quad \sum_{j=1}^N \frac{m_j}{\rho_j} \mathbf{x}_{ji}^\alpha \mathbf{x}_{ji}^\beta \nabla_i^2 W_{ij} \approx \delta^{\alpha\beta} \quad (27)$$

Note that one can completely eliminate these errors in a way similar to the case of the first derivative. However, the issue associated with the above SPH operator for the second derivatives, i.e. Equation (25), is that it involves the second derivatives of the kernel function. Unfortunately, for most existing kernel functions, their second derivatives changes sign within the kernel influence domain, as shown in Figure 3 for the two most popular Gaussian and Cubic-spline kernel functions. This makes the conditions in Equation (27) to be extremely hard to be satisfied. Therefore, for practical SPH applications, it is recommended to avoid the use of the second derivatives of the kernel function. Accordingly, a different way to approximate the second derivatives of a function by SPH is needed.

Perhaps, the simplest method to get away from the second derivative of the kernel function is to apply Taylor series expansion of a function f_j around $\mathbf{x}_i$ up to the second-order of accuracy, giving:

$$f_j = f_i + \frac{\partial f_i}{\partial \mathbf{x}^\alpha} \mathbf{x}_{ji}^\alpha + \frac{1}{2} \frac{\partial^2 f_i}{\partial \mathbf{x}^\alpha \partial \mathbf{x}^\beta} \mathbf{x}_{ji}^\alpha \mathbf{x}_{ji}^\beta + O(h^3) \quad (28)$$

² An alternative way to derive this SPH operator is to replace the function f in Equation (13) by $\nabla^2 f$ and applying the Gaussian theorem as done for the first derivative.

Next, multiply Equation (28) by $\mathbf{x}_{ji} \nabla_i W_{ij} / |\mathbf{x}_{ji}|^2$ and taking the integral of the equation over the entire domain results:

$$\begin{aligned} & \int \frac{(f_j - f_i) \mathbf{x}_{ji} \nabla_i W_{ij}}{|\mathbf{x}_{ji}|^2} d\mathbf{x}_j \\ &= \frac{\partial f_i}{\partial \mathbf{x}^\alpha} \int \mathbf{x}_{ji}^\alpha \frac{\mathbf{x}_{ji} \nabla_i W_{ij}}{|\mathbf{x}_{ji}|^2} d\mathbf{x}_j + \frac{1}{2} \frac{\partial^2 f_i}{\partial \mathbf{x}^\alpha \partial \mathbf{x}^\beta} \int \mathbf{x}_{ji}^\alpha \mathbf{x}_{ji}^\beta \frac{\mathbf{x}_{ji} \nabla_i W_{ij}}{|\mathbf{x}_{ji}|^2} d\mathbf{x}_j \end{aligned} \quad (29)$$

From the integral theory, the first term on the right-hand side of Equation (29) is vanished for a symmetric kernel function W , while the second term should result in a delta function, $\delta^{\alpha\beta}$, which ultimately gives $\frac{1}{2} \nabla^2 f_i$. Accordingly, by rearranging Equation (29), we have:

$$\nabla^2 f_i = 2 \int \frac{(f_j - f_i) \mathbf{x}_{ji} \nabla_i W_{ij}}{|\mathbf{x}_{ji}|^2} d\mathbf{x}_j \quad (30)$$

Finally, by discretising the above integral onto a finite set of particles, the following SPH operator for the second derivative of a function can be obtained:

$$\nabla^2 f_i = 2 \sum_{j=1}^N \frac{m_j}{\rho_j} \frac{(f_j - f_i) \mathbf{x}_{ji} \nabla_i W_{ij}}{|\mathbf{x}_{ji}|^2} \quad (31)$$

which only involves the first derivative of the kernel function, and thus in principle, could produce better accuracy compared to the SPH operator in Equation (25). We acknowledge that in the derivation of the above SPH operator for the second derivative of a function, we have ignored the error introduced by the interpolation theory, and this will be discussed in due course.

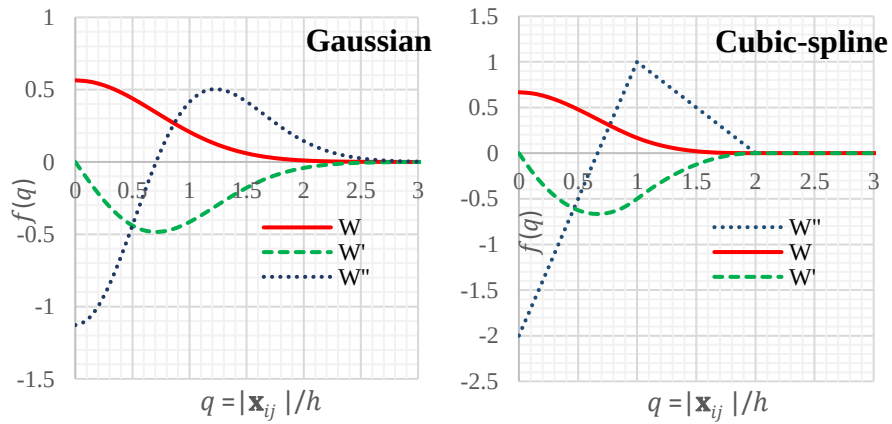


Figure 3. Gaussian and Cubic-spline kernel functions and its derivatives, respectively.

2.3 Selection of kernel functions and associated issues

The selection of appropriate kernel function in SPH will directly affect the accuracy, efficiency and the stability of the SPH algorithm. As discussed in Section 2.1, a good kernel function needs to satisfy several key requirements, which are summarised below:

1. The kernel function must be positive, symmetric with respect to particle distance and have smooth first and second derivatives.
2. It should have a compact domain and smoothly reduces as the distance from the centre of the kernel function increases.
3. It must satisfy the normalised condition, which requires $\int W(\mathbf{x}_i - \mathbf{x}_j, h) dV = 1$

Most existing kernel functions in the literature satisfy the above requirements, and the two most popular kernel functions are the Gaussian kernel function and cubic-spline function. For the Gaussian kernel function:

$$W(q, h) = \alpha_d \exp[-q^2] \quad (32)$$

where $q = |\mathbf{x}_{ij}|/h$ is the ratio between the distance between two particles and the smoothing length h , which defines the rate of falling-off of W or the area of the kernel influence domain; and α_d is the normalisation factor given as $\alpha_d = [1/h\sqrt{\pi}, 1/\pi h^2, 1/(h^2\pi\sqrt{\pi})]$ for one-, two- and three-dimensions, respectively. The cubic-spline function takes the following form:

$$W(q, h) = \alpha_d \begin{cases} \frac{2}{3} - q^2 + \frac{1}{2}q^3 & 0 \leq q < 1 \\ \frac{1}{6}(2 - q)^3 & 1 \leq q < 2 \\ 0 & q \geq 2 \end{cases} \quad (33)$$

where α_d is the dimensional normalising factor defined by $\alpha_d = [1/h, 15/7\pi h^2, 3/2\pi h^2]$ for one-, two- and three-dimensions, respectively. The graphical representation of these kernel functions and its derivatives were shown in Figure 3. Compared to the cubic-spline function, the Gaussian kernel function does not have a compact domain³, so all particles will make contribution to the SPH approximation in the computation, resulting in an extremely unnecessary large computational cost, i.e. in the order of $O(N^2)$ with N being the total number of particles in the system. In contrast, the cubic-spline function drops quickly and approaches zero as $q = 2$ and thus allowing to reduce the calculation to a sum over closely neighbouring particles, which dramatically reduces the cost to $O(nN)$ with n being the number of contributing neighbours, although there is an additional cost of finding the neighbouring particles.

In addition to the computational issue, the selection of kernel function will have a direct impact on the stability of SPH simulation. For instance, in the areas of compu-

³ Note that the plot of Gaussian kernel function and its derivatives in Figure 3 are truncated at $q = 3$

tational fluid mechanics or astrophysics, the SPH estimation of density is very important as this quantity is subsequently used to compute the pressure, which governs the motion of the entire system. The SPH kernel approximation controls the accuracy of density calculation and thus has a direct influence on the numerical stability of the application. An earlier study conducted by Dehnen and Aly [38] on the stability of SPH concluded that the misuse of Gaussian and Cubic-spline kernel functions would facilitate the so-call pairing instability for a randomly disordered particle system, in which particles tend to form a clump in the numerical simulations. It is noted that the pairing instability is different from the tensile instability, which is caused by negative stresses/pressures. Dehnen and Aly [38] argues that the pairing issue in SPH is mainly caused by the SPH density estimator error resulted from the misuse of kernel estimations. In particular, each kernel function has a compacted domain, which can accommodate a limited number of “neighbouring” particles in the kernel estimation. When the number of “neighbouring” particles within the kernel domain exceed a certain threshold (i.e. in a highly disordered system or chaotic system), the kernel estimation would result in significant errors. One way to mitigate these estimation errors, as well as to repair the pairing instability issue, is to use the Wendland C^2 kernel function, which takes the following form for 1D condition:

$$W(q, h) = \alpha_d \begin{cases} (1 - 0.5q)^3(1.5q + 1) & 0 \leq q \leq 2 \\ 0 & q > 2 \end{cases} \quad (34)$$

and the following form for 2D & 3D conditions

$$W(q, h) = \alpha_d \begin{cases} (1 - 0.5q)^4(2q + 1) & 0 \leq q \leq 2 \\ 0 & q > 2 \end{cases} \quad (35)$$

where α_d is the dimensional normalising factor defined by $\alpha_d = [5/8h, 7/4\pi h^2, 21/2\pi h^3]$ for one-, two- and three-dimensions, respectively.

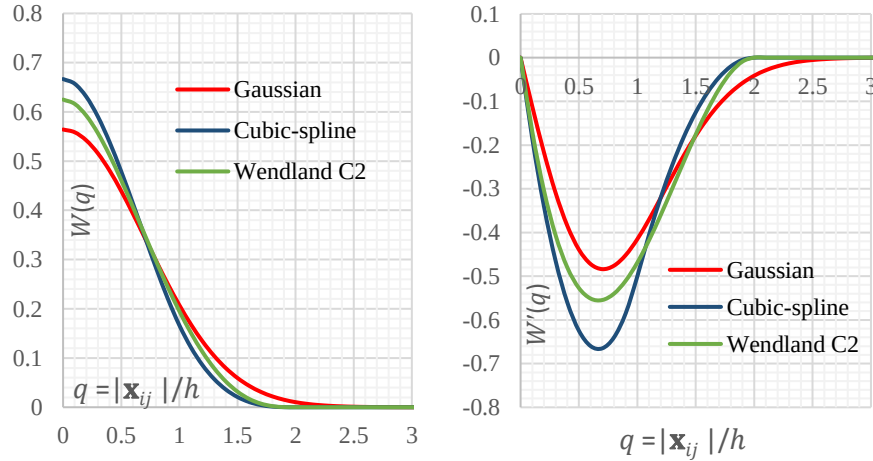


Figure 4. Comparison of Wendland C^2 kernel function and its first derivatives against the Gaussian and Cubic-spline kernel function

Figure 4 shows the comparison between Wendland C^2 kernel function against the other two popular ones. It can be seen that, similar to the Cubic-spline function, the

Wendland C^2 kernel function also features a compact support domain. Furthermore, it is obvious from the figure that the Wendland C^2 kernel function can slightly accommodate more “neighbouring particles” than the Cubic-spline function. All three kernel functions also feature the so-called inflection point (i.e. the zero gradient point at peak of the kernel function), which was attributed to the source of the pairing instability [38] because particles located near the inflection point would not gain enough repulsive force due to the kernel gradient. *It is important to note that this pairing instability only occurs in a situation where there are more neighbouring particles in the influence domain than a kernel function can accommodate.* Nevertheless, even with the presence of the inflection point, the Wendland C^2 kernel function does not show any sign of pairing instability. This can be demonstrated by conducting a simple numerical test, consisting of an initially random distribution of SPH particles in a square box. The initial velocity of all particles are set to zero, and to avoid the tensile instability issue caused by negative pressure, a positive background pressure was assigned to all particles. To facilitate the pairing instability, we have intentionally designed the tests in such a way that both Gaussian and Cubic-spline functions will have more neighbouring particles than the standard number of particles that these kernels can accommodate. The simulations were then run for a long period of time (again to facilitate the pairing instability), and the results are shown in Figure 5. The particle system in the Cubic-spline kernel function suffers the pairing instability the most and the situation is getting worse as the number of neighbouring particles is increased, i.e. $kh/\Delta x = 5.7$ with Δx being the initial distance between particle and k being a scalar parameter, together with h defining the influence domain of the kernel function. This is not surprising because in both tests we have intentionally forced the kernel function to take more neighbouring particles than the actual number of particles that it can accommodate, which is around $kh/\Delta x = 2.4$. The Gaussian kernel function works better when the number of neighbouring particles is sufficiently small, which can be attributed to the fact that the Gaussian kernel function can accommodate more neighbouring particles due to the infinite kernel domain, but still show pairing instability when the number of neighbouring particles increases to an excessive number (i.e. $kh/\Delta x = 5.7$). In contrast, the Wendland C^2 kernel function was able to maintain the relatively good particle distributions throughout the numerical test, and this can be theoretically explained by the linear stability analysis for conservative SPH in spatial dimensions [38]. In particular, Dehnen and Aly [38] demonstrated that SPH kernel functions whose Fourier transform is negative for some wave vector will inevitably trigger the SPH pairing instability at sufficient large number of neighbouring particles, which are the cases for the Gaussian and Cubic-spline functions. To sufficiently use these kernel functions, a number of neighbouring particle needs to be sufficiently maintained to not exceed a certain threshold, which depend on specific applications. In contrast, the Wendland C^2 kernel function shown non-negative Fourier transform and demonstrated a remarkable feature in removing the pairing instability. This suggests that the Wendland C^2 kernel function is a good candidate for dealing with problems involved highly disordered particles. Nevertheless, the drawback of Wendland C^2 kernel function is that it suffers comparably large errors when the number of neighbouring particles is low. Thus, when using Wendland C^2 kernel function, it is important to maintain a good number of neighbouring particles.

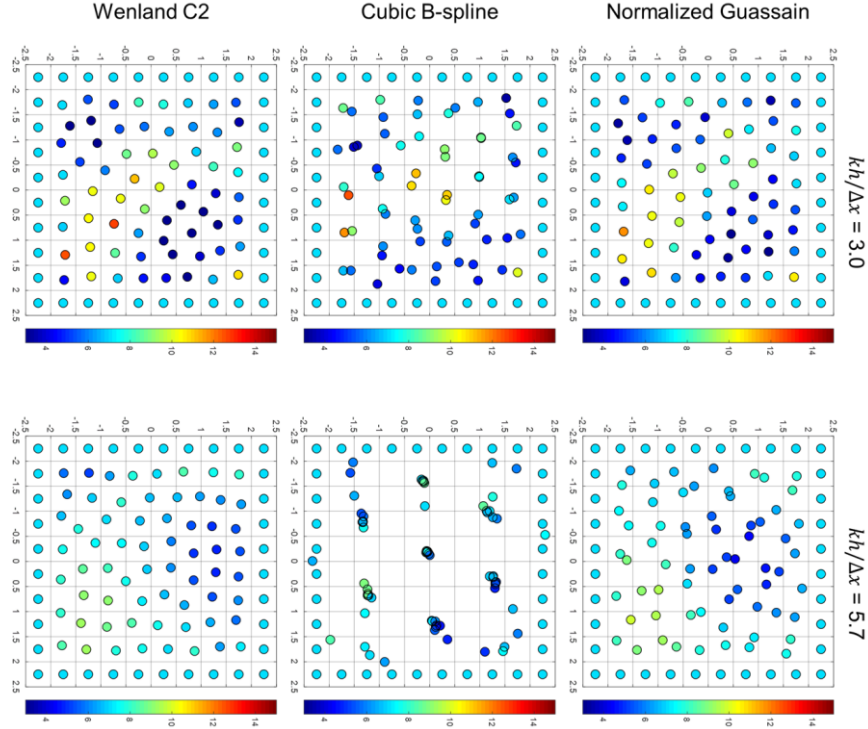


Figure 5. Misuses of kernel functions causing pairing instability in SPH.

2.4 Choosing smoothing length for kernel function

In SPH simulations, each particle is assigned with a smoothing length, which controls the size of the kernel supporting domain and thus the number of neighbouring particles. In addition, depending on specific kernel functions, the smoothing length should be set to maximise its benefit. For example, the recommended smoothing length for the Cubic-spline function is within $kh/\Delta x = 2.0 - 2.6$ and that for the Gaussian kernel functions is 2.0-3.0. Failure to maintain these numbers will facilitate the pairing stability issue, as shown in Figure 5. Furthermore, in early SPH applications, the smoothing length of each particle was often kept constant, but gradually found to be no longer suitable for applications involved highly disordered particles such as complex free-surface flows or debris flows. In such applications, SPH particles might concentrate at some regions, while scattering at others within the computational domain. Keeping the constant smoothing length will result in less number of neighbouring particles in the scatter regions and thus losing the accuracy of SPH kernel estimation. In contrast, the number of neighbouring particles would be too large in the concentrated areas, causing pairing instability as discussed in the previous section. Therefore,

it is generally a good practice to design an adaptive smoothing length, which can automatically adjust depending on the level of particle concentration or density. A simple approach is to link the variable smoothing length to the density is to take the time derivative of Equation (2), which leads to:

$$\begin{aligned}
\frac{d\rho_i}{dt} &= \frac{d}{dt} \sum_{j=1}^N m_j W(\mathbf{x}_i - \mathbf{x}_j, h_i) \\
&= \sum_{j=1}^N m_j \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h_i)}{\partial \mathbf{r}_{ij}} \cdot \frac{d\mathbf{r}_{ij}}{dt} + \sum_{j=1}^N m_j \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h_i)}{\partial h_i} \cdot \frac{dh_i}{dt} \\
&= \sum_{j=1}^N m_j (\mathbf{v}_i - \mathbf{v}_j) \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial \mathbf{r}_{ij}} + \sum_{j=1}^N m_j \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial h_i} \cdot \frac{dh_i}{dt}
\end{aligned} \tag{36}$$

The rearrangement of the above equation leads to the following interesting time-dependent smoothing length equation, which can be evolved with the particle density:

$$\frac{dh_i}{dt} = \frac{\frac{d\rho_i}{dt} - \sum_{j=1}^N m_j (\mathbf{v}_i - \mathbf{v}_j) \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial \mathbf{r}_{ij}}}{\sum_{j=1}^N m_j \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial h_i}} \tag{37}$$

It is noted that we have not tested the above equation. However, one can see that the mathematical derivation of the equation is conceptually correct and, indeed, it links the rate of change of the smoothing length to the change of the rate of change of the density, rather than the rate of change of the density. Alternatively, the reader can use the following equation to link the smoothing length to the rate of change of the density [39, 40]:

$$\frac{dh}{dt} = -\frac{1}{v} \frac{h}{\rho} \frac{d\rho}{dt} \tag{38}$$

Since each particle now has its own smoothing length, the kernel influence domain of particle i might cover particle j but not necessarily vice versa. Therefore, it is possible for particle i to exert a force on particle j without j exerting the same corresponding reaction on particle i . As a result, the momentum equation will not conserve exactly. To overcome this problem, some measures must be taken to preserve the symmetric of particle interactions. One simple approach to preserve the symmetry of particle interaction is to modify the smoothing length by taking the arithmetic mean or the average of the smoothing length of a pair of interacting particles [39]:

$$h_{ij} = \frac{h_i + h_j}{2} \tag{39}$$

Other ways can also be used to get the symmetric smoothing length using the geometric mean of the smoothing lengths of the pair of the interaction particles:

$$h_{ij} = \frac{2h_i h_j}{h_i + h_j} \tag{40}$$

Alternatively, one can take the maximum value of the smoothing lengths $h_{ij} = \max(h_i, h_j)$ or minimum of the smoothing lengths $h_{ij} = \min(h_i, h_j)$. The kernel function can then be obtained by using the symmetric smoothing length $W_{ij} = W(\mathbf{x}_i - \mathbf{x}_j, h_{ij})$. It is noted that there are some advantages and disadvantages associated with each of the above approaches to average the smoothing length. For example, taking the arithmetic mean or maximum smoothing length tends to use more neighbouring particles and sometimes may overly smooth out the interaction with surrounding particles. Taking geometric or minimum smoothing length, on the other hand, tends to possess less neighbouring particles. Another approach to preserve the symmetry of particle interaction is to directly use the average of kernel function values without using a symmetric smoothing length [39, 41]:

$$W_{ij} = \frac{W(\mathbf{r}_{ij}, h_i) + W(\mathbf{r}_{ij}, h_j)}{2} \quad (41)$$

Finally, it is noted that, while it is preferable to use the variable smoothing length, many SPH applications in geotechnical engineering areas does not require this update, but still achieving reasonable results. Readers who are new to SPH is strongly recommended to start with a constant smoothing length. Nevertheless, the use of symmetric smoothing length or symmetric kernel average is very important to guarantee the conservation of momentum equation, which controls the stability and accuracy of SPH.

3 General SPH framework for geomechanics applications

The reader at this point should have developed some basic understanding of the key concepts of the SPH method. The next question would be how these concepts can be applied to solve geotechnical problems and in what capacity the method can produce results comparable to those by existing numerical methods, besides its advantages in some specific areas. Before we start this discussion, it is important to remind the reader that, in SPH, the computational domain is represented by a set of moving particles (or material points), each of which occupies a given volume in the continuum space and carries field variables. Therefore, SPH is a continuum-based numerical method, which is very similar to FEM, although SPH does not require any background mesh and solve the strong-form governing differential equations, unlike FEM solving weak-form differential equations. We will first establish the continuum governing equations for a single-phase system of general geomaterials (assuming isothermal). We will then present some potential applications of SPH in this area and discussed potential issues associated with these applications as well as with SPH in general.

3.1 SPH approximation of governing equations

The governing equations for solving general geomechanics and geotechnical engineering problems consist of the continuity and momentum balance equations. The

continuity equation describes the change of material density, and thus void ratio, during the deformation process, while the momentum equation describes how the materials undergo deformation under external loads. These two equations are written as follows [42], respectively:

$$\frac{d\rho_i}{dt} = -\rho \nabla \cdot \mathbf{v}|_i = \sum_{j=1}^N m_j (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} \quad (42)$$

$$\frac{d\mathbf{v}_i}{dt} = \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma} + \mathbf{g}|_i = \sum_{j=1}^N m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij} + \mathbf{g} \quad (43)$$

where $\boldsymbol{\sigma}$ is the stress tensor, which will be defined later, and $\mathbf{g}$ is the acceleration due to the gravity.

The reader will have immediately noticed that Equation (42) can be achieved by adopting the following simple transformation $[-\rho \nabla \cdot \mathbf{v} = \nabla \cdot (\rho \mathbf{v}) - \mathbf{v} \nabla \rho]$ then applying Equations (15) and (16), or simply applying the SPH operator in Equation (20) to the $\nabla \cdot \mathbf{v}$ term, which also results in a slightly different version of the continuity density equation. Alternatively, the continuity equation can be also derived by taking derivative of Equation (2), leading to the following continuity equations:

$$\frac{d\rho_i}{dt} = \frac{1}{\vartheta_i} \sum_{j=1}^N m_j (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} \quad (44)$$

where ϑ_i is an extra term introduced to the continuity equation as a result of the spatial derivative of the smoothing length and is defined as follows:

$$\vartheta_i = \left[1 - \frac{\partial h_i}{\partial \rho_i} \sum_{j=1}^N m_j \frac{\partial W(\mathbf{x}_i - \mathbf{x}_j, h)}{\partial h_i} \right] \quad (45)$$

For a constant smoothing length, Equation (44) simply returns to Equation (42), suggesting that the SPH continuity equation can be simply derived from the SPH estimation of density, which was discussed in Section 2.1. On the other hand, the SPH momentum equation⁴ was obtained by applying the symmetric SPH operator, i.e. Equation (23), to the $\nabla \cdot \boldsymbol{\sigma}$ term. The reader will have wondered why we apply the “bad” SPH operator, which has poor results of SPH approximation for the gradient of a constant function, to approximate the momentum equation, instead of using a “good” SPH operator such as Equation (20) or Equation (21). Indeed, this is one of the interesting features of SPH as it appears that the “good” SPH operators do not reproduce the SPH momentum equation, which exactly conserves both the total linear and angular momenta, while the “bad” SPH operator does well in this aspect. The conservation of the

⁴ Note that an alternative popular SPH momentum equation can be also derived by applying the SPH operator (24). Both approaches similar results and thus here we only focus on one of the two popular SPH equations for the momentum balance.

total linear momentum of the above governing equation can be straightforwardly proved by taking derivative of the total momentum of the entire system [32]:

$$\frac{d}{dt} \sum_i m_i \mathbf{v}_i = \sum_i \sum_j m_i m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij} = 0 \quad (46)$$

where the double summation is equal to zero because $\nabla_i W_{ij} = -\nabla_j W_{ij}$. Similarly, the conservation of the total angular momentum can also be proven in a similar manner by:

$$\begin{aligned} \frac{d}{dt} \sum_i \mathbf{x}_i \times m_i \mathbf{v}_i &= \sum_i m_i \left(\frac{d\mathbf{x}_i}{dt} \times \mathbf{v}_i \right) + \sum_i m_i \left(\mathbf{x}_i \times \frac{d\mathbf{v}_i}{dt} \right) \\ &= \sum_i \sum_j m_i m_j \left\{ \mathbf{x}_i \times \left[\left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij} \right] \right\} = 0 \end{aligned} \quad (47)$$

which again equals to zero because of the symmetric features of the kernel function. On the other hand, if one prefers to use a “good” SPH operator such as Equation (20), the following momentum equation can be obtained:

$$\frac{d\mathbf{v}_i}{dt} = \sum_j m_j \left(\frac{\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j}{\rho_i \rho_j} \right) \cdot \nabla_i W_{ij} = 0 \quad (48)$$

which guarantees the vanishing of gradient of a constant stress field. Unfortunately, the above equation does not exactly conserve both linear and angular momentums and thus failing to maintain the stability of numerical simulations. To the best of our knowledge, we have not yet achieved an SPH formulation for the momentum equation that exactly conserves both linear and angular momentum, while maintaining exact derivatives. And this conclusion extends to all existing particle numerical methods.

3.2 Material constitutive models

One of the most interesting features of SPH is its capability to simulate both fluid-like materials and solid-like materials undergoing extremely large deformation and flow behaviour. Early SPH applications in the field of geomechanics [43-45] explored the traditional SPH approach developed for computational fluid mechanics and elastic solid [46-48], hereafter referred to as CFD approach. In this approach, the total stress tensor ($\boldsymbol{\sigma}$) was decomposed into the hydrostatic pressure (p) and shear stress ($\boldsymbol{\tau}$), which can be computed using equation of state (EoS) and rheological type of constitutive model, respectively. A more rigorous approach was subsequently developed [8, 42, 49], in which advanced constitutive models based on the plasticity theory were adopted and successfully simulate a range of applications in geomechanics [4, 5, 50-58]. In this section, we will provide a brief description of these two approaches. For the CFD approach, we will present the visco-plastic $\mu(I)$ model [59], which can be thought of as an extension of the Bingham fluid model with pressure and friction dependent yield stress for application to dense granular flows. As for the more rigorous approach, we will first present a general elastoplastic constitutive model following the

Drucker-Prager yield criterion [50]. This will follow by an advanced scale-dependent constitutive model, capable of capturing localised failure of general geomaterials [60-63].

3.2.1 CFD approach – $\mu(I)$ rheological constitutive model

The $\mu(I)$ rheological model was developed to capture the inertial effects of granular materials in the dense regime [64]. It assumes the granular material behaves as a viscoplastic fluid, following Drucker-Prager like yielding condition. The material does not flow when the stress state of the material is beneath the yielding stress, but above which material flows like a non-Newtonian fluid. The stress tensor in the $\mu(I)$ model was decomposed into the pressure and shear stress tensor: $\boldsymbol{\sigma} = p\mathbf{I} + \boldsymbol{\tau}$ with $\mathbf{I}$ being the unit tensor. The following equation of state can be used to compute the isotropic pressure:

$$p = c^2(\rho - \rho_0), \quad (49)$$

where c is the speed of sound, ρ is the density of an SPH particle, and ρ_0 is the reference density of the material. The shear stress tensor is determined by,

$$\boldsymbol{\tau} = 2\eta\dot{\boldsymbol{\epsilon}}, \quad (50)$$

$$\eta = \frac{\mu p}{\sqrt{\dot{\boldsymbol{\epsilon}} : \dot{\boldsymbol{\epsilon}}^T}} \quad (51)$$

$$\mu = \mu_s + \frac{\mu_p - \mu_s}{I_0/I_i + 1} \quad (52)$$

where η is an apparent viscosity; $\dot{\boldsymbol{\epsilon}}$ is the strain-rate tensor; μ is a frictional function dependent on the inertial number $I_i = d\sqrt{\dot{\boldsymbol{\epsilon}} : \dot{\boldsymbol{\epsilon}}}/\sqrt{p/\rho_0}$ with d being the real grain diameter and μ_s , μ_p , and I_0 being materials constants. The model includes a Drucker Prager-like yield criterion such that no flow occurs when [59]:

$$\sqrt{\frac{1}{2}\boldsymbol{\tau} : \boldsymbol{\tau}} \leq \mu_s p \quad (53)$$

To avoid unphysical behaviour, the shear component of the stress tensor is assumed to be 0 when the pressure is negative, and the strain rate tensor is initialised as 10^{-7} as zero strain rates can result in mathematically undefined behaviour.

3.2.2 General elasto-plastic constitutive model

While the CFD approach derives the stress tensor from instantaneous density and strain-rate, while the general elasto-plastic approach evolves the stress tensor over time using a stress-strain relationship that relates the stress-increment to the strain-increment. Plasticity theory dictates that for an elastoplastic material, the total strain-rate tensor is decomposed into elastic and plastic components:

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}_e + \dot{\boldsymbol{\epsilon}}_p \quad (54)$$

The stress is then calculated from the generalized Hooke's Law:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}^e : (\dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}_p) \quad (55)$$

where $\mathbf{D}^e$ is the elastic stiffness matrix [50]. The plastic strain rate can be computed using the general plastic flow rule:

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial g}{\partial \boldsymbol{\sigma}} \quad (56)$$

where $\dot{\lambda}$ is the rate of the change of the plastic-multiplier and g is the plastic potential function.

Plastic deformation occurs when the yield criterion is satisfied. In principle, any existing elasto-plastic constitutive models developed for FEM can be implemented in SPH. Herein, we present the simplest case for an elasto-plastic constitutive model that follows the Drucker-Prager criterion, which takes the following general form:

$$f(I_1, J_2, \kappa) = \alpha_\phi I_1 + \sqrt{J_2} - \beta_\phi c(\kappa) = 0 \quad (57)$$

where I_1 and J_2 are the first and second invariants of the stress tensor; α_ϕ and β_ϕ are Drucker-Prager constants related to the Coulomb internal friction angle (ϕ); and $c(\kappa)$ is related to soil cohesion and is assumed to be a function of plastic strain.

In three-dimensional condition, α_ϕ and k_c are calculated as, respectively:

$$\alpha_\phi = \frac{2 \sin \phi}{\sqrt{3}(3 - \sin \phi)} \quad \text{and} \quad k_c = \frac{6c \times \cos \phi}{\sqrt{3}(3 - \sin \phi)} \quad (58)$$

And the following non-linear softening law is adopted to describe the cohesion reduction process during the post-failure process:

$$c(\kappa) = c_0 - c_0 \cdot a(1 - e^{-b\kappa}) \quad (59)$$

$$d\kappa = \sqrt{\frac{3}{2}} d\boldsymbol{\varepsilon}^p : d\boldsymbol{\varepsilon}^p$$

where c_0 is the initial cohesion and a and b are constants. The plastic flow function can be simply defined as follow:

$$g = \alpha_\psi I_1 + \sqrt{J_2} \quad (60)$$

where α_ψ is a Drucker-Prager constant and is determined the same as Equation (58) where ϕ is substituted for the dilation angle, ψ . It is well-known that the value of dilation angle in granular materials evolves with the material state and tends to vanish at a critical state corresponding to zero volume change with material deformation [65]. To reproduce the evolution of dilation towards the critical state in this SPH framework, the dilation angle ψ is related to the development of accumulated plastic displacement by a presumed exponential function as follows:

$$\psi = \psi_0 e^{s_f |\boldsymbol{\varepsilon}^p|} \quad (61)$$

where ψ_0 is the initial dilation angle and s_f is the scale factor. Equation (61) implies that $\psi = \psi_0$ at the initial state and gradually approaches zero as the accumulated plastic strain develops, which corresponds to the progressive failure of granular columns. The rate of change of ψ toward zero is controlled by the scale factor s_f .

To solve the above constitutive equation for the stress update, it is preferable to adopt an advanced stress-return mapping algorithm [58]. On the other hand, the fully explicit solution of the above constitutive model takes the following form:

$$\dot{\boldsymbol{\sigma}} = \left(\mathbf{D}^e : - \frac{\mathbf{D}^e : \frac{\partial g}{\partial \boldsymbol{\sigma}} : \frac{\partial f^T}{\partial \boldsymbol{\sigma}} : \mathbf{D}^e}{\frac{\partial f^T}{\partial \boldsymbol{\sigma}} : \mathbf{D}^e : \frac{\partial g}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial \kappa} \sqrt{\frac{3}{2} \frac{\partial g}{\partial \boldsymbol{\sigma}} : \frac{\partial g^T}{\partial \boldsymbol{\sigma}}}} \right) : \dot{\boldsymbol{\epsilon}} \quad (62)$$

For large deformation analyses, an invariant stress rate with respect to rigid-body rotation must be enforced to the stress-strain relation. Therefore, the Jaumann stress-rate formulation is often adopted:

$$\dot{\boldsymbol{\sigma}}^J = \dot{\boldsymbol{\sigma}} - \boldsymbol{\omega} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \boldsymbol{\omega}^T \quad (63)$$

where $\boldsymbol{\omega}$ is the spin-rate tensor. Finally, the above stress-strain relation is discretised onto SPH particles and updated for every particle each time increment following the same procedure presented in [50].

3.2.3 Capturing pre- and post-localisation behaviour at particle level: a double scale approach to constitutive modelling

Classical continuum constitutive models can be written for a unit volume element, thanks to the assumption of homogeneous deformation, and hence can be used for a volume element of any size. In relation to the SPH, the particle size does not affect the behaviour of the constitutive model it uses, given homogenous deformation over the volume of the particle is the implicit assumption. However, localised failure in the form of fracture or localisation band makes the assumption of homogeneous deformation that continuum constitutive models are based on invalid. The deformation and nonlinear processes inside the localisation band dominate the inelastic response of the material, while the material outside this band usually undergoes elastic or negligible inelastic deformation. In such cases of localised failure, the behaviour of the volume element crossed by the localisation band is governed by behaviour of the localisation band, its size and orientation, in addition to the size and behaviour of the zone outside the band. A length scale related to the thickness of the localisation band is involved in the behaviour. Classical continuum models do not possess such a length scale and hence fails to correctly describe post-localisation behaviour. In the analysis of Boundary Value Problems involving localised failure, the material stability in such cases is lost, leading to the dependence of numerical solutions on the discretisation. Without enhancements, these classical continuum models cannot give correct and converging numerical solutions upon refinement of the discretisation and this is a common issue with any numerical method, including the SPH. A range of available different enhancements can be selected, such as higher-order theories [66-70], or simply artificial scaling of constitutive behaviour using smeared crack/deformation approach [71-73]. However, they are not always suitable in terms of versatility, simplicity and computational efficiency for SPH simulations of complex failure processes that usually involve the activation and deactivation of several cracks or localisation bands [60, 61]. A generic and systematic enrichment based on the mechanism of localised failure that can be applied to any existing constitutive model and particularly suitable for SPH is presented in this sub-section, based on our earlier developments [60, 61]. The struc-

ture of constitutive model is enriched to accommodate mesoscale details of the localisation band, including its orientation, thickness and behaviour. Given the fact that the localisation band thickness is usually very small, it is physically reasonable and computationally efficient to consider the case of a volume element represented by an SPH particle crossed by a localisation band.

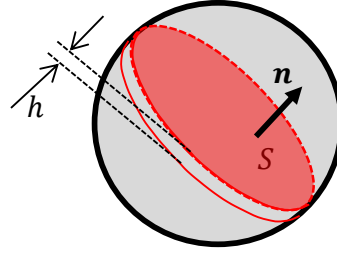


Figure 6. An SPH particle crossed by a localisation band of thickness h .

The strain rate inside the band $\dot{\epsilon}^i$ can take the following form [74]:

$$\dot{\epsilon}^i = \dot{\epsilon}^o + \frac{1}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} = \dot{\epsilon}^o + \frac{1}{2h} (\mathbf{n} \otimes \dot{\mathbf{u}} + \dot{\mathbf{u}} \otimes \mathbf{n}) \quad (64)$$

where $\mathbf{n}$ is the normal vector of the band, $\dot{\mathbf{u}}$ the velocity jump across the localisation band and $\dot{\epsilon}^o$ the strain rate outside the localization band. It is noted that all rate terms in this sub-section are pseudo rates, as all equations can be written in incremental forms. Rate forms are used just for the sake of simplicity in the presentation.

The volume averaged strain rate $\dot{\epsilon}$ is:

$$\dot{\epsilon} = f \dot{\epsilon}^i + (1 - f) \dot{\epsilon}^o \quad (65)$$

where f is the volume fraction of the localization zone. If an effective size H of the particle can be defined as $H = \frac{V}{S}$, where V is the volume of the particle and S the surface area of the localization zone (Figure 6), then the volume fraction f can be expressed as the ratio between the thickness of the localization band and the particle size H :

$$f = \frac{Sh}{V} = \frac{Sh}{SH} = \frac{h}{H} \quad (66)$$

Equations (64) and (65) can be used to obtain strain rates $\dot{\epsilon}^i$, and $\dot{\epsilon}^o$ in terms of the macro strain rate $\dot{\epsilon}$ and velocity jump $\dot{\mathbf{u}}$:

$$\dot{\epsilon}^o = \dot{\epsilon} - \frac{f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \quad (67)$$

In the same way, the strain rate inside the band can also be expressed in terms of $\dot{\epsilon}$ and $\dot{\mathbf{u}}$, as:

$$\dot{\epsilon}^i = \dot{\epsilon} + \frac{1-f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \quad (68)$$

Equations (67) and (68) indicate different strain rates outside and inside the localization zone, generated by the macro strain rate and the velocity jump between two surfaces of the localization band and reflecting the discontinuity of strain rates due to

localization. Associated with these strain rates are corresponding stress tensors outside and inside the localization band, denoted as $\boldsymbol{\sigma}^o$ and $\boldsymbol{\sigma}^i$, and different constitutive responses outside and inside the band. The relationships between macro stress $\boldsymbol{\sigma}$ and stresses outside ($\boldsymbol{\sigma}^o$) and inside ($\boldsymbol{\sigma}^i$) the localization band can be obtained using the virtual work equation, expressed as:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} = f \boldsymbol{\sigma}^i : \dot{\boldsymbol{\epsilon}}^i + (1 - f) \boldsymbol{\sigma}^o : \dot{\boldsymbol{\epsilon}}^o \quad (69)$$

Substituting equations (89)-(90) into the above expression of the virtual work and rearranging the obtained expression, we obtain:

$$\frac{1-f}{H} (\mathbf{t}^o - \mathbf{t}^i) \cdot \dot{\mathbf{u}} + [\boldsymbol{\sigma} - f \boldsymbol{\sigma}^i - (1 - f) \boldsymbol{\sigma}^o] : \dot{\boldsymbol{\epsilon}}^o = 0 \quad (70)$$

where $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$, $\mathbf{t}^i = \boldsymbol{\sigma}^i \cdot \mathbf{n}$ and $\mathbf{t}^o = \boldsymbol{\sigma}^o \cdot \mathbf{n}$ are the tractions associated with macro stress $\boldsymbol{\sigma}$, stress $\boldsymbol{\sigma}^i$ inside and stress $\boldsymbol{\sigma}^o$ outside the localisation zone, respectively. Since condition (70) must be met for any arbitrary rates $\dot{\mathbf{u}}$, and $\dot{\boldsymbol{\epsilon}}^o$, the following relationships are obtained:

$$\mathbf{t}^o = \mathbf{t}^i \quad (71)$$

$$\boldsymbol{\sigma} = f \boldsymbol{\sigma}^i + (1 - f) \boldsymbol{\sigma}^o \quad (72)$$

It can be proved that the above two relationships also lead to $\mathbf{t} = \mathbf{t}^o$ as continuity of traction across the whole volume element. As can be seen, there are three stress-strain relationships associated with the macro behaviour and the responses inside and outside the localisation band. While the macro strain rate exhibits a jump across the localization band, it is reasonable to assume homogeneous deformation inside and outside the localization band, and corresponding constitutive relationships in the following generic forms:

$$\dot{\boldsymbol{\sigma}}^o = \mathbf{D}^o : \dot{\boldsymbol{\epsilon}}^o = \mathbf{D}^o : \left[\dot{\boldsymbol{\epsilon}} - \frac{f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \quad (73)$$

$$\dot{\boldsymbol{\sigma}}^i = \mathbf{D}^i : \dot{\boldsymbol{\epsilon}}^i = \mathbf{D}^i : \left[\dot{\boldsymbol{\epsilon}} + \frac{1-f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \quad (74)$$

in which $\mathbf{D}^o$ and $\mathbf{D}^i$ are the tangent stiffnesses outside and inside the localization band, respectively.

Equations (71)-(74) can be used to obtain the macro stress – macro strain relationship as functions of constitutive responses inside and outside the localization band and the geometrical properties of the band (thickness and orientation). Substituting the rate constitutive equations (73) and (74) into the rate form of volume averaged stress, we obtain the macro stress:

$$\dot{\boldsymbol{\sigma}} = f \mathbf{D}^i : \left[\dot{\boldsymbol{\epsilon}} + \frac{1-f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] + (1 - f) \mathbf{D}^o : \left[\dot{\boldsymbol{\epsilon}} - \frac{f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \quad (75)$$

It can be seen that the velocity jump $\dot{\mathbf{u}}$ is needed for the calculation of the macro stress rate in the above equation, given macro strain rate $\dot{\boldsymbol{\epsilon}}$ as the input at the particle (or constitutive) level from the numerical methods for the solution of BVPs. The traction continuity $\mathbf{t}^i = \mathbf{t}^o$ in rate form is used for the determination of $\dot{\mathbf{u}}$. From the condition $\dot{\mathbf{t}}^i = \dot{\mathbf{t}}^o$ and constitutive relationships (73) and (74), we can write:

$$\mathbf{D}^i : \left[\dot{\boldsymbol{\epsilon}} + \frac{1-f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \cdot \mathbf{n} = \mathbf{D}^o : \left[\dot{\boldsymbol{\epsilon}} - \frac{f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \cdot \mathbf{n} \quad (76)$$

The above can be rearranged to obtain the velocity jump $\dot{\mathbf{u}}$ in term of macro strain rate $\dot{\boldsymbol{\epsilon}}$:

$$\dot{\mathbf{u}} = \left[\frac{1-f}{h} (\mathbf{n} \cdot \mathbf{D}^i \cdot \mathbf{n}) + \frac{f}{h} (\mathbf{n} \cdot \mathbf{D}^o \cdot \mathbf{n}) \right]^{-1} \cdot (\mathbf{D}^o - \mathbf{D}^i) : \dot{\boldsymbol{\epsilon}} \cdot \mathbf{n} \quad (77)$$

The described algorithm is an explicit stress return algorithm, based on the rate form of traction continuity, $\mathbf{t}^i = \mathbf{t}^o$. This is also used to obtain the tangent stiffness of the volume element crossed by a shear band. The readers can refer to Nguyen et al. [60] and Nguyen & Bui [61] for details and examples on an implicit stress return algorithm. The approach presented can be used with any existing constitutive models, given the generic forms (73) and (74) for constitutive responses outside and inside the localization zone, respectively. As can be seen in equations (75) and (77), the size H of the volume element, thickness h of the localization band, its orientation and constitutive responses of two separate regions (the band and the outside zone) appear in the constitutive structure. Models derived from this approach automatically possess a length scale h that is invariant with the discretization and can be considered as an intrinsic material property, and behavior at the mesoscale of the localization band. Therefore they can describe and correctly capture both pre- and post-localization responses at the constitutive (or particle) level [60, 61]. As a result, no ad hoc regularization is needed in the analysis of BVPs. This approach is suitable for any numerical methods for the solution of BVPs, and particularly the SPH, given it does not require any modification beyond the constitutive level, and can be used straightforwardly for an SPH particle. This also forms the basis for more advanced ones, with both elastic and inelastic responses outside the localisation band associated with the activation and deactivation of more than one localisation bands [75], or evolution of localisation band thickness associated with the transition from diffuse to localised failure [61]. From this general approach, simplified ones can be derived using assumption on the thickness of the localization band in relation to the size of the volume element containing it.

For localisation zone of very small thickness, if this thickness is also very small compared to the size of the volume element (or SPH particle) considered then the volume fraction f is very small: $f = \frac{h}{H} \ll 1$. Therefore $\dot{\boldsymbol{\epsilon}}^i$ in equation (68) can be approximated as [61-63]:

$$\dot{\boldsymbol{\epsilon}}^i = \dot{\boldsymbol{\epsilon}} + \frac{1-f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \approx \frac{1}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \quad (78)$$

The strain rate outside the localization zone can be rewritten as:

$$\dot{\boldsymbol{\epsilon}}^o = \dot{\boldsymbol{\epsilon}} - \frac{f}{h} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} = \dot{\boldsymbol{\epsilon}} - \frac{1}{H} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \quad (79)$$

Examples that are suitable for the above simplification include, but are not limited to, localised failure of geomaterials such as rocks, concrete under tension or shearing under sufficiently low confining pressures. In such cases, given very small physical thickness of the localization band, its responses can be described by a cohesive-frictional model for an idealised zero-thickness interface, using traction $\mathbf{t}^i$ and displacement jump $\mathbf{u}$. Therefore the stress $\boldsymbol{\sigma}^i$ and strain $\boldsymbol{\epsilon}^i$ are no longer needed. This cohesive-frictional interface model can be described in the following incremental form:

$$\mathbf{t}^i = \mathbf{K}^i \dot{\mathbf{u}} \quad (80)$$

where $\mathbf{t}^i = \boldsymbol{\sigma}^i \mathbf{n}$ is the traction and $\mathbf{K}^i$ the corresponding tangent stiffness of the interface.

For $f \rightarrow 0$, the macro stress $\boldsymbol{\sigma}$ coincides with the stress $\boldsymbol{\sigma}^o$ for the zone outside the localisation band:

$$\boldsymbol{\sigma} = f \boldsymbol{\sigma}^i + (1 - f) \boldsymbol{\sigma}^o \approx \boldsymbol{\sigma}^o \quad (81)$$

and the traction continuity (71) is expressed in the following form:

$$\boldsymbol{\sigma}^o \mathbf{n} - \mathbf{t}^i = \mathbf{0} \quad (82)$$

As traction and displacement jump are used to describe the behaviour inside the localisation zone, the simplified system now contains the following three key relationships:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^o = \mathbf{D}^o : \dot{\boldsymbol{\epsilon}}^o = \mathbf{D}^o : \left[\dot{\boldsymbol{\epsilon}} - \frac{1}{H} (\mathbf{n} \otimes \dot{\mathbf{u}})^{\text{sym}} \right] \quad (83)$$

$$\mathbf{t}^i = \mathbf{K}^i \dot{\mathbf{u}} \quad (84)$$

$$\boldsymbol{\sigma}^o \mathbf{n} - \mathbf{t}^i = \mathbf{0} \quad (85)$$

This simplified model, with the effects of thickness h of the localization band lumped into the fracture behaviour of the cohesive-frictional model (via fracture energies in both pure and mixed modes) has been extensively used in our groups for modelling geomaterial failure using the SPH [54, 57, 58], MPM [60-63, 76], and also the Finite Element Method (FEM; [77-79]).

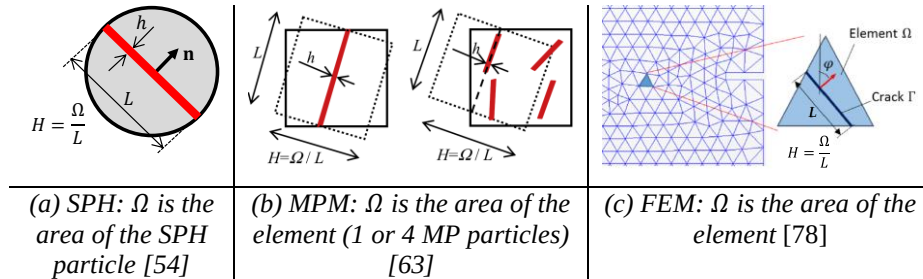


Figure 7. Determination of size H for 2D applications using SPH (a), MPM (b) and FEM (c).

The length H , as an effective size of an SPH particle, naturally appears in the structure of the constitutive model (Equations (83)-(85)) and allows scaling of the constitutive behavior of the SPH particle to correctly describe post-localization stage of failure. This is particularly an appealing characteristic for SPH, a truly mesh-free numerical method, as everything required for the proposed approach can be accessed at the particle level and interaction between constitutive models derived from the proposed approach and the SPH-based discretization is through the effective size H of the SPH particle, which is also the resolution of the discretization (Figure 11). This is different from FEM [77-79] and MPM applications [60-63, 76] in which involvement of element size in interfacing models derived from this approach with mesh-based methods

is required, given the resolution of the discretization is governed by the element size, not the size of the integration (or material) point (Figure 11).

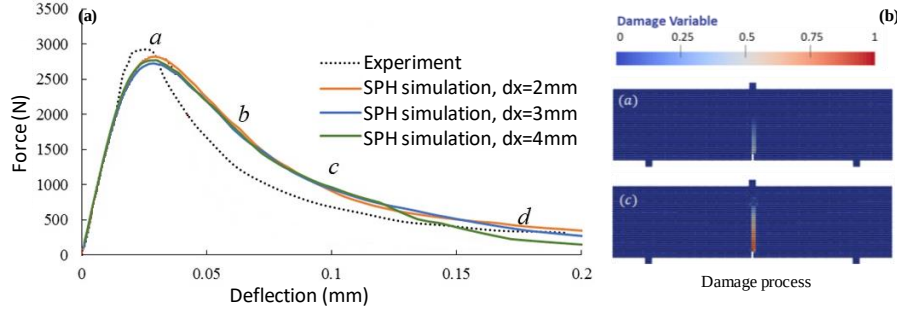


Figure 8. SPH simulation of three-point bending fracture [58].

The results of our SPH simulation of failure of a notched beam under three-point bending test in Figure 8a shows the insensitiveness of the numerical solution with respect to the resolution of the SPH discretization (Figure 8a), and damage contour at different stages of failure (Figure 8b). The constitutive behaviour for SPH in that simulation is based on the approach described above Equations (83)-(85), in combination with a mixed-mode cohesive-frictional model to describe the behaviour of the localization band idealized as a zero-thickness surface and embedded in the SPH particle. The behaviour of the fracturing SPH particle in such cases automatically scales with its size, thanks to the appearance of its size H in the constitutive equation.

3.2.4 How do I test the constitutive models implemented in SPH?

Once a particular constitutive model is implemented in SPH, it is important to ensure the SPH code can correctly reproduce the constitutive response. The reader would have noticed that it is not straightforward in SPH to perform an element test, like FEM. Thus, an alternative approach should be used. In our view, one of the first SPH tests that needs to pass to ensure the SPH code can correctly reproduce the constitutive response is to conduct the simple shear test [56, 80]. The geometry and setting of this test are shown in Figure 9. In this test, a representative soil element, which is formed by a group of SPH particles, is placed at the centrally located area and surrounded by boundary areas which are also modelled by a set of SPH particles with the same properties. Particles within the central area are allowed to move freely, while those located within the boundary area are enforced by a constant velocity field defined by:

$$v_{xi} = \zeta y_i \quad \text{and} \quad v_{yi} = 0 \quad (86)$$

where v_{xi} and v_{yi} is the horizontal velocity of particles within the boundary area, respectively; and ζ is a constant parameter defining the loading rate, which can be taken to be 0.01 [56].

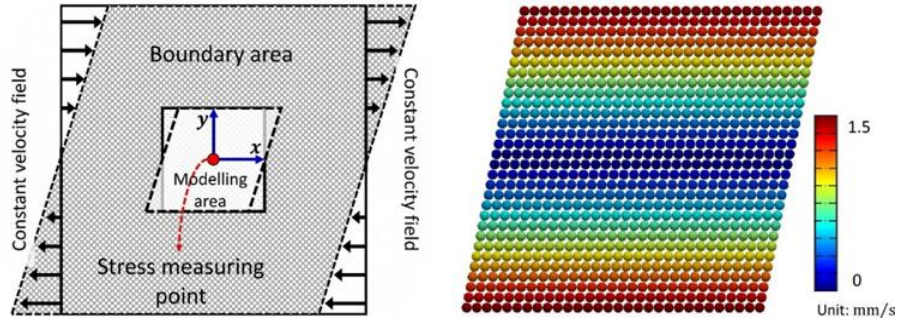


Figure 9. Setting of simple shear test for SPH simulations.

The responses of a constitutive model in SPH can be then checked by calculating the averaged normal and shear stresses of all SPH particles located within the central area, and comparing these results against those obtained from a single-element test using standard stress-updating algorithms. Figure 10 illustrates the performance of the MCG-SPH code⁵ for an advanced critical state-based constitutive model for sandy materials [81] through the simple shear tests for three different states of materials, i.e. dense, medium and loose sands. It can be seen that, under the current setting conditions, the simple test represents the undrained simple shear test conditions. The results indicate that the SPH method could reproduce well the stress-strain relationship and stress loading path of an advanced constitute model.

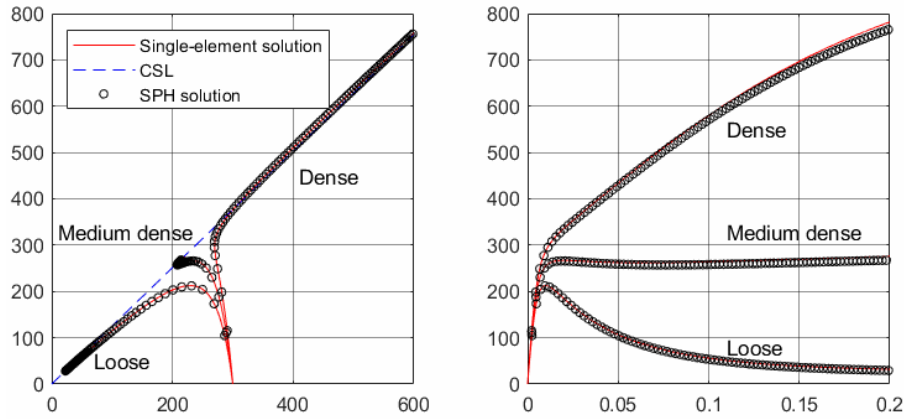


Figure 10. SPH modelling of simple shear test for SIMSAND model.

⁵ MCG-SPH code refers to the SPH code developed by the Monash Computational Geomechanics (MCG) Lab at Monash University, Australia.

3.3 Dissipated terms in SPH

The reader may have noticed that the SPH motion equation formulated in Section 3.1 is a fully dynamic equation⁶, i.e. Equation (43). In the absence of any dissipated terms, particles are subjected to free oscillations due to unbalanced forces, part of which is contributed by the errors introduced by the symmetric SPH operator such as Equation (23) and the rest is attributed by the zero-energy mode produced by the anti-symmetric kernel function with zero kernel gradient. Missing these dissipated terms can ultimately lead to the complete termination of the SPH computational process. It is noted that this is a common issue in dynamic simulations using numerical methods. A common way to suppress this numerical oscillations in SPH is to introduce the artificial viscosity term, which was originally proposed by Monaghan and Gingold [82]:

$$\mathbf{D}_{disp}|_i = \sum_{j=1}^N m_j \left(\frac{\alpha_d c_{ij} \pi_{ij} + \beta_d \pi_{ij}^2}{\rho_{ij}} \right) \cdot \nabla_i W_{ij} \quad (87)$$

with $\pi_{ij} = \frac{h_{ij} \mathbf{v}_{ij} \cdot \mathbf{r}_{ij}}{|\mathbf{r}_{ij}| + \epsilon h_{ij}^2}$

where α_d and β_d are two unknown constants, which are usually taken to be unity [40] or equal to 0.01 and 0 for granular materials [42], respectively; ρ_{ij} and h_{ij} are the mean density and smoothing length; $\epsilon = 0.01$ is a numerical parameter introduced to prevent numerical divergences; and c_{ij} is the sound velocity, which for solid materials is computed by $c_i = \sqrt{E_i/\rho_i}$ with E_i is the material elastic modulus. The artificial viscosity is added to the motion equation as follows:

$$\frac{d\mathbf{v}_i}{dt} = \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma} + \mathbf{g} \Big|_i = \sum_{j=1}^N m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij} - \mathbf{D}_{disp}|_i + \mathbf{g} \quad (88)$$

The introduction of the artificial viscosity to the momentum equation not only helps to suppress the numerical oscillations, but also mitigates issues related to pairing instability between SPH particles. However, the main drawback of this approach is that it introduces a large amount of dissipated energy to the system when a high value of α_d is adopted. Therefore, it is preferable to minimise the influence of this dissipated term in SPH simulations by setting these unknown parameters as small as possible. Bui et al. [42], through the investigation of the influence of this dissipated term on the granular flow, suggested that the second term involved β_d does not have strong influence on the behaviour of granular materials. They suggested that, for SPH applications adopting Cubic-spline function with $h = 1.2\Delta x$, $\alpha_d = 0.1$ seems to be suitable to most cases.

In view of the dissipated mechanism, an alternative approach was to replace the artificial viscosity with a viscous damping force per unit mass defined by [52]:

⁶ Dissipation due to plastic deformation is different from the dissipation discussed in this section. This raises an interesting question if visco-plastic constitutive models would help to suppress these numerical oscillations, which could be an interesting topic for future investigations of SPH.

$$\mathbf{D}_d|_i = c_d \mathbf{v}_i \quad (89)$$

where c_d is a damping coefficient, which can be computed by $c_d = \xi \sqrt{E/\rho h^2}$ [10] with ξ being a non-dimensional damping coefficient that requires calibrations for different applications.

It is argued that the above viscous damping force has more physical meaning compared to the artificial viscosity because the damping coefficient is directly linked to material properties. Thus, once the non-dimensional parameter is calibrated for a certain type of material, the damping coefficient will purely depend on the material properties, unlike the artificial viscosity. Nevertheless, this viscous damping force needs to be used together with the stress regularisation to avoid the inherent short-length-scale noise in the stress profile of SPH simulations [52].

3.4 Tensile instability issue in SPH

Different from the pairing instability discussed in Section 2.3, which is mainly caused by the misuse of the kernel function, the SPH tensile instability is caused by negative pressures/stresses, resulting in the attraction force between a pair of SPH particles causing particles to move closely to each other (i.e. clumping). This instability was originally studied by Swegle et al. [31], who related it to the sign of the stress and the second derivative of the interpolating kernel. However, they did not recognise the mechanism of pairing instability caused by the misuse of the kernel function, and thus incorrectly described both instability mechanisms using the same criterion. Furthermore, the cubic-spline kernel function used in their study appears to be suffered the most from pairing instability, as demonstrated in Section 2.3. There have been several attempts to remove this instability using different approaches [83, 84]. However, in our view, the most effective and successful has been the artificial pressure/stress method proposed by Monaghan [85] for fluids and was subsequently generalised by Gray & Monaghan [47] for elastic solid. The key idea of this method is to introduce a small repulsive force between a pair of neighbouring particles by using an artificial stress term to prevent them from getting closer when two particles are in a state of tensile stress.

Within the context of geomechanics applications, Bui et al. [42] was the first who demonstrated that, for non-cohesive granular materials, tensile instability issues is almost unrecognised and can be completely removed by adopting a tension cracking treatment, which removes undesirable negative stresses from the numerical simulation. This treatment is physically correct for non-cohesive granular materials as these materials in principle cannot carry any tensile stress, unless they are under unsaturated

conditions, which is out of the scope of this discussion. On the other hand, for cohesive frictional granular materials, it is inevitable to avoid the possibility of tensile instability in SPH simulations because there always exists a tension zone in the yield surface space of these materials, which is corresponding to the negative stress zone.

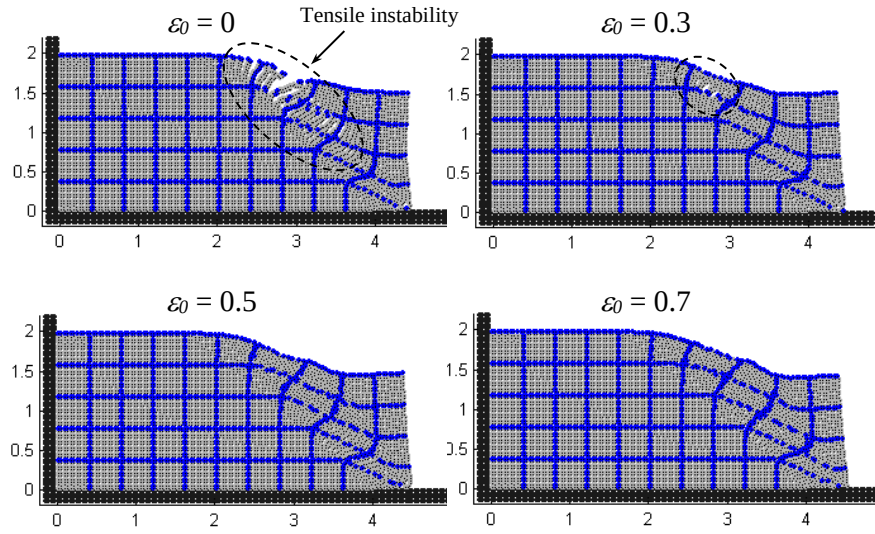


Figure 11. The tensile instability in cohesive-frictional granular materials was removed by the artificial stress method. The exponent n was kept constant at 2.55 [42].

To mitigate this issue, the artificial stress method can be adopted and is defined as follows [47]:

$$\mathbf{F}_\sigma|_i = \sum_{j=1}^N m_j f_{ij}^n (\mathbf{R}_i + \mathbf{R}_j) \cdot \nabla_i W_{ij} \quad \text{with} \quad f_{ij} = \frac{W_{ij}(\mathbf{x}_{ij}, h)}{W(\Delta x, h)} \quad (90)$$

where n is the exponential factor depended on the smoothing kernel, which can be chosen from the dispersion equation analysis [47]; and Δx is the initial particle spacing. For the cubic-spline kernel function, the ratio $W_{ij}/W(\Delta x, h)$ has the value 4 if $h = \Delta x$, and if $h = 1.2\Delta x$ (the typical h for the cubic-spline function), the ratio is about 2.55. Gray and Monaghan [47] suggested the best choice of n when applying SPH for elastic solid is 4. However, Bui et al. [42] found that this choice cannot be used for cohesive-frictional soil as f_{ij} will increase by a factor of about 42 as $|\mathbf{x}_{ij}|$ decreases from Δx to zero. This may sometimes lead to numerical instability. For most of general SPH applications to simulate cohesive-frictional granular materials, the ex-

ponential factor n should be chosen to be 2.55, and therefore for $h = 1.2\Delta x$, f_{ij} increases by a factor of about ~ 11 as $|\mathbf{x}_{ij}|$ decreases from Δx to 0; while this force decreases rapidly according to $(|\mathbf{x}_{ij}| - 2h)^{3n}$ in the domain $h \leq |\mathbf{x}_{ij}| \leq 2h$. This ensures that the effect of the artificial stress is confined to nearest neighboring particles. The effectiveness of the artificial stress method in removing the tensile instability in non-cohesive frictional granular materials was demonstrated in Bui et al. [42], as shown in Figure 11 for different value of constant parameter ε_0 . The recommended value was $\varepsilon_0 = 0.5$ for SPH simulations adopting the cubic-spline kernel function with the smoothing length of $h = 1.2\Delta x$. It is noted that although this is the recommended value for cohesive granular materials, sensitive studies are required for different kernel functions with a different range of interpolation domain. Also, when investigating the tensile instability issue, it is important to distinguish this issue from the pairing stability, which is mainly caused by the misuse of smoothing length of a particular kernel function.

Here, we further present the procedure to extend this artificial stress method to 3D condition. The artificial stress tensor $\mathbf{R}_i$ for particle i is calculated according to the following procedure:

$$\hat{\mathbf{R}}_i = -\varepsilon_0 \frac{\langle \hat{\boldsymbol{\sigma}}_i \rangle}{\rho_i^2} \quad (91)$$

where $\langle \cdot \rangle$ indicates the Macaulay brackets; $\hat{\mathbf{R}}_i$ is the diagonal component of the artificial stress tensor $\mathbf{R}_i$; ε_0 is a constant parameter ranging from 0 to 1, though the recommended value for granular materials is 0.5 [42]; and $\hat{\boldsymbol{\sigma}}_i$ is the diagonal stress tensor of the particle i , with non-diagonal component of $\hat{\boldsymbol{\sigma}}_i$ being zero; and the hat indicates that the tensors are taken in coordinate where $\boldsymbol{\sigma}_i$ is a diagonal. Consequently, the procedure to obtain $\mathbf{R}_i$ is as follows:

1. $\hat{\boldsymbol{\sigma}}_i$ is obtained by diagonalising $\boldsymbol{\sigma}_i$
2. $\hat{\mathbf{R}}_i$ is calculated from $\hat{\boldsymbol{\sigma}}_i$
3. $\mathbf{R}_i$ is obtained by rotating $\hat{\mathbf{R}}_i$ back to the original coordinate system

Given $\boldsymbol{\sigma}_i$ is a symmetric matrix, we have $\boldsymbol{\sigma}_i = \mathbf{Q}_i: \hat{\boldsymbol{\sigma}}_i: \mathbf{Q}_i^T$, where $\hat{\boldsymbol{\sigma}}_i$ is a diagonal matrix containing the eigenvalues of $\boldsymbol{\sigma}_i$ and the columns of $\mathbf{Q}_i$ corresponding eigenvectors. The eigenvalue (3×3) matrix are the zeros of the polynomial of degree 3, and thus can be computed by direct methods, i.e. by Cardano's formula and the eigenvectors by vector cross product [86]. However, if the eigenvalues differ very much in size, this method computes the small eigenvalues with a low relative accuracy due to rounding errors. Therefore, one can use the hybrid method defined in [86]: Cardano's formula is used as the default method, but if an error estimate indicates that the resulting eigenvalue may be inaccurate, the eigenvalues are calculated iteratively by the QL

algorithm, where $\boldsymbol{\sigma}_i$ is decomposed into an orthogonal matrix $\mathbf{Q}_i$ and a lower triangular matrix $\mathbf{L}$ by a sequence of plane rotations and using implicit shifting to accelerate the convergence. Once evaluated, the artificial stress $\mathbf{F}_\sigma|_i$ can be simply added to the momentum equation, we have:

$$\frac{d\mathbf{v}_i}{dt} = \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma} + \mathbf{g} \Big|_i = \sum_{j=1}^N m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla_i W_{ij} - \mathbf{D}_{disp} \Big|_i + \mathbf{F}_\sigma \Big|_i + \mathbf{g} \quad (92)$$

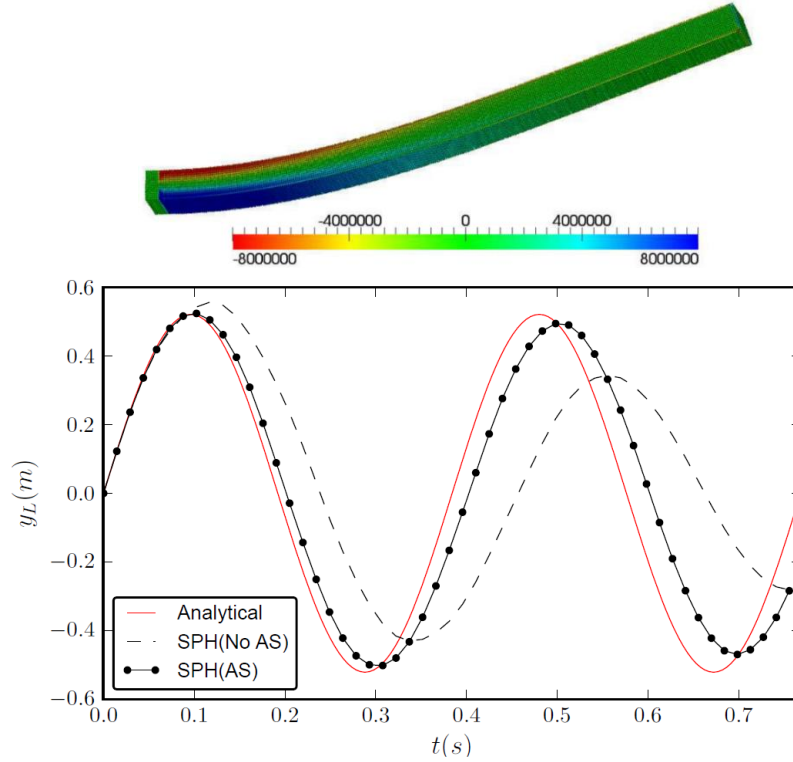


Figure 12. Distribution of horizontal stress in an oscillating elastic beam shown at maximum deformation and the time evolution of the end bar (AS=Artificial Stress)⁷.

The robustness of the artificial stress method in removing the tensile instability under 3D conditions is shown in Figure 12. In this test, an elastic beam with a rectangular cross-section of $(b \times d) = (0.2 \times 0.1)m$ and length of $L = 2m$ is fixed at one end

⁷ This result was a part of the collaborative works (unpublished) between MCG Lab and Prof. D. Roose from KU Leuven University. The work was conducted by Y.R. Lopez under the supervision of Bui and Roose in 2014.

and free at the other end. Initially, the beam is excited by an initial velocity field, following its natural frequency. The elastic material properties of the beam are set to the shear modulus of $G = 0.22\rho c^2$ and Poisson's ratio $\nu = 0.3$. The results are then compared to the standard analytical solution for an elastic beam oscillation. With the help of the artificial stress method, the stress profile shown in Figure 12 does not show any sign of tensile instability (i.e. particle separation and stress noise). Furthermore, the oscillation of the free-end shows a reasonable agreement with the analytical solution. The difference in the frequency was attributed to the dissipated term, which can be further fine-tuning to match the analytical solution.

3.5 *Boundary conditions in SPH*

Like any other numerical methods, the treatment of boundary conditions in SPH is required to facilitate its applications to a wide range of engineering problems. Several specific boundary conditions that are commonly encountered when applying SPH to the geotechnical engineering field are discussed below.

3.5.1 **Solid boundary conditions**

Fully-fixed and free-slip (or free-roller) conditions are two typical boundary conditions commonly encountered in geotechnical applications. In FEM and other numerical methods, these boundary conditions can be straightforwardly imposed by specifying specific conditions on material nodes/points on the solid interface. In SPH, although it is possible to directly impose such prescribed boundary values to particles, there exist issues associated with particles close to the solid boundary. For example, when an SPH particle approaches the solid boundary, the kernel interpolation domain of the particle will be truncated by the boundary and resulting in the low accuracy of SPH interpolation. Two typical methods, which are the root of all existing boundary treatment methods, have been developed to deal with these type of SPH solid boundary conditions, including the ghost-particle approach [87] and virtual-particle approach [88, 89]. The former approach is more suitable for free-slip (or symmetric) boundary conditions, while the latter one is suitable for modelling fully-fixed boundary conditions. While the ghost-particle approach [87] can be directly used to replicate the free-slip boundary conditions suitable for most geotechnical problems [42], the virtual-particle approach [88, 89] required further improvement to accommodate stress boundary conditions suitable for wider geomechanics applications. This was achieved in the work of Bui et al. [42] and thus will not be repeated here.

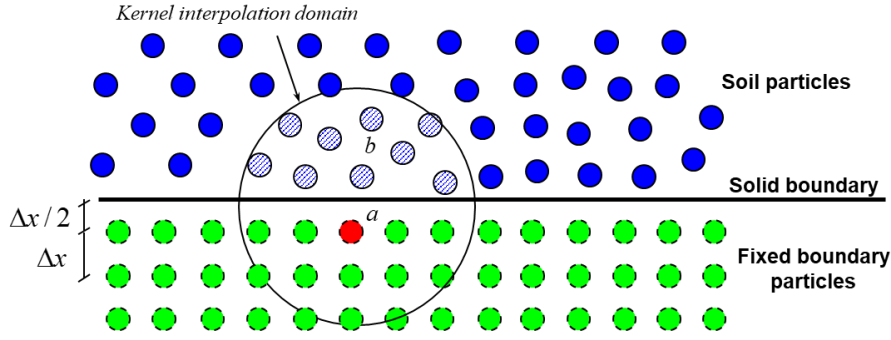


Figure 13. Arrangement of boundary and real particles in SPH.

Alternative to the combined approach that requires to create ghost- and virtual-particles to model the free- and fully fixed-boundary conditions, respectively, a simpler approach which makes use of one set of particles (namely fixed boundary particles), can be used to replicate both boundary conditions [49, 90]. Figure 13 outlines the setup for this type of boundary condition. In this approach, three or four layers of fixed boundary particles (depending on the extent of the kernel interpolation domain) are used to represent the solid boundary, with the first layer placed at a distance of $0.5\Delta x$ away from the boundary in the normal direction. These boundary particles carry all essential information as required for material particles, but their properties are directly interpolated from adjacent material particles [49, 90]. For fully fixed boundary condition, the following conditions are imposed to fixed boundary particles:

$$\mathbf{v}_a = - \sum_j \frac{m_b}{\rho_b} \mathbf{v}_b \tilde{W}_{ij} \quad \text{and} \quad \boldsymbol{\sigma}_a = \sum_j \frac{m_b}{\rho_b} \boldsymbol{\sigma}_b \tilde{W}_{ab} \quad (93)$$

For free-slip boundary condition, the following conditions are imposed to fixed boundary particles:

$$\mathbf{v}_{a,n} = \sum_b \frac{m_b}{\rho_b} (\mathbf{v}_{a,n} - 2\mathbf{v}_{b,n}) \tilde{W}_{ab} \quad \text{and} \quad \mathbf{v}_{a,t} = \sum_b \mathbf{v}_{b,t} \tilde{W}_{ab} \quad (94)$$

$$\sigma_a^{\alpha\beta} = \begin{cases} \sum_b \frac{m_b}{\rho_b} \sigma_b^{\alpha\beta} \tilde{W}_{ab} & \alpha = \beta \\ - \sum_b \frac{m_b}{\rho_b} \sigma_b^{\alpha\beta} \tilde{W}_{ab} & \alpha \neq \beta \end{cases} \quad (95)$$

where α and β represent the Cartesian coordinate; $\tilde{W}_{ab} = W_{ab}/(\sum_b m_b/\rho_b W_{ab})$ is the normalised kernel operator; $\mathbf{v}_{a,n}$ and $\mathbf{v}_{a,t}$ are the normal and shear velocity components with respect to the boundary surface of material particle b ; and σ_a is the stress tensor of boundary particle a .

3.5.2 Flexible confined stress boundary

While the solid boundary conditions can be reasonably well modelled using either ghost or virtual particles, it is not straightforward to extend this approach to model flexible confining stress boundaries. One of the key reasons is because this type of boundary condition often involves complex moving surface boundary, making it difficult to create a required number of boundary layers of ghost/virtual particles. Therefore, it is desirable to develop a robust approach that does not require creating ghost/virtual particles, while can still impose the required confining stress to flexible boundaries. Such an approach was recently proposed in [56] by making use of kernel truncation properties of SPH kernel approximations near boundaries [10]. The key idea behind this approach is illustrated in Figure 14. Consider a continuum body Ω of arbitrary shape represented by a set of SPH particles. If one wants to automatically impose a constant confining pressure σ_c on the interface of the continuum domain, all they need to do is to assign a constant pressure field to all SPH particles representing the body Ω , and adding the following confining stress term to the momentum equation of each SPH particle:

$$\mathbf{P}_{\sigma_c}|_i = \sum_{j=1}^N \frac{m_j}{\rho_i \rho_j} (\sigma_{ci} + \sigma_{cj}) \cdot \nabla_i W_{ij} \quad (96)$$

The reader would have wondered why the above additional term produces the constant confining stress σ_c on the surface S of the continuum body Ω , while not altering the internal forces acting on SPH particles located inside the interface (i.e. particle represents an element dV). To demonstrate this concept, let us rewrite Equation (96) in the following kernel integral form:

$$\mathbf{P}_{\sigma_c}|_i = \sum_{j=1}^N \frac{m_j}{\rho_i \rho_j} (\sigma_{ci} + \sigma_{cj}) \nabla_i W_{ij} = \frac{1}{\rho_i} \int_{\Omega} (\sigma_{ci} + \sigma_{cj}) \nabla_i W_{ij} dV_j \quad (97)$$

where dV_j is the volume of particle j or a volume element j . The above kernel integral can be further extended as follows:

$$\begin{aligned} & \frac{1}{\rho_i} \int_{\Omega} (\sigma_{ci} + \sigma_{cj}) \nabla_i W_{ij} dV_j \\ &= \frac{1}{\rho_i} \int_{\Omega} (\sigma_{cj} - \sigma_{ci}) \nabla_i W_{ij} dV_j + \frac{1}{\rho_i} \int_{\Omega} (2\sigma_{ci}) \nabla_i W_{ij} dV_j \end{aligned} \quad (98)$$

Because the confining pressure is constant everywhere on the domain Ω , the first term on the right-hand side of Equation (98) vanishes for every particle representing Ω . The remaining term can be further analysed by applying the divergence theorem, which converts the volume integral to the surface integral, we have:

$$\frac{1}{\rho_i} \int_{\Omega} (2\sigma_{ci}) \nabla_i W_{ij} dV_j = -\frac{2\sigma_{ci}}{\rho_i} \left(\int_S W_{ij} \vec{n} ds \right) \quad (99)$$

where S is the surface of the volume Ω and $\vec{n}$ is unit vector normal to S . The above surface integral is zero everywhere within Ω , such as for SPH particle i representing element dV in Figure 14, which can be attributed to the symmetric property of the kernel function W_{ij} . In order words, if the kernel interpolation domain of a particle

representing Ω is closed or not truncated, its surface integral will theoretically vanish⁸. However, this is not the case for particle representing element dV' , which located close to the surface boundary S of the domain Ω . In this case, the above surface integral can be written as follows:

$$-\frac{2\sigma_{ci}}{\rho_i} \left(\int_{S'} W_{ij} \vec{n} ds \right) = -\frac{2\sigma_{ci}}{\rho_i} \int_{ac} W_{ij} \vec{n}_2 ds - \frac{2\sigma_{ci}}{\rho_i} \int_{abc} W_{ij} \vec{n}_3 ds \quad (100)$$

where $\vec{n}_2$ and $\vec{n}_3$ are unit vectors normal to surface sections ac and abc as shown in Figure 14, respectively. The reader can immediately see that the last term in Equation (100) is again vanished due to the closed surface abc , while the first term is indeed the surface integral of the confining stress over the surface ac . This results in the confining force acting on the element dV' in the direction opposite to the normal vector $\vec{n}_2$. As a result, the additional confining stress term in Equation (96) is simplified to:

$$\mathbf{P}_{\sigma_c}|_i = \sum_{j=1}^N \frac{m_j}{\rho_i \rho_j} (\sigma_{ci} + \sigma_{cj}) \nabla_i W_{ij} = -\frac{2\sigma_{ci}}{\rho_i} \int_S W_{ij} \vec{n} ds \quad (101)$$

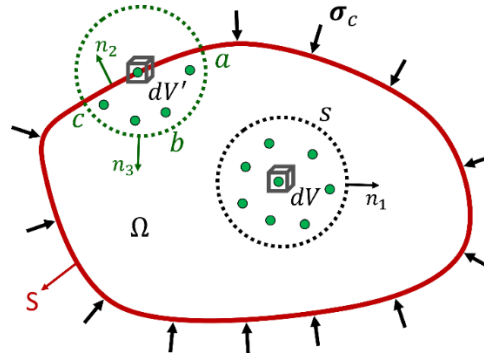


Figure 14. Illustration of the proposed confining boundary condition [56].

Equation (101) indicates that the confining stress term only works on particles located close to the interface surface of the domain Ω , and thus can be used to impose the confining stress to the surface of the domain Ω . At this point, the reader may have noticed that the above confining stress is multiplied by 2 and wonders if the above equation exactly reproduces a constant confining stress σ_c on the surface of the domain Ω . Our numerical investigation [56] has confirmed that this multiplication is required to exactly reproduce the desirable confining stress. Finally, since all we need in this approach is the locations of particles and a constant confining stress σ_c assigned to all SPH particles, the above method can be applied to any complex and moving surface interfaces without any difficulty. However, in practical applications of SPH,

⁸ Here we have ignored the interpolation error.

it is recommended that the above confining stress term is only applied to particles located close on the surface area to avoid numerical errors introduced by the errors associated with the SPH kernel estimation. This involves an additional step to specify those particles located close to the confining stress boundary. A straightforward approach to specify these SPH particles is to again make use of the SPH kernel truncation, which results in the following empirical criteria [56]:

$$f_i = \begin{cases} \leq 0.55 & \text{in } 2D \\ \leq 0.70 & \text{in } 3D \end{cases} \quad (102)$$

where f_i is an index parameter calculated by $f_i = \sum_{j=1}^N m_j / \rho_j W_{ij}$.

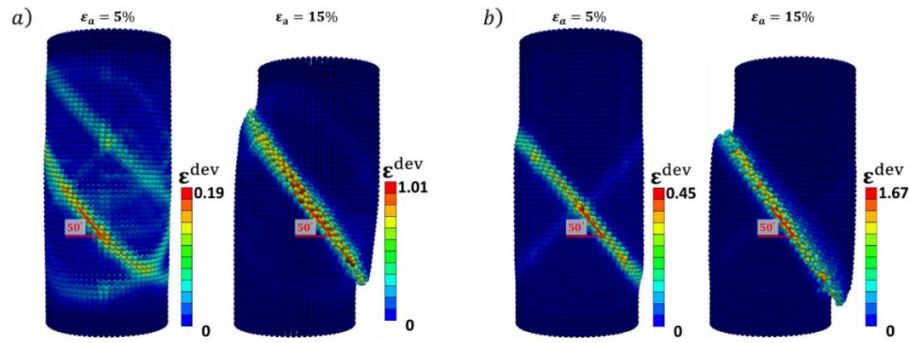


Figure 15. Deformation of soil specimens in triaxial shear tests under a) 50kPa confining stress b) 100kPa confining stress [56]⁹;

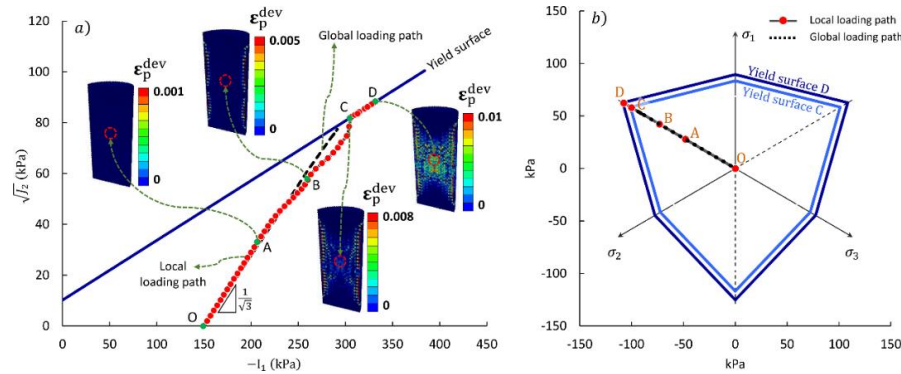


Figure 16. Stress loading paths in the triaxial test [56].

⁹ Details of model setting and material properties for simulations presented in this section can be found S. Zhao, H. H. Bui, V. Lemiale, G. D. Nguyen, and F. Darve, "A generic approach to modelling flexible confined boundary conditions in SPH and its application," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 43, no. 5, pp. 1005-1031, 2019.

The effectiveness of this approach in capturing a complex moving interface subjected to a constant confining stress can be demonstrated in SPH simulations of a triaxial test shown in Figure 15 [56]. In this test, a cylinder soil specimen with a dimension of 25mm in diameter and 100mm in height was subjected to shearing under a constant confining stress of 50kPa. The soil was modelled by the general elasto-plastic constitutive model with the Mohr-Coulomb yielding criterion. The confining stress was facilitated by the constant confining pressure to all SPH particles at the beginning of the simulation and kept constant throughout the simulation. Thanks to SPH kernel approximation features, the confining stress was automatically enforced to all particles located close to the membrane boundary and automatically updated as the sample deformed (Figure 15). The reader would have noticed that this method does not require any extra computational efforts to determine normal vectors of the confining curvature boundary, which are commonly required in other numerical methods to enforce the confining stress boundary. The loading path was well maintained until the structural failure of the soil specimens occurred (i.e. localised failure) where the stress loading path was slightly off the expected loading path. Nevertheless, it was well maintained under the three-dimensional space as shown in Figure 16.

3.6 Time integrations

The SPH governing equations written in the form of time-dependent ordinary differential equations can be integrated using standard numerical techniques such as the second-order accurate leapfrog (LF), predictor-corrector and Runge-Kutta (RK) schemes. In practice, the leapfrog algorithm is very popular for its low memory storage required in the computation and the efficiency for one force per step and hence it is used in all applications presented in this note. In the LF scheme, field variables ($\mathbf{A}$) such as velocities, density and stresses are advanced at mid time-steps, while the positions ($\mathbf{x}$) are advanced in a full time-steps:

$$\mathbf{A}_{t+\Delta t/2} = \mathbf{A}_{t+\Delta t/2} + \Delta t \left(\frac{d\mathbf{A}}{dt} \right)_{t+\Delta t/2} \quad (103)$$

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \Delta t \left(\frac{d\mathbf{x}}{dt} \right)_{t+\Delta t/2} \quad (104)$$

The stability of the LF time integration scheme is governed by the so-called CFL (Courant-Friedrichs-Levy) condition, which results in a time-step proportional to the smoothing length:

$$\Delta t \leq C_{CFL} h / c \quad \text{with} \quad c = \sqrt{E/\rho} \quad (105)$$

where c is the sound speed of the material; E is the elastic modulus of the material; and C_{CFL} is a constant, which is typically taken to be 0.1.

3.7 Parallel computing with SPH

One of the key advantages of SPH in geotechnical applications is its capability to handle large deformation and flow failure behaviour of geomaterials. However,

because of the mesh-free nature, the method generally leads to more computational cost and becomes very expensive for large-scale applications. In such case, it is desirable to develop a scalable parallel computing SPH code to broaden its use cases. Of many existing parallelisation approaches which can be used to speed up an SPH code, we are interested in developing distributed-memory parallelism using the Message Passing Interface (MPI). The choice of MPI is common for short-range interaction particle methods such as SPH as it is relatively straightforward to parallelise, allows us to access more computational resources, and can be extendable to hybrid MPI-GPU approaches (reserved for future work). The readers are referred to our recent publication in [90] for the detailed algorithm. Here, we only summary key steps required to develop an MPI code and demonstrate the performance of our high-performance MCG-SPH code suitable for large scale geophysical applications. The key steps required to develop a scalable parallel SPH code include:

1. **Domain participation:** We adopted the Orthogonal Recursive Bisection (ORB) algorithm, which subdivides the domain into bounding boxes whose faces/edges are co-axial with the Cartesian axes and each MPI process is assigned a box (Figure 17). The boundaries of these domains are updated occasionally, depending on the motion of the particles in the simulation.
2. **Physical particle distribution:** This step, which occurs every time-step, involves the redistribution of real SPH particles that have crossed subdomain boundaries.
3. **Halo distribution:** The step involves the redistribution of halo particle information, which also occurs every time-step. The halo particles are copies of real particles that are located within a kernel radius of another subdomain boundary (Figure 17). Halo particles are necessary for ensuring that real particles within subdomains have the necessary particle neighbours to perform SPH interpolations. In some cases, where SPH particles' stress tensor is updated based on strain-rate, a second exchange of information is required to update halo particles' stress tensor.

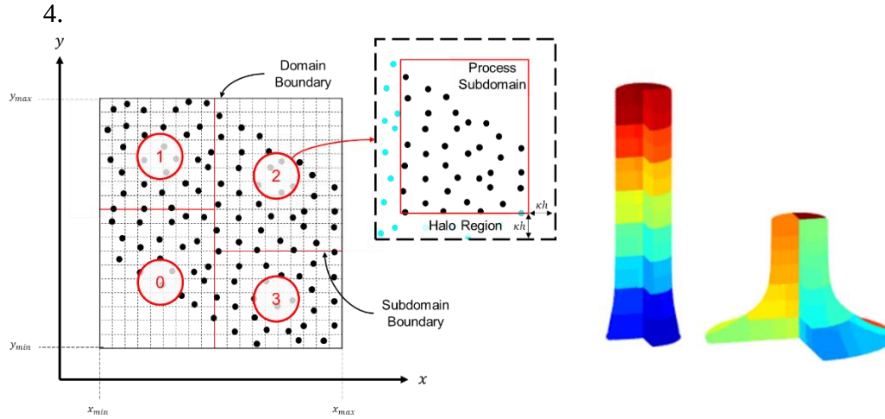


Figure 17. Computational domain participation strategy in SPH

Figure 18 demonstrates the efficiency of the code for a test case of 32 million real SPH particles, the parallel scheme obtains a speedup of more than 900 times (~90%

efficiency) at 1,024 CPU cores. A demonstration of a use case is the simulation of the Mt St Helens debris flow event that occurred in 1980, which involved 2.9 billion cubic meters of deposit over 62 million square meters and over \$3 billion in damages (USD, inflation adjusted) and 57 lives lost.

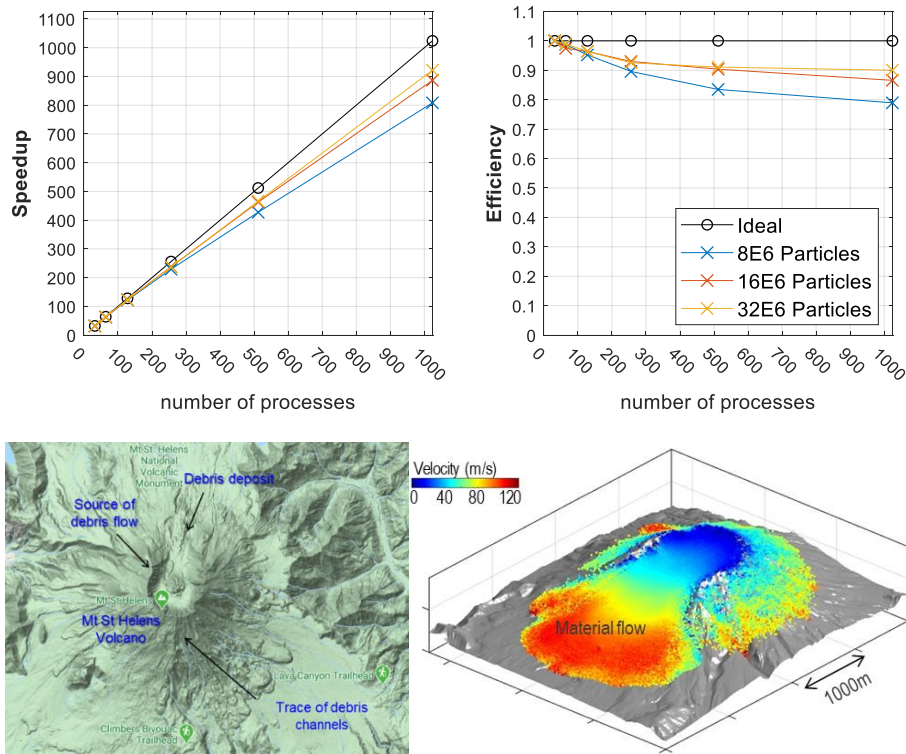


Figure 18. Computing efficiency and application of SPH to simulate field-scale applications

4 Some specific applications in geomechanics

4.1 Traditional geomechanics applications, basic tests

When it comes to assessing a new numerical method, the first question we would ask is: *how is the new method compared with the existing ones?* The finite element method (FEM) is well-known for its capability to predict high-accurate solutions for small deformation problems. Therefore, it is a good idea to benchmark SPH against FEM for small deformation problems such as the bearing capacity and slope stability problems. Figure 19 shows a comparison between SPH and FEM (Plaxis) for the prediction of load-bearing capacity and shear-banding development in the soil, which was

previously reported in [91]. In both models, the soil was simulated using an elastic-perfectly plastic model following the Drucker-Prager yield criterion. The FEM analysis was conducted using Plaxis with two different FEM elements (6-node and 15-node elements). It can be seen that the SPH code could reproduce very well both the load-displacement curve and the shear band development in the model predicted by FEM. The SPH result was even closer to the FEM result using high-accuracy elements (i.e. 15-node).

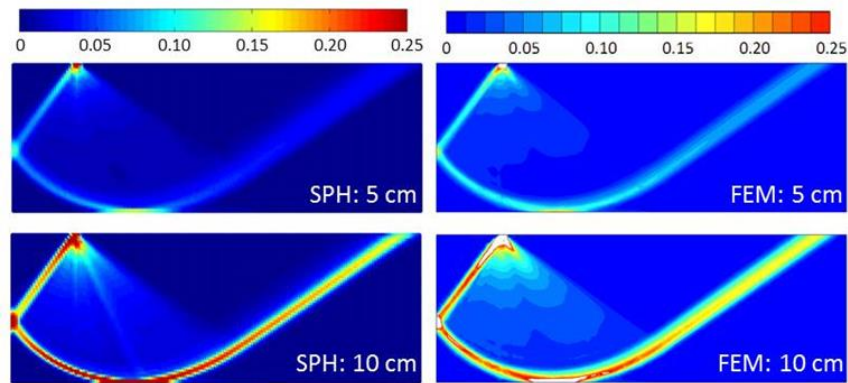
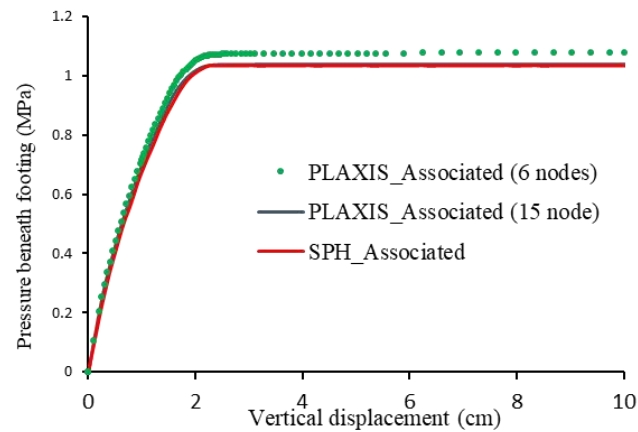


Figure 19. Comparison between SPH and FEM for bearing capacity problems

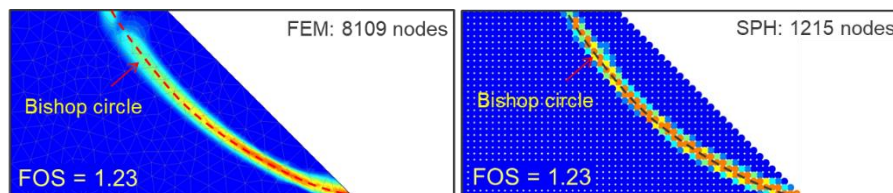


Figure 20. Comparison between SPH and FEM for slope stability problems

Figure 21 shows the comparison between SPH and FEM for the slope stability problem. In both methods, a simple cut-slope was analysed using the Mohr-Coulomb elasto-plastic constitutive model with a friction of 31.2° and cohesion of 0.55kPa . FEM (Plaxis) used 8109 nodes to represent the slope, while SPH only utilised 1215 particles. The slope was subjected to gravity load and the shear strength reduction method [92] was applied to bring the slope to failure. It can be seen that SPH can exactly reproduce the potential failure surface predicted by FEM. Both methods result in the same factor of safety of $\text{FOS} = 1.23$. However, the FEM could not simulate the post-failure process of the slope, as shown in Figure 21, while SPH can simulate the entire failure process. This suggests that SPH could reproduce similar results to FEM for small deformation problems, while having advantages in predicting large deformation and flow-failure problems, which will be demonstrated in subsequent sections.

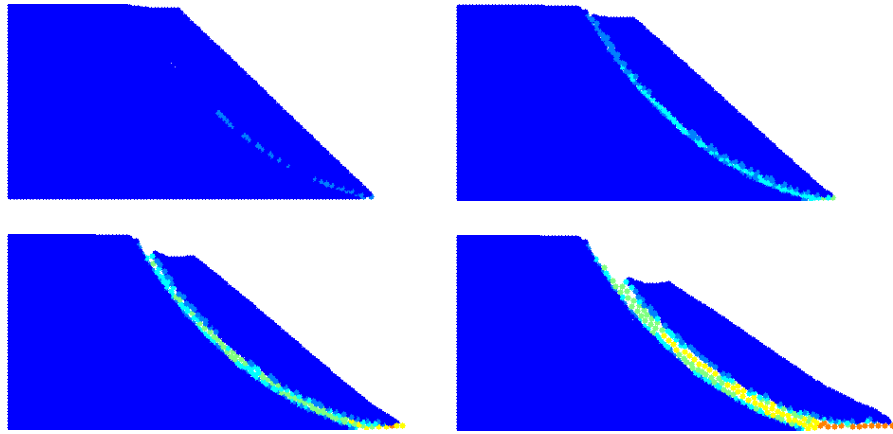


Figure 21. Progressive failure of a cut-slope predicted by SPH.

4.2 SPH applications to model granular flows¹⁰

One of the attractive features of SPH is its capability to simulate large deformation and post-failure behaviour of geomaterials. In this section, the capability of SPH in simulating granular flows is demonstrated by simulating column collapse of non-cohesive frictional granular materials, and numerical results are benchmarked against experimental data. First, the 2D progressive collapse and deposit morphologies of granular columns predicted by SPH simulations are compared with the 2D flow experiment of aluminium bars reported in [12] for two initial aspect ratios a of 0.5 and 1.0 (i.e. the ratio of column high to column width). The granular material is modelled using the general elasto-plastic constitutive model following the Drucker-Prager

¹⁰ Details of model setting and material properties for simulations presented in this section can be found in N.H.T. Nguyen, H.H. Bui and G.D. Nguyen, "Effects of material properties on the mobility of granular flow," *Granular Matter*, vol. 22, p. 59, 2020.

yielding criterion described in Section 3.2.2. Figure 22 presents a comparison between SPH simulations and the 2D experiments for the progressive collapse of granular columns with the initial aspect ratios a of 0.5 and 1, respectively. The SPH model can predict fairly well the collapse process of the granular columns in both experiments, both in term of the evolution of surface morphology and the run-out distance. To further demonstrate the capability of SPH in predicting the run-out distance of granular flows, a series of SPH simulations of granular collapse test was conducted for a range of initial aspect ratios (from 0.25 to 10), and the results are compared with data obtained from the 2D experiments [12] and the literature, as shown in Figure 23. The SPH results (red squares) agree well with their experimental counterparts (blue diamonds) when the initial aspect ratio a ranges from 0.25 to 10, and falling well within a range of data collected in the literature. This suggests that SPH with the Ducker-Prager elasto-plastic constitutive model can predict well the behaviour of granular flows under the plane-strain condition.

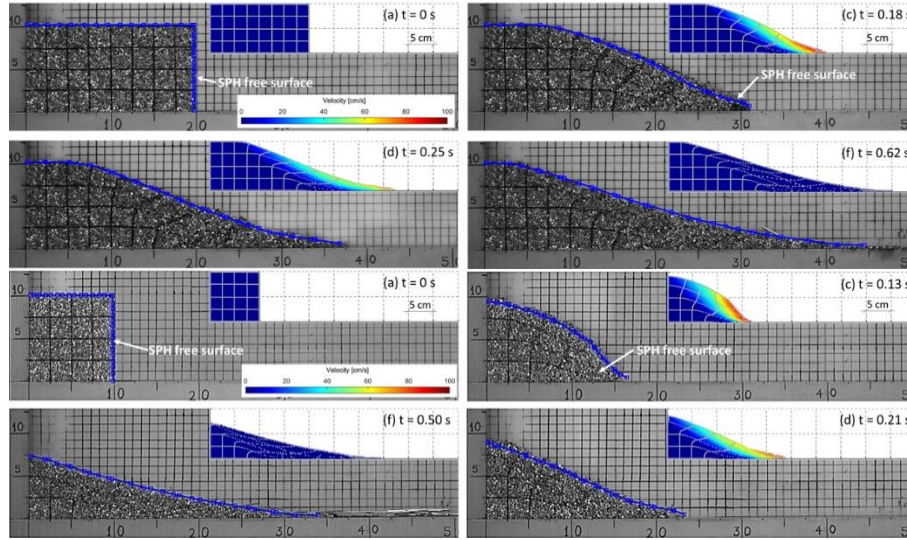


Figure 22. Progressive failure of 2D granular column with the initial aspect ratio $a = 0.5$ and 1.0 . Blue line represents free surface extracted from the SPH simulation [93].

The capability of SPH in modelling 3D granular column collapse was also demonstrated in Figure 24, where the results of SPH simulation of a cylinder granular column collapse experiment are compared with the experimental data reported by Lube et al. [94]. Excellent agreements between SPH and the experiment are obtained for both the surface morphology and final run-out distance. The undisturbed zone observed on the top surface of the material sample in the experiment was well captured by SPH. Furthermore, a smooth distribution of the vertical stress profile at large deformation was also achieved, thanks to the stress regularisation technique [52].

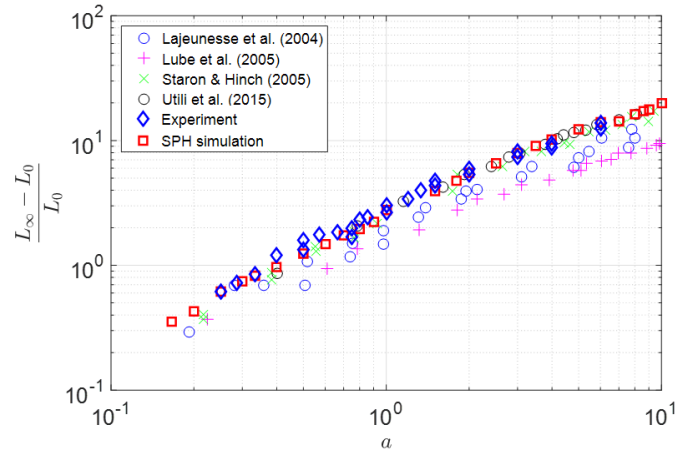


Figure 23. Comparison of the final run-out distances of 2D granular flow with different aspect ratios obtained from experiments and simulations.

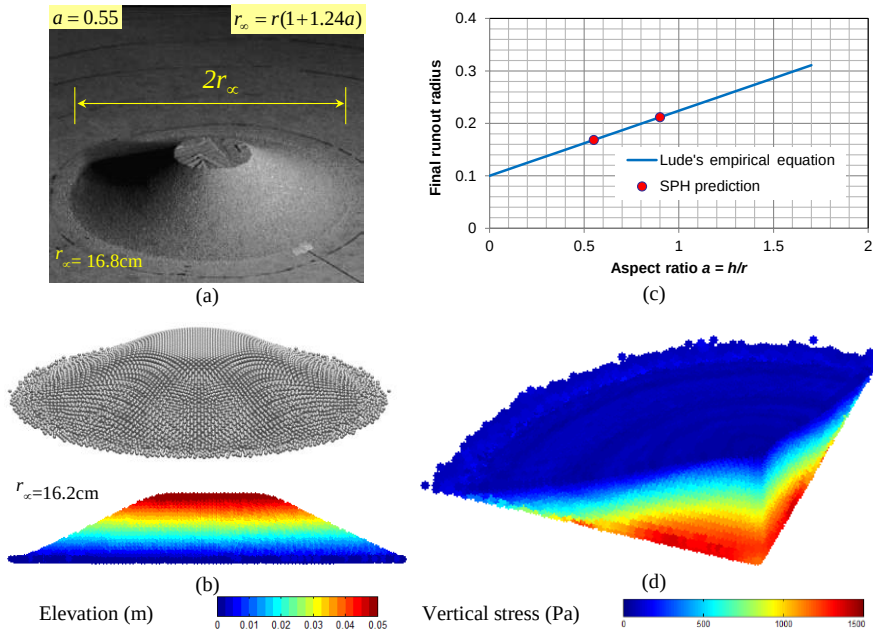


Figure 24. Comparisons between 3D SPH simulation¹¹ and experiment for the granular columns collapse.

¹¹ Details of model setting and material properties for simulations can be found in H. H. Bui and G. D. Nguyen, "Numerical predictions of post-flow behaviour of granular materials using an improved

4.3 SPH applications to model soil-structure interactions

Soil-structure interaction is an interesting topic which has been extensively investigated in the literature. Given the capability of SPH in predicting large deformation and flow failure of granular materials, as demonstrated in the earlier section, it is interesting to discuss how SPH can be extended to model soil-structure interactions. We will first present our latest development of SPH for large-scale simulations of the interaction between the granular flows and control structures [95]. Figure 25 shows the application of the high-performance computing MCG-SPH code [42, 90] to investigate the interaction of granular flows against check-dams and baffles [95], which are commonly used as the control structures to slow down debris flows. In the model, the debris flow was modelled using the $\mu(I)$ rheological constitutive model described in Section 3.2.1, the validation of which has been previously reported in [90] and demonstrated to be suitable for this type of problem. The simulations involve more than 3 millions material particles and over 800 thousand boundary particles and are simulated on using 192 CPU cores on NCI-Gadi or Pawsey Magnus of the National Computing Infrastructure (NCI), Australia. The reader can immediately see from Figure 25 that the high-performance computing model can be effectively used to assess the performance of different control structures without involving substantial costs required to conduct large-scale experiments. For example, the SPH simulation results in Figure 25 demonstrated that the taller baffle system appears to be more efficient than the shorter system and there exists a critical height above which the baffle system does not gain more benefit. The check dams appear to be better in slowing down the debris flows. However, if one looks at the total forces acting on the check dams, it is an order of magnitude larger than the individual baffle of the same height as the dam experiences [95].

At this point, the reader would have asked what if we have a deformable or moving rigid structures and how one can extend the current SPH model to simulate such a system. First, we will discuss how SPH can be extended to model the interaction between soil and rigid structures, as in the segmental retaining wall system, which is commonly used in practice to reinforce soil slopes due to its capability to tolerate minor ground movement and settlement without causing damage the retaining wall structure. To model this type of problems, one would need to find a way to represent the retaining wall blocks in SPH as well as to describe their rigid body motions in SPH. Such a model has been developed by Bui et al. [51], which was dated back to the original work by Monaghan [96], and will be briefly summarised this model here. In their SPH model, the retaining wall blocks (or rigid structures) are simulated by placing SPH boundary particles on the surface boundary of each wall block, as shown

SPH model," in *CIGOS 2019, Innovation for Sustainable Infrastructure*: Springer, 2020, pp. 895-900.

in Figure 26. The dynamic motions of retaining wall blocks can be then described through the motion of their central mass, which obeys Newton's second law. The translational and rotational motion equations for the centre of mass of a block can be written as follows, respectively:

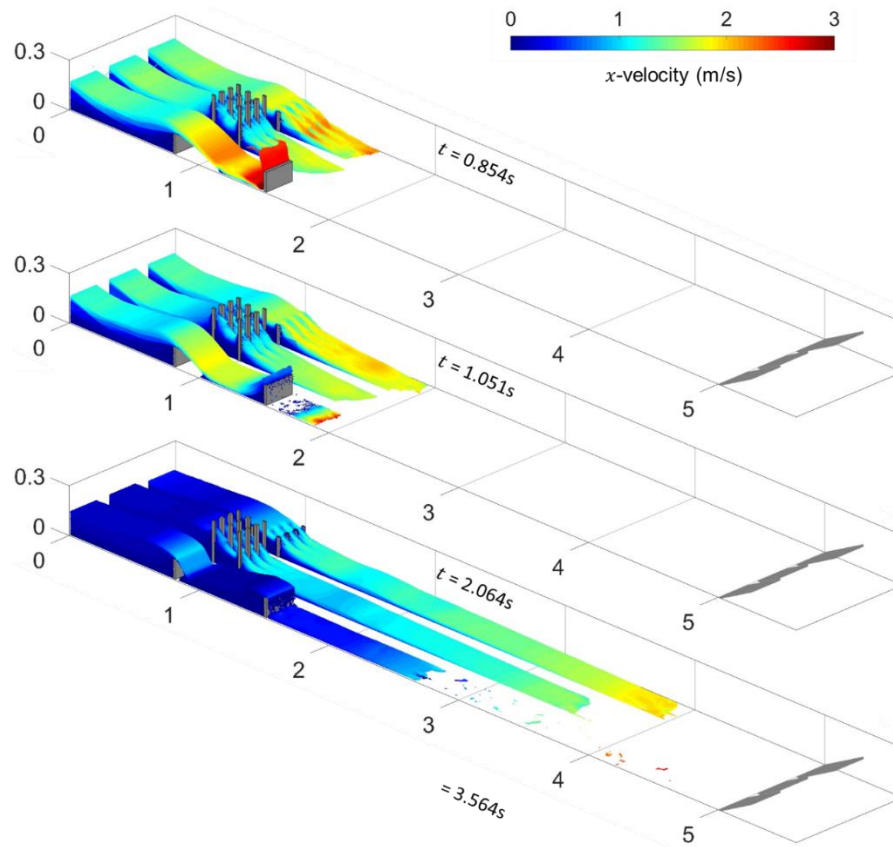


Figure 25. Large-scale simulation¹² of the interaction between SPH and protective structures [95].

¹² Details of model setting and material properties for simulations can be found in E. Yang, H. H. Bui, H. De Sterck, G. D. Nguyen, and A. Bouazza, "Numerical investigation of the mechanism of granular flow impact on rigid control structures," *Acta Geotechnica*, (Under review), 2020

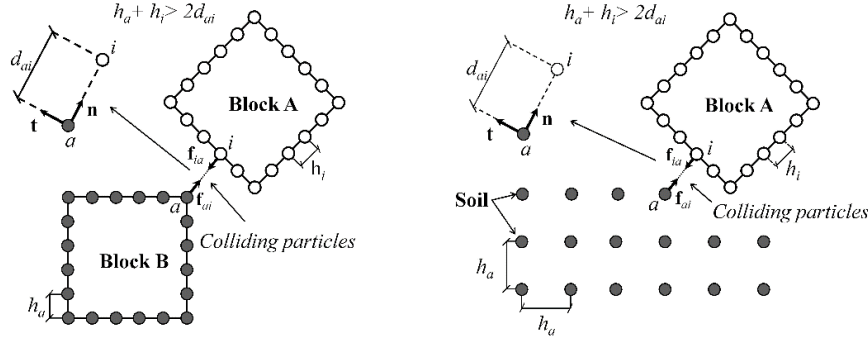


Figure 26. Representation of wall blocks in SPH and their interactions with soil and other blocks [51].

$$M_k \frac{d\mathbf{V}_k}{dt} = \sum_{i \in S_k} \mathbf{f}_i \quad (106)$$

$$I_k \frac{d\boldsymbol{\Omega}_k}{dt} = \sum_{i \in S_k} (\mathbf{r}_i - \mathbf{R}_k) \times \mathbf{f}_i \quad (107)$$

where M_k and $\mathbf{V}_k$ are the central mass and velocity of block k ; I_k and $\boldsymbol{\Omega}_k$ are the inertial moment and angular velocity about the centre of mass of block k ; $\mathbf{f}_i$ is the force vector acting on boundary particle i representing the block; and $\mathbf{r}_i$ and $\mathbf{R}_k$ are vector coordinates of boundary particle i and the centre of mass of block k , respectively. To complete the model, one needs to adopt a contact model to describe the interaction between soil and block or block and block, which was discussed at length in Bui et al. [51]. Finally, once such a contact model is selected, and the velocity and rotation of the central are specified, the motion of boundary particles on each block can be updated as follows:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{V}_k + \boldsymbol{\Omega}_k \times (\mathbf{r}_i - \mathbf{R}_k) \quad (108)$$

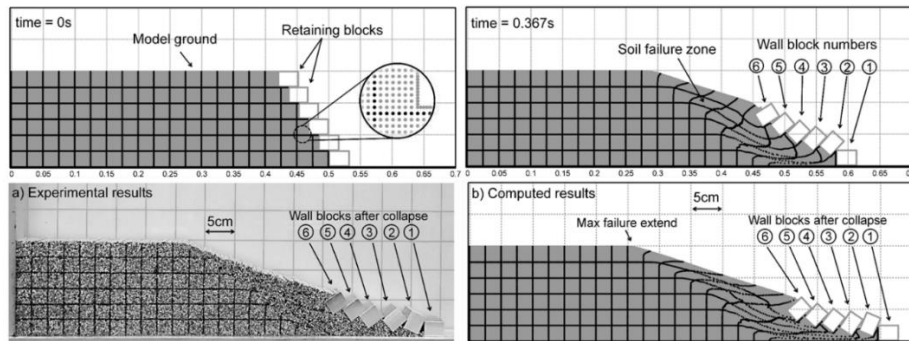


Figure 27. SPH simulation of the progressive collapse of the retaining wall system consisting of six rigid wall blocks and its comparison against experiment

The application¹³ of this SPH framework to model the progressive collapse of a retaining wall system consisting of six retaining wall blocks and its comparison against experiment is shown in Figure 27. It can be seen that the model can capture well the dynamic movement of each retaining wall block and very good agreement with experiment was achieved [51]. Further application of this model to a high retaining wall structure consisting of multiple blocks is illustrated in Figure 28, showing the capability of SPH in modelling a highly complex soil-structure interaction system.

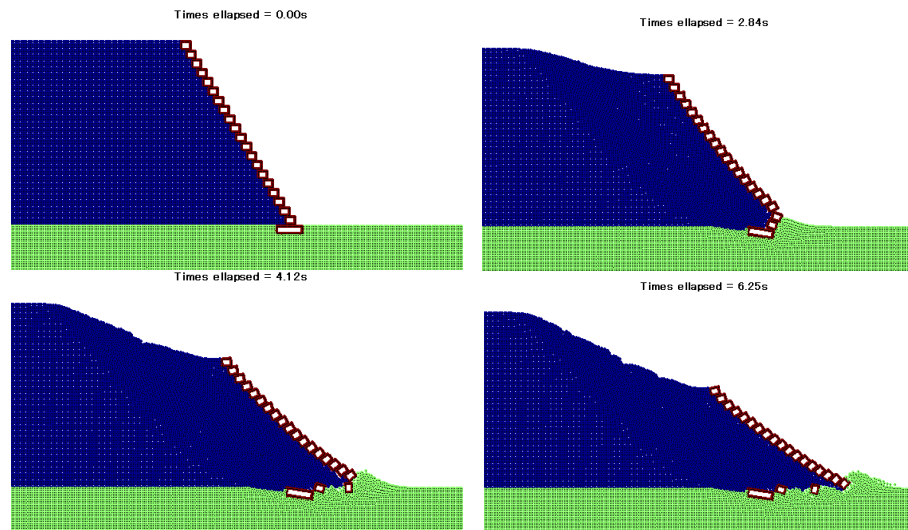


Figure 28. Progressive failure of a high retaining system consisting of multiple wall blocks reinforced at the base.

4.4 SPH applications to fracturing in geomechanics¹⁴

The capability of SPH in modelling complex fracturing problems in geomechanics is demonstrated in this section. Two typical rock fracturing tests, namely semi-circular bending test and circular ring test, undergoing mixed-mode fractures are simulated by using SPH combined with the novel two-scale constitutive model, and numerical results are compared against experimental data available in the literature. The detailed

¹³ Details of model setting and material properties for simulations can be found H. H. Bui, J. K. Kodikara, A. Bouazza, A. Haque, and P. G. Ranjith, "A novel computational approach for large deformation and post-failure analyses of segmental retaining wall systems," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 38, pp. 1321-1340.

¹⁴ Details of model setting and material properties for simulations presented in this section can be found in Y. Wang, H. T. Tran, G. D. Nguyen, P. G. Ranjith, and H. H. Bui, "Simulation of mixed-mode fracture using SPH particles with an embedded fracture process zone," *International Journal for Numerical and Analytical Methods in Geomechanics*, 2020.

model setting, SPH boundary conditions and material properties required for the two-scale model were documented in [58] and thus will not be repeated here. We will only provide some key results obtained from our latest SPH developments in this section. Figure 29 illustrates the progressive development of fracture and the horizontal velocity profile at the failure stage for the semi-circular specimen with the notch inclination angle of 30° . As expected, the damage process initiated at particles near the notch tip and propagated toward the loading point.

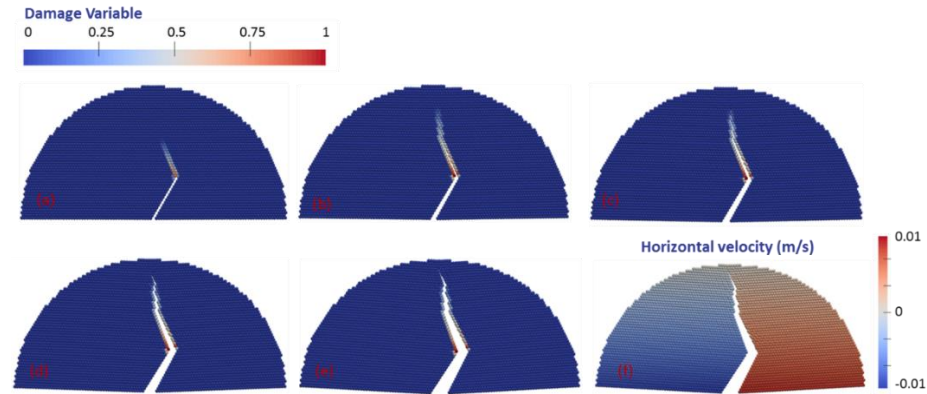


Figure 29. Fracture pattern for notch inclination angle of 30° in the semi-circular bending test: (a-e) fracture development and (f) horizontal velocity for final fracture pattern [58].

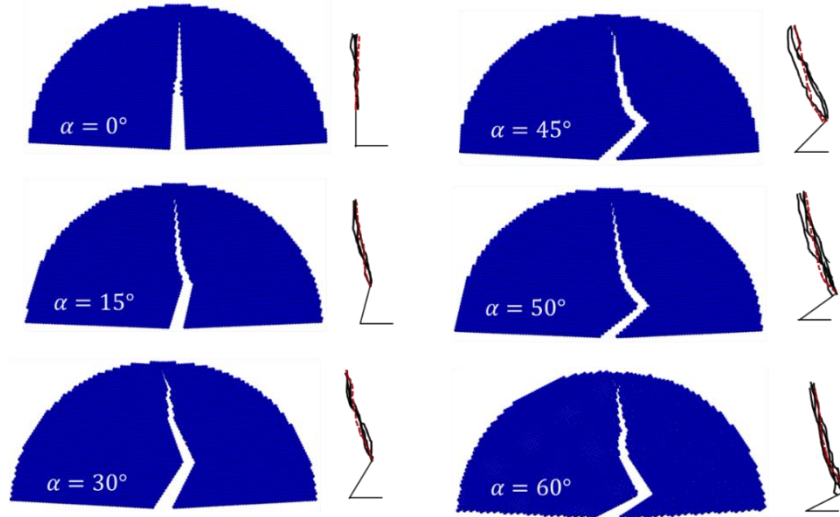


Figure 30. Comparison of final fracture pattern between experimental and numerical results in the semi-circular bending test for various notch angles [58].

Figure 30 shows a comparison of mixed-mode fracture envelope between experiments and SPH simulations for different notch inclination angles $\alpha_n = 0^\circ, 15^\circ, 30^\circ, 45^\circ, 50^\circ$ and 60° . The SPH simulations (i.e. red lines) match well with the experimental results (i.e. black lines). Finally, the comparison of peak loads between experiments and simulations for the notch inclination angles varying from 0° to 60° with an internal increment of 5° is plotted in Figure 31. Again, the SPH simulations can well capture the increasing trend of the peak load with the increasing notch angles in the experiment. This suggests that the combination of SPH and the two-scale constitutive model with an embed fracture process zone could accurately predict the mixed-mode fracture behaviour of rocks.

Figure 32 shows a comparison between SPH and experiment for fracture development in circular ring specimens with different inner-to-outer diameter ratios (d/D). The results again demonstrate the capability of SPH in capturing the complex fracturing pattern developed in rock materials. For the inner-to-outer diameter ratio of less than 0.3 (i.e. $d/D \leq 0.2$), both SPH simulations and experiments show a single crack (i.e. primary crack) initiated from the inner ring along the central loading line and propagated toward the loading zones on the top and bottom of the specimen. As the inner-to-outer diameter ratio increases beyond 0.3 (i.e. $d/D \geq 0.3$), the secondary crack developed in both SPH simulations and experiments, forming in the direction perpendicular to the loading line. In contrast to the primary crack, the secondary crack is initiated from the outer ring and propagated toward the inner ring, but always lagging behinds the primary crack. Overall, the results show good agreements between SPH simulation and experiment, suggesting that the combination of SPH with the two-scale constitutive model with an embedded fracture process zone could capture well the fracture developments in rocks or rock-like materials.

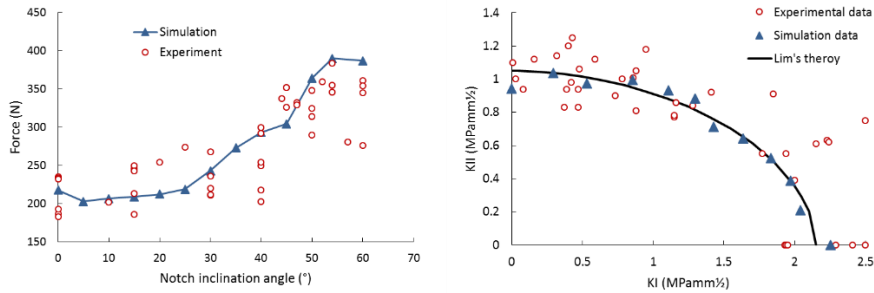


Figure 31. Comparison between SPH and experiment for the predictions of peak force and fracture toughness in the semi-circular bending test [58].

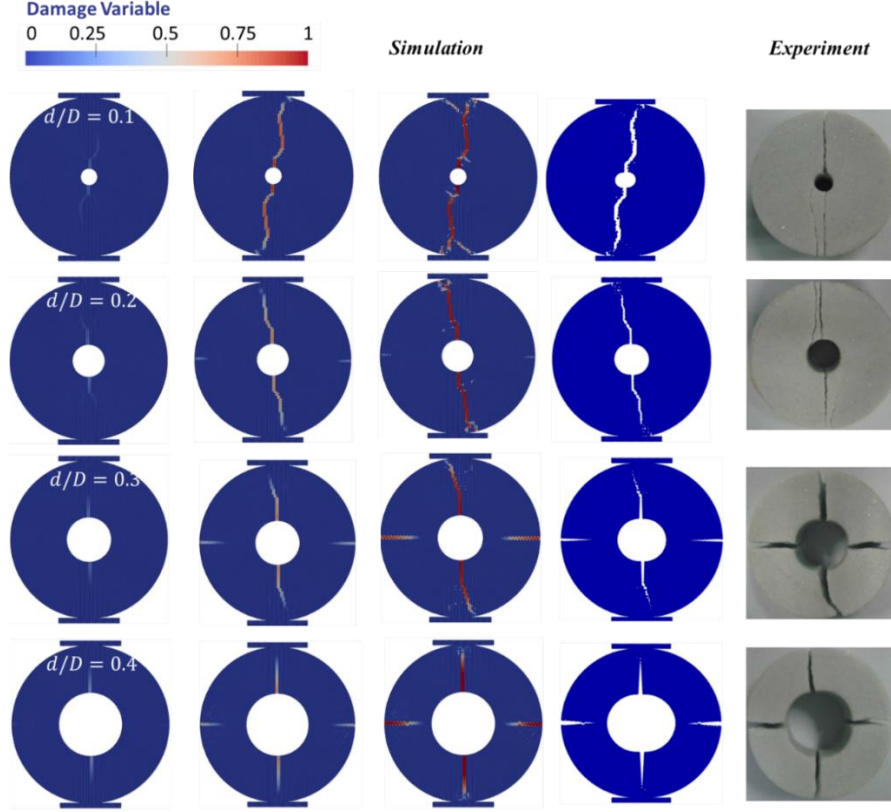


Figure 32. Comparison of final fracture pattern between experiments and SPH simulations for the final fracture patterns developed in circular ring tests with different diameter ratios (d/D)

4.5 Modelling of coupled multiphase flow and geomechanics in porous media by SPH

In this section, we will demonstrate the capability of SPH in the coupled behaviour of fluid and solid in a deformable porous medium. To achieve this, the SPH governing equations described in Section 3.1 will be generalised to accommodate the interaction among phases in the porous medium. In general, the governing equations of the fluid-solid mixture consists of the mass and momentum balance equations, which can be written as follows [4]:

$$\frac{d^\alpha \bar{\rho}_\alpha}{dt} + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha = 0 \quad (109)$$

$$\bar{\rho}_\alpha \frac{d^\alpha \mathbf{v}_\alpha}{dt} = \nabla \cdot \bar{\boldsymbol{\sigma}}_\alpha + \bar{\rho}_\alpha \mathbf{b} - \Sigma \mathbf{R}^{\alpha\beta} \quad (110)$$

where $\mathbf{v}_\alpha$ is the velocity vectors of phase α in the mixture; $\bar{\rho}_\alpha = n_\alpha \rho_\alpha$ is the partial density of phase components in the mixture corresponding to the volume fraction n_α ; $\bar{\sigma}_\alpha$ is the partial stress $n_\alpha \sigma_\alpha$ of each phase; and (d^α/dt) denotes the material derivative of a field quantity (π) on phase α , which can be written in a general form as follows:

$$\frac{d^\alpha \pi}{dt} = \frac{\partial \pi}{\partial t} + \mathbf{v}_\alpha \cdot \nabla \pi \quad (111)$$

To solve the above equations by SPH, one needs to discretise these equations onto SPH particles using suitable SPH operators, as discussed in Section 2. This forms the basics of two existing SPH approaches to solve multiphase flow problems in geomechanics, as outlined in Figure 24. In the first approach (i.e. single-layer approach), a single set of SPH particles is used to represent the multiphase porous media, which in general consists of air, water and solid. Each SPH particle then carries the information of three phases and the fully coupled governing equations of these phases are solved in this single set of SPH particles [8, 97]. In the second approach (i.e. multiple-layers approach), two or three sets of SPH particles are used to represent the porous media [4, 43-45, 98]. The governing equations of each phase are then solved separately on each set of SPH particles. The interactions among phases are then considered through several coupled physical processes [4].

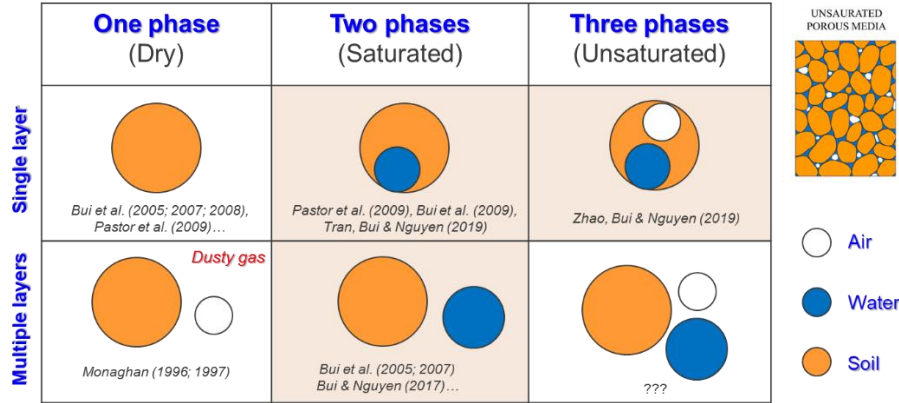


Figure 33. Different strategies to solve multiphase flow problems in SPH.

Here, we will illustrate the multi-layers SPH approach, which was previously developed by Bui and Nguyen [4] for solving fully coupled fluid-solid problem. In our view, this is one of the most rigorous multi-layer SPH models for multiphase flow through deformable porous media, considering the fully coupled hydro-mechanical

processes. The governing equations for water and soil phases in a fully saturated porous system can be derived from the above general mixture theory. For the water phase, the following governing equations hold [4]¹⁵:

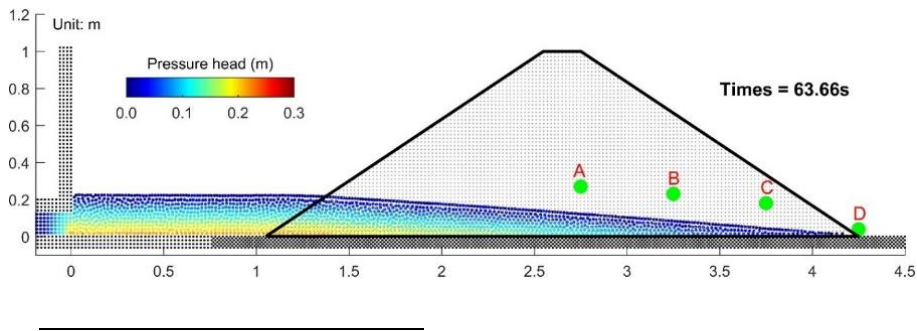
$$\begin{aligned} n_w \frac{d^w(\rho_w)}{dt} &= -\rho_w \nabla \cdot (n_s \mathbf{v}_s + n_w \mathbf{v}_w) \\ \bar{\rho}_w \frac{d^w(\mathbf{v}_w)}{dt} &= -\nabla(n_w p_w) + \bar{\rho}_w \mathbf{g} + \mathbf{R}^{ws} \end{aligned} \quad (112)$$

And the governing equations for soil phase are:

$$\begin{aligned} \frac{d^s n_s}{dt} &= -n_s (\nabla \cdot \mathbf{v}_s) \\ \bar{\rho}_s \frac{d^s(\mathbf{v}_s)}{dt} &= \nabla \cdot (\boldsymbol{\sigma}' - n_s p_w \mathbf{I}) + \bar{\rho}_s \mathbf{g} - \mathbf{R}^{ws} \end{aligned} \quad (113)$$

where $\boldsymbol{\sigma}'$ is the effective soil stress $\mathbf{R}^{ws}$ is the seepage force. The reader is referred to Bui and Nguyen [4] for a more detailed descriptions of mathematical models and numerical conditions required for simulations shown in this section.

The above governing equations are then solved separately for water and soil phases. Figure 34 and Figure 35 show the progressive development of seepage flow through a rock-field dam experiment [99], which is assumed to be rigid. The two-phase SPH model [4] was able to capture a smooth and stable pressure profile of water flow for a very long physical time of testing (i.e. >300s), which is not a straightforward task for many existing SPH codes. Furthermore, the model was able to capture well the phreatic surface and the pore-water pressure measured in the experimental data reported in [99]. Figure 36 shows the application of the two-phase SPH model to predict the progressive failure of an embankment as compared against experiments. The SPH model could capture the overall failure mechanism of the embankment, though further work still required to include more advanced constitutive model and take into consideration of unsaturated soils.



¹⁵ Note that Equation (112) can be further simplified if the spatial gradient of the porosity is assume to be constant, which returns to the simplified form as in Bui and Nguyen (2017).

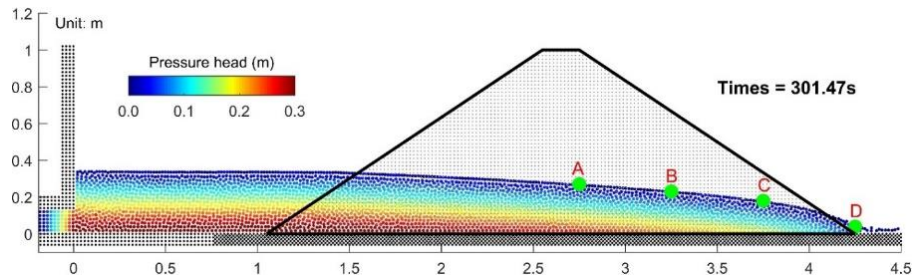


Figure 34. Modelling of seepage flow through rock-filled dam using the two-layer SPH framework

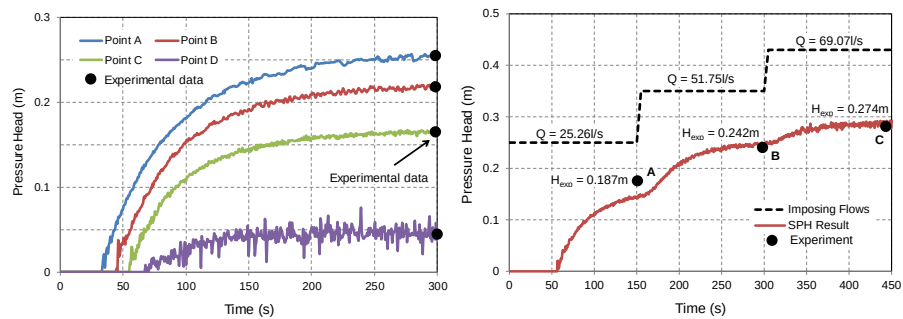


Figure 35. Modelling of seepage flow through rock-filled dam using the two-layer SPH framework

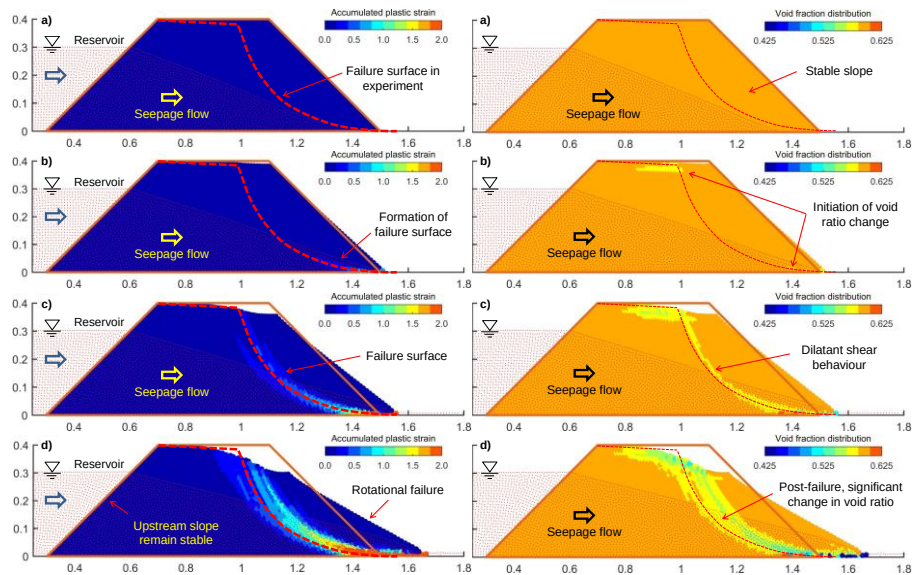


Figure 36. Modelling of progressive failure of slope embankment by the two-layer SPH framework

5 Conclusions

Fundamentals and applications of SPH have been presented with sufficient details covering a range of problems in geomechanics. Misconceptions on tensile instability and challenges inherent to the method (such as numerical accuracy, pairing instability and stress boundary conditions) have been addressed and solutions discussed to provide readers insights into SPH, in addition to the fundamentals and applications. Other issues that are not intrinsic to SPH, but are essential for the applications of the method have also been given attentions. They include parallelisation to tackle field-scale applications, and material models for SPH. The latter is central to geomechanics applications and provides the readers with a range of constitutive models suitable for different applications involving solid deformation and flow of both fluid and granular materials. Along this line, of interest is our recent developments of a double-scale approach to tackle material instability issues related to softening and localization that is particularly suitable for SPH applications in geomechanics, thanks to the truly meshfree nature of the method. The presented examples provide a wide spectrum of problems in geomechanics, illustrating great capacity, versatility and potential of the method for geomechanics applications.

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References

- [1] R. A. Gingold and J. J. Monaghan, "Smoothed Particle Hydrodynamics - Theory and Application to Non-Spherical Stars," (in English), *Monthly Notices of the Royal Astronomical Society*, vol. 181, no. 2, pp. 375-389, 1977.
- [2] L. B. Lucy, "Numerical Approach to Testing of Fission Hypothesis," (in English), *Astronomical Journal*, vol. 82, no. 12, pp. 1013-1024, 1977.
- [3] H. H. Bui, K. Sako, and R. Fukagawa, "Numerical simulation of soil–water interaction using smoothed particle hydrodynamics (SPH) method," *Journal of Terramechanics*, vol. 44, no. 5, pp. 339-346, 11// 2007.

- [4] H. H. Bui and G. D. Nguyen, "A coupled fluid-solid SPH approach to modelling flow through deformable porous media," *International Journal of Solids and Structures*, vol. 125, pp. 244-264, 2017/10/15/ 2017.
- [5] H. H. Bui, K. Sako, R. Fukagawa, and J. Wells, "SPH-based numerical simulations for large deformation of geomaterial considering soil-structure interaction," in *The 12th International Conference of International Association for Computer Methods and Advances in Geomechanics (IACMAG)*, 2008, vol. 1, pp. 570-578.
- [6] C. Nguyen, H. H. Bui, and R. Fukagawa, "Two-dimensional numerical modelling of modular-block soil retaining walls collapse using meshfree method," *Int J Geomate*, vol. 5, no. 1, pp. 647-652, 2013.
- [7] J. Wang and D. Chan, "Frictional contact algorithms in SPH for the simulation of soil-structure interaction," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 38, no. 7, pp. 747-770, 2014.
- [8] M. Pastor, B. Haddad, G. Sorbino, S. Cuomo, and V. Drempetic, "A depth-integrated, coupled SPH model for flow-like landslides and related phenomena," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 33, no. 2, pp. 143-172, 2009.
- [9] H. H. Bui, R. Fukagawa, K. Sako, and J. C. Wells, "Slope stability analysis and discontinuous slope failure simulation by elasto-plastic smoothed particle hydrodynamics (SPH)," *Géotechnique*, vol. 61, no. 7, pp. 565-574, 2011.
- [10] H. H. Bui and R. Fukagawa, "An improved SPH method for saturated soils and its application to investigate the mechanisms of embankment failure: Case of hydrostatic pore-water pressure," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 37, no. 1, pp. 31-50, 2013/01/01 2013.
- [11] X. Xu and X.-L. Deng, "An improved weakly compressible SPH method for simulating free surface flows of viscous and viscoelastic fluids," *Computer Physics Communications*, vol. 201, pp. 43-62, 4// 2016.
- [12] C. T. Nguyen, H. H. Bui, and R. Fukagawa, "Failure Mechanism of True 2D Granular Flows," *JOURNAL OF CHEMICAL ENGINEERING OF JAPAN*, vol. 48, no. 6, pp. 395-402, 2015 2015.
- [13] A. H. Fávero Neto and R. I. Borja, "Continuum hydrodynamics of dry granular flows employing multiplicative elastoplasticity," *Acta Geotechnica*, journal article vol. 13, no. 5, pp. 1027-1040, October 01 2018.

- [14] C. Peng, W. Wu, H.-s. Yu, and C. Wang, "A SPH approach for large deformation analysis with hypoplastic constitutive model," *Acta Geotechnica*, vol. 10, no. 6, pp. 703-717, 2015/12/01 2015.
- [15] S. Zhao, H. H. Bui, V. Lemial, and G. D. Nguyen, "SPH Simulation of Strain Localisation in Geomaterials Using a Visco-Plastic Constitutive Model," in *Poromechanics VI*, 2017.
- [16] C. T. Nguyen, C. T. Nguyen, H. H. Bui, G. D. Nguyen, and R. Fukagawa, "A new SPH-based approach to simulation of granular flows using viscous damping and stress regularisation," *Landslides*, pp. 1-13, 2016// 2016.
- [17] H. Bui, R. Fukagawa, and K. Sato, "Smoothed particle hydrodynamics for soil mechanics," *proceedings of Numerical Methods in Geotechnical Engineering, Graz*, pp. 275-281, 2006.
- [18] L. Libersky and A. G. Petschek, "Smooth particle hydrodynamics with strength of materials," in *Advances in the Free-Lagrange Method Including Contributions on Adaptive Gridding and the Smooth Particle Hydrodynamics Method*, vol. 395, H. Trease, M. Fritts, and W. P. Crowley, Eds. (Lecture Notes in Physics: Springer Berlin Heidelberg, 1991, pp. 248-257.
- [19] J. K. Chen, J. E. Beraun, and T. C. Carney, "A corrective smoothed particle method for boundary value problems in heat conduction," *International Journal for Numerical Methods in Engineering*, vol. 46, no. 2, pp. 231-252, 1999.
- [20] H. Takeda, S. M. Miyama, and M. Sekiya, "Numerical Simulation of Viscous Flow by Smoothed Particle Hydrodynamics," *Progress of Theoretical Physics*, vol. 92, no. 5, pp. 939-960, 1994.
- [21] H. H. Bui, G. D. Nguyen, J. Kodikara, and M. Sanchez, "Soil cracking modelling using the mesh-free SPH method," *12th Australia New Zealand Conference on Geomechanics*, 2015.
- [22] T. Douillet-Grellier, B. D. Jones, R. Pramanik, K. Pan, A. Albaiz, and J. R. Williams, "Mixed-mode fracture modeling with smoothed particle hydrodynamics," *Computers and Geotechnics*, vol. 79, pp. 73-85, 2016/10/01/ 2016.
- [23] Y. Wang, H. H. Bui, G. D. Nguyen, and P. G. Ranjith, "A new SPH-based continuum framework with an embedded fracture process zone for modelling rock fracture," *International Journal of Solids and Structures*, 2018/09/15/ 2018.
- [24] H. T. Tran, H. H. Bui, G. D. Nguyen, J. Kodikara, and M. Sanchez, "A Continuum Based Approach to Modelling Tensile Cracks in Soils," in *Poromechanics VI*, 2017.

- [25] Y. Wang, H. H. Bui, G. D. Nguyen, and P. G. Ranjith, "A Mesh-Free Continuum Based Computational Approach to Modelling Rock Fracture," in *Poromechanics VI*, 2017, pp. 2041-2048.
- [26] T. Blanc and M. Pastor, "Towards SPH modelling of failure problems in geomechanics A fractional step Taylor-SPH model," (in English), *European Journal of Environmental and Civil Engineering*, vol. 15, pp. 31-49, 2011.
- [27] T. Blanc and M. Pastor, "A stabilized Fractional Step, Runge-Kutta Taylor SPH algorithm for coupled problems in geomechanics," (in English), *Computer Methods in Applied Mechanics and Engineering*, vol. 221, pp. 41-53, 2012.
- [28] T. Blanc and M. Pastor, "A stabilized Smoothed Particle Hydrodynamics, Taylor-Galerkin algorithm for soil dynamics problems," (in English), *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 37, no. 1, pp. 1-30, Jan 2013.
- [29] X. Y. Hu and N. A. Adams, "A multi-phase SPH method for macroscopic and mesoscopic flows," (in English), *Journal of Computational Physics*, vol. 213, no. 2, pp. 844-861, Apr 10 2006.
- [30] X. Y. Hu and N. A. Adams, "An incompressible multi-phase SPH method," (in English), *Journal of Computational Physics*, vol. 227, no. 1, pp. 264-278, Nov 10 2007.
- [31] J. Swegle, D. Hicks, and S. Attaway, "Smoothed particle hydrodynamics stability analysis," *Journal of computational physics*, vol. 116, no. 1, pp. 123-134, 1995.
- [32] D. J. Price, "Smoothed particle hydrodynamics and magnetohydrodynamics," *Journal of Computational Physics*, vol. 231, no. 3, pp. 759-794, 2012.
- [33] J. J. Monaghan, "Smoothed Particle Hydrodynamics and Its Diverse Applications," (in English), *Annual Review of Fluid Mechanics*, Vol 44, vol. 44, pp. 323-346, 2012.
- [34] J. J. Monaghan, "Theory and applications of smoothed particle hydrodynamics," (in English), *Frontiers of Numerical Analysis*, pp. 143-194, 2005.
- [35] M. Liu and G. Liu, "Smoothed particle hydrodynamics (SPH): an overview and recent developments," *Archives of computational methods in engineering*, vol. 17, no. 1, pp. 25-76, 2010.
- [36] J. J. Monaghan and D. J. Price, "Variational principles for relativistic smoothed particle hydrodynamics," (in English), *Monthly Notices of the Royal Astronomical Society*, vol. 328, no. 2, pp. 381-392, Dec 1 2001.

- [37] J. J. Monaghan, "Smoothed particle hydrodynamics," (in English), *Reports on Progress in Physics*, vol. 68, no. 8, pp. 1703-1759, Aug 2005.
- [38] W. Dehnen and H. Aly, "Improving convergence in smoothed particle hydrodynamics simulations without pairing instability," *Monthly Notices of the Royal Astronomical Society*, vol. 425, no. 2, pp. 1068-1082, 2012.
- [39] L. A. Richards, "Capillary conduction of liquids through porous mediums," (in English), *Physics-a Journal of General and Applied Physics*, vol. 1, no. 1, pp. 318-333, Jul-Dec 1931.
- [40] J. J. Monaghan, "Smoothed particle hydrodynamics," *Annual review of astronomy and astrophysics*, vol. 30, no. 1, pp. 543-574, 1992.
- [41] L. Hernquist and N. Katz, "TREESPH-A unification of SPH with the hierarchical tree method," *The Astrophysical Journal Supplement Series*, vol. 70, pp. 419-446, 1989.
- [42] H. H. Bui, R. Fukagawa, K. Sako, and S. Ohno, "Lagrangian meshfree particles method (SPH) for large deformation and failure flows of geomaterial using elastic-plastic soil constitutive model," (in English), *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 32, no. 12, pp. 1537-1570, Aug 25 2008.
- [43] H. H. Bui, R. Fukagawa, and K. Sako, "Smoothed particle hydrodynamics for soil mechanics," in *Proceedings of the 6th European Conference on Numerical Methods in Geotechnical Engineering - Numerical Methods in Geotechnical Engineering*, 2006, pp. 278-281.
- [44] H. H. Bui, K. Sako, and R. Fukagawa, "Numerical simulation of soil-water interaction using smoothed particle hydrodynamics (SPH) method," in *15th International Conference of the International Society for Terrain Vehicle Systems 2005, ISTVS 2005*, 2005, pp. 126-140.
- [45] K. MAEDA and M. SAKAI, "Development of seepage failure analysis procedure of granular ground with Smoothed Particle Hydrodynamics (SPH) method," *Journal of applied mechanics*, vol. 7, pp. 775-786, 2004.
- [46] J. J. Monaghan, "Simulating Free-Surface Flows with Sph," (in English), *Journal of Computational Physics*, vol. 110, no. 2, pp. 399-406, Feb 1994.
- [47] J. P. Gray, J. J. Monaghan, and R. P. Swift, "SPH elastic dynamics," (in English), *Computer Methods in Applied Mechanics and Engineering*, vol. 190, no. 49-50, pp. 6641-6662, 2001.

- [48] P. W. Randles and L. D. Libersky, "Smoothed particle hydrodynamics: Some recent improvements and applications," (in English), *Computer Methods in Applied Mechanics and Engineering*, vol. 139, no. 1-4, pp. 375-408, Dec 15 1996.
- [49] B. H. Ha, "Lagrangian mesh-free particle method (SPH) for large deformation and post-failure of geomaterial using elasto-plastic constitutive models," 立命館大学, 2007.
- [50] H. H. Bui, R. Fukagawa, K. Sako, and S. Ohno, "Lagrangian meshfree particles method (SPH) for large deformation and failure flows of geomaterial using elastic-plastic soil constitutive model," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 32, no. 12, pp. 1537-1570, 2008.
- [51] H. H. Bui, J. K. Kodikara, A. Bouazza, A. Haque, and P. G. Ranjith, "A novel computational approach for large deformation and post-failure analyses of segmental retaining wall systems," (in English), *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 38, no. 13, pp. 1321-1340, Sep 2014.
- [52] C. T. Nguyen, C. T. Nguyen, H. H. Bui, G. D. Nguyen, and R. Fukagawa, "A new SPH-based approach to simulation of granular flows using viscous damping and stress regularisation," (in English), *Landslides*, vol. 14, no. 1, pp. 69-81, Feb 2017.
- [53] A. H. F. Neto and R. I. Borja, "Continuum hydrodynamics of dry granular flows employing multiplicative elastoplasticity," *Acta Geotechnica*, vol. 13, no. 5, pp. 1027-1040, 2018.
- [54] Y. Wang, H. H. Bui, G. D. Nguyen, and P. Ranjith, "A new SPH-based continuum framework with an embedded fracture process zone for modelling rock fracture," *International Journal of Solids and Structures*, vol. 159, pp. 40-57, 2019.
- [55] H. Tran, Wang, Y., Nguyen, G.D, Kodikara, J, Sanchez, M, Bui, HH, "Modelling 3D desiccation cracking in clayey soils using a size-dependent SPH computational approach," *Computers and Geotechnics*, vol. (in press), 2019.
- [56] S. Zhao, H. H. Bui, V. Lemiale, G. D. Nguyen, and F. Darve, "A generic approach to modelling flexible confined boundary conditions in SPH and its application," *International Journal for Numerical and Analytical Methods in Geomechanics*, vol. 43, no. 5, pp. 1005-1031, 2019.
- [57] H. T. Tran, Y. Wang, G. D. Nguyen, J. Kodikara, M. Sanchez, and H. H. Bui, "Modelling 3D desiccation cracking in clayey soils using a size-dependent SPH computational approach," *Computers and Geotechnics*, vol. 116, p. 103209, 2019.

- [58] Y. Wang, H. T. Tran, G. D. Nguyen, P. G. Ranjith, and H. H. Bui, "Simulation of mixed-mode fracture using SPH particles with an embedded fracture process zone," *International Journal for Numerical and Analytical Methods in Geomechanics*, 2020.
- [59] P. Jop, Y. Forterre, and O. Pouliquen, "A constitutive law for dense granular flows," *Nature*, vol. 441, p. 727, 06/08/online 2006.
- [60] G. D. Nguyen, C. T. Nguyen, V. P. Nguyen, H. H. Bui, and L. Shen, "A size-dependent constitutive modelling framework for localised failure analysis," *Computational Mechanics*, vol. 58, no. 2, pp. 257-280, 2016.
- [61] G. D. Nguyen and H. H. Bui, "A thermodynamics- and mechanism-based framework for constitutive models with evolving thickness of localisation band," *International Journal of Solids and Structures*, vol. 187, pp. 100-120, 2020/03/15/ 2020.
- [62] G. D. Nguyen, I. Einav, and A. M. Korsunsky, "How to connect two scales of behaviour in constitutive modelling of geomaterials," (in English), *Geotechnique Letters*, vol. 2, pp. 129-134, Jul-Sep 2012.
- [63] G. D. Nguyen, A. M. Korsunsky, and I. Einav, "A constitutive modelling framework featuring two scales of behaviour: Fundamentals and applications to quasi-brittle failure," (in English), *Engineering Fracture Mechanics*, vol. 115, pp. 221-240, Jan 2014.
- [64] P. Jop, Y. Forterre, and O. Pouliquen, "A constitutive law for dense granular flows," *Nature*, vol. 441, no. 7094, pp. 727-730, 2006.
- [65] M. D. Bolton, "Strength and dilatancy of sands," *Geotechnique*, vol. 36, no. 1, pp. 65-78, 1986.
- [66] G. Pijaudier-Cabot and Z. P. Bažant, "Nonlocal Damage Theory," *Journal of Engineering Mechanics*, vol. 113, no. 10, pp. 1512-1533, 1987.
- [67] Z. Chen and H. L. Schreyer, "Simulation of Soil‐Concrete Interfaces with Nonlocal Constitutive Models," *Journal of Engineering Mechanics*, vol. 113, no. 11, pp. 1665-1677, 1987.
- [68] Z. P. Bažant, "Why Continuum Damage is Nonlocal: Micromechanics Arguments," *Journal of Engineering Mechanics*, vol. 117, no. 5, pp. 1070-1087, 1991.
- [69] I. Vardoulakis and E. C. Aifantis, "A gradient flow theory of plasticity for granular materials," *Acta Mechanica*, vol. 87, no. 3, pp. 197-217, 1991/09/01 1991.
- [70] R. D. Borst and J. Pamin, "Gradient plasticity in numerical simulation of concrete cracking," *European Journal of Mechanics - A/Solids*, vol. 15, no. 2, pp. 295-320, 1996.

- [71] L. Cedolin and Z. P. Bažant, "Effect of finite element choice in blunt crack band analysis," *Computer Methods in Applied Mechanics and Engineering*, vol. 24, no. 3, pp. 305-316, 1980.
- [72] A. Crook, S. Willson, J. Yu, and D. Owen, "Predictive modelling of structure evolution in sandbox experiments," *Journal of Structural Geology*, vol. 28, no. 5, pp. 729-744, 2006.
- [73] F. Zabala and E. Alonso, "Progressive failure of Aznalcóllar dam using the material point method," *Géotechnique*, vol. 61, no. 9, pp. 795-808, 2011.
- [74] M. Neilsen and H. Schreyer, "Bifurcations in elastic-plastic materials," *International Journal of Solids and Structures*, vol. 30, no. 4, pp. 521-544, 1993.
- [75] C. T. Nguyen, G. D. Nguyen, A. Das, and H. H. Bui, "Constitutive modelling of progressive localised failure in porous sandstones under shearing at high confining pressures," *International Journal of Rock Mechanics and Mining Sciences*, vol. 93, pp. 179-195, 2017.
- [76] G. D. Nguyen, "An enriched constitutive model for fracture propagation analysis using the material point method," in *Applied Mechanics and Materials*, 2014, vol. 553, pp. 731-736: Trans Tech Publ.
- [77] L. A. Le, G. D. Nguyen, H. H. Bui, A. H. Sheikh, A. Kotousov, and A. Khanna, "Modelling jointed rock mass as a continuum with an embedded cohesive-frictional model," *Engineering Geology*, vol. 228, pp. 107-120, 2017/10/13/ 2017.
- [78] L. A. Le, G. D. Nguyen, H. H. Bui, A. H. Sheikh, and A. Kotousov, "Localised failure mechanism as the basis for constitutive modelling of geomaterials," *International Journal of Engineering Science*, vol. 133, pp. 284-310, 2018/12/01/ 2018.
- [79] L. A. Le, G. D. Nguyen, H. H. Bui, A. H. Sheikh, and A. Kotousov, "Incorporation of micro-cracking and fibre bridging mechanisms in constitutive modelling of fibre reinforced concrete," *Journal of the Mechanics and Physics of Solids*, vol. 133, p. 103732, 2019/12/01/ 2019.
- [80] H. Nonoyama, S. Moriguchi, K. Sawada, and A. Yashima, "Slope stability analysis using smoothed particle hydrodynamics (SPH) method," *Soils and foundations*, vol. 55, no. 2, pp. 458-470, 2015.
- [81] Y.-F. Jin, Z.-X. Wu, Z.-Y. Yin, and J. S. Shen, "Estimation of critical state-related formula in advanced constitutive modeling of granular material," *Acta Geotechnica*, vol. 12, no. 6, pp. 1329-1351, 2017.
- [82] J. J. Monaghan and R. A. Gingold, "Shock Simulation by the Particle Method Sph," (in English), *Journal of Computational Physics*, vol. 52, no. 2, pp. 374-389, 1983.

- [83] P. W. Randles and L. D. Libersky, "Normalized SPH with stress points," (in English), *International Journal for Numerical Methods in Engineering*, vol. 48, no. 10, pp. 1445-+, Aug 10 2000.
- [84] C. Dyka, P. Randles, and R. Ingel, "Stress points for tension instability in SPH," *International Journal for Numerical Methods in Engineering*, vol. 40, no. 13, pp. 2325-2341, 1997.
- [85] J. J. Monaghan, "SPH without a tensile instability," (in English), *Journal of Computational Physics*, vol. 159, no. 2, pp. 290-311, Apr 10 2000.
- [86] J. Kopp, "Efficient numerical diagonalization of hermitian 3×3 matrices," *International Journal of Modern Physics C*, vol. 19, no. 03, pp. 523-548, 2008.
- [87] L. D. Libersky, A. G. Petschek, T. C. Carney, J. R. Hipp, and F. A. Allahdadi, "High-Strain Lagrangian Hydrodynamics - a 3-Dimensional Sph Code for Dynamic Material Response," (in English), *Journal of Computational Physics*, vol. 109, no. 1, pp. 67-75, Nov 1993.
- [88] H. Takeda, S. M. Miyama, and M. Sekiya, "Numerical-Simulation of Viscous-Flow by Smoothed Particle Hydrodynamics," (in English), *Progress of Theoretical Physics*, vol. 92, no. 5, pp. 939-960, Nov 1994.
- [89] J. P. Morris, P. J. Fox, and Y. Zhu, "Modeling low Reynolds number incompressible flows using SPH," (in English), *Journal of Computational Physics*, vol. 136, no. 1, pp. 214-226, Sep 1 1997.
- [90] E. Yang, H. H. Bui, H. De Sterck, G. D. Nguyen, and A. Bouazza, "A scalable parallel computing SPH framework for predictions of geophysical granular flows," *Computers and Geotechnics*, vol. 121, p. 103474, 2020.
- [91] H. H. Bui and H. D. V. Khoa, "Bearing capacity of shallow foundation by Smoothed Particle Hydrodynamics (SPH) analysis," in *Computational Geomechanics, COMGEO II - Proceedings of the 2nd International Symposium on Computational Geomechanics*, 2011, pp. 457-468.
- [92] H. H. Bui, R. Fukagawa, K. Sako, and J. C. Wells, "Slope stability analysis and discontinuous slope failure simulation by elasto-plastic smoothed particle hydrodynamics (SPH)," *Geotechnique*, vol. 61, no. 7, pp. 565-574, JUL 2011 2011.
- [93] N. H. Nguyen, H. H. Bui, and G. D. Nguyen, "An approach to calculating large strain accumulation for discrete element simulations of granular media," *International Journal for Numerical and Analytical Methods in Geomechanics*, 2020.

- [94] G. Lube, H. E. Huppert, R. S. J. Sparks, and M. A. Hallworth, "Axisymmetric collapses of granular columns," *Journal of Fluid Mechanics*, vol. 508, p. 175, 2004.
- [95] E. Yang, H. H. Bui, H. De Sterck, G. D. Nguyen, and A. Bouazza, "Numerical investigation of the mechanism of granular flow impact on rigid control structures," *Acta Geotechnica*, vol. (Under review), 2020.
- [96] J. J. Monaghan, A. Kos, and N. Issa, "Fluid motion generated by impact," (in English), *Journal of Waterway Port Coastal and Ocean Engineering-Asce*, vol. 129, no. 6, pp. 250-259, Nov-Dec 2003.
- [97] H. H. Bui and R. Fukagawa, "A first attempt to solve soil-water coupled problem by SPH," *Japanese Terramechanics*, vol. 29, pp. 33-38, 2009.
- [98] H. H. Bui, K. Sako, and R. Fukagawa, "Numerical simulation of soil-water interaction using smoothed particle hydrodynamics (SPH) method," (in English), *Journal of Terramechanics*, vol. 44, no. 5, pp. 339-346, Nov 2007.
- [99] A. Larese De Tetto and R. Rossi, *A coupled Eulerian-PFEM model for the simulation of overtopping in rockfill dams*. Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE), 2012.

Constitutive modelling for fast granular flow

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Granular material may behave like solid, liquid or gas. We present a unified constitutive theory for the solid-, fluid- and gas-like behaviour. The theory is formulated in rate form by decomposing the total stress into a frictional (inviscid) stress and a collisional (viscous) stress. This decomposition applies to both the stress and its rate. We make use of the hypoplastic constitutive model for the frictional stress by replacing the total stress with the frictional stress. The viscous stress rate is obtained by time-differentiating a non-Newtonian model, which gives rise to a strain acceleration tensor. Our theory shows a smooth transition between solid and fluid. We demonstrate the model performance by considering simple shear under constant normal stress.

1 Introduction

We consider cohesionless granular material like pure sand and confine ourselves to a purely phenomenological approach without resort to the micromechanical aspect. The study of constitutive models depends on observations from the so-called element tests. An element test is characterized by uniform stress and strain. The study of granular material at low and high strain rate have been developed along different lines.

The solid-like behaviour with flow deformation has been the domain of soil mechanics. Here, we are in a lucky position to have quite some element tests at disposal, e.g. isotropic compression, oedometer compression, triaxial test, plane strain, true triaxial and simple shear test. The experimental observations are well documented, which helps to develop the constitutive models. Some salient features of the solid-like behaviour are irreversible deformation, dilatancy, Coulomb failure mechanism and rate independence. A major contribution is the introduction of critical state, which is characterized by the friction angle in a critical state and the pressure. Granular material approaches the critical state under large deformation. Many constitutive models have been proposed with the majority being elastic-plastic theory. We will make use of the hypoplastic model, which is based on non-linear tensor functions and does not decompose the deformation into elastic and plastic part. This offers some advantage to deal with fast granulation flow. The study of fast granular flow was initiated by the

pioneer experimental work of Bagnold [Bag84]. Bagnold carried out shear tests in a Couette cell using naturally buoyant particles in fluid. He found out that fast flowing granular materials behave like a non-Newtonian fluid. His work ignited relevant research in the following decades. Sometimes differentiation is made between fast and very fast flow, or between dense and dilute flow. The fluid-like and gas-like behaviour is usually considered as non-Newtonian fluid, where the stress is related to the strain rate. The material behaviour is mainly characterized by rate dependence and viscosity, which depends on density and strain rate. Until now granular material in slow flow (solid-like) and fast flow (fluid-like) has been developed along different lines. We try to bring these two lines together in a unified framework by considering the salient features of granular materials in slow and fast flow.

Fast flow: difficulty in testing Because of the large deformation, the only feasible element test is the simple shear. Such test can be conducted either under constant normal stress or constant volume. The latter is known as undrained test in soil mechanics. In soil mechanics lab there are two kinds of simple shear devices after Norwegian Geotechnical Institute and Cambridge. However, these devices allow only limited deformation. For fast granular flow, there are two kinds of devices, i.e. the Couette cell [Sav84, Han85] and the ring shear device [Boy11]. Neither of them is element test because the strain is not uniform. Another difficulty in testing is the gravity. Because the stress level is extremely low, particles tend to settle under gravity. This difficulty can be circumvented by using materials with the same density as the interstitial fluid [Bag84]. Often the tests gave no information about the deformation distribution in the specimen, and the formation of shear zones is suspected. Such tests represent boundary value problems and are not very useful for constitutive modelling. In all, the data are rather scarce. An alternative is to do numerical simulations with Discrete element method (DEM). With the help of periodic boundary conditions, granular material is subjected to virtually unlimited deformation in simple shear. Moreover, gravity can be switched off in such simulations. Most calculations assume spherical particles and simple contact laws. In spite of the simplicity, however, the numerical simulations reveal some major features of fast granular flow, i.e. fast granular flow is viscous and the viscosity depends on the density [Chi12, Nes15]

$$\mathbf{T} = \eta(\mathbf{D}) \mathbf{D} \quad (1)$$

Fast flow: dilute vs. dense Following Bagnold [Bag84] and inspired by the similarity between molecules and granular materials, kinetic theory has been developed for fast granular flow. The theory is developed for dilute granular flow with spherical and elastic particles without gravity. In analogy to molecules, granular temperature was introduced. A constitutive equation relating stress with strain rate can be derived. The dependence of stress on the square of strain rate is reminiscent of the experimental finding of Bagnold [Bag84]

$$\mathbf{T} \propto \mathbf{D}^2 \quad (2)$$

However, fast and dilute granular flows are but rare. Flying particles with pure elastic collisions free from gravity can be hardly found in the real world. Recently, the

research on granular materials has been more focused on dense granular flow with enduring contacts among the particles [Gdr04, Jop06].

Fast flow: how fast? We have been using the term “fast flow” without further specification. We now recapitulate the various numbers to differentiate between slow, fast and very fast flow. A well-known number in fluid dynamics is the Reynold number R_e , which is defined by the ratio between inertial force and viscous force in fluid flow. Reynold number is used to discriminate between laminar and turbulent flow. For $R_e < 2300$ laminar flow was observed, and for $R_e > 2900$ turbulent flow was observed. Note that there is no clear demarcation between laminar and turbulent flow. Some colleagues in the UK were able to raise the critical Reynold number substantially by more carefully repeating the test of Reynold using the same device. Bagnold introduced a dimensionless number to characterize the ratio between collisional and viscous stresses.

Bagnold number The Bagnold number B_a is the ratio between the stress due to grain collisions and the viscous stress for granular flow with interstitial Newtonian fluid:

$$N_B = \frac{T_{collision}}{T_{viscous\ stress}} = \frac{\rho d^2 \lambda^{1/2} \dot{\gamma}}{\mu} \quad (3)$$

where $T_{collision}$ and $T_{viscous}$ denote the stress caused by collision of grains and viscous response of the granular flow, respectively. The linear concentration is defined by

$$\lambda = \frac{1}{\left(\frac{\phi_{max}}{\phi}\right)^{1/3} - 1} \quad (4)$$

The collision stress is $T_{collision} = \rho v^2$ (dimension consideration). The particle velocity v can be assumed equal to $d\dot{\gamma}$ with the viscous stress being equal to $\mu\dot{\gamma}$.

2 Behaviours of fast granular flow

2.1 Experimental observations

Simple shear is the only feasible motion for element tests. However, the devices in soil mechanics lab allow only limited deformation. Therefore, most observations were made with Couette cell [Bag84, Han85] or ring shear device [Sav84]. Figure 1 shows the test data reported by Bagnold [Bag84] in a Couette cell. The tests were carried out by submerging granular material in fluid (water and glycerine). The data show two distinct regimes, which are called the macro-viscous regime (fast flow) and the grain inertia regime (very fast flow). In the macro-viscous regime with $N_B < 40$, the flow is dominated by the viscous stress and the stress due to grain collisions is negligible. The granular flow in the macro-viscous regime can be described as Newtonian fluid with the stress proportional to the strain rate. In the grain-inertia regime with $N_B > 450$ the stress due to grain collisions is much larger than the viscous stress, and the stress is proportional to the square of the strain rate.

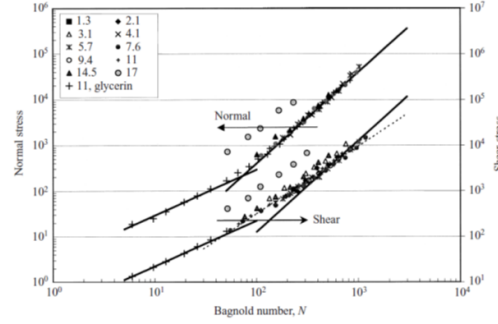


Figure 1: Experimental shear and normal stresses as reported by Bagnold [Bag84] for linear different linear concentrations (from Hunt et al. 2020 [Hun02])

Note that the different solid fractions are only feasible in suspended granular materials with neutral buoyancy in a fluid. In air, the particles would settle to the bottom. A closer look at the test data shows that the behaviour depends only weakly on the solid fraction when it is under some threshold. Obviously, the particles are so dilute that the collisions do not affect the overall behaviour. Recently, improved testing showed that the exponent in the grain inertia regime is not 2 but about 1.5 at high strain rate [Hun02]. Note further that both the shear and normal stresses increase the strain rate. This normal stress effect is also known as shear thickening, which is well known for non-Newtonian fluids. The opposite is called shear thinning. Moreover, the ratio between the shear stress and the normal stress mimics granular materials under quasi-static loading (Figure 1).

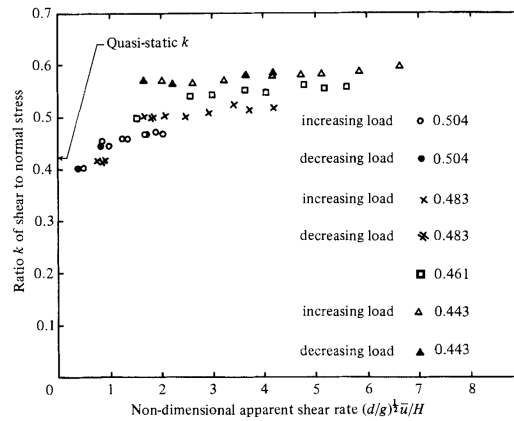


Figure 2: Experimental data for 1.32 mm mean diameter spherical polystyrene beads (Savage and Sayed 1984 [Sav84])

Fast flow of dry granular materials was studied in an annular shear device (ring shear device) by Savage and Sayed [Sav84]. Obviously the Couette cell is not suitable for dry granular materials due to gravity. The major findings are summarized below. At lower solid concentration, the stress depends linearly on the solid fraction and quadratically on the shear rate, which agrees well with Bagnold's observation on suspended granular materials. Both dry and suspended granular materials seem to follow the same dependence. At high concentration, however, the exponent is less than 2, which agrees with the refined tests by Hunt et al. [Hun02]. Figure 2 shows that the ratio increases with the rate and approaches an asymptote at high shear rate [Sav84].

It is extremely difficult to generate uniform deformation in the presence of gravity. The displacement profiles often show stagnation zones near the fixed bottom so that the test cannot be regarded as an element test. This means that the strain rate is often underestimated. Moreover, the density variation over the specimen height due to gravity was not provided.

Hanes and Inman [Han85] reported tests on glass spheres in a Couette shear cell similar to Bagnold [Bag84]. The observations by Bagnold was confirmed. The viscosity is dependent on the solid fraction, which agrees fairly well with the kinetic theories.

2.2 Observations from DEM simulations

It is extremely difficult to realize element tests for fast granular flow in laboratory. An alternative is to perform numerical simulations (numerical tests). Such tests can be performed under ideal conditions, i.e. simple shear without gravity. There are many such tests reported in the literature. We select two publications by Chialvo et al. [Chi12] for dry granular flow and by Ness and Sun [Nes15] for wet granular flow. Their results are summarized by Vescovi et al. [Ves20] and given in Figure 3. The DEM simulations were carried out with spherical particles and simple contact laws. The simple shear tests were performed using periodic boundary conditions under constant normal stress without considering gravity. Obviously, both dry and wet granular material show viscous behaviour at high shear rate. The viscous behaviour depends strongly on the solid fraction. The observations by Bagnold [Bag84] are confirmed for low solid fraction. For very high shear rate the shear stress curves of all densities collapse to a single curve. Obviously, the simulation for low density would not be possible under gravity, since the particles would sink to the bottom.

2.3 Viscosity and solid fraction

The viscosity of granular materials is known to depend on the solid fraction. The following relationship by Krieger and Dougherty [Kri59] for suspended granular materials is often used.

$$\eta = \alpha \left(1 - \frac{\phi}{\phi_m} \right)^{-\beta} \quad (5)$$

where α and β are fitting parameters and ϕ_m is the maximum solid fraction.

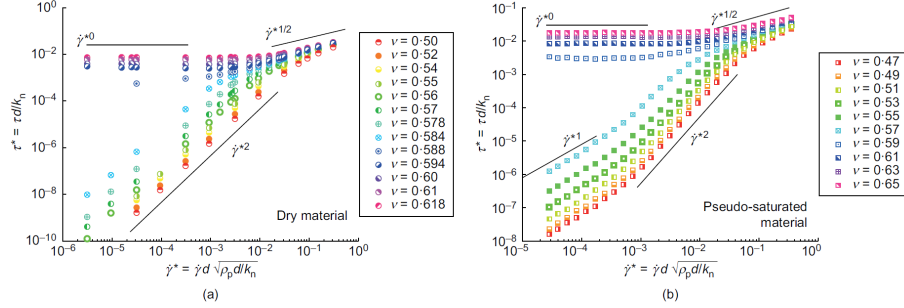


Figure 3: Scaled shear stress over scaled shear rate with k_n : normal stiffness between particles, d : particle diameter, ρ_p : particle density

2.4 Recent work by Gdr MiDi

Recently, the French group Gdr MiDi has carried out intensive research on fast granular flows. Their work was first focused on dry granular flow [Gdr04, Jop06, For08] and later was extended to suspended granular flow [Boy11, Gua18]. They introduced the following dimensionless number to characterize the ratio between the inertial force and external force.

2.5 Inertial number

The inertia number I was introduced by the Gdr MiDi-group in France and quantifies the significance of dynamic effects in a granular material. It measures the ratio of inertial forces of grains to imposed external forces. A small value corresponds to the quasi-static state, while a high value corresponds to the inertial state or even the “dynamic” state

$$I = \frac{\text{Inertial force}}{\text{External force}} = \frac{\dot{\gamma} d}{\sqrt{P/\rho}} \quad (6)$$

The flow regimes according to I are (i) quasi static flow with $I < 10^{-3}$, (ii) dense flow (fast) with $10^{-3} < I < 10^{-1}$ and (iii) collisional flow (very fast) with $I > 10^{-1}$. The inertia number is equal to the square root of the Savage number. This inertia number was proposed for dry granular materials. Recently it is modified to consider saturated granular material [Gua18]. Consider fast flow in simple shear. The solid fraction depends only on the inertial number and the relationship between the shear stress and normal stress obeys a Coulomb-like friction law, i.e.,

$$\tau = \mu(I) p \quad \text{and} \quad \phi = \phi(I) \quad (7)$$

where p is the normal stress; μ is the friction coefficient. The above relationships can be shown graphically as follows:

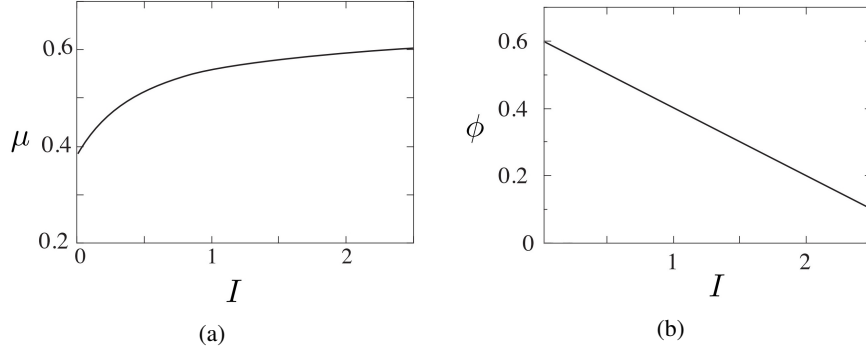


Figure 4: Friction law and volume fraction law against inertial number I (Forterre and Pouliquen 2008 [For08])

Note that the friction coefficient starts from the quasi-static state and increases with the inertial number to approach asymptotically a limit at high shear rate. The relationships are obtained based on two dimensional DEM simulations and later three dimensional DEM simulations. The Gdr MiDi model has been applied to several boundary value problems such as Couette cell, vertical silo, flow down inclined plane, heap flow, rotating drum.

2.6 Jamming and critical state

For both dry and suspended granular materials, the shear stress increases with the solid fraction (density) until the jamming point, which is supposed to mark the turning point from fluid to solid. However, jamming is usually studied in a Couette cell with constant volume. Obviously, jamming is not expected in simple shear under constant normal stress, because the dilatancy is not completely confined. This has some resemblance with the critical state with constant stresses and constant volume. Once a critical state is reached, granular material may further deform without inducing any change in stress and density. It is not yet quite clear how jamming is related to the critical state. We believe that the boundary conditions play an important role.

2.7 Why do we need a new model?

Gdr MiDi model can describe the salient behaviour of granular materials during fast flow. However, it does not consider the initiation of flow. Nor can it describe the behaviour during a shear reversal [Gua18].

Consider the following gedanken experiment of a simple shear under constant normal stress. A specimen with an initial density subjected to simple shear will either dilate or contract depending on the initial density relative to the critical state. For continuing

deformation, the density will approach the critical density, which depends on the normal stress (not on the initial density). Once the critical state is reached and the shear rate is further elevated, the material changes from solid-like behaviour to the fluid-like behaviour. The Gdr MiDi model can be used to describe the steady state of the fluid-like behaviour at high shear rate. Fast granular flow can be maintained at certain shear rate. This is a steady state characterized by constant stresses and constant solid fraction. Note that acceleration is needed to move from one steady state to the other steady state. Obviously, the Gdr MiDi model cannot describe the initiation of flow, which is an unsteady process.

Now let us consider a shear reversal from a steady shear flow. We need first to decelerate to reduce the shear rate to zero and then accelerate in the opposite direction to reach fast flow. Obviously, the Gdr MiDi model cannot account for this process either. Do we need to account for the unsteady processes? To answer this question, let us have a look at the development of debris flows. A debris flow usually starts as a result of slope failure (landslide). The slope failure is mainly dictated by the soil-like behaviour. Afterwards, the failure soil mass slides down the slope and accelerate to reach fast flow, which is dictated by the fluid-like behaviour. Upon reaching the plane at the toe of the slope, the soil mass decelerates, spreads out and changes back to the solid state.

Whereas slope stability has been modelled mainly in the realm of soil mechanics (solid-like), the modelling of debris flows has been developed mainly along the line of fluid mechanics (fluid-like). It is desirable for a unified modelling of landslides and debris flows within one single consistent numerical model. Such a numerical model requires a constitutive model for both the solid-like and the fluid-like behaviour, i.e. both unsteady and steady processes.

3 Constitutive model for fast granular flow

3.1 Model framework

In order to describe the the steady and unsteady processes in one single framework, we make the fundamental assumption, as in previous studies [Peng16, Wang18, Xu16, Wu06], that the inviscid and the viscous stresses coexist in granular flows i.e.

$$\mathbf{T} = \mathbf{T}_i + \mathbf{T}_v \quad (8)$$

in which $\mathbf{T}_i$ and $\mathbf{T}_v$ denote the inviscid and viscous stress, representing the frictional behaviour between the particles and the viscous behaviour due to grain collision during fast granular flows, respectively. To obtain a concrete formulation, some fundamental restrictions should be imposed on equation (8). Firstly, the proposed constitutive model should be able to capture the salient behaviours of granular material in a steady state, such as frictional behaviour, dilatancy, and critical state. Secondly, the formulation of the viscous part should consider the influence of strain acceleration and strain history. Thirdly, the proposed model should be able to describe the whole

process of granular flow from initiation to fast flow in a unified way, which is realised by the coupled evolution of the two stress components. To this end, we make use of a critical state enhanced hypoplastic constitutive model and non-newtonian rheology to formulate the new constitutive model. The rate form of the new model is expressed as follows:

$$\dot{\mathbf{T}} = \dot{\mathbf{T}}_i + \dot{\mathbf{T}}_v \quad (9)$$

where $\dot{\mathbf{T}}$, $\dot{\mathbf{T}}_i$ and $\dot{\mathbf{T}}_v$ denote the Cauchy, inviscid, and viscous stress rates, respectively. An important assumption is that the inviscid stress and the viscous stress are accumulated separately according to the respective constitutive equations. The sum of these two stresses gives rise to the total stress, which enters into the equilibrium condition.

3.2 Hypoplastic model with critical state for inviscid behaviour

Hypoplasticity is a nonlinear rate-form constitutive theory that has long been used for analysing mechanical behaviours and other boundary value problems in granular material. In the framework of hypoplasticity, the constitutive equation is written in two parts, representing reversible and irreversible behaviours of soils. According to Kolymbas and Wu [Wu90], the hypoplastic rate constitutive equation can be written as the sum of linear and nonlinear terms of the strain rate $\mathbf{D}$:

$$\dot{\mathbf{T}} = \mathcal{L}(\mathbf{T}) : \mathbf{D} + \mathbf{N}(\mathbf{T}) \|\mathbf{D}\| \quad (10)$$

where the tensorial functions $\mathcal{L}$ and $\mathbf{N}$ are of the 4th and 2nd order, respectively. The colon $:$ denotes an inner product between two tensors. $\mathbf{T}$ is the Cauchy stress tensor, which can be used to replace the inviscid stress in equation (8), and $\mathbf{D}$ is the stretching tensor. $\|\mathbf{D}\|$ stands for the Euclidean norm of the stretching tensor. The Jaumann stress rate tensor $\dot{\mathbf{T}}$ is defined in terms of the material time-derivative of the Cauchy stress tensor $\dot{\mathbf{T}}_i$ and the spin tensor $\mathbf{W}$:

$$\dot{\mathbf{T}} = \dot{\mathbf{T}}_i + \mathbf{T}\mathbf{W} - \mathbf{W}\mathbf{T} \quad (11)$$

The stretching and spin tensors are related to the velocity gradient tensor through

$$\mathbf{D} = \frac{1}{2} [\nabla \dot{\mathbf{x}} + (\nabla \dot{\mathbf{x}})^T], \quad \mathbf{W} = \frac{1}{2} [\nabla \dot{\mathbf{x}} - (\nabla \dot{\mathbf{x}})^T] \quad (12)$$

where $\dot{\mathbf{x}}$ is the velocity and ∇ is the gradient operator.

The functions $\mathcal{L}$ and $\mathbf{N}$ must be isotropic to remain invariant under rigid body rotations. Since $\mathcal{L}$ is independent of $\mathbf{D}$, constitutive equations in the form of equation (10) are necessarily rate independent. This can be easily ascertained by the fact that equation (10) is positively homogeneous of the first degree in strain rate $\mathbf{D}$. To show this, we can write equation (10) in the following form by making use of Euler's theorem for homogeneous functions.

$$\dot{\mathbf{T}} = [\mathcal{L} + \mathbf{N} \otimes \vec{\mathbf{D}}] : \mathbf{D} \quad (13)$$

where $\vec{\mathbf{D}} = \mathbf{D}/\|\mathbf{D}\|$ is the direction of strain rate and $\otimes$ stands for the dyadic product. The term in the square brackets in equation (13) is the directional stiffness tensor, which can be viewed as the counterpart of the tangential stiffness of elastoplastic models. Obviously, the directional stiffness tensor depends on the direction of strain rate $\vec{\mathbf{D}}$. Therefore, loading and unloading in the hypoplastic model (13) are implicitly stated without additional loading criterion. This is different from elastoplastic models, where two stiffness tensors, one for loading and the other for unloading, are used. Furthermore, elastoplastic models need explicit loading criterion to decide which stiffness shall be used.

Although not defined a priori as in elastoplastic models, a failure criterion can be obtained from equation (10) by searching for the pair of stress and strain rates that produces a vanishing stress rate. By using the fact that $\vec{\mathbf{D}} : \vec{\mathbf{D}} = 1$, the failure criterion can be derived:

$$f(\mathbf{T}) = \mathbf{N}^T : (\mathcal{L}^T)^{-1} : \mathcal{L}^{-1} : \mathbf{N} - 1 = 0 \quad (14)$$

Details of the derivation of the failure criterion can be found in Wu and Niemunis [Wu96].

Based on the above concept, a simple hypoplastic constitutive equation for granular materials was proposed by Wu and Bauer [Wu94]. The model is able to capture the main behaviour of granular material in the quasi-static regime. The constitutive model is formulated as follows:

$$\dot{\mathbf{T}} = C_1(\text{tr}\mathbf{T})\mathbf{D} + C_2 \frac{\text{tr}(\mathbf{T}\mathbf{D})\mathbf{T}}{\text{tr}\mathbf{T}} + (C_3 \frac{\mathbf{T}^2}{\text{tr}\mathbf{T}} + C_4 \frac{\mathbf{T}^{*2}}{\text{tr}\mathbf{T}})\|\mathbf{D}\| \quad (15)$$

where $C_j (j = 1, \dots, 4)$ are dimensionless material parameters; $\mathbf{T}^*$ is the stress deviator expressed by

$$\mathbf{T}^* = \mathbf{T} - \frac{1}{3}(\text{tr}\mathbf{T})\mathbf{1} \quad (16)$$

with $\mathbf{1}$ being the second order unit tensor. The hypoplastic model (15) possesses simple mathematical formulation and contains only four material parameters. These parameters can be related to some well-established parameters in soil mechanics. To calibrate these parameters, two stress states, i.e., the initial hydrostatic and the state at failure, are considered based on a single drained triaxial compression test with constant confining pressure [Wu94]. To this end, the following parameters are introduced:

- the stress ratio: $R = \mathbf{T}(1, 1)/\mathbf{T}(3, 3)$
- the initial tangent modulus: $E_i = (\dot{\mathbf{T}}_i(1, 1) - \dot{\mathbf{T}}_i(3, 3))/\mathbf{D}(1, 1)$
- the initial Poisson's ratio: $\nu_i = [\mathbf{D}(3, 3)/\mathbf{D}(1, 1)]_{R=1}$
- the failure stress ratio: $R_f = [\mathbf{T}(1, 1)/\mathbf{T}(3, 3)]_{max}$

- the failure Poisson's ratio: $\nu_f = [\mathbf{D}(3, 3)/\mathbf{D}(1, 1)]_{R=R_f}$

Note that the failure stress ratio R_f and the failure Poisson's ratio ν_f are related to the friction angle ϕ_c and the dilatancy angle ψ , respectively, through the following relations: 17

$$R_f = \frac{1 + \sin\phi_c}{1 - \sin\phi_c} \quad (17)$$

and

$$\nu_f = \frac{1 + \tan\psi}{2} \quad (18)$$

Taking the four material constants C_1 , C_2 , C_3 and C_4 as unknowns, a system of four linear equations can be obtained by substituting the corresponded stress and strain rate of the two stress states into the model (15). Therefore, the material constants are related to the initial tangent modulus E_i , the initial Poisson's ratio ν_i , the friction angle ϕ_c and the dilatancy angle ψ . It should be pointed out that these parameters are obtained under a specific confining pressure, e.g., $\mathbf{T}(3, 3) = 100$ kPa. Bering in mind that the model (15) is homogeneous in stress tensor $\mathbf{T}$, the calibrated parameters can be used at arbitrary confining pressures. In addition, the deviatoric loading in the initial hydrostatic state can be considered to be zero, i.e., the initial Poisson's ratio $\nu_i = 0$.

Now, we consider a granular flow in the quasi-static regime. The evolution of solid fraction has a major influence on the stress behaviour before it reaches the critical state. To account for the effects of void ratio, the following density function was introduced into the nonlinear part of model (15) by Wu et al. [Wu96].

$$f_d = (a - 1)D_c + 1 \quad (19)$$

where a is a material parameter related to the stress level and

$$D_c = \frac{e_{crt} - e}{e_{crt} - e_{min}} \quad (20)$$

is the modified relative density; e is the void ratio; e_{min} and e_{crt} are the minimum and the critical void ratio, respectively. The effect of void ratio and stress level on the behaviour of granular materials is taken into account by using the following expressions:

$$e_{crt} = p_1 + p_2 \exp(p_3 |\text{tr} \mathbf{T}|) \quad (21)$$

and

$$a = q_1 + q_2 \exp(q_3 |\text{tr} \mathbf{T}|) \quad (22)$$

where $p_j (j = 1, \dots, 3)$ and $q_j (j = 1, \dots, 3)$ are material parameters and can be determined by fitting the experimental data at the critical state situation; and $|\cdot|$ denotes absolute value. About the material parameters $p_i (i = 1, \dots, 3)$ and $q_i (i = 1, \dots, 3)$, some theoretical and experimental analysis are presented in [Wu96]. p_1 is the critical void ratio when the confining pressure approaches infinity, since p_3 is negative. The value of p_1 should be close to the minimum void ratio under a high confining pressure.

For the case of zero confining pressure, the critical void ratio is equal to $p_1 + p_2$ which may close to the maximum void ratio measured with very low confining pressure. q_1 is assumed to be always equal to 1 and q_3 is a negative value. For the case of $\text{tr}\mathbf{T} \rightarrow \infty$, the difference between dense and loose packing tends to disappear since the parameter $a \rightarrow 1$. Based on the numerical parametric study [Wu96], q_2 is suggested to lie in the range $(-0.4, 0.0)$. p_3 and q_3 for quartz sand are assumed to be -0.0001 kPa. In the case of very low confining pressure, such as the state of liquefaction, relatively higher values of q_2 , p_3 and q_3 may be needed to keep the sensitivity of f_d to the stress level.

Then the constitutive model representing the inviscid stress rate can be written as follows:

$$\dot{\mathbf{T}}_i = C_1(\text{tr}\mathbf{T}_i)\mathbf{D} + C_2 \frac{\text{tr}(\mathbf{T}_i\mathbf{D})\mathbf{T}_i}{\text{tr}\mathbf{T}_i} + f_d \left(C_3 \frac{\mathbf{T}_i^2}{\text{tr}\mathbf{T}_i} + C_4 \frac{\mathbf{T}_i^{*2}}{\text{tr}\mathbf{T}_i} \right) \|\mathbf{D}\| \quad (23)$$

with the critical state function f_d and inviscid stress rate $\mathbf{T}_i$ in equation (15). The inclusion of the critical state function makes the hypoplastic model an attractive choice for describing the rate-independent behaviours of granular material with density dependent softening and hardening features. Note that the candidate for the frictional part is not limited by the equation (23). Some updated hypoplastic models for granular materials, such as the models in [Her04, Von96, Wang18], can serve the same purpose.

3.3 Acceleration-based formulation for viscous behaviour

The description of the viscous behaviour has been developed independently of the theories for the inviscid behaviour. One is tempted to treat granular flow as a non-Newtonian fluid with a single viscosity, i.e.

$$\mathbf{T}_v = \eta \mathbf{D} \quad (24)$$

where η is the viscosity coefficient.

Most viscous models proposed until now are based on a relationship between stress and strain rate. Such models cannot account for the different behaviour for loading and unloading which requires constitutive models formulated in rates [Wu06]. Therefore, the viscous part has to be formulated in rate form as well. Note further that the viscous part is assumed to be dependent on stress, which is supported by some experiments [Jop06]. Moreover, a higher order derivative of strain rate included in the constitutive equations may be able to model the acceleration effect of granular materials. To this end, the equation for the viscous part can be rewritten formally as follows:

$$\dot{\mathbf{T}}_v = \mathbf{H}(\mathbf{T}, \mathbf{D}, \dot{\mathbf{D}}) \quad (25)$$

where the $\mathbf{T}$ is total stress tensor, $\dot{\mathbf{D}}$ is the Jaumann stretching-rate tensor, and can be obtained according the scheme in equation (12) defined as:

$$\dot{\mathbf{D}} = \dot{\mathbf{D}} + \mathbf{D}\mathbf{W} - \mathbf{W}\mathbf{D} \quad (26)$$

in which $\dot{\mathbf{D}}$ is the second time-derivation of strain rate expressed as

$$\dot{\mathbf{D}} = \frac{1}{2} \left[\nabla \ddot{\mathbf{x}} + (\nabla \ddot{\mathbf{x}})^T \right] \quad (27)$$

with $\ddot{\mathbf{x}}$ being the second time-derivation of displacement.

By using the representation theorem for isotropic functions [Wang70] and considering stress dependence, the following terms can be used to compile a workable constitutive equation:

$$\dot{\mathbf{T}}_v = \eta_1 \dot{\mathbf{D}} + \eta_2 (\mathbf{T} \dot{\mathbf{D}} + \dot{\mathbf{D}} \mathbf{T}) + \eta_3 \dot{\mathbf{D}}^2 \quad (28)$$

The last two terms are included to describe the so-called normal-stress effect. In order to see this, let us consider an undrained simple shear motion with constant volume (the constitutive equations for simple shear tests can be found in Section 4.1). To make it simple, we confine ourselves to the material time differentiation and write out the terms $\dot{\mathbf{D}}$, $\mathbf{T} \dot{\mathbf{D}} + \dot{\mathbf{D}} \mathbf{T}$ and $\dot{\mathbf{D}}^2$ in matrices as follows:

$$\dot{\mathbf{D}} = \begin{pmatrix} 0 & \ddot{\gamma} & 0 \\ \ddot{\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{T} \dot{\mathbf{D}} + \dot{\mathbf{D}} \mathbf{T} = \begin{pmatrix} 2\tau \ddot{\gamma} & \bar{p} \ddot{\gamma} & 0 \\ \bar{p} \ddot{\gamma} & 2\tau \ddot{\gamma} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \dot{\mathbf{D}}^2 = \begin{pmatrix} \ddot{\gamma}^2 & 0 & 0 \\ 0 & \ddot{\gamma}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (29)$$

where $\ddot{\gamma}$ and τ are the shear acceleration and shear stress, respectively, in the simple shear test; $\bar{p}$ denotes the sum of normal stress and lateral stress during shearing. The stress $\bar{p}$ can be obtained by $\bar{p} = (1 + K_0)P_n$ with $K_0 \approx 1 - \sin \phi$ and P_n being the earth pressure at rest and the normal stress, respectively.

It is clear that the first and last two terms give rise to only shear and normal stresses, respectively. The second term leads to both normal and shear stress effect. Therefore, we take the second term to describe the viscous behaviour during fast granular flows, and the following simple formula is proposed for the viscous part:

$$\dot{\mathbf{T}}_v = \eta (\mathbf{T} \dot{\mathbf{D}} + \dot{\mathbf{D}} \mathbf{T}) \quad (30)$$

As might be expected, the viscosity coefficient η may depend on the strain rate $\mathbf{D}$, the solid fraction ϕ , and the gradient of volume fraction in granular flow [Wang01]. In some recent models for dense granular flows, the viscosity coefficient is allowed to depend on the normal stress P_n [Jop06]

$$\eta = \tilde{\eta}(\mathbf{I}_D, \mathbf{II}_D, \mathbf{III}_D, \phi, \text{grad} v, P_n \dots) \quad (31)$$

where $\mathbf{I}_D$, $\mathbf{II}_D$ and $\mathbf{III}_D$ are the three invariants of the stretching tensor $\mathbf{D}$ given by $\mathbf{I}_D = \text{tr}(\mathbf{D})$, $\mathbf{II}_D = [\text{tr}(\mathbf{D})^2 - \text{tr}(\mathbf{D}^2)]/2$ and $\mathbf{III}_D = \det \mathbf{D}$.

Since the effect of stress level has been included in equation (30), in this work, we propose the following simple expression for the viscosity:

$$\eta = A \sqrt{m_1 + m_2 \|\mathbf{D}\|^2} \quad (32)$$

in which A , m_1 and m_2 are the material parameters to be determined by fitting experimental data. The above expression describes fairly well the dependence of viscosity on shear rate in granular flow, namely linear dependence at low shear rate and quadratic dependence at high shear rate.

3.4 The complete constitutive model for granular flow

Combining equations (23), (30) and (32), the complete form of the new model is obtained:

$$\begin{aligned} \dot{\mathbf{T}} = & C_1(\text{tr}\mathbf{T}_i)\mathbf{D} + C_2\frac{\text{tr}(\mathbf{T}_i\mathbf{D})\mathbf{T}_i}{\text{tr}\mathbf{T}_i} + f_d\left(C_3\frac{\mathbf{T}_i^2}{\text{tr}\mathbf{T}_i} + C_4\frac{\mathbf{T}_i^{*2}}{\text{tr}\mathbf{T}_i}\right)\|\mathbf{D}\| \\ & + A\sqrt{m_1 + m_2\|\mathbf{D}\|^2}(\mathbf{T}\mathbf{D} + \mathbf{D}\mathbf{T}) \end{aligned} \quad (33)$$

The above constitutive equation applies to the entire process from solid-like to fluid-like behaviour. Unlike most conventional models, where constitutive equations for the static and dynamical regimes are formulated and applied separately, the above constitutive equation makes no distinction between them. Rather, the transition from solid-like to fluid-like behaviour turns out as an outcome.

To explain the above mechanism, let us consider planar granular flow with infinite length down an inclined plane. The granular flow is initiated by increasing the inclination of the plane. Initially, the granular material is in the quasi-static regime with friction dominating the behaviour. The collision between grains is negligible. Along with increasing inclination, the granular material will start to move towards fully developed flow. The inviscid stress increases along with increase of the flow rate. With further increasing the plane angle, the intergranular collision increases leading to the increase of the viscous stress. Meanwhile, the interplay between particles gives rise to mutually repulsion, resulting in reduction of the grains friction and inviscid stress until a critical point is achieved, where the inviscid stress decreases and the viscous stress becomes dominant.

4 Model Performance in simulating fast flow

The performance of the proposed model is examined by simulating simple shear under a constant normal stress. This type of test has been long utilized to study the fast granular flow since the 1960s. For simulating boundary value problems, the constitutive model can be combined with some advanced numerical methods, such as smooth particle hydrodynamic method (SPH) and particle finite element method (PFEM). This is beyond the scope of our lecture. For simulating debris flow and the creep of geomaterials with a similar framework, the readers may refer to our previous works [Peng16, Guo16, Wang18, Xu16].

4.1 Constitutive equation for simple shear test

The simple shear test is commonly performed on cohesive and granular soils in order to study various soil characteristics. The specimen in simple shear apparatus is laterally confined and placed between two rigid plates, with one on the top and other at the bottom. While the plates remain parallel, the upper one moves horizontally and causes shear deformation in the sample. The sketch for a simple shear test is shown in Figure 5.

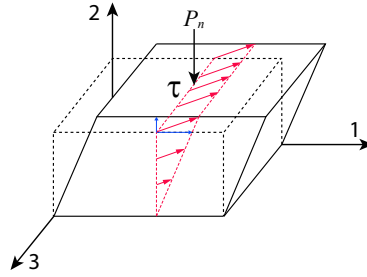


Figure 5: Sketch of a simple shear test, P_n and τ are the normal and shear stresses

Then the stress, strain rate and spin tensors for such a test can be expressed in the following matrix form:

$$\mathbf{T} = \begin{pmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} & 0 \\ \mathbf{T}_{12} & \mathbf{T}_{22} & 0 \\ 0 & 0 & \mathbf{T}_{33} \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 0 & \mathbf{D}_{12} & 0 \\ \mathbf{D}_{12} & \mathbf{D}_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \mathbf{W} = \begin{pmatrix} 0 & \mathbf{W}_{12} & 0 \\ \mathbf{W}_{12} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (34)$$

The motion and displacement in a simple shear test can be described as follows:

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{X}_1 + \mathbf{X}_2 f_1 \\ \mathbf{x}_2 &= \mathbf{X}_2 + \mathbf{X}_3 f_2 \\ \mathbf{x}_3 &= \mathbf{X}_3 \end{aligned} \quad (35)$$

where f_1 and f_2 represent functions of the shear displacement and volume change, respectively. According to equation (12), the strain rate and spin tensors in the simple shear tests are:

$$\mathbf{D} = \frac{1}{2(1+f_2)} \begin{pmatrix} 0 & \dot{f}_1 & 0 \\ \dot{f}_1 & 2\dot{f}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{W} = \frac{1}{2(1+f_2)} \begin{pmatrix} 0 & \dot{f}_1 & 0 \\ -\dot{f}_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (36)$$

By making use of equations (26), (35) and (36), the Jaumann rate of the stretching tensor can be derived as:

$$\dot{\mathbf{D}} = \frac{1}{2(1+f_2)} \begin{pmatrix} 0 & \ddot{f}_1 & 0 \\ \ddot{f}_1 & 2\ddot{f}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2(1+f_2)^2} \begin{pmatrix} -\dot{f}_1^2 & -\dot{f}_1 \dot{f}_2 & 0 \\ -\dot{f}_1 \dot{f}_2 & \dot{f}_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (37)$$

where $\ddot{f}_1$ and $\ddot{f}_2$ are the accelerations along the coordinate 1 and 2, respectively. The first coordinate stands for the shear component and the second for the dilatancy component. Note that the second part of equation (37) has negligible influence on a simple shear tests, leaving only the first part, which denotes the material time-derivation of strain rate $\dot{\mathbf{D}}$. This is because the shear rate is usually rather low and the higher order terms need not be considered.

4.2 Numerical simulation

In the laboratory, a simple shear test can be performed either drained or undrained. The undrained condition is simulated by continuously adjusting the vertical stress so that the specimen height is kept constant (thereby keeping constant volume). The change in vertical stress is assumed to be equal to the change in pore water pressure that would have occurred during a truly undrained test. On the other hand, a drained test can be performed by applying a constant normal stress to the shear plane. During the shearing, the normal stress is kept constant to allow volume change. To show the evolution of solid fraction during the granular flow in a simple shear test, we confine our attention on the drained condition with a constant normal stress (see Figure 5).

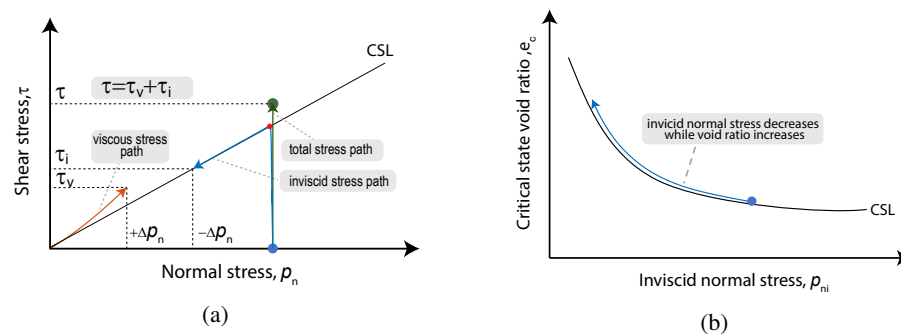


Figure 6: (a) the stress path in the drained simple shear test and (b) inviscid normal stress P_{ni} versus critical state void ratio e_c

Simple shear tests are usually carried out under constant shear rate. Usually, no statement is made as to how this shear rate is reached (acceleration). Since our constitutive model includes the acceleration, we need to specify how a strain rate changes with time. To be more exact, when a test machine is turned out to reach a certain strain rate. The speed of the machine will increase from zero until a given value is reached. Afterwards, the machine will move with this speed till the test end. This is simulated by defining the displacement function f_1 with a positive acceleration. As shown in Figure 6a, at the onset of the test, the material is shear under a low shear rate. The material is in a quasi-static regime and its behaviour is predominated by the friction between grains. This frictional behaviour is described by the rate independent model (33) with an accumulation of the inviscid stress (shear stress). With increasing shear

rate, the viscous stress is continuously accumulated and the viscous part begins to take effect. Since the normal stress is constant, the inviscid part of the normal stress begins to decrease while the viscous normal and shear stress increase. It is interesting to note that the critical state of the frictional behaviour is still existing during the shearing. After reaching the critical state, the inviscid stresses will decrease along the critical state line. Another important mechanism is the increase of the void ratio (or decrease of the solid fraction) during fast shearing. The increase of the shear rate gives rise to increasing viscous stresses, which in turn leads to decreasing inviscid stresses. The critical state line relates the critical void ratio with the pressure of the inviscid stress. As shown in Figure 6b, the critical void ratio increases with decreasing pressure. This means that higher shear rate is related with larger void ratio (smaller solid fraction).

Table 1: Parameters for simulating the simple shear test

C_1	C_2	C_3	C_4	p_1	p_2	p_3
[-]	[-]	[-]	[-]	[-]	[-]	[kPa ⁻¹]
-1.70	-283.4	-283.4	2419.3	0.5	0.5	-0.0005
q_1	q_2	q_3	A	m_1	m_2	e_i
[-]	[-]	[kPa ⁻¹]	[s]	[s]	[s ²]	[-]
1.0	-0.4	-0.0001	-0.0008	0.5	0.001	0.2

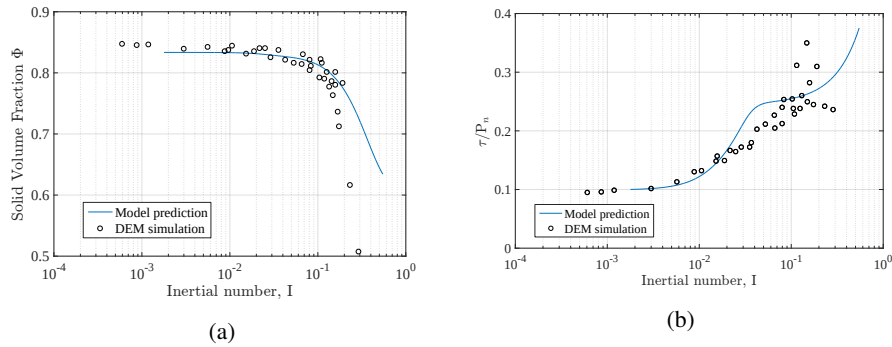


Figure 7: Comparison between model prediction and DEM simulation of fast granular flow in the simple shear test: (a) inertial number I versus solid volume fraction Φ (b) inertial number I versus stress ratio τ/P_n

To examine the above mechanism, we simulate the drained simple shear tests and compare the model prediction with DEM simulations from the literature [Gdr04, Cru03, Cru04a, Cruz04b]. The parameters used in this simulation are given in Table 1, and the comparison between model prediction and DEM simulation is shown in Figure 7. Obviously the solid volume fraction decreases with the shear rate, denoted by the inertial number I (Figure 7a). Moreover, the DEM simulation suggests that the ratio between

normal and shear stress increases with the inertial number I (Figure 7b). Generally, the variation of solid fraction and shear stress ratio are well captured by our model. Note that the parameters for the viscous part listed in Table 1 are constant during the granular flow in the test. Since these parameters may vary with solid fraction, a better prediction might be expected by properly linking these parameters with solid fraction.

5 Conclusions

A new approach to fast granular flow is presented. The main assumption is the decomposition of stress into a frictional (inviscid) stress and a collisional (viscous) stress and the formulation of the constitutive model in rate form. For the inviscid stress rate we make use of our rate independent hypoplastic constitutive equation. The viscous stress rate is obtained by time differentiating the non-newtonian viscous fluid, which leads to the strain acceleration. We show that our model may reproduce some salient features of fast granular flow. More phenomena in fast granular flow are to be explored, e.g. the effect of various accelerations, the transient behaviour from a constant shear rate to zero shear rate, and the behaviour of unloading and reloading.

A further interesting area is the numerical implementation of our model. Most FEM codes use stress and strain rates, while most SPH codes use stress. Our model requires the acceleration in addition to the strain rate.

References

- [Bag84] Ralph Alger Bagnold. *Experiments on a gravity-free dispersion of large solid spheres in a Newtonian fluid under shear*, Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 225.1160: 49-63, 1954.
- [Boy11] Boyer François, Guazzelli Élisabeth and Pouliquen Olivier. *Unifying suspension and granular rheology*, Physical Review. Letters, 107, 188301, 2011.
- [Cam06] Charles S. Campbell. *Granular material flows—an overview*, Powder Technology 162.3: 208-229, 2006.
- [Cam90] Charles S. Campbell. *Rapid granular flows*, Annual Review of Fluid Mechanics 22.1: 57-90, 1990.
- [Cru04a] Frédéric da Cruz, Michaël Prochnow, Jean-Noël Roux, François Chevoir. *Dense granular flows: friction and jamming*, Proceedings of the 17th ASCE Engineering Mechanics Conference, University of Delaware, Newark, DE, USA, June 13-16, 2004.
- [Chi12] Sebastian Chialvo, Sun Jin, Sundaresan Sankaran. *Bridging the rheology of granular flows in three regimes*, Physical review E 85.2: 021305, 2012.

- [Cru03] Frédéric da Cruz, François Chevoir, Jean-Noël Roux, Ivan Iordanoff. *Macroscopic friction of dry granular materials*, In Tribology series, vol. 43, pp. 53-61. Elsevier, 2003.
- [Cruz04b] Frédéric da Cruz. *Friction and jamming in granular flows*, PhD Thesis, Ecole Nationale des Ponts et Chaussees, Marne la vallee, France, 2004.
- [For08] Yoël Forterre, Olivier Pouliquen. *Flows of dense granular media*, Annu. Rev. Fluid Mech. 40: 1-24, 2008.
- [Gdr04] GDR MiDi. *On dense granular flows*, The European Physical Journal E 14, no. 4: 341-365, 2004.
- [Gua18] Élisabeth Guazzelli, Olivier Pouliquen. *Rheology of dense granular suspensions*, Journal of Fluid Mechanics 852, 2018.
- [Guo16] Xiaogang Guo, Chong Peng, Wei Wu, Yongqi Wang. *A hypoplastic constitutive model for debris materials*, Acta Geotechnica 11, no. 6: 1217-1229, 2016.
- [Her04] Ivo Herle, Dimitrios Kolymbas. *Hypoplasticity for soils with low friction angles*, Computers and Geotechnics, 31(5), pp.365-373, 2004.
- [Han85] Daniel M. Hanes, Douglas L. Inman. *Observations of rapidly flowing granular-fluid materials*, Journal of Fluid Mechanics 150 (1985): 357-380, 1985.
- [Hun02] Melany Hunt, Roberto Zenit, Charles S. Campbell, Christopher E. Brennen. *Revisiting Bagnold's 1954 suspension experiments*, Journal of Fluid Mechanics 452: 1-24, 2002.
- [Jop06] Pierre Jop, Yoël Forterre, and Olivier Pouliquen. *A constitutive law for dense granular flows*, Nature 441.7094: 727-730, 2006.
- [Kri59] Irvin M. Krieger, Thomas J. Dougherty. *A mechanism for non-Newtonian flow in suspensions of rigid spheres*, Transactions of the Society of Rheology 3.1: 137-152, 1959.
- [Nes15] Christopher Ness, Jin Sun. *Flow regime transitions in dense non-Brownian suspensions: Rheology, microstructural characterization, and constitutive modeling*, Physical Review E 91.1: 012201, 2015.
- [Peng16] Chong Peng, Xiaogang Guo, Wei Wu, Yongqi Wang. *Unified modelling of granular media with smoothed particle hydrodynamics*, Acta Geotechnica 11, no. 6: 1231-1247, 2016.
- [Sav84] Stuart Savage, Mohamed Sayed. *Stresses developed by dry cohesionless granular materials in an annular shear cell*, Journal of Fluid Mechanics, 142, 391-430, 1984.

- [Ves20] Dalila Vescovi, Pietro Marveggio, Claudio Giulio Di Prisco. *Saturated granular flows: constitutive modelling under steady simple shear conditions* Géotechnique 70.7: 608-620, 2020.
- [Von96] Peter-Andreas Von Wolffersdorff. *A hypoplastic relation for granular materials with a predefined limit state surface*, Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures 1, no. 3: 251-271, 1996.
- [Wang70] Chao Cheng Wang. *A new representation theorem for isotropic functions: An answer to Professor GF Smith's criticism of my papers on representations for isotropic functions*, Archive for rational mechanics and analysis, Jan 1:36(3):166-9, 1970.
- [Wang18] Shun Wang, Wei Wu, Zhen-Yu Yin, Chong Peng, Xuzhen He. *Modelling the time-dependent behaviour of granular material with hypoplasticity*, International Journal for Numerical and Analytical Methods in Geomechanics 42, no. 12: 1331-1345, 2018.
- [Wang01] Yongqi Wang, Columban Hutter. *Granular material theories revisited*, In Geomorphological Fluid Mechanics, pp. 79-107. Springer, Berlin, Heidelberg, 2001.
- [Wu06] Wei Wu. *On high-order hypoplastic models for granular materials*, Journal of engineering mathematics 56, no. 1: 23, 2006.
- [Wu96] Wei Wu, Erich Bauer, Dimitrios Kolymbas. *Hypoplastic constitutive model with critical state for granular materials*, Mechanics of materials, 23(1), 45-69, 1996.
- [Wu96] Wei Wu, Andrzej Niemunis. *Failure criterion, flow rule and dissipation function derived from hypoplasticity*, Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures, 1(2), pp.145-163, 1996.
- [Wu94] Wei Wu, Erich Bauer. *A simple hypoplastic constitutive model for sand*, International Journal for Numerical and Analytical Methods in Geomechanics 18, no. 12: 833-862, 1994.
- [Wu90] Wei Wu, Dimitrios Kolymbas. *Numerical testing of the stability criterion for hypoplastic constitutive equations*, Mechanics of materials, 9(3), 245-253, 1990.
- [Xu16] Guofang Xu, Wei Wu, Jilin Qi. *Modeling the viscous behavior of frozen soil with hypoplasticity*, International Journal for Numerical and Analytical Methods in Geomechanics 40.15: 2061-2075, 2016.15):2061–2075.

Coupled depth integrated two phase SPH models for fast landslides

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Once that readers are familiar with fundamentals of SPH modeling and how this technique can be applied to model geotechnical problems involving large deformations, we will address a special technique which can be applied to a special group of problems, where one dimension - depth, for instance- is much smaller than the other two. This technique consists on integrate the partial differential equations describing the 3D problem along depth, and thus, reducing the problem to 2D. This technique provides a reasonable compromise between cost and efficiency and has been extensively used in other areas such as open channel hydraulics and coastal, harbor and ocean engineering. Its application to fast fluidized landslides is relatively new in comparison with the other areas. This Chapter is devoted to describing depth integrated models for landslide propagation.

1 Introduction

Fundamental aspects of SPH and its application to geomechanical problems have been described in previous chapters of this book. There, SPH has been shown to be a method able to cope with large deformation problems without the need of expensive remeshing operations.

SPH is a technique suitable for both solids and fluids, and for problems where there are transitions from solid to fluid. This is the case of fast catastrophic landslides, where an initial solid mass of soil becomes a fluid which propagates with large velocity, until it comes to rest again, coming back to the solid-state.

Engineers are concerned with predicting the behavior of geostructures before a failure happens, obtaining information on deformations, and also on how far are the service

conditions from failure, which is usually described by a factor of safety. Knowing failure conditions, the design can be improved, or the structure reinforced.

In other cases, such as large landslides, the scale of the involved geostructures and the large forces acting on them make it difficult to avoid failure. Such is the case of earthquakes in mountainous regions, volcanic eruptions, etc. This is the case of large landslides that, once triggered, propagate long distances downhill, runouts being sometimes of the order of tens of kilometers.

The objective of the analysis in these cases is to study the consequences of such failures, assessing their risks and designing protection and mitigation measures.

Of course, a detailed 3D coupled analysis using meshless methods such as SPH would be the optimal solution. However, this can be extremely expensive in terms of the time of computations. The situation is much the same as that of coastal and ocean engineering, where 3D formulations are available, even though not used because of the cost. The method used there is based on using depth integrated equations, which provide a good compromise between cost and accuracy.

The method we propose consists of (i) using full 3D models for triggering and at singular points where the 3D structure of the flow is needed, and (ii) using depth integrated models to analyze propagation. Therefore, the method is based on using a series of models, the resulting accuracy being limited by that of the weakest link in the chain. This is the reason for devoting effort to develop depth integrated models based on sound coupled mathematical models, using suitable constitutive/rheological laws, discretized with the SPH method.

One important feature of the models we will describe here is the use of (i) two sets of SPH nodes for solid and fluid phases, together with finite difference meshes associated to SPH nodes where the evolution of pore water pressure (pwp) is studied.

The two phase / two layer approach has been applied to (i) debris flow problems, and (ii) waves entering a reservoir. In the former, nodes represent solid and fluid phases, while in the latter, they represent two layers, the solid avalanche and the water in the reservoir.

As this Chapter deals with depth integrated models for fast landslide propagation, the material is arranged as follows:

- (i) After this introductory section, we will provide a short description of depth integrated models, focusing on the nature of the system of hyperbolic equations.
- (ii) The third Section will be devoted to describing the general mathematical model, and how some interesting simplifying assumptions lead to simpler models.
- (iii) Material behavior plays a paramount role in the propagation of landslide. Here, we will provide an overview of the models describing it, including frictional, viscous and cohesive models.

- (iv) SPH has already been described in the preceding Chapters, so we will concentrate here on specific features of depth integrated models.
- (v) Finally, we have chosen a set of examples, including some different types of fast landslides which will be presented in the last Section.

2 Hyperbolic PDEs and systems: basic aspects

Depth integrated models are a convenient simplification of 3D models, providing an acceptable compromise between computational cost and accuracy. They have been extensively used in the fields of coastal, harbor, oceanographic and hydraulics engineering since the work of Barré de Saint Venant [SV71] in 1871.

Let us start by showing the eulerian form of shallow water equations written in a reference system $OX_1X_2X_3$, which for simplicity can be assumed to coincide with two axes on a horizontal plane OX_1 and OX_2 .

$$\frac{\partial \phi}{\partial t} + \text{div } F = D + S \quad (1)$$

where ϕ , D , S are the vector of unknowns, D a vector of diffusive terms and S a vector of sources. $F = (F_1, F_2)$ is a matrix of flux vectors along axes 1 and 2. In a 1D case, the equation simplifies to:

$$\frac{\partial \phi}{\partial t} + \frac{\partial F_1}{\partial x_1} = D + S \quad (2)$$

We will come back later to this equation, but what matters so far is the structure of the PDE (partial differential equation), where we can observe 4 terms:

- (i) A partial derivative with respect to time of a vector which includes the unknowns of our problem, which is the rate of change of the unknowns at a fixed point in space,
- (ii) the divergence of a flux vector, and (iii) two terms including diffusive and source terms. The former includes second order derivatives with respect to space, hence the name of diffusive.

The problem we are considering is a system of first order hyperbolic equations. In order to better understand the nature of depth integrated equations, we will consider first some "toy" or "model" equation.

2.1 The 1D scalar convection equation

Let us consider the convective transport along a 1D channel or pipe of magnitude with a concentration given by $\phi(x, t)$. In Figure 1, we describe the balance of the concen-

tration in a control section of length dx . We will further assume that the convective velocity u is constant.

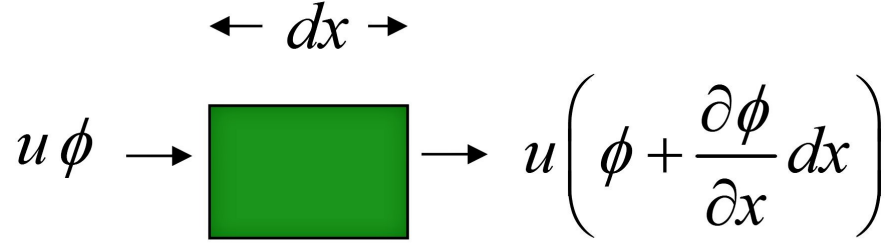


Figure 1: Convection of a scalar magnitude.

The equation describing the balance of mass (concentration) is

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} = 0 \quad (3)$$

which is known as primitive variable formulation.

If we introduce the flux F as $F = u\phi$, the equation can be written in its conservative form:

$$\frac{\partial\phi}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (4)$$

We can compare now this equation with the general form, and observe the physical meaning of the flux term F .

This is the simplest PDE in 1D. Its solutions are functions (waves) of the form:

$$\phi = f(x - ut) \quad (5)$$

which are waves propagating to the right. The shape of the function does not change.

Regarding the conditions for this type of problem being well-posed, and for a domain $(0,L)$ we need to add:

- (i) An initial condition $\phi(x, t = 0) = h_0(x)$ $0 < x < L$

- (ii) Only one boundary condition at the boundary where the information enters the domain, which is $x = 0$: $\phi(x = 0, t) = g(t)$ $0 < t < T$ and no boundary condition at $x = L$.

A general 1D scalar equation can be written as:

$$a \frac{\partial \phi}{\partial t} + b \frac{\partial \phi}{\partial x} = c \quad (6)$$

When all the coefficients a , b and c are either constants or depend only on x, t , the equation is said to be linear. A particular case of the nonlinear equations where the coefficients may depend on the unknown but not on its derivatives x, t is called quasi-linear.

Any discontinuity present on the initial shape will not be damped. We can think that the general model includes this wave propagation property, in some cases the solution being a wave which propagates without changing its amplitude. Moreover, if we want to develop a new model for depth integrated equations, it is advisable to assess its performance with this simple toy model. Diffusive terms for this equation would describe, for instance, molecular diffusion, the equation being written as:

$$\frac{\partial \phi}{\partial t} + \frac{\partial F}{\partial x} = D \frac{\partial^2 \phi}{\partial x^2} \quad (7)$$

where D is the diffusion coefficient. Now the propagating wave will be damped, the nature of the solution depending on the relative importance of diffusion and convection.

Finally, source terms describe how the concentration increases or decreases along time. One possible form for the contribution of the source term is $-s\phi$ which describes a negative source (sink) proportional to the concentration. It can represent, for instance, the decrease rate of a bacteria population. Source terms acting with convection without diffusion, result only on a change of the propagating wave amplitude. The resulting equation is:

$$\frac{\partial \phi}{\partial t} + \frac{\partial F}{\partial x} = D \frac{\partial^2 \phi}{\partial x^2} - s\phi \quad (8)$$

This simple equation includes all the terms shown in the general equation but has the limitation of being linear, while in most cases we will be interested in nonlinear phenomena.

So far, we have considered the eulerian formulation. The lagrangian formulation is obtained by considering the material derivative (or derivative following a particle).

$$\frac{d}{dt}\phi(x, t) = \frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial x} \frac{\partial x}{\partial t} = \frac{\partial\phi}{\partial t} + u \frac{\partial\phi}{\partial x} \quad (9)$$

From here, we can write the lagrangian form of the 1D convective transport equation as:

$$\frac{d\phi}{dt} = D \frac{\partial^2 \phi}{\partial x^2} + S \quad (10)$$

We have to remember that this is the description of how a magnitude changes for an observer traveling with the moving material at the same speed. In case no diffusive nor source terms exist, the equation results on:

$$\frac{d\phi}{dt} = 0 \quad (11)$$

which describes how for our traveling observer the concentration at a material point does not change.

2.2 The quasi linear equation. Burgers equation

So far we have assumed a simple 1D linear model describing convection of a magnitude ϕ with a velocity u . If we recall now a typical fluid dynamics equation, we will find terms of the form $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \dots = \dots$ where we find a similitude with the 1D hyperbolic equation studied in the preceding subsection. The difference is that this equation is nonlinear. The simplest nonlinear 1D hyperbolic PDE is the Burgers equation, given by:

$$\frac{\partial\phi}{\partial t} + \phi \frac{\partial\phi}{\partial x} = 0 \quad (12)$$

The interest of this equation is that the shape of the propagating function can change, featuring shock waves or rarefaction waves. The primitive variables form can be easily transformed into the conservative form by introducing the flux $F = \frac{1}{2}\phi^2$.

$$\frac{\partial\phi}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (13)$$

2.3 1D systems of hyperbolic equations

We will consider now a simplified form of the 1D nonlinear shallow water equations,

$$\frac{\partial}{\partial t} \begin{pmatrix} h \\ \bar{u}h \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \bar{u}h \\ \bar{u}^2h + \frac{1}{2}gh^2 \end{pmatrix} = \begin{pmatrix} 0 \\ -gh\frac{\partial Z}{\partial x} + \frac{1}{\rho}\tau_{bx} \end{pmatrix} \quad (14)$$

where we have introduced the depth averaged velocity ($\bar{u}$):

$$\bar{u} = \frac{1}{h} \int_z^h u dx_3 \quad (15)$$

The coordinate system is sketched in Figure 2 below.

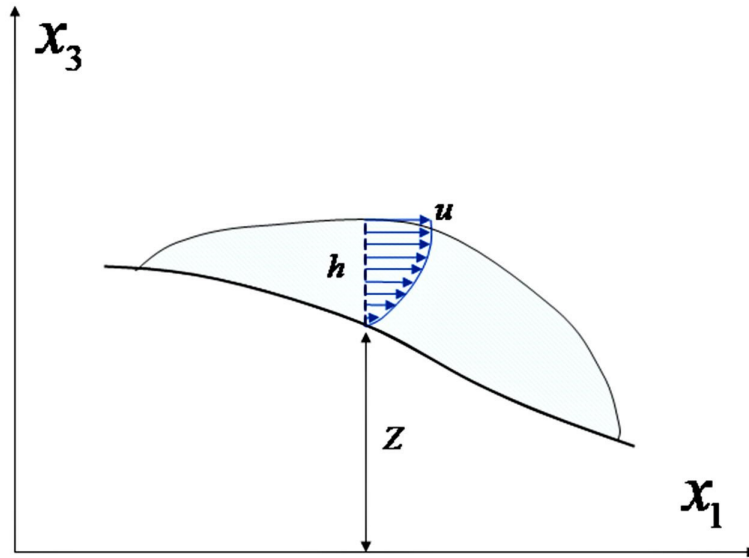


Figure 2: Sketch of the reference axes and main magnitudes.

The unknowns vector, flux, and source terms are:

$$\phi = \begin{pmatrix} h \\ \bar{u}h \end{pmatrix} \quad F = \begin{pmatrix} \bar{u}h \\ \bar{u}^2h + \frac{1}{2}gh^2 \end{pmatrix} \quad S = \begin{pmatrix} 0 \\ -gh\frac{\partial Z}{\partial x} + \frac{1}{\rho}\tau_{bx} \end{pmatrix} \quad (16)$$

The above equations are the depth integrated equations obtained from integrating along depth balance of mass and balance of momentum equations. They can be applied to a variety of problems, such as:

- (i) long wave propagation in coastal regions,
- (ii) transients in open channels,
- (iii) fast landslides and avalanches, and
- (iv) flood waves resulting from breaking of dams, just to mention a few.

The above equation is the eulerian, conservation form. The primitive variables formulation is

$$\frac{\partial \phi}{\partial t} + A \frac{\partial \phi}{\partial x} = S \quad A = \begin{pmatrix} 0 & 1 \\ gh - \bar{u}^2 & 2\bar{u} \end{pmatrix} \quad (17)$$

This formulation, though not convenient for discretization, provides valuable information regarding the possible wave speeds, the characteristic lines and the Riemann invariants which characterize the two existing waves allowing to develop boundary conditions of absorbing type, for instance.

In our case, the discretization method that we will use is the SPH, which requires a lagrangian formulation. To obtain it, we begin by writing separately balance of mass and momentum equations as:

$$\begin{aligned} \frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \bar{u}h &= 0 \\ \frac{\partial}{\partial t} \bar{u}h + \frac{\partial}{\partial x} (\bar{u}^2 h + \frac{1}{2} gh^2) &= -gh \frac{\partial Z}{\partial x} + \frac{1}{\rho} \tau_{bx} \end{aligned} \quad (18)$$

From the balance of mass, and taking into account the definition of the material derivative, we obtain:

$$\frac{\partial h}{\partial t} + \bar{u} \frac{\partial h}{\partial x} + h \frac{\partial \bar{u}}{\partial x} = 0 \quad (19)$$

from where it follows:

$$\frac{dh}{dt} + h \frac{\partial \bar{u}}{\partial x} = 0 \quad (20)$$

Regarding the balance of momentum, we expand the left-hand side term as:

$$\begin{aligned}
\frac{\partial}{\partial t} \bar{u}h + \frac{\partial}{\partial x} (\bar{u}^2h + \frac{1}{2}gh^2) = \\
\bar{u} \frac{\partial h}{\partial t} + h \frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial}{\partial x} (\bar{u}h) + \bar{u}h \frac{\partial \bar{u}}{\partial x} + \frac{\partial}{\partial x} \left(\frac{1}{2}gh^2 \right) \quad (21) \\
\bar{u} \left(\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} (\bar{u}h) \right) + h \left(\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial x} \left(\frac{1}{2}gh^2 \right)
\end{aligned}$$

The first term is the balance of mass equation, hence it is zero, and the second contains the material derivative of the velocity. We obtain:

$$h \frac{d\bar{u}}{dt} = -\frac{\partial}{\partial x} p - gh \frac{\partial Z}{\partial x} + \frac{1}{\rho} \tau_{bx} \quad \text{where } p = \left(\frac{1}{2}gh^2 \right) \quad (22)$$

The lagrangian form of the depth integrated equations is, therefore:

$$\begin{aligned}
\frac{dh}{dt} + h \frac{\partial \bar{u}}{\partial x} &= 0 \\
h \frac{d\bar{u}}{dt} &= -\frac{\partial p}{\partial x} - gh \frac{\partial Z}{\partial x} + \frac{1}{\rho} \tau_{bx} \quad (23)
\end{aligned}$$

3 Two-phase depth integrated mathematical models including pwp for landslide propagation

3.1 Introduction

So far, we have presented hyperbolic PDEs and systems, of which shallow water (or depth integrated) equations are a particular case. These models can be obtained from the 3D continuum models describing the flow of fluids, and describe a variety of problems for which the depth is small in comparison with length and width. They have been extensively used in the fields of coastal, harbour, oceanographic and hydraulics engineering since the work of Barré de Saint Venant in 1871[SV71]. In the case of avalanche dynamics, Savage and Hutter [SH89, SH91] proposed their much-celebrated 1D lagrangian model, where a simple Mohr-Coulomb model allowed a description of the granular material behaviour. This work was extended to 2D and more complex terrains in Hutter et al. [HSSN93], Gray et al. [GWH99]. It has been applied by Laigle and Coussot [LC97], Mc Dougall and Hungr [MH04], Pastor et al. [PQM⁺02, PBP09] and Quecedo et al. [QPH04]. Concerning limitations of the model, Hutter et al. [HWP05] provide a detailed discussion, being worth mentioning the textbook by Pudasaini and Hutter [PH07].

In many cases, there is an important coupling of pore water and air with the solid grains. As soil skeleton dilates (or contracts), pore pressures change, and so do effective stresses. In consequence, basal friction and mobility of the soil mass will be much affected. The first models addressing this issue are those of Hutchinson [Hut86], who proposed a simple sliding-consolidation mechanism for a block, Iverson [Ive97], Iverson and Denlinger [ID01]. A more general approach was proposed by Wang and Hutter [WH99], based on mixture theory.

These models are limited in the sense that they consider only a one phase fluid, while in many problems, such as debris flows there exists an important mobility of one phase relative to the other. Porosity can change and the fluid, in some cases, can abandon the solid skeleton.

3.2 Assumptions, equations and relevant magnitudes

We will recall here equations and magnitudes defined in preceding Chapters devoted to 3D modeling of multiphase problems. The general formulation which can be applied to describe debris flows was proposed by Zienkiewicz and Shiomi [ZS84], following previous work by Biot [Bio41]. It is important to notice that in the area of granular media, Anderson and Jackson [AJ67] proposed a similar model which has been applied to industrial problems such as fluidized beds. Pitman and Le [PL05], and Pudasaini [Pud12] have proposed two phase models for debris flows.

Regarding the 3D coupled model, the basic magnitudes and concepts are:

- (i) the porosity n ,
- (ii) the phase densities for solid and fluid, which depend on the porosity and on the densities of soil grains ρ_s and pore fluid ρ_w as:

$$\begin{aligned}\rho^{(s)} &= (1 - n) \rho_s \\ \rho^{(w)} &= n \rho_w\end{aligned}\tag{24}$$

- (iii) The material derivatives for soil and water phases are used:

$$\begin{aligned}\frac{d^{(s)}}{dt} &= \frac{\partial}{\partial t} + \mathbf{v}_s^T \cdot \text{grad} \\ \frac{d^{(w)}}{dt} &= \frac{\partial}{\partial t} + \mathbf{v}_w^T \cdot \text{grad}\end{aligned}\tag{25}$$

where $\mathbf{v}_s$ and $\mathbf{v}_w$ are the velocities of solid and fluid particles. They are related by:

$$\frac{d^{(w)}}{dt} = \frac{d^{(s)}}{dt} + (\mathbf{v}_w - \mathbf{v}_s)^T \cdot \text{grad}\tag{26}$$

(iv) Regarding the stresses, the total stress acting on the mixture is decomposed as:

$$\boldsymbol{\sigma} = (1 - n) \boldsymbol{\sigma}_s + n \boldsymbol{\sigma}_w = \boldsymbol{\sigma}^{(s)} + \boldsymbol{\sigma}^{(w)} \quad (27)$$

where the partial stresses $\boldsymbol{\sigma}^{(s)}$ and $\boldsymbol{\sigma}^{(w)}$ have been introduced as:

$$\boldsymbol{\sigma}^{(s)} = (1 - n) \boldsymbol{\sigma}_s \quad \boldsymbol{\sigma}^{(w)} = n \boldsymbol{\sigma}_w \quad (28)$$

The stress in the fluid can be decomposed as:

$$\boldsymbol{\sigma}^{(w)} = -n p_w \mathbf{I} + n \boldsymbol{\tau}_w \quad (29)$$

where p_w is the total pressure in the fluid (hydrostatic plus excess pore water pressure) and $\boldsymbol{\tau}_w$ characterizes viscous behavior. We will neglect it in what follows.

The effective stress can be written as

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + p_w \mathbf{I} = (1 - n) (\boldsymbol{\sigma}_s + p_w \mathbf{I}) \quad (30)$$

From here, partial stresses result on:

$$\begin{aligned} \boldsymbol{\sigma}^{(s)} &= \boldsymbol{\sigma}' - (1 - n) p_w \mathbf{I} \\ \boldsymbol{\sigma}^{(w)} &= -n p_w \mathbf{I} \end{aligned} \quad (31)$$

(v) Balance of mass equations for fluid and solid phases can be cast as:

$$\begin{aligned} -\frac{d^{(s)}n}{dt} + (1 - n) \operatorname{div} \mathbf{v}_s &= 0 \\ \frac{1}{Q} \frac{d^{(w)}p_w}{dt} + \frac{d^{(w)}n}{dt} + n \operatorname{div} \mathbf{v}_w &= 0 \end{aligned} \quad (32)$$

where the mixed volumetric stiffness (Q) depends on volumetric stiffnesses of solid grains and water as:

$$\frac{1}{Q} = \frac{(1 - n)}{K_s} + \frac{n}{K_w} \approx \frac{n}{K_w} \quad (33)$$

(vi) Balance of momentum for solid and fluid phases:

$$\begin{aligned} n\rho_w \frac{d^{(w)}\mathbf{v}_w}{dt} &= \{-n \operatorname{grad} p_w\} + n\rho_w \mathbf{b} - \mathbf{R} \\ (1-n)\rho_s \frac{d^{(s)}\mathbf{v}_s}{dt} &= \operatorname{div} \boldsymbol{\sigma}' - (1-n) \operatorname{grad} p_w + (1-n)\rho_s \mathbf{b} + \mathbf{R} \end{aligned} \quad (34)$$

where $\mathbf{b}$ is the gravity acceleration, $\mathbf{R}$ is the interaction solid-fluid forces,

$$\mathbf{R} = -n\mathbf{R}_w = (1-n)\mathbf{R}_s \quad (35)$$

, and $\mathbf{R}_{(\alpha)}$ that acting on phase (α) .

Regarding interaction laws, for a Darcy flow, $\mathbf{R}$ is given by:

$$\mathbf{R} = n^2 \mathbf{k}_w^{-1} (\mathbf{v}_w - \mathbf{v}_s) = n \mathbf{k}_w^{-1} \mathbf{w} \quad (36)$$

where $\mathbf{k}_w$ is the permeability tensor. Other alternatives, such as that used by Pitman and Le [PL05] (see Anderson and Jackson [AJ67]), can be used for a wider range of porosities, and when the relative velocity is larger:

$$\mathbf{R} = \frac{n(1-n)}{V_T n^m} (\rho_s - \rho_w) \mathbf{g} (\mathbf{v}_w - \mathbf{v}_s) \quad (37)$$

where V_T is the terminal velocity of solid particles falling in the fluid, $\mathbf{g}$ the acceleration of gravity and m a constant.

It is convenient to express the interaction term as:

$$\mathbf{R} = C_d (\mathbf{v}_w - \mathbf{v}_s) \quad (38)$$

where C_d is:

$$C_d = n^2 \mathbf{k}_w^{-1} \quad (\text{Darcy}) \quad (39)$$

or

$$C_d = \frac{n(1-n)}{V_T n^m} (\rho_s - \rho_w) \mathbf{g} \quad (\text{Anderson}) \quad (40)$$

3.3 Depth integrated equations for two phase flows

We will use the reference system with axes $\{x_1, x_2, x_3\}$ sketched in Figure 2. Z will denote the basal surface elevation, and h the depth of flowing mass. Velocities will be denoted as $\{v_1, v_2, v_3\}$, and sub-indexes s and w will refer to solid and fluid phases.

An overbar over a magnitude indicates it is a depth averaged value. For instance:

$$\bar{\theta} = \frac{1}{h} \int_Z^{Z+h} \theta(x_1, x_2, x_3) dx_3 \quad (41)$$

We will define the mixture averaged velocity ($\bar{v}$) as:

$$\bar{v} = (1 - \bar{n})\bar{v}_s + \bar{n} \bar{v}_w \quad (42)$$

and the “quasi material derivative” as:

$$\frac{\bar{d}}{dt} = \frac{\partial}{\partial t} + \bar{v}_j \frac{\partial}{\partial x_j} \quad j = 1, 2 \quad (43)$$

Depth integration is performed taking into account Leibnitz’s rule:

$$\int_a^b \frac{\partial}{\partial s} F(r, s) dr = \frac{\partial}{\partial s} \int_a^b F(r, s) dr - F(b, s) \frac{\partial b}{\partial s} + F(a, s) \frac{\partial a}{\partial s} \quad (44)$$

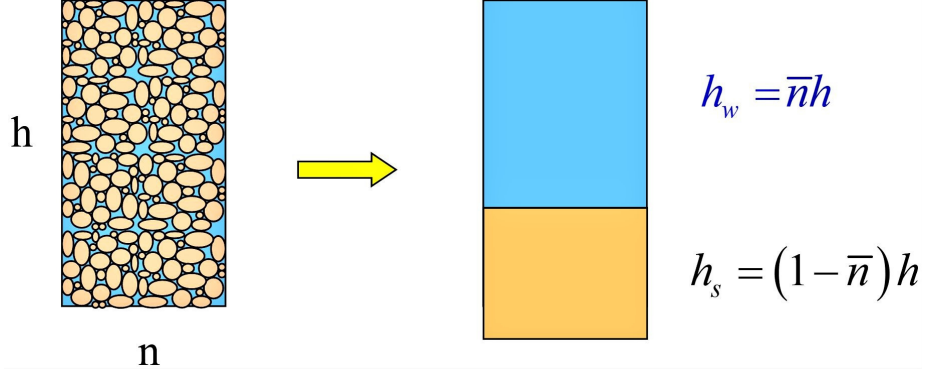
We will introduce next two auxiliary variables h_s and h_w which characterize the solid and fluid contents in a column of total height (h) (see Figure 3).

$$\begin{aligned} h &= h_s + h_w \\ h_s &= (1 - n)h \quad h_w = nh \end{aligned} \quad (45)$$

After applying Leibnitz’s rule to balance of mass equations, we obtain the balance of mass equations for both phases solid (s) and fluid (w) as:

$$\frac{\bar{d}^{(\alpha)}}{dt} (h_\alpha) + h_\alpha \operatorname{div} \bar{v}_\alpha = \bar{n}_\alpha e_R \quad (46)$$

where $\alpha = \{s, w\}$ $h_\alpha = \bar{n}_\alpha h$ and $\bar{n}_s = (1 - \bar{n})$ $\bar{n}_w = \bar{n}$

Figure 3: Definition of auxiliary variables h_s and h_w .

In above equations, α refers to the phase, $\frac{d^{(\alpha)}}{dt}$ is the derivative following phase α , $\bar{n}_\alpha$ the volume fraction, h the depth of the flow, $\bar{v}_\alpha$ the depth averaged velocity and e_R the erosion rate, defined as the increment of height of the moving soil per unit time. There are laws such as that proposed by Hungr et al. [?], which relate it to the depth averaged velocity of the flowing material.

Regarding the **balance of momentum equations** for both phases, after integrating along depth (local x_3 axis), we arrive to:

$$\begin{aligned}
 \rho_s h_s \frac{d^{(s)} \bar{v}_s}{dt} &= \operatorname{div} \left(h \bar{\sigma}^{(s)} \right) - h \bar{p}_w \operatorname{grad} \bar{n} \\
 &\quad - \tau_b^{(s)} + \rho_s h_s \mathbf{b} + h_s \bar{\mathbf{R}}_s - (1 - \bar{n}) \rho_s \left(\bar{v}_s - \bar{v}_s^{(b)} \right) e_R \\
 \rho_w h_w \frac{d^{(w)} \bar{v}_w}{dt} &= -\operatorname{grad} (h \bar{p}_w) + h \bar{p}_w \operatorname{grad} \bar{n} \\
 &\quad - \tau_b^{(w)} + \rho_w h_w \mathbf{b} + h_w \bar{\mathbf{R}}_w - \bar{n} \rho_w \left(\bar{v}_w - \bar{v}_w^{(b)} \right) e_R
 \end{aligned} \tag{47}$$

where we have introduced the shear basal stresses of the solid and fluid phases as:

$$\tau_{bi}^{(s)} = -\sigma_{i3}^{(s)} \Big|_Z \quad \tau_{bi}^{(w)} = -\sigma_{i3}^{(w)} \Big|_Z \tag{48}$$

The terms $\bar{v}_s^{(b)}$ and $\bar{v}_w^{(b)}$ denote the basal slip velocities of solid and water phases.

The depth averaged pore pressure ($\bar{p}_w$) will be decomposed as described when presenting the 3D mathematical model into a hydrostatic part and an excess pore pressure as:

$$\bar{p}_w = \bar{p}_{w,hydr} + \Delta\bar{p}_w \quad (49)$$

One special case of particular interest is where the stresses in the solid phase can be considered as hydrostatic, the pore fluid being inviscid.

$$\begin{aligned} \sigma_{ii} &= ((1-n)\rho_s + n\rho_w) b_3 (h - x_3) \quad i = 1..3 \\ \sigma_{ii}^{(w)} &= n\rho_w b_3 (h - x_3) - n \Delta p_w \end{aligned} \quad (50)$$

from where we obtain:

$$\begin{aligned} \sigma_{ii}^{(s)} &= (1-n)\rho_s b_3 (h - x_3) + n\Delta p_w \quad i=1..3 \\ \sigma'_{ii} &= (1-n)(\rho_s - \rho_w) b_3 (h - x_3) + \Delta p_w \quad i=1..3 \end{aligned} \quad (51)$$

The depth integrated equations are then:

$$\begin{aligned} \rho_s h_s \frac{d^{(s)} \bar{\mathbf{v}}_s}{dt} &= \text{grad} \left\{ \frac{1}{2} (1 - \bar{n}) \rho_s h^2 b_3 \right\} + \text{grad} (\bar{n} h \Delta \bar{p}_w) \\ &\quad + \frac{1}{2} \rho_w h^2 b_3 \text{grad} \bar{n} - h \Delta \bar{p}_w \text{grad} \bar{n} \\ &\quad - \boldsymbol{\tau}_b^{(s)} + \rho_s b h_s + h_s \bar{\mathbf{R}}_s - (1 - \bar{n}) \rho_s (\bar{\mathbf{v}}_s - \bar{\mathbf{v}}_s^{(b)}) e_R \end{aligned} \quad (52)$$

for the solid phase, and

$$\begin{aligned} \rho_w h_w \frac{d^{(w)} \mathbf{v}_w}{dt} &= \text{grad} \left\{ \frac{1}{2} \bar{n} \rho_w h^2 b_3 \right\} - \text{grad} (h_w \Delta \bar{p}_w) \\ &\quad - \frac{1}{2} \rho_w h^2 b_3 \text{grad} \bar{n} + h \Delta \bar{p}_w \text{grad} \bar{n} \\ &\quad - \boldsymbol{\tau}_b^{(w)} + \rho_w b h_w + h_w \bar{\mathbf{R}}_w - \bar{n} \rho_w (\bar{\mathbf{v}}_w - \bar{\mathbf{v}}_w^{(b)}) e_R \end{aligned} \quad (53)$$

for the fluid.

Above equations can be written in a more compact manner by introducing

(i) the pressure terms P_s and P_w defined as:

$$\begin{aligned} P_s &= \left\{ -\frac{1}{2} (1 - \bar{n}) h^2 b_3 - \frac{1}{\rho_s} \bar{n} h \Delta \bar{p}_w \right\} \\ P_w &= \left\{ -\frac{1}{2} \bar{n} h^2 b_3 + \frac{1}{\rho_w} \bar{n} h \Delta \bar{p}_w \right\} \end{aligned} \quad (54)$$

(ii) F_s and F_w :

$$\begin{aligned} F_s &= \left\{ \frac{1}{2} \frac{\rho_w}{\rho_s} h^2 b_3 - h \frac{1}{\rho_s} \Delta \bar{p}_w \right\} \\ F_w &= \left\{ \frac{1}{2} h^2 b_3 + h \frac{1}{\rho_w} \Delta \bar{p}_w \right\} \end{aligned} \quad (55)$$

(iii) and the source terms:

$$\begin{aligned} S_s &= \frac{1}{\rho_s h_s} \left\{ \tau_b^{(s)} + \rho_s \mathbf{b} h_s + h_s \bar{\mathbf{R}}_s - (1 - \bar{n}) \rho_s (\bar{\mathbf{v}}_s - \mathbf{v}_s^b) e_R \right\} \\ S_w &= \frac{1}{\rho_w h_w} \left\{ \tau_b^{(w)} + \rho_w \mathbf{b} h_w + h_w \bar{\mathbf{R}}_w - \bar{n} \rho_w (\bar{\mathbf{v}}_w - \mathbf{v}_w^b) e_R \right\} \end{aligned} \quad (56)$$

The balance of momentum equations are now written as:

$$\begin{aligned} \frac{d^{(s)} \bar{\mathbf{v}}_s}{dt} &= \frac{1}{h_s} \text{grad } P_s + \frac{1}{h_s} F_s \text{grad } \bar{n} + S_s \\ \frac{d^{(w)} \bar{\mathbf{v}}_w}{dt} &= \frac{1}{h_w} \text{grad } P_w + \frac{1}{h_w} F_w \text{grad } \bar{n} + S_w \end{aligned} \quad (57)$$

From the above equations we can obtain those proposed by Pitman and Le [PL05] just by assuming that excess pore pressures ($\Delta \bar{p}_w$) are zero.

For convenience, from now on, we will drop the overbar, all magnitudes being depth integrated unless otherwise stated.

Regarding the excess pore pressure evolution, it is given by:

$$\begin{aligned} \frac{d^{(s)} \Delta p_w}{dt} &= -\rho' b_3 \frac{d^{(s)} h}{dt} \left(1 - \frac{x_3}{h} \right) \\ &+ \frac{K_v}{\alpha} \frac{\partial}{\partial x_3} \left(\frac{n}{C_d} \frac{\partial \Delta p_w}{\partial x_3} \right) - \frac{K_v}{\alpha} \frac{1}{1 - \bar{n}} \frac{d^{(s)} \bar{n}}{dt} \end{aligned} \quad (58)$$

where $K_v = \frac{E}{3(1-2\nu)}$ is the volumetric stiffness of soil skeleton, E the Young's modulus, ν the Poisson's ratio, α being a constitutive parameter and $\bar{C}_d = \frac{C_d}{n}$. If the state of stress is purely hydrostatic, $\alpha = 1$, while under an state of stress $(k_0\sigma_1, k_0\sigma_1, \sigma_3)$ $\alpha = k_0$.

It consists of three terms:

- (i) the increment of excess pore pressure caused by an increase of the debris flow height (see Figure 4).
- (ii) the consolidation along x_3 , and
- (iii) the changes of averaged porosity obtained in the depth integrated equations.

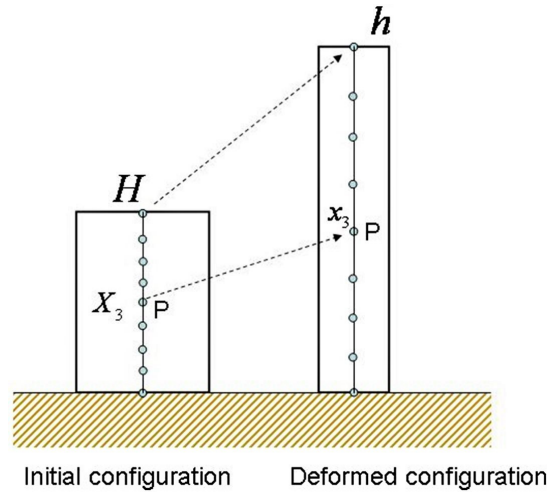


Figure 4: Deformation of a soil column.

4 A short note on constitutive and rheological modeling

4.1 Introduction

Rheology describes the relations between stress and rate of deformation in fluids, while constitutive relations provide suitable relations between stress, rate of stress, and rate of strain. Landslide triggering is usually modeled with constitutive equations, while the propagation of fluidized material is described by rheological laws. One possible solution has been explored by Pastor et al. [PBH⁺15] and applied to both flowslides and rock avalanches.

4.2 Pure cohesive viscoplastic fluid: Bingham model

Bingham model includes two material parameters, the yield stress below which the material does not flow, and the viscosity. The expression for the Bingham model is written as:

$$\tau = \tau_y + \mu \left(\frac{\partial v_1}{\partial x_3} \right) \quad (59)$$

where τ_y is the yield stress.

Depending on the fluid phase viscosity, mudflows, lahars and debris flow can be modeled as viscoplastic fluids with Bingham-like models. Considering a Bingham fluid initially at rest and increasing the shear stress, the fluid will start moving only when the shear stress reaches. This behavior creates what is generally called a "plug" or a zone where the velocity is constant and the rate of deformation is zero.

Concerning the bottom friction, it is assumed that it can be approximated under the hypothesis of simple shear flow conditions. The shear stress at the bottom can be related to the depth-averaged velocity with the following expression:

$$\bar{v} = \frac{\tau_b h}{6\mu} \left(1 - \frac{\tau_y}{\tau_b} \right)^2 \left(2 + \frac{\tau_y}{\tau_b} \right) \quad (60)$$

In order to obtain the basal shear stress, a third-order polynomial has to be solved at every material node and time step. A possible solution was proposed by Pastor et al. [PQG⁺04b]. It consists on obtaining the best second-order polynomial approximating a third-order one.

4.3 Frictional and viscous-frictional fluids

Frictional viscoplastic fluids are used to model fast landslides where friction is important. If the cohesion is assumed to be zero, and the shear behavior is described by:

$$\tau(z) - s(z) = \mu \left(\frac{\partial v_1}{\partial x_3} \right)^m \quad (61)$$

from where the basal shear stress becomes:

$$\tau_b = s_b + \left(\frac{1 + 2m}{m} \right)^m \frac{1}{h^m} \mu \bar{v}^m \quad (62)$$

where s_b is the shear strength at the bottom. In the case, $m = 2$, the above expression reduces to:

$$\tau_b = s_b + \frac{25}{4} \frac{1}{h^2} \mu \bar{v}^2 \quad (63)$$

It is interesting to note the similarity with Voellmy's law:

$$\tau_b = \left\{ \rho g h \cos \theta \tan \varphi + \rho g \frac{\bar{v}^2}{\varsigma} \right\} \quad (64)$$

The difference with the proposed model consists on the Voellmy coefficient being dependent on h .

5 SPH discretization

In previous Chapters the fundamentals of SPH, together with the discretization of two phase, coupled, geotechnical problems have been described. Here, we will focus on depth integrated modeling for two phase materials.

SPH based depth averaged models for landslide propagation have been used by Rodriguez-Paz and Bonet [RPB05], McDougall and Hungr [MH04] and Pastor et al. [PBP09]. An improved method for pore pressure dissipation based on combining the SPH nodes with finite difference (FD) 1D meshes associated to them has been recently proposed by Pastor et al. [PBH⁺15].

Pastor et al. [PYS⁺18] proposed a two phase SPH depth integrated model, which was basically the one proposed in 2005 by Pitman and Le [PL05], the originality being its formulation using a SPH model. The model has been recently extended to include excess pore water dissipation (Tayyebi [Tay19], Tayyebi et al. [TPY⁺20])

The depth integrated mathematical model which we have chosen to describe these phenomena consists of a set of five equations dealing with the balance of mass and momentum for both phases and pore pressures. The unknowns are solid and fluid heights and velocities, depending upon position and time, i.e.

$$h_\alpha(x_1, x_2, t), \bar{v}_\alpha(x_1, x_2, t) \quad \alpha = s, w \quad (65)$$

and pore pressures in excess to hydrostatic:

$$\Delta p_w(x_1, x_2, x_3, t) \quad (66)$$

which will depend on x_3 too. This general model can be hierarchically simplified to obtain most of depth integrated models which are currently applied to landslide propagation problems.

Following the procedure outlined in previous Sections we will introduce:

- (i) two sets of nodes $\{x_{\alpha K}\}$ with $K = 1..N_{\alpha}$ where N_s and N_w are the number of SPH nodes in the solid and fluid phases, and,
- (ii) the nodal variables:
 - $h_{\alpha I}$ heights of phases at node I ,
 - $\bar{v}_{\alpha I}$ depth averaged, 2D velocities, and
 - $\tau_{bI}^{(\alpha)}$ shear stress at the bottom,

In Figure 5, we sketch the SPH soil and water nodes together with the finite difference meshes associated to each solid point to describe pore pressure evolution.

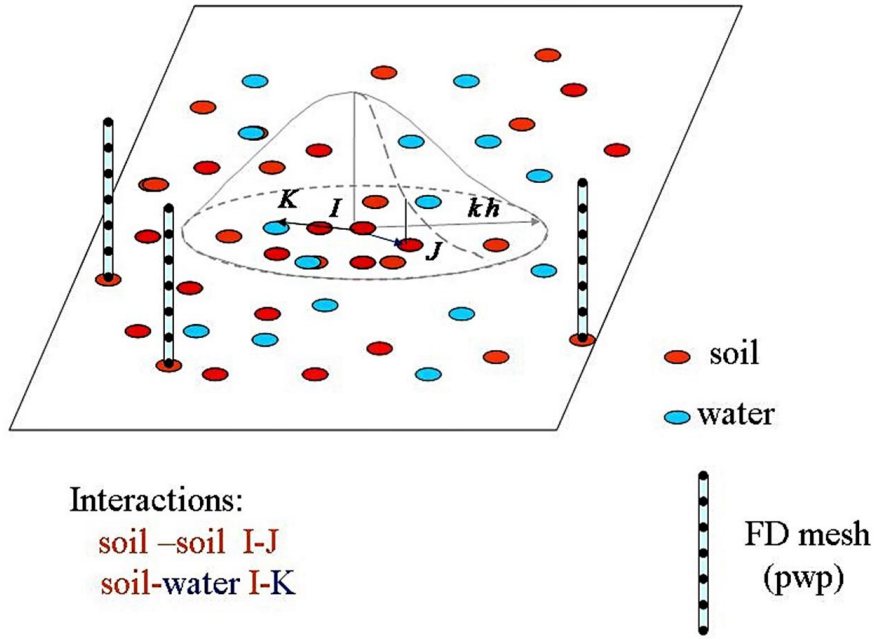


Figure 5: SPH nodes with FD meshes at solid nodes.

If the 2D area associated to a general fluid or solid node I is Ω_I , we will introduce for convenience, a fictitious volume m_I with dimensions L^3 moving with this node:

$$m_I = \Omega_I h_I \quad (67)$$

The SPH approximation of the balance of mass equation for both phases is built from:

$$\left\langle \frac{\bar{d}h_\alpha}{dt} + h_\alpha \operatorname{div} \bar{\mathbf{v}}_\alpha \right\rangle = \langle \bar{n}_\alpha e_R \rangle \quad (68)$$

from which:

$$\frac{\bar{d}}{dt} \langle h_\alpha \rangle + \langle h_\alpha \rangle \langle \operatorname{div} \bar{\mathbf{v}}_\alpha \rangle = \langle \bar{n}_\alpha e_R \rangle \quad (69)$$

From now on, when possible, we will drop the sub-indexes for the sake of simplicity. The equation is written at node I as:

$$\frac{\bar{d}}{dt} h_I + h_I \langle \operatorname{div} \bar{\mathbf{v}} \rangle_I = \langle \bar{n} e_R \rangle_I \quad (70)$$

where the divergence term is approximated as:

$$\operatorname{div} \bar{\mathbf{v}}_I = - \sum_J \Omega_J \mathbf{v}_J \operatorname{grad} W_{IJ} \quad (71)$$

or

$$\operatorname{div} v_I = - \sum_J \frac{m_J}{h_J} \mathbf{v}_J \operatorname{grad} W_{IJ} \quad (72)$$

The discretized balance of mass equation is written as:

$$\begin{aligned} \frac{\bar{d}h_I}{dt} &= -h_I \sum_J \frac{m_J}{h_J} \mathbf{v}_J \operatorname{grad} W_{IJ} + \langle \bar{n} e_R \rangle_I & \text{(Basic form)} \\ \frac{\bar{d}h_I}{dt} &= \sum_J m_J \mathbf{v}_{IJ} \operatorname{grad} W_{IJ} + \langle \bar{n} e_R \rangle_I & \text{(1st form)} \\ \frac{\bar{d}h_I}{dt} &= h_I \sum_J \frac{m_J}{h_J} \mathbf{v}_{IJ} \operatorname{grad} W_{IJ} + \langle \bar{n} e_R \rangle_I & \text{(3rd form)} \end{aligned} \quad (73)$$

where we have introduced (v_{IJ}):

$$\mathbf{v}_{IJ} = \mathbf{v}_I - \mathbf{v}_J \quad (74)$$

Alternatively, the height can be obtained once the position of the nodes is known as:

$$h_I = \langle h(x_I) \rangle = \sum_J h_J \Omega_J W_{IJ} = \sum_J m_J W_{IJ} \quad (75)$$

The height can be normalized, which allows improving the approximation close to the boundary nodes:

$$h_I = \frac{\sum_J m_J W_{IJ}}{\sum_J \left(\frac{m_J}{h_J} \right) W_{IJ}} \quad (76)$$

Next, we will discretize the balance of linear momentum equation. We will recall here for convenience the momentum equations, writing them in a more compact form as:

$$\frac{d^{(\alpha)} \bar{v}_\alpha}{dt} = \frac{1}{h_\alpha} \text{grad } P_\alpha + \frac{1}{h_\alpha} F_\alpha \text{grad } \bar{n} + S_\alpha \quad \alpha = \{s, w\} \quad (77)$$

where the pressure terms are:

$$\begin{aligned} P_s &= \left\{ -\frac{1}{2} (1 - \bar{n}) h^2 b_3 - \frac{1}{\rho_s} \bar{n} h \Delta \bar{p}_w \right\} \\ P_w &= \left\{ -\frac{1}{2} \bar{n} h^2 b_3 + \frac{1}{\rho_w} \bar{n} h \Delta \bar{p}_w \right\} \end{aligned} \quad (78)$$

and

$$\begin{aligned} F_s &= \left\{ \frac{1}{2} \frac{\rho_w}{\rho_s} h^2 b_3 - h \frac{1}{\rho_s} \Delta \bar{p}_w \right\} \\ F_w &= \left\{ \frac{1}{2} h^2 b_3 + h \frac{1}{\rho_w} \Delta \bar{p}_w \right\} \end{aligned} \quad (79)$$

Finally, the source terms are:

$$\begin{aligned} S_s &= \frac{1}{\rho_s h_s} \left\{ \tau_b^{(s)} + \rho_s \mathbf{b} h_s + h_s \bar{\mathbf{R}}_s - (1 - \bar{n}) \rho_s (\bar{\mathbf{v}}_s - \mathbf{v}_s^b) e_R \right\} \\ S_w &= \frac{1}{\rho_w h_w} \left\{ \tau_b^{(w)} + \rho_w \mathbf{b} h_w + h_w \bar{\mathbf{R}}_w - \bar{n} \rho_w (\bar{\mathbf{v}}_w - \mathbf{v}_w^b) e_R \right\} \end{aligned} \quad (80)$$

We will consider next how to discretize each of the three terms $\text{grad } P_\alpha$, $\frac{1}{h_\alpha} F_\alpha \text{grad } \bar{n}$ and S_α .

Regarding the gradient terms, we will write only one of the symmetrized forms, (see Monaghan [MG83, Mon00, Mon92]):

$$\begin{aligned} \frac{1}{h_{\alpha I}} \text{grad } P_{\alpha I} &= - \sum_1^{N_{\alpha h}} m_J \left(\frac{P_{\alpha I}}{h_{\alpha I}^2} + \frac{P_{\alpha J}}{h_{\alpha J}^2} \right) \\ \frac{1}{h_{\alpha I}} \text{grad } \bar{n}_{\alpha I} &= - \sum_1^{N_{\alpha h}} m_J \left(\frac{\bar{n}_{\alpha I}}{h_{\alpha I}^2} + \frac{\bar{n}_{\alpha J}}{h_{\alpha J}^2} \right) \end{aligned} \quad (81)$$

which results on:

$$\begin{aligned} \frac{d^{(\alpha)}}{dt} \bar{\mathbf{v}}_{\alpha I} &= \sum_J m_J \left(\frac{P_{\alpha I}}{h_I^2} + \frac{P_{\alpha J}}{h_J^2} \right) \text{grad } W_{IJ} \\ &+ F_{\alpha I} \sum_J m_J \left(\frac{n_{\alpha I}}{h_I^2} + \frac{n_{\alpha J}}{h_J^2} \right) \text{grad } W_{IJ} + S_{\alpha I} \end{aligned} \quad (82)$$

The scheme is explicit, and we use a time step limit given by the CFL condition:

$$\Delta t_{SPH} \leq \frac{h_{\min}}{(\max(\sqrt{gh_I} + |v_I|))} \quad (83)$$

In above equations, there is a term describing basal excess pore pressure (Δp_{wbI}) at node I which has to be obtained at each node and time step. One alternative is to use simple shape functions fulfilling boundary conditions at the surface and the basal surface. This has been used by Iverson and Denlinger [ID01], Pastor et al. [PQM⁺02, PQG⁺04a, PSD⁺15] and Quecedo et al. [QPH04]. This approach presents the limitation of not being able to model changes of boundary conditions at the bottom. For instance, when a landslide runs over a very permeable basal layer -or a rack- pore

pressure becomes zero there, while in the body of the landslide is not zero. If a single shape function is used, once the basal value is set to zero, the pressure becomes zero in the whole depth.

To overcome this limitation, we have proposed to introduce FD meshes associated to each SPH solid node [PBH⁺15]. Figure 5 provides a sketch of the SPH nodes and FD meshes layout. Pastor et al. [PYS⁺18] has been extended the model, proposed for 1-phase modeling of flowslides, to 2-phase modeling of debris flows.

The analysis of excess pore pressure evolution is based on equation 58, which is a classical parabolic partial differential equations which include two source terms related to variations of height and porosity.

Initial conditions describe the excess pore pressure distribution in all FD meshes. Here, we have assumed simple linear laws with values of zero at the top and $\Delta p_{wp,0}^{(b)}$ at the basal surface. The latter has to be estimated, either from field data or from the results of a model describing triggering of the landslide. This initial condition plays a fundamental role in debris flow propagation characteristics. When no data are available, it has to be estimated.

Concerning boundary conditions, we have assumed a zero value at the top, while at the base it is usual to assume an impermeable boundary (zero flow). However, these are the situations where the debris flow arrives to mitigation structures such as basal grids, where total pore pressure will be dissipated and become equal to the atmospheric. This makes the flow to slow down or even to stop, as basal friction will increase. Once the flow exits the grid, the flux is made zero again. Here, we have boundary conditions which depend on the position of the nodes on the terrain.

A variable smoothing length formula proposed by Benz [Ben90] is considered in the present work.

$$h_I h_{SMLI}^{NDIM} = const \quad (84)$$

where h_{SMLI} denotes the smoothing length at node I .

The algorithm is explicit and less accurate than the approach proposed by Bonet et al. [BKRPP04], where both the mass conservation and balance of momentum equations were solved using a Newton Raphson algorithm.

The resulting equations are ODEs which can be integrated in time using a scheme such as Leap Frog or Runge Kutta (2nd or 4th order).

One important issue is the representation of the terrain over which the avalanche moves, as it greatly influences the results. If we denote the height of the terrain by Z_I at node I , we have to obtain (i) its gradient ($\text{grad } Z_I$), and (ii) the radius of curvature along the tangent to the node path, which can be obtained from the second-order derivatives of Z .

In the case of fast landslides, the terrain information is given on a digital terrain model (DTM), which consists of a series of values (x_k, y_k, z_k) at the nodes of a structured grid. From here we can obtain both gradients and second derivatives at the grid nodes using a classical nodal recovery technique on a finite element mesh which nodes are those of the DTM grid.

Concerning the neighbor search, we have used an auxiliary structured grid covering the part of the terrain where the SPH particles are. Spacing is taken as the minimum smoothing length. For a given SPH node, the search is restricted to the cell it belongs and its neighbors. This temporary grid is valid only for a given time step. In cases where the flow is elongated, the grid can be oriented automatically following the main inertia axes of the set of SPH nodes on the plane.

6 Benchmarks and applications

Finally, we have selected some benchmarks which illustrate the behavior of the models described in this Chapter.

6.1 Shocks and expansion waves

The first example we will study is illustrated in Figure 6 (Yagüe [Her18], Pastor et al. [PYS⁺18]). It consists of a domain enclosed by two walls located at $x = -10m$ and $x = 10m$ filled with two masses having different heights and porosities:

$$\begin{aligned} h_L &= 1.04 \quad h_{sL} = 0.32 \quad h_{wL} = 0.72 \quad n_L = 0.69 \\ h_R &= 1.38 \quad h_{sR} = 0.84 \quad h_{wR} = 0.54 \quad n_R = 0.39 \end{aligned} \quad (85)$$

We have depicted in the profile, the total height $h = h_s + h_w$ and the height of the solid fraction h_s . The solid is assumed to have no strength, with particles of density $\rho_s = 2000 \text{ Kg/m}^3$ the water being inviscid. The interaction forces are given by Anderson formula,

$$\begin{aligned} R &= -nR_w = (1 - n)R_s \\ R &= C_d (v_w - v_s) \\ C_d &= \frac{n(1 - n)}{V_T n^m} (\rho_s - \rho_w) g \end{aligned} \quad (86)$$

where we have chosen $V_T = 1.e - 3 \text{ m/s}$ and $m = 1$.

This test has been used in Pelanti et al. [PBM08] to show the complex pattern of rarefaction and shock waves in both solid and fluid phases. Debris flows having two

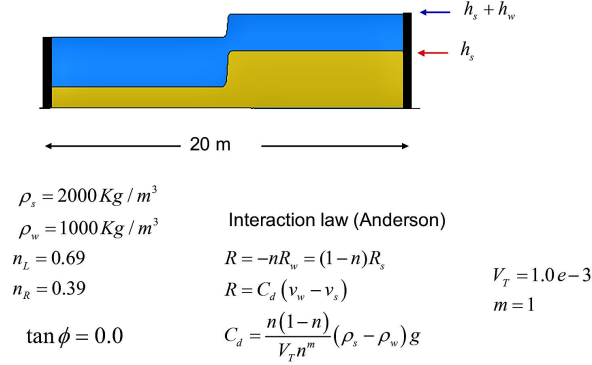


Figure 6: Two phase dam break problem.

phases with important relative mobility present a rich structure of shocks and rarefaction waves, which has to be properly modeled. Otherwise, the model will have numerical damping or dispersion.

At time zero, the wall separating both masses is removed. as soil and water have different heights, a complex pattern of shocks and rarefaction waves is produced. This is depicted in Figure 7, where we show the profiles of total height and soil fraction at times 0.5, 1.0, 1.5, 2.0, 3.5 and 6s.

Finally, we depict in Figure 8 the profiles of porosity at times 0 and 2s.

6.2 Dambreak of a frictional fluid over a dry horizontal plane

We have chosen a 1D dam break problem to assess factors upon which runout and propagation depend. It consists of the dam sketched in Figure 9, with a initial height of the material equal to $10m$. and a length of $10m$.

The dam is filled with a saturated loose granular material with densities of solid particles and fluid $\rho_s = 2500 \text{ Kg/m}^3$ $\rho_w = 2500 \text{ Kg/m}^3$ and an initial porosity of 0.4, for which the mixture density is $\rho = 2050 \text{ Kg/m}^3$.

The material is contained by two walls, and at time 0s, the wall on the right is removed, which causes the material to liquefy. Then, the debris flow propagates along the horizontal plane.

It is interesting to note, when analyzing the results we are presenting, that:

- (i) the runout of a dry material with the same friction angle and porosity is 11.80 m, the flow coming to rest at time 1.75s, and
- (ii) in case the material is fully saturated, one-phase models predict a runout of 24.5m, with a stopping time close to 3s.

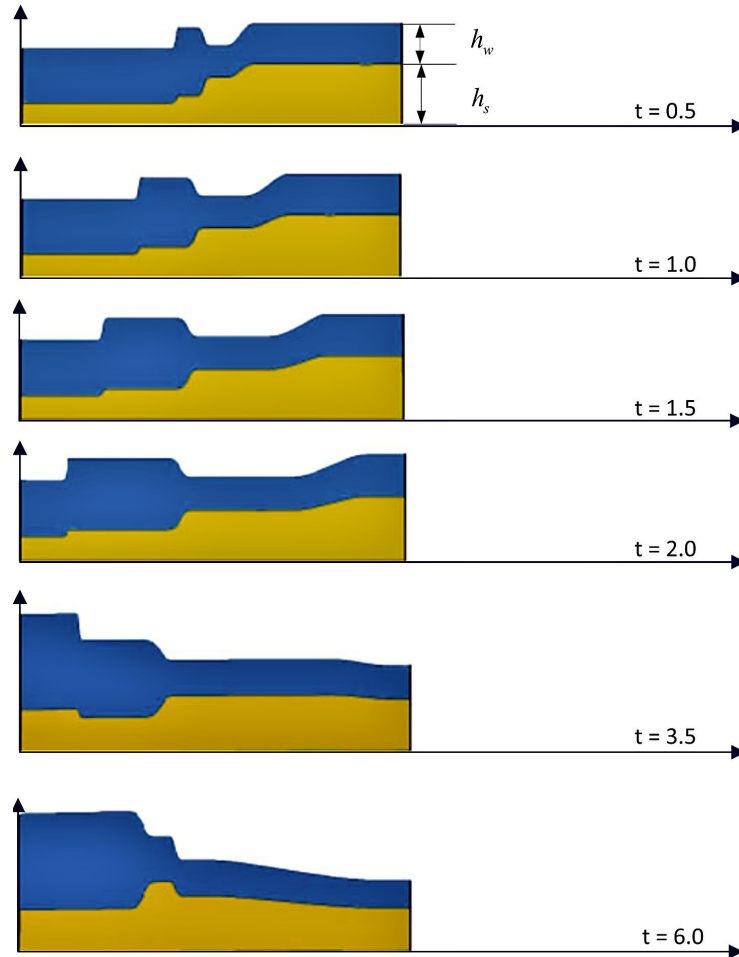


Figure 7: Profiles of h_s and $h_s + h_w$ at times 0.5, 1.0, 1.5, 2.0, 3.5 and 6s.



Figure 8: Profiles of porosity at times 0 and 2s.

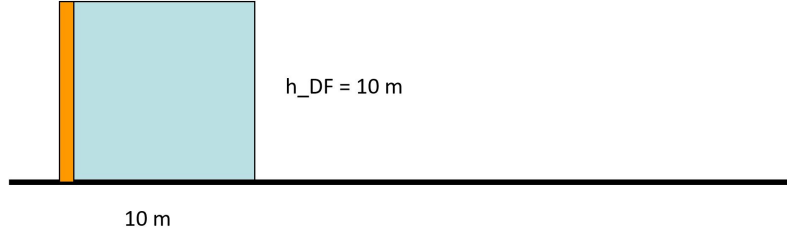


Figure 9: The 1D dam break problem.

In order to assess the predictions of the proposed model, we have selected a control case having similar consolidation and propagation times. The model describing the interaction between phases is that of Anderson and Jackson [AJ67], with $V_T = 1.e - 3 \text{ m/s}$ and exponent $m = 1$. This corresponds to a darcy's permeability of $8.57 \cdot 10^{-5} \text{ m/s}$ with a consolidation coefficient $C_V = 2.92 \text{ m}^2/\text{s}$ for $h = 5\text{m}$.

We depict in Figure 10 the profiles of the fluidized material at times 0, 0.5, 1.0, 2.0, 3.0, and 4.0s. We have followed the convention described in Section 5 to characterize solid and fluid fractions, solid being the darker shade of green. We can see in the figure how solid and fluid components travel with the same speed.

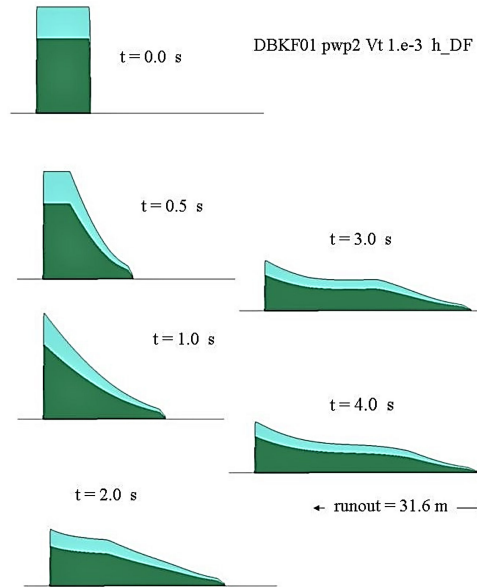


Figure 10: Dam break problem: profiles of debris flow height at times 0, 0.5, 1.0, 2.0, 3.0, and 4.0s. Dark and light shades describe the phases, darker being the solid.

One way to characterize propagation is by plotting the position along time of the front. In this case, we depict in Figure 11 the coordinate x of the leading soil and fluid particles along time.

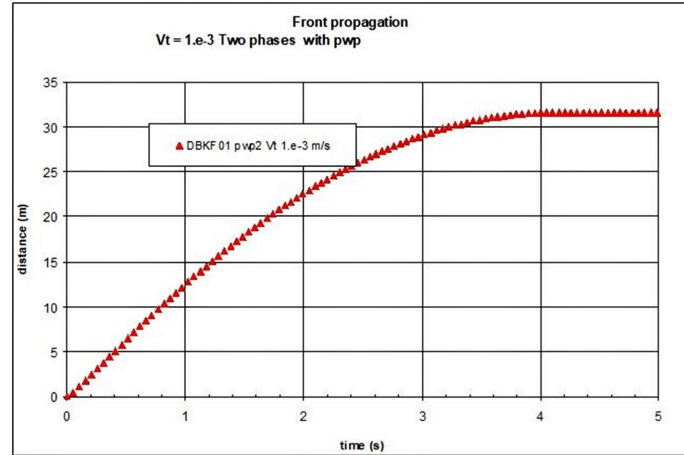


Figure 11: Runout of solid and fluid leading nodes.

We can observe how at $3.5s$ approximately the flow has stopped, the runout being $31.6m$, much larger than those of one-phase or dry materials, the reason being the basal pore pressures.

Next, we will consider the evolution on this reference case of the pore pressures (in excess of hydrostatic). We plot in Figure 12 the profiles of pore-water pressure superimposed on the deformed mass of fluidized soil at times $0.5, 1, 2, 3$ and $4s$.

We can observe how basal pore pressure decrease along time, reaching values close to zero at $3s$ approximately. In addition to pore pressure dissipation, the effect of the decreasing height of the debris flow contributes to decreasing the pressure.

In order to study this effect, we depict in Figure 13 the evolution of basal pore pressure and height as node 501, located at the middle of the reservoir, along time. We have made to coincide the vertical scales of debris flow height and excess pore-water pressure, the latter being measured in m . When the pwp has a value h , the material is in a liquefied state.

Analyzing both curves, we can observe a first period of $0.5s$ with a value of height which has not changed as the rarefaction wave has not reached this point. At this period, pore-water pressure changes are only caused by consolidation. Later, the soil node we are considering starts moving, its height decreasing as time increases. This results on an additional decrease of the excess pore-water pressure. Finally, at time $3.2s$ approximately, the pore-water pressure is fully dissipated and the height is constant.

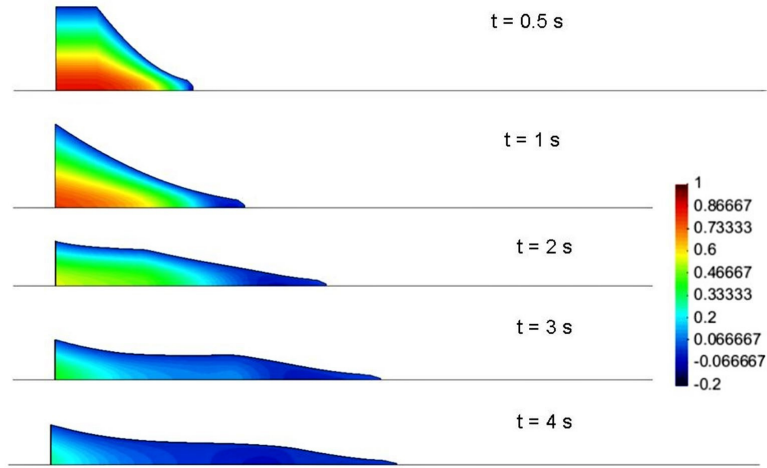


Figure 12: Excess pore pressure profiles along time, depicted on the deformed geometry.

We recall here that the profiles of pore-water pressure have been obtained from the finite difference meshes associated to SPH solid nodes, which move with them. In this way, the profiles of pore-water pressure correspond to a material point.

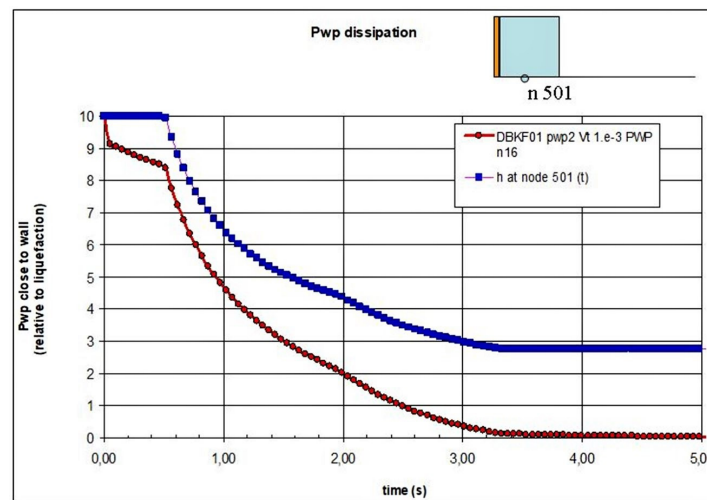


Figure 13: Pore pressure evolution along time at node 501, located initially at the middle of the reservoir.

In order to assess the effect of pwp on the runout, we compare in Figure 14 the runout of 2 phases debris flows with and without pore water pressure. Both arrive to equilibrium, but the case without pwp stops before, its runout being smaller.

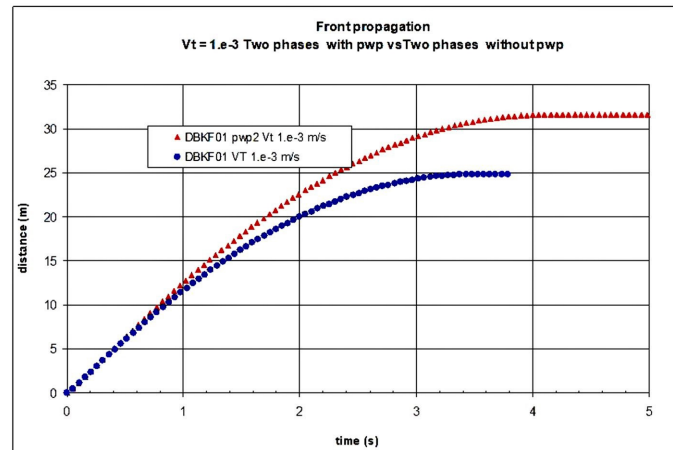


Figure 14: Comparison of the runouts of 2 phase debris flow models with and without pore-water pressure.

6.3 Yu Tung road debris flow

On 7 June 2008, an intense rainstorm triggered a debris flow on the natural hillside in Lantau Island, Hong Kong (Figure 15).



Figure 15: Aerial View of the debris flow event after the landslide incident.

Over $3000m^3$ of debris ran down the hillside and traveled $510m$ at an apparent travel angle of 17° to the Yu Tung Road which resulted in significant entrainment and deposition along the debris path and serious road blockage.

For the analysis, we have used the debris flow two phase model including pore water pressure evolution. We provide in Figure 16, a topographical map showing the landslide path and positions of the flowing mass from initial to final deposition. The rheological parameters of the basal friction angle of 40° with a Voellmy coefficient equal to $600 m/s^2$ has been considered.

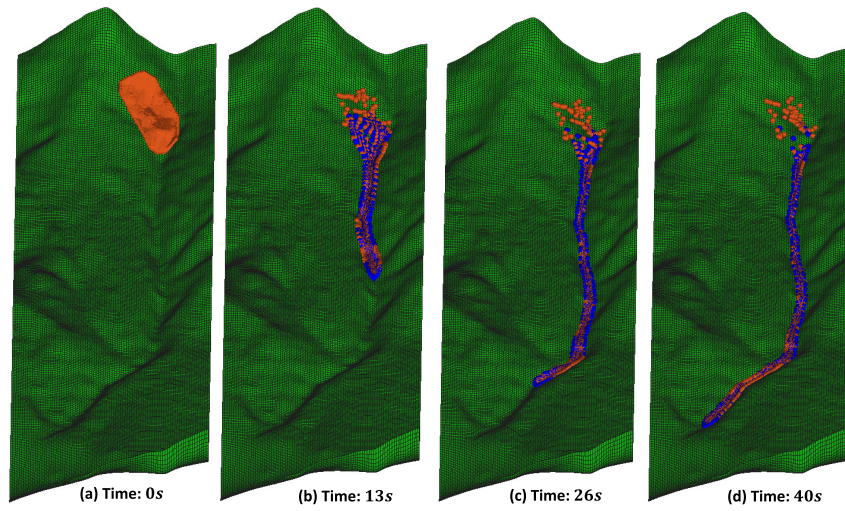


Figure 16: Results sequence of the debris flow simulation at different positions.

The velocity distribution at different times is shown in Figure 17. The frontal velocity of the debris was computed to be about $12m/s$ at the time of $4s$ and a distance of $100m$ from the source location. Then, the debris flow traveled at a higher speed with an average velocity of about $17m/s$ at propagation time of $13s$ and a distance of $350m$. Finally, it slows down to $11m/s$ at the time of $23s$.

Field mapping revealed that significant entrainment of loose materials and erosion of the side slopes had occurred. It is estimated that the active volume increased to about $3400m^3$ which implies that the bed entrainment was a key aspect in effecting the dynamics of the moving mass.

The model takes into account bed entrainment along the landslide path and decreasing of the ground surface elevation consistently over time. Figure 18 shows the amount of erosion. We have used Hungr's erosion law [Hun95], with an entrainment coefficient of $0.0011 ms^{-1}$.

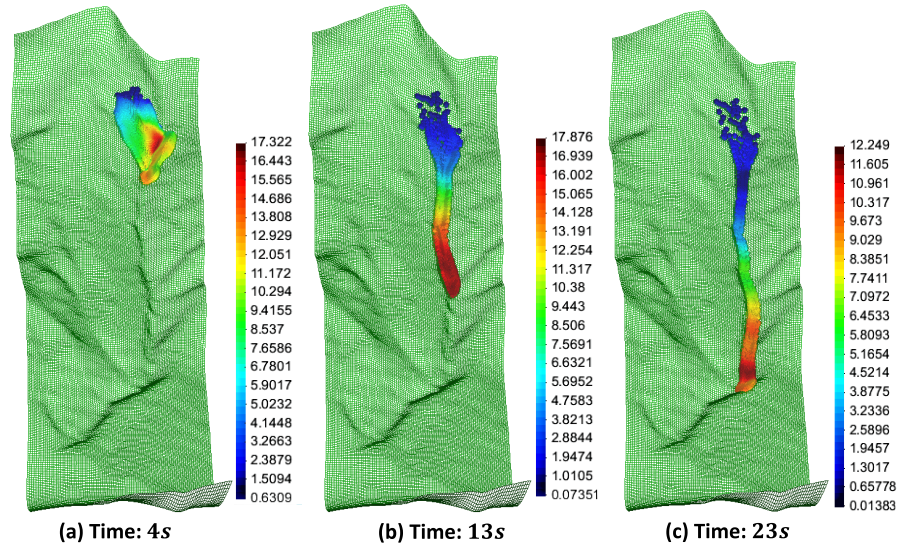


Figure 17: Computed velocities at times 7s, 15s and 25s.

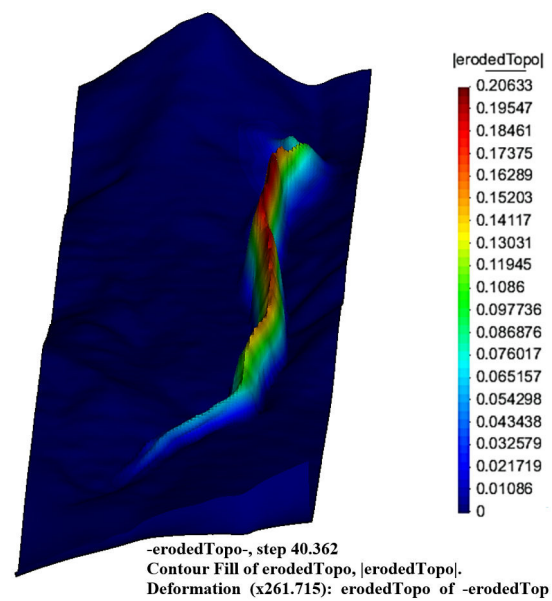


Figure 18: Final erosion depths at time 40s.

Debris flow velocities were estimated at various locations along the flow path by using super-elevation data and a video record which captured the whole debris flow process. Figure 19 shows the observed frontal velocities (shown in red dots) along chainage and the profile of frontal velocities computed by the proposed model.

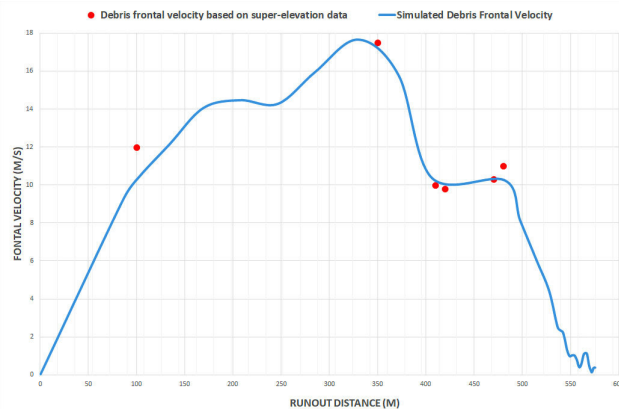


Figure 19: Comparison between observed and computed frontal velocities.

7 Conclusions

Depth integrated models are a suitable complement of 3D techniques. They can cope with complex two flows where relative mobility of the phases is large and where water pressure evolution inside the flowing mass control its behavior. There exist different alternative formulations -eulerian, lagrangian, finite elements, SPH, etc- of which we have chosen SPH within a lagrangian framework. SPH models such as the one described here can use a double set of nodes to represent both fluid and solid phases. Moreover, pore water pressure evolution can be dealt with a set of finite difference meshes associated to each SPH node.

In our opinion, this class of models can be used together with a full 3D approximation, the latter dealing with triggering and particular parts of the flow, where knowing its 3D structure is necessary.

We would like to close the Chapter by stating that models have to be validated against (i) problems having a known analytical solution (ii) laboratory flume small scale tests, and (iii) real cases for which consistent data is available.

References

- [AJ67] T. B. Anderson and R. Jackson. Fluid Mechanical Description of Fluidized Beds. Equations of Motion. *Ind. Eng. Chem. Fundam.*, 6(4):527–539, nov 1967.
- [Ben90] W. Benz. Smooth Particle Hydrodynamics: A Review. In J.-R. Buchler, editor, *Numer. Model. Nonlinear Stellar Pulsations*, pages 269–288, Dordrecht, 1990. Springer Netherlands.
- [Bio41] M. A. Biot. General Theory of Three-Dimensional Consolidation. *J. Appl. Phys.*, 12(2):155–164, feb 1941.
- [BKRPP04] J. Bonet, S. Kulasegaram, M. X. Rodriguez-Paz, and M. Profit. Variational formulation for the smooth particle hydrodynamics (SPH) simulation of fluid and solid problems. *Comput. Methods Appl. Mech. Eng.*, 193(12-14):1245–1256, mar 2004.
- [GWH99] J. M. Gray, M. Wieland, and K. Hutter. Gravity-driven free surface flow of granular avalanches over complex basal topography. *Proc. R. Soc. London. Ser. A Math. Phys. Eng. Sci.*, 455(1985):1841–1874, may 1999.
- [Her18] A.Y. Hernán. Modelización de flujos de derrubios mediante SPH. 2018.
- [HSSN93] K. Hutter, M. Siegel, S. B. Savage, and Y. Nohguchi. Two-dimensional spreading of a granular avalanche down an inclined plane Part I. theory. *Acta Mech.*, 100(1-2):37–68, mar 1993.
- [Hun95] O. Hungr. A model for the runout analysis of rapid flow slides, debris flows, and avalanches. *Can. Geotech. J.*, 32(4):610–623, aug 1995.
- [Hut86] J. N. Hutchinson. A sliding–consolidation model for flow slides. *Can. Geotech. J.*, 23(2):115–126, may 1986.
- [HWP05] K. Hutter, Y. Wang, and S. P. Pudasaini. The Savage–Hutter avalanche model: how far can it be pushed? *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.*, 363(1832):1507–1528, jul 2005.
- [ID01] R. M. Iverson and R. P. Denlinger. Flow of variably fluidized granular masses across three-dimensional terrain: 1. Coulomb mixture theory. *J. Geophys. Res. Solid Earth*, 106(B1):537–552, jan 2001.
- [Ive97] R. M. Iverson. The physics of debris flows. *Rev. Geophys.*, 35(3):245–296, aug 1997.
- [LC97] D. Laigle and P. Coussot. Numerical Modeling of Mudflows. *J. Hydraul. Eng.*, 123(7):617–623, jul 1997.
- [MG83] J. J. Monaghan and R. A. Gingold. Shock simulation by the particle method SPH. *J. Comput. Phys.*, 52(2):374–389, nov 1983.

- [MH04] S. McDougall and O. Hungr. A model for the analysis of rapid landslide motion across three-dimensional terrain. *Can. Geotech. J.*, 41(6):1084–1097, dec 2004.
- [Mon92] J. J. Monaghan. Smoothed Particle Hydrodynamics. *Annu. Rev. Astron. Astrophys.*, 30(1):543–574, sep 1992.
- [Mon00] J. J. Monaghan. SPH without a Tensile Instability. *J. Comput. Phys.*, 159(2):290–311, apr 2000.
- [PBH⁺15] M. Pastor, T. Blanc, B. Haddad, V. Dremptic, M. S. Morles, P. Dutto, M. M. Stickle, P. Mira, and J. A. Merodo. Depth Averaged Models for Fast Landslide Propagation: Mathematical, Rheological and Numerical Aspects. *Arch. Comput. Methods Eng.*, 22(1):67–104, jan 2015.
- [PBM08] M. Pelanti, F. Bouchut, and A. Mangeney. A Roe-type scheme for two-phase shallow granular flows over variable topography. *ESAIM Math. Model. Numer. Anal.*, 42(5):851–885, sep 2008.
- [PBP09] M. Pastor, T. Blanc, and M. J. Pastor. A depth-integrated viscoplastic model for dilatant saturated cohesive-frictional fluidized mixtures: Application to fast catastrophic landslides. *J. Nonnewton. Fluid Mech.*, 158(1-3):142–153, may 2009.
- [PH07] S. P. Pudasaini and K. Hutter. *Avalanche dynamics: Dynamics of rapid flows of dense granular avalanches*. Springer Berlin Heidelberg, Berlin, Heidelberg, 2007.
- [PL05] E. B. Pitman and L. Le. A two-fluid model for avalanche and debris flows. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.*, 363(1832):1573–1601, jul 2005.
- [PQG⁺04a] M. Pastor, M. Quecedo, E. Gonzalez, M. I. Herreros, J. A. Merodo, and P. Mira. Modelling of Landslides: (II) Propagation. In *Degrad. Instab. Geomaterials*, pages 319–367. Springer Vienna, Vienna, 2004.
- [PQG⁺04b] M. Pastor, M. Quecedo, E. González, M. I. Herreros, J. A. Merodo, and P. Mira. Simple Approximation to Bottom Friction for Bingham Fluid Depth Integrated Models. *J. Hydraul. Eng.*, 130(2):149–155, feb 2004.
- [PQM⁺02] M. Pastor, M. Quecedo, J. A. Merodo, M. I. Herreros, E. Gonzalez, and P. Mira. Modelling tailings dams and mine waste dumps failures. *Géotechnique*, 52(8):579–591, oct 2002.
- [PSD⁺15] M. Pastor, M. M. Stickle, P. Dutto, P. Mira, J. A. Fernández Merodo, T. Blanc, S. Sancho, and A. S. Benítez. A viscoplastic approach to the behaviour of fluidized geomaterials with application to fast landslides. *Contin. Mech. Thermodyn.*, 27(1-2):21–47, jan 2015.
- [Pud12] S. P. Pudasaini. A general two-phase debris flow model. *J. Geophys. Res. Earth Surf.*, 117(F3), sep 2012.

- [PYS⁺18] M. Pastor, A. Yague, M. M. Stickle, D. Manzanal, and P. Mira. A two-phase SPH model for debris flow propagation. *Int. J. Numer. Anal. Methods Geomech.*, 42(3):418–448, feb 2018.
- [QPH04] M. Quecedo, M. Pastor, and M. I. Herreros. Numerical modelling of impulse wave generated by fast landslides. *Int. J. Numer. Methods Eng.*, 59(12):1633–1656, 2004.
- [RPB05] M. Rodriguez-Paz and J. Bonet. A corrected smooth particle hydrodynamics formulation of the shallow-water equations. *Comput. Struct.*, 83(17-18):1396–1410, jun 2005.
- [SH89] S. B. Savage and K. Hutter. The motion of a finite mass of granular material down a rough incline. *J. Fluid Mech.*, 199:177 – 215, 1989.
- [SH91] S. B. Savage and K. Hutter. The dynamics of avalanches of granular materials from initiation to runout. Part I: Analysis. *Acta Mech.*, 86(1-4):201–223, mar 1991.
- [SV71] A. Saint-Venant. Theorie du mouvement non permanent des eaux, avec application aux crues des rivières et a l’introduction de marées dans leurs lits. *Comptes-Rendus l’Académie Des Sci*, pages 147–273, 1871.
- [Tay19] S. M. Tayyebi. *A two-phase SPH depth integrated model for debris flow propagation considering pore water pressure evolution*. PhD thesis, Universidad Politécnica de Madrid, 2019.
- [TPY⁺20] S. M. Tayyebi, M. Pastor, A. L. Yifru, V. K. Thakur, and M.M. Stickle. Two-phase SPH-FD depth integrated model for debris flows: application to basal grid brakes. *Géotechnique*, 2020.
- [WH99] Y. Wang and K. Hutter. A constitutive theory of fluid-saturated granular materials and its application in gravitational flows. *Rheol. Acta*, 38(3):214–223, aug 1999.
- [ZS84] O. C. Zienkiewicz and T. Shiomi. Dynamic behaviour of saturated porous media; The generalized Biot formulation and its numerical solution. *Int. J. Numer. Anal. Methods Geomech.*, 8(1):71–96, jan 1984.

Modeling snow and avalanches with the Material Point Method and finite strain elastoplasticity

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Snow is a complex and fascinating material which can sustain stresses like a solid or flow like a fluid depending upon the load it is subjected to. The transition from solid to fluid state can lead to catastrophic snow slab avalanches. Modeling large deformations, compaction, fractures and contacts involved in snow and avalanche mechanics requires both suitable constitutive models and an appropriate numerical framework. Recently, the Material Point Method (MPM), a hybrid Eulerian-Lagrangian continuum approach, has shown great promise in modeling complex processes involved in snow avalanche release and flow in a unified manner. This includes compaction hardening, anticrack nucleation and propagation during slab avalanche release and flow regime transition reported in avalanche dynamics. In this Chapter, we first introduce the state of the art in snow and avalanche mechanics as well as related modeling challenges. Second, we recall finite strain elastoplasticity theory and the MPM algorithm. Third, we describe different constitutive snow models based on damage or critical state soil mechanics. Finally, we show the application of MPM to snow microstructure compression, anticrack propagation in avalanche release as well as avalanche dynamics.

1 Introduction

Snow is one of nature's most fascinating and complex material which can behave like a solid or flow like a fluid depending on the applied loading. Snow complexity arises from i) its porous character, as it is made of ice, air and possibly water and ii) the



Figure 1: A snow slab avalanche triggered by a snowboarder in Haines, Alaska. ©Oli Gagnon.

fact that it is a ‘hot’ material, i.e. exists close to its melting point. The solid-to-fluid transition in snow can have dramatic consequences, such as snow avalanches (Fig. 1).

A lot of progress has been made in snow and avalanche mechanics over the past decade. Science barriers have been pushed by modern experimental methods coupled with multiscale models, which are encouraged by the fast increase of computational capabilities. In particular, some researchers have characterized the important and complex role of snow microstructural network on snow mechanics [e.g. [HCN15](#), [SCMP16](#), [WGF15](#), [KS14](#), [GLTT17](#)] while others have helped in better understanding how snow mechanical behavior affects crack propagation and slab avalanche release at the slope scale [[HGZ08](#), [vHH09](#), [vHSH10](#), [MKC10](#), [GvHC⁺15](#), [GvHC⁺17](#)].

Concerning snow failure, recent laboratory experiments highlighted that failure initiation in typical weak snow layers is not in pure shear as previously assumed but mixed-mode (shear and compression) [[RGS15](#), [CSM15](#)] with lower strengths in shear than in compression [[RS10](#)]. With respect to crack propagation, the development of the Propagation Saw Test (PST) [[SS07](#), [GJ08](#)] highlighted the importance of the structural collapse of the weak layer after failure as well as the crucial influence of slab elasticity and strength on crack propagation propensity [[vHGB⁺16](#)].

While the yield surface of snow is now better characterized, the post-peak behavior is usually oversimplified, assuming either brittle or quasi-brittle behavior. Yet, snow has a more complex plastic behavior with hardening in compression, promoting irreversible compaction (compressibility) and softening in shear and tension, facilitating fracture. In addition, most models neglect the volumetric collapse of the weak layer and thus fail in reproducing field observations. In classical continuum methods for

fracture (standard mesh-based discretization schemes) as well as in standard materials, the concept of collapse under compressive stresses (or anticrack) is physically impossible due to mesh or material inter-penetration induced by volume loss. So far, no standalone continuum constitutive model exists for anticrack types of fractures to simulate dynamic crack propagation in porous cohesive materials.

Each of the processes required for the release of a slab avalanche has been investigated using different numerical approaches. Failure initiation and crack propagation are classically modeled using the Finite Element Method [GCEN13, GSvH⁺14, MJ08, MKC10], the Fiber Bundle Model [RSDH09] or Cellular Automata [FLG04, FZ07]. More recently the Discrete Element Method has enabled the simulation of both avalanche release [initiation and propagation, GvHC⁺15, GvHC⁺17, GR17] and flow processes [snow granulation, SGH⁺15]. However, due to the high computational cost, this method is used only for relatively small scales. Popular classical numerical tools developed for avalanche dynamics simulation primarily apply two-dimensional (2D) depth-averaged methods based on shallow water theory [NDEC13, RKHF18], which fail to capture important flow characteristics along the surface-normal direction such as velocity distribution [EYZ20]. Hence, a unified and continuum approach to simulate both avalanche release and flow at the slope scale accounting for all important mechanical processes is necessary.

In this Chapter, we will describe the Material Point Method [MPM, SZS95, see § 3], a numerical framework capable of integrating all essential physical ingredients mentioned above into a single framework. MPM has recently gained interest in computational mechanics, geotechnics [e.g. BBS00, ASB13, SAY⁺15, BFL16, VWH17] and graphics [e.g. NGL10, SSC⁺13, DBD16, JST⁺16, KGP⁺16, TGK⁺17]. MPM is a continuum and hybrid Eulerian-Lagrangian method which has the particular and major advantage of dissociating Lagrangian material particles and Eulerian calculation points allowing it to be an ideal numerical framework for simulating fractures, collisions and coexistence between solid- and fluid-like behaviors. The recent developments of MPM has allowed to overcome a critical science barrier in snow and avalanche research, namely simulating the whole avalanche process, from quasi-static snow failure to dynamic fracture propagation and flow at the slope scale in a unified and multiscale physically-based framework using constitutive models based on critical state soil mechanics.

2 Finite Strain Elastoplasticity

This section gives a brief introduction to continuum mechanics in the framework of finite strain elastoplasticity, and its content is to a large extent based on the textbooks of [BW08], [GS08] and [Mal69], as well as [JST⁺16]. The reader is referred to these references for more details.

At the core of continuum mechanics, we make the assumption that a material body can be modeled as a continuum. A separation is made between (initial) undeformed material body, which is described by a set of material coordinates $\mathbf{X}$, and the deformed

material body, which is described by a set of spatial coordinates $\mathbf{x}$. These are referred to as the Lagrangian and Eulerian descriptions of the body, respectively.

2.1 Strains and stresses

A deformation of a body over a time t is described by the mapping ϕ which takes a Lagrangian coordinate $\mathbf{X}$ to an Eulerian coordinate $\mathbf{x} = \phi(\mathbf{X}, t)$. The strain experienced by a body under deformation can be quantified through the deformation gradient, which is a second-order tensor defined as

$$\mathbf{F}(\mathbf{X}, t) = \frac{\partial \phi(\mathbf{X}, t)}{\partial \mathbf{X}}. \quad (1)$$

The determinant of the deformation gradient $J \equiv \det(\mathbf{F})$ quantifies the body's (infinitesimal) volume change such that $J = 1$ represents no volume change, $J < 1$ represents volume decrease and $J > 1$ represents volume increase. We remark that for a deformation to be admissible one must require the mapping ϕ to be one-to-one and $J > 0$. Thus, $\mathbf{F}$ is invertible.

Several strain measures can be defined. For example, the Green tensor is defined as

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{I}) \quad (2)$$

and can be interpreted as the finite strain version of the small strain tensor

$$\mathbf{E}_s = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad (3)$$

where $\mathbf{u}$ is the displacement field. Another strain measure is the Hencky strain tensor, defined as

$$\boldsymbol{\epsilon} = \frac{1}{2} \ln \mathbf{F} \mathbf{F}^T \quad (4)$$

which can be interpreted as an extension of the natural (logarithmic) strain measure in small strain theory to the finite strain context.

As with strain, there exist several definitions of stress measures, e.g., the familiar Cauchy stress defined by the second-order tensor $\boldsymbol{\sigma}$ which measures the force on the body per unit *deformed* area. In finite strain theory, it is common to work with the first Piola-Kirchhoff stress tensor

$$\mathbf{P}(\mathbf{X}, t) = J(\mathbf{X}, t) \boldsymbol{\sigma}(\mathbf{X}, t) \mathbf{F}(\mathbf{X}, t)^{-T} \quad (5)$$

which, unlike the Cauchy stress, measures the force per unit *undeformed* area. Note that we made no symbolic distinction between the Cauchy stress in Eulerian $\boldsymbol{\sigma}(\mathbf{x}, t)$ and Lagrangian $\boldsymbol{\sigma}(\mathbf{X}, t)$ description. The reader should be able to distinguish them based on the context (in particular, from its arguments). Moreover, the second Piola-Kirchhoff stress tensor is given by $\mathbf{S}(\mathbf{X}, t) = \mathbf{F}(\mathbf{X}, t) \mathbf{P}(\mathbf{X}, t)$. Finally, we mention the Kirchhoff stress tensor

$$\boldsymbol{\tau}(\mathbf{X}, t) = J(\mathbf{X}, t) \boldsymbol{\sigma}(\mathbf{X}, t). \quad (6)$$

The Lagrangian velocity $\mathbf{V}$ and acceleration $\mathbf{A}$ are defined through

$$\mathbf{V}(\mathbf{X}, t) = \frac{\partial \phi(\mathbf{X}, t)}{\partial t} \quad (7)$$

$$\mathbf{A}(\mathbf{X}, t) = \frac{\partial \mathbf{V}(\mathbf{X}, t)}{\partial t} \quad (8)$$

respectively. We note the difference compared to the Eulerian acceleration $\mathbf{a}$,

$$\mathbf{a}(\mathbf{x}, t) = \frac{D\mathbf{v}(\mathbf{x}, t)}{Dt} \quad (9)$$

which is given by the material derivative ($D/Dt = \partial/\partial t + \mathbf{v} \cdot \nabla_{\mathbf{x}}$) of the Eulerian velocity $\mathbf{v}(\mathbf{x}, t)$.

2.2 Balance laws

In our context, the governing balance laws of interest are conservation of mass and conservation of momentum. We state them here without derivation. In the Eulerian description under the assumption of no external body forces other than that resulting from gravity $\mathbf{g}$, the balance law for mass and linear momentum are respectively given by

$$\frac{D\rho(\mathbf{x}, t)}{Dt} + \rho(\mathbf{x}, t) \nabla_{\mathbf{x}} \cdot \mathbf{v}(\mathbf{x}, t) = 0 \quad (10)$$

$$\rho(\mathbf{x}, t) \frac{D\mathbf{v}(\mathbf{x}, t)}{Dt} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}(\mathbf{x}, t) + \rho(\mathbf{x}, t) \mathbf{g} \quad (11)$$

where ρ is the mass density. Equivalently, in the Lagrangian description, these equations are given by

$$\rho(\mathbf{X}, t) J(\mathbf{X}, t) = \rho(\mathbf{X}, 0) \quad (12)$$

$$\rho(\mathbf{X}, 0) \frac{\partial \mathbf{V}(\mathbf{X}, t)}{\partial t} = \nabla_{\mathbf{X}} \cdot \mathbf{P}(\mathbf{X}, t) + \rho(\mathbf{x}, 0) \mathbf{g} \quad (13)$$

where no symbolic distinction between the Eulerian and Lagrangian mass density ρ has been made.

Furthermore, conservation of angular momentum require the Cauchy stress to be symmetrical, i.e., $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$. In the Lagrangian view, this corresponds to symmetry of the second Piola-Kirchhoff tensor, i.e., $\mathbf{S} = \mathbf{S}^T$. Thus, we have in total 9 unknowns (3 velocity components and 6 stress components). However, the above equations for conservation of mass and linear momentum, Eq. (10)-(13), represent only 6 equations. We need constitutive equations in order to close the system. These equations must fulfill material frame-indifference, i.e., invariance under rigid body transformations. In other words, if we view the same configuration from a rotated point of view, the stress must transform by the same rotation.

2.3 Elasticity

Here, we present constitutive models for elastic materials. Common to all elastic materials is that the stress at one point of the material depends only on the current strain at that point, in particular $\boldsymbol{\sigma}(\mathbf{X}, t) = \hat{\boldsymbol{\sigma}}(\mathbf{F}(\mathbf{X}, t), \mathbf{X})$, where $\hat{\boldsymbol{\sigma}}$ denotes the stress response function. Notably, it does not depend on past deformation history or the rate at which deformation is applied. If the elastic material is homogeneous, which will be the assumption in the following, then $\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$. Moreover, frame-indifference implies that the stress must depend on the deformation through the right Cauchy-Green strain tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F}$. Furthermore, the elastic material is isotropic if $\hat{\boldsymbol{\sigma}}(\mathbf{F}) = \hat{\boldsymbol{\sigma}}(\mathbf{F}\mathbf{Q})$ for all rotation tensors $\mathbf{Q}$. In fact, it can be shown that the stress response function for a frame-indifferent isotropic elastic material can be completely defined through the principal invariants of $\mathbf{C}$.

An elastic material is said to be hyperelastic if the first Piola-Kirchhoff stress can be derived from a strain energy density function $\Psi(\mathbf{F})$ through

$$\mathbf{P}(\mathbf{F}) = \frac{\partial \Psi(\mathbf{F})}{\partial \mathbf{F}}. \quad (14)$$

An example of a frame-indifferent isotropic hyperelastic constitutive model is the St. Venant-Kirchhoff model,

$$\Psi = \frac{1}{2} \lambda (\text{tr} \mathbf{E})^2 + \mu \text{tr}(\mathbf{E}^2) \quad (15)$$

where λ and μ are the two Lamé parameters and $\mathbf{E}$ is the Green finite strain tensor introduced earlier. The latter model results in the second Piola-Kirchhoff tensor on the form

$$\mathbf{S} = \mathcal{C} : \mathbf{E} = \lambda (\text{tr} \mathbf{E}) \mathbf{I} + 2\mu \mathbf{E} \quad (16)$$

which highlights the analogy with the well-known (small strain) linear isotropic elasticity,

$$\boldsymbol{\sigma} = \mathcal{C} : \mathbf{E}_s = \lambda (\text{tr} \mathbf{E}_s) \mathbf{I} + 2\mu \mathbf{E}_s \quad (17)$$

where $\mathcal{C}$ is a fourth-order tensor defined as $\mathcal{C} = 2\mu \mathbf{I} + \lambda \mathbf{1}\mathbf{1}^T$. A variant of the St. Venant-Kirchhoff model can be expressed in terms of Hencky strain $\boldsymbol{\epsilon}$, making several numerical aspects more convenient,

$$\Psi = \frac{1}{2} \lambda (\text{tr} \boldsymbol{\epsilon})^2 + \mu \text{tr}(\boldsymbol{\epsilon}^2) \quad (18)$$

which results in the Kirchhoff stress $\boldsymbol{\tau}$ on the familiar form

$$\boldsymbol{\tau} = \mathcal{C} : \boldsymbol{\epsilon} = \lambda (\text{tr} \boldsymbol{\epsilon}) \mathbf{I} + 2\mu \boldsymbol{\epsilon}. \quad (19)$$

This elastic model has been successfully used in various publications on material point method modeling [Mas13, KGP⁺16, GGT⁺18].

2.4 Plasticity

We separate between elastic and plastic, i.e, permanent/non-reversible, deformations. The finite strain equivalent of the additive decomposition of elastic and plastic strain in the small deformation theory, is the multiplicative decomposition of the deformation gradient,

$$\mathbf{F} = \mathbf{F}_E \mathbf{F}_P \quad (20)$$

where $\mathbf{F}_E$ refers to the deformation arising from the elastic forces, while $\mathbf{F}_P$ is the permanent, plastic, component. It is important to note that stress due to the elastic forces discussed in the previous section, is only a result of the elastic deformation $\mathbf{F}_E$. Thus, in many equations presented in Section 2.3 we must replace $\mathbf{F}$ with $\mathbf{F}_E$ to be consistent. In particular, the hyperelastic strain energy density is only a function of $\mathbf{F}_E$, e.g.,

$$\Psi(\mathbf{F}_E) = \frac{1}{2} \lambda (\text{tr} \boldsymbol{\epsilon}_E)^2 + \mu \text{tr}((\boldsymbol{\epsilon}_E)^2) \quad (21)$$

the St. Venant-Kirchhoff model. Here, $\boldsymbol{\epsilon}_E = \frac{1}{2} \ln(\mathbf{F}_E(\mathbf{F}_E)^T)$. Moreover, the Kirchhoff, Cauchy and first Piola-Kirchhoff stress tensor can be written

$$\boldsymbol{\tau} = \frac{\partial \Psi(\mathbf{F}_E)}{\partial \mathbf{F}_E} (\mathbf{F}_E)^T, \quad (22)$$

$$\boldsymbol{\sigma} = \frac{1}{J} \boldsymbol{\tau} = \frac{1}{J} \frac{\partial \Psi(\mathbf{F}_E)}{\partial \mathbf{F}_E} (\mathbf{F}_E)^T, \quad (23)$$

$$\mathbf{P} = \boldsymbol{\tau} \mathbf{F}^{-T} = \frac{\partial \Psi(\mathbf{F}_E)}{\partial \mathbf{F}_E} (\mathbf{F}_E)^T \mathbf{F}^{-T} = \frac{\partial \Psi(\mathbf{F}_E)}{\partial \mathbf{F}_E} (\mathbf{F}_P)^{-T}, \quad (24)$$

respectively.

The onset of plastic deformations is characterized by a yield function y which depends on the stress state and possible hardening parameters. Conventionally, $y < 0$ defines admissible states, and $y > 0$ is said to be non-admissible. The yield surface $y = 0$ defines the limit where deformations are no longer elastic. Thus, plastic deformations can only occur on the yield surface.

An elastoplastic model is not complete without a flow rule. Let us define the elastic right Cauchy-Green strain tensor $\mathbf{C}_E$ and the elastic left Cauchy-Green strain tensor $\mathbf{b}_E$ as $\mathbf{C}_E = (\mathbf{F}_E)^T \mathbf{F}_E$ and $\mathbf{b}_E = \mathbf{F}_E (\mathbf{F}_E)^T$ [BW08]. Furthermore, $\mathbf{C}_P = (\mathbf{F}_P)^T \mathbf{F}_P$ denotes the plastic right Cauchy-Green strain tensor. The associative plastic flow rule is given by [Sim92] and [SM93]

$$-\frac{1}{2} \mathcal{L}_{\mathbf{v}} \mathbf{b}_E = \dot{\gamma} \frac{\partial y}{\partial \boldsymbol{\tau}} \mathbf{b}_E, \quad (25)$$

$$\dot{\gamma} \geq 0, y \leq 0, \dot{\gamma} y = 0, \quad (26)$$

where $\mathcal{L}_{\mathbf{v}} \mathbf{b}_E = \mathbf{F} \frac{\partial}{\partial t} (\mathbf{C}_P)^{-1} \mathbf{F}^T$ is the Lie derivative of $\mathbf{b}_E$, $\dot{\gamma}$ is the plastic consistency parameter and Eq. (26) are the Kuhn-Tucker conditions. The associativity corresponds to the direction choice of $\frac{\partial y}{\partial \boldsymbol{\tau}}$. This choice is also known as the principle

of maximum plastic dissipation [BW08], leading to a plastic flow that maximizes the plastic dissipation rate. We refer to the derivation by [KGP⁺16] for more detailed discussion of the associative flow rule and non-associative flow rule. More details about the derivation of Eq. (25) can be found in [GGT⁺18].

3 MPM Algorithm

Given a continuous material, MPM discretizes it into a set of particles (material points) to track mass, position, momentum and deformation gradient as shown in Fig. 2. Since the mass of each Lagrangian particle is constant in time, the mass conservation is naturally fulfilled. The position, momentum and deformation gradient of the particles are solved and updated with a background Eulerian grid. Both implicit and explicit formulations of MPM can be used to solve the system [KGP⁺16]. We follow the explicit MPM algorithm in [SSC⁺13]. Various basis functions can be implemented for the grid, such as quadratic splines. Here, we take the dyadic products of one-dimensional cubic B-splines in [SSC⁺13] as an example.

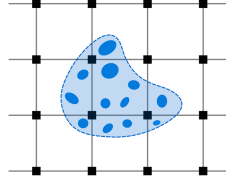


Figure 2: A continuous material described with Lagrangian particles and an Eulerian grid.

$$N_{\mathbf{i}}^h(\mathbf{x}_p) = N\left(\frac{1}{h}(x_p - ih)\right)N\left(\frac{1}{h}(y_p - jh)\right)N\left(\frac{1}{h}(z_p - kh)\right) \quad (27)$$

where h is the grid spacing, $\mathbf{i} = (i, j, k)$ is the grid index, $\mathbf{x}_p = (x_p, y_p, z_p)$ is the evaluation position, and the interpolation function $N(x)$ is

$$N(x) = \begin{cases} \frac{1}{2}|x|^3 - x^2 + \frac{2}{3}, & 0 \leq |x| < 1 \\ -\frac{1}{6}|x|^3 + x^2 - 2|x| + \frac{4}{3}, & 1 \leq |x| < 2 \\ 0, & \text{otherwise} \end{cases} \quad (28)$$

The interpolating weights and their gradients can then be obtained as $w_{ip} = N_{\mathbf{i}}^h(\mathbf{x}_p)$ and $\nabla w_{ip} = \nabla N_{\mathbf{i}}^h(\mathbf{x}_p)$, respectively. These weighting functions are needed in the information transfer between the particles and the grid. The detailed procedure of updating the particle states is presented in Fig. 3 and interpreted in the following.

1. Transfer particle states to the grid

The mass and velocity of the particles are transferred to the grid nodes to obtain

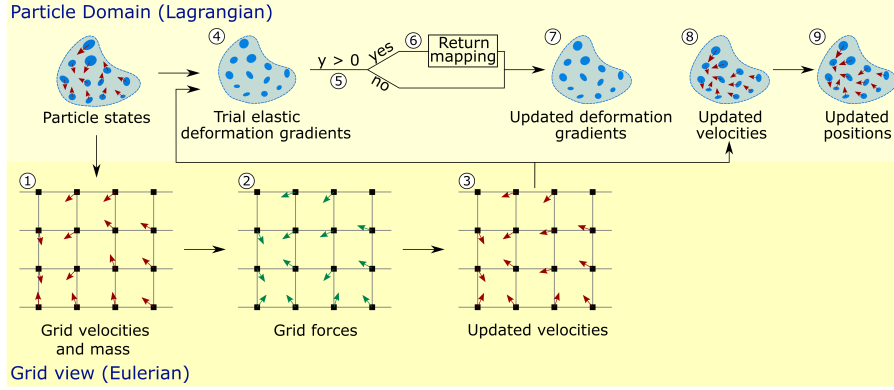


Figure 3: Overview of the MPM algorithm. Modified based on [GGT⁺18, SSC⁺13].

the grid mass and velocities according to the following expressions

$$m_i^n = \sum_p m_p w_{ip}^n \quad (29)$$

$$\mathbf{v}_i^n = \sum_p \mathbf{v}_p^n m_p w_{ip}^n / m_i^n \quad (30)$$

where m_i^n and $\mathbf{v}_i^n$ are the mass and velocity of grid node i at time step n , respectively, m_p is the mass of particle p , and $\mathbf{v}_p^n$ is the velocity of particle p at time step n . For each grid node i , its mass and velocity is calculated from the particles in the grid cells sharing the grid node i . While the particle mass is transferred using the weighting functions, the transfer of particle velocity uses both the weighting functions and the particle mass to conserve momentum.

2. Compute grid forces

The force at each grid node comes from elastic stresses of the particles close to the node, which can be calculated based on the energy density function

$$\mathbf{f}_i^n = - \sum_p V_p^0 \left(\frac{\partial \Psi_p(\mathbf{F}_{E,p}^n)}{\partial \mathbf{F}_{E,p}^n} \right) (\mathbf{F}_{E,p}^n)^T \nabla w_{ip}^n \quad (31)$$

where V_p^0 is the initial volume of particle p , $\Psi_p(\mathbf{F}_{E,p}^n)$ is the energy density of particle p calculated from the elastic particle deformation gradient $\mathbf{F}_{E,p}^n$. Knowing the Cauchy stress tensor $\boldsymbol{\sigma}_p^n$ from Eq. (23), the grid force can be expressed as

$$\mathbf{f}_i^n = - \sum_p V_p^n \boldsymbol{\sigma}_p^n \nabla w_{ip}^n \quad (32)$$

where $V_p^n = J V_p^0$ is the particle volume at time step n .

3. Update grid velocities

The grid velocity at time step $n + 1$ is updated based on the grid velocity and acceleration at the previous time step n as follows

$$\mathbf{v}_i^{n+1} = \mathbf{v}_i^n + \Delta t \mathbf{f}_i^n / m_i^n \quad (33)$$

where Δt is the time interval between the time steps. Furthermore, boundary conditions need to be considered before the update of the grid velocity. For example, a grid node in contact with a fixed ground surface might need to take ground friction into account if the grid velocity is pointing towards the ground surface. In case of occurrence of the frictional behavior, the grid velocity along the tangential direction of the ground surface might be adjusted based on the friction coefficient of the ground surface.

4. Compute trial elastic deformation gradients

Assuming the deformation of the particles is fully elastic, their trial elastic deformation gradients can be obtained based on the previous deformation gradient $\mathbf{F}_E^n$ and the updated motion of the grid $\mathbf{v}_i^{n+1}$

$$\mathbf{F}_E^{\text{trial}} = \left(\mathbf{I} + \Delta t \sum_i \mathbf{v}_i^{n+1} (\nabla w_{ip}^n)^T \right) \mathbf{F}_E^n \quad (34)$$

where $\mathbf{I}$ is the identity matrix.

5. Check yield condition

Having the trial elastic deformation gradients, the trial elastic strains and stresses can be obtained. Taking the Hencky strain and the Kirchhoff stress in [GGT⁺18] as an example, the trial Hencky strain and trial Kirchhoff stress can be calculated as

$$\boldsymbol{\epsilon}_E^{\text{trial}} = \frac{1}{2} \ln \left(\mathbf{F}_E^{\text{trial}} (\mathbf{F}_E^{\text{trial}})^T \right) \quad (35)$$

$$\boldsymbol{\tau}_E^{\text{trial}} = \mathcal{C} : \boldsymbol{\epsilon}_E^{\text{trial}} \quad (36)$$

where $\mathcal{C}$ is the fourth-order elastic modulus tensor. With the obtained elastic stress, the yield function of the material y can then be computed and checked. If the state is non-admissible ($y > 0$), the assumption of pure elasticity has failed, and parts of the deformation must be plastic. The plastic deformation needs to be computed through return mapping detailed in step (6). If the state is admissible ($y \leq 0$), the trial elastic deformation gradients will be updated as the new deformation gradients in step (7).

6. Perform return mapping

When the assumption of pure elastic deformation is failed, plastic deformation needs to be introduced by projecting the trial state back to the yield surface.

The difference between the trial state and the projected state gives the amount of plastic strain

$$\epsilon_P^{n+1} = \epsilon_E^{\text{trial}} - \epsilon_E^{n+1} = \dot{\gamma} \Delta t \frac{\partial g}{\partial \tau} \quad (37)$$

where the plastic multiplier $\dot{\gamma}$ gives the magnitude of the plastic strain and the plastic potential function g defines the direction of the plastic strain occurring during the time interval Δt . The choice of the function g results in different flow rules. A possible choice is $g = y$, meaning that the change of the plastic strain coincides with the gradient of the yield surface. This is known as an associated flow rule, and all other choices are called non-associative. In pure elasticity, the total energy of the system remains constant. Plasticity can only decrease the total energy, otherwise we are in violation of the second law of thermodynamics. A flow rule should be shown to result in a non-negative plastic rate of dissipation

$$\dot{\epsilon}_P = \tau : l_P \geq 0 \quad (38)$$

where l_P is the plastic rate of deformation. An associated flow rule is a consequence of the principle of maximum plastic dissipation, ensuring the material dissipates energy due to plastic deformation as efficiently as possible. Moreover, the so-called Kuhn-Tucker conditions (Eq. 26) must be fulfilled.

7. Update deformation gradients

As mentioned in step (5), the trial elastic deformation gradients are taken as the updated ones if the assumption of pure elastic deformation holds. In case that plastic deformation occurs, the elastic deformation gradients should be updated based on the singular value decomposition of the elastic strain ϵ_E^{n+1} obtained in step (6).

$$\mathbf{F}_E^{n+1} = \mathbf{U}_E \Sigma_E \mathbf{V}_E^T \quad (39)$$

where

$$\Sigma_E = \exp(\epsilon_E^{n+1}) \quad (40)$$

8. Update particle velocities

The updated grid velocities are transferred to the particles to get updated particle velocities. The transfer scheme combines Particle-In-Cell (PIC) and Fluid-Implicit-Particle (FLIP) schemes by assigning different weights as below

$$\mathbf{v}_p^{n+1} = (1 - \alpha) \mathbf{v}_{\text{PIC}p}^{n+1} + \alpha \mathbf{v}_{\text{FLIP}p}^{n+1} \quad (41)$$

where

$$\mathbf{v}_{\text{PIC}p}^{n+1} = \sum_i \mathbf{v}_i^{n+1} w_{ip}^n \quad (42)$$

$$\mathbf{v}_{\text{FLIP}p}^{n+1} = \mathbf{v}_p^n + \sum_i (\mathbf{v}_i^{n+1} - \mathbf{v}_i^n) w_{ip}^n \quad (43)$$

PIC is simple and effective to implement. However, it suffers from significant dissipation/damping during frequent particle/grid transfers. In comparison,

FLIP addresses the dissipation by transferring incremental grid velocities to particles, instead of directly interpolating from grid to particles. Nevertheless, FLIP gives notable noise due to accumulated instability [JSS⁺15]. Thus, PIC and FLIP is normally combined to get stable simulations with negligible numerical damping. The value of α typically ranges from 0.95 to 0.99 [JSS⁺15, SSC⁺13].

9. Update particle positions

The new particle positions can be computed based on the updated grid positions

$$\mathbf{x}_p^{n+1} = \sum_i \mathbf{x}_i^{n+1} w_{ip} \quad (44)$$

where

$$\mathbf{x}_i^{n+1} = \mathbf{x}_i^n + \mathbf{v}_i^{n+1} \Delta t \quad (45)$$

4 Constitutive Snow Models

In this section, we focus on the description of three snow plasticity models. The first one is a damaged-based model developed for the graphics needs of the Disney movie Frozen [SSC⁺13]. The two other models are based on critical state soil mechanics and were developed to simulate dense cohesive snow as well as highly porous weak snowpack layers involved the release of snow slab avalanches [GGT⁺18].

4.1 Damage-based model: insights from Disney Animation Studios

The constitutive model developed by [SSC⁺13] for the needs of the Disney movie Frozen relies on an update of elastic constants involved in the Hooke's law μ and λ based on the amount of plastic deformation as follows:

$$\mu(\mathbf{F}_P) = \mu_0 e^{\xi(1-J_P)} \quad \text{and} \quad \lambda(\mathbf{F}_P) = \lambda_0 e^{\xi(1-J_P)}, \quad (46)$$

where $J_P = \det \mathbf{F}_P$, μ_0, λ_0 are the initial Lamé coefficients and ξ is the hardening coefficient. Note that J_P characterizes the amount of irreversible volume change such that $J_P = V^{\text{sf}}/V^0$ with V^{sf} is the current stress-free volume and V^0 is the initial volume. To compute J_P , [SSC⁺13] defines critical stretch θ_s and compression θ_c thresholds to start fracture or plastic compaction, respectively. Hence, the singular values of $\mathbf{F}_E$ are restricted to the $[1 - \theta_c, 1 + \theta_s]$ range. If the deformation exceeds the critical compression, J_P will decrease leading to compaction hardening (volume decrease and increasing of elastic constants). On the other hand if the deformation exceeds the critical stretch, J_P will increase leading to expansion softening (volume increase and decrease of elastic constants) promoting fracture.

We present below how the deformation gradient is updated. The procedure first assumes that all the deformation is elastic, i.e. that $\tilde{\mathbf{F}}_E^{n+1} = \mathbf{F}_E^{\text{trial}}$ (Eq. 34) and

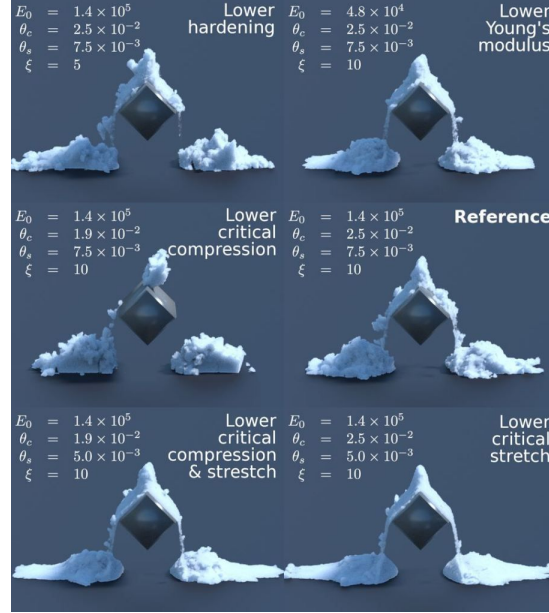


Figure 4: Snow drop test for different parameters of the model [SSC⁺13].

$\tilde{\mathbf{F}}_P^{n+1} = \mathbf{F}_P^n$. This implies

$$\mathbf{F}^{n+1} = \tilde{\mathbf{F}}_E^{n+1} \mathbf{F}_P^n \quad (47)$$

and thus

$$\tilde{\mathbf{F}}_E^{n+1} = \mathbf{F}^{n+1} (\mathbf{F}_P^n)^{-1} \quad (48)$$

Then, the procedure of [SSC⁺13] consists in computing the part of $\tilde{\mathbf{F}}_E^{n+1}$ that is outside of the admissible deformation range and use it to update $\tilde{\mathbf{F}}_P^{n+1}$. This is performed by limiting the range of the singular values of $\tilde{\mathbf{F}}_E^{n+1}$. The singular values are the diagonal terms of $\tilde{\Sigma}_E$ computed according to the singular value decomposition

$$\tilde{\mathbf{F}}_E^{n+1} = \mathbf{U}_E \tilde{\Sigma}_E \mathbf{V}_E^T. \quad (49)$$

The singular values are updated by clamping them to the admissible range according to

$$\Sigma_E = \text{clamp} \left(\tilde{\Sigma}_E, [1 - \theta_c, 1 + \theta_s] \right). \quad (50)$$

At this stage, one can compute the final elastic deformation gradients as

$$\mathbf{F}_E^{n+1} = \mathbf{U}_E \Sigma_E \mathbf{V}_E^T, \quad (51)$$

and the final plastic deformation gradient can be computed owing that the total deformation remains unchanged i.e.

$$\mathbf{F}^{n+1} = \mathbf{F}_E^{n+1} \mathbf{F}_P^{n+1} \quad (52)$$

which leads to

$$\mathbf{F}_P^{n+1} = (\mathbf{F}^{n+1})^{-1} \mathbf{F}_E^{n+1}. \quad (53)$$

As show in Fig. 4, this model, which has been designed for visual animation of snow can mimic the behavior of different snow types. Strength, elasticity and brittleness can be controlled by tuning the critical deformation, Young's modulus and hardening coefficient.

4.2 Critical state soil mechanics: a cohesive Cam Clay model for snow and weak snow layers

We present here the recent constitutive models based on critical state soil mechanics developed by [GGT⁺18]. For plasticity, the yield function $y(\boldsymbol{\tau}) \leq 0$ defines admissible stress states in an elastoplastic continuum. We model snow based on the critical state plasticity theory for soil mechanics [SW68, Par72]. For any stress $\boldsymbol{\tau}$, there exist a mean effective stress (or pressure) p and a deviatoric stress $\mathbf{s}$. They are given by

$$p = -\frac{1}{d} \text{tr}(\boldsymbol{\tau}), \quad (54)$$

$$\mathbf{s} = \boldsymbol{\tau} + p\mathbf{I}, \quad (55)$$

respectively, where $d = 2$ or 3 is the problem dimension, $\mathbf{I}$ is the identity matrix and compression corresponds to $p > 0$. According to the Von Mises theory [Mis13], we can derive the Mises equivalent stress q , given by $q = (3/2 \mathbf{s} : \mathbf{s})^{1/2}$.

Recent experiments [RGS15] and simulations based on X-ray microtomography [HCN15, CSM15, Hag17, SCM17] highlighted the mixed-mode nature of snow failure including tensile, shear and compression failure modes. Given these past studies, it appears that an ellipsoid yield function is appropriate to reproduce this mixed-mode character. Hence we chose to start from the Modified Cam Clay (MCC) yield surface [RB68] which has been widely used in the area of soil mechanics. Note that the analogy between snow and clay was already made by [McC79] who extended the clay model of [PR73] to model shear fractures induced by strain softening. However, the MCC model is originally cohesionless and does not exhibit any stress under extension, similar to dry sand. Hence, cohesion was added to the yield function by shifting the MCC model along the p -axis. We thus propose a new Cohesive Cam Clay (CCC) model similar to that of [MLM96] with the following yield surface:

$$y(p, q) = q^2(1 + 2\beta) + M^2(p + \beta p_0)(p - p_0), \quad (56)$$

where p_0 represents the consolidation pressure and M is the slope of the cohesionless Critical State Line (CSL) which controls the amount of friction, β represents the ratio between tensile and compressive strength and controls the amount of cohesion ($\beta \geq 0$). This yield surface is represented in Fig. 5a. Both MCC and our model are ellipsoids and are symmetric around the hydrostatic axis.

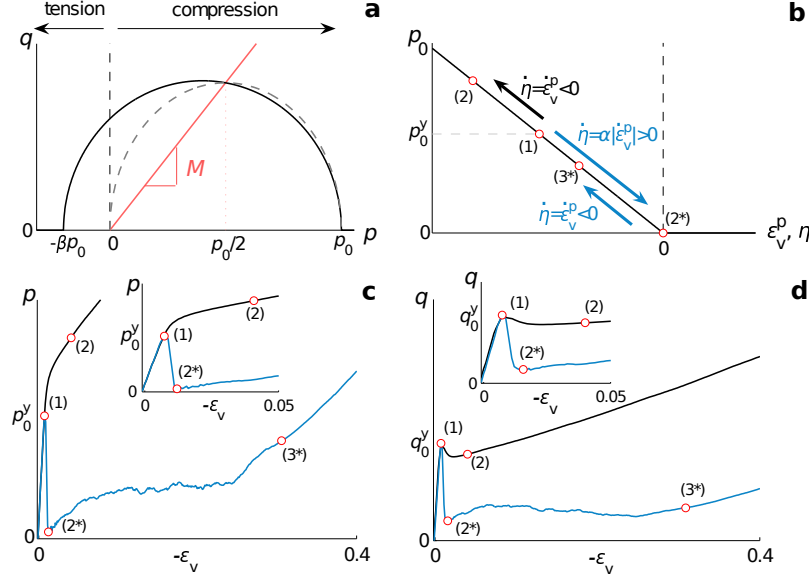


Figure 5: Overview of the elastoplastic model. **a** Cohesive (black line) and cohesionless (dashed gray line) Cam Clay yield surface in the $p-q$ space. The red line corresponds to the Critical State Line. **b** Illustration of the hardening models $p_0(\epsilon_P^V)$ (for the slab) and $p_0(\eta)$ (for the weak layer): the black arrow shows the classical hardening law used for the snow slab in which p_0 increases in compression ($\dot{\epsilon}_P^V < 0$); the blue arrows represent the new softening model for the weak layer for which p_0 decreases under compression ($\dot{\eta} = \alpha|\dot{\epsilon}_V^P| > 0$) until $\epsilon_P^V = 0$ after which the classical hardening law is used with $\beta = 0$. **c** Typical $p - \epsilon_V$ curve obtained for the unconfined compression of the weak layer in experiment n° 2 (see Methods section for model parameters) for the classical hardening law (in black) and the new softening one (in blue). **d** Same as **c** but for the $q - \epsilon_V$ curve. In **c** and **d**, p and q in the weak layer (blue curves) do not perfectly reach zero after softening due to a loss of homogeneity (failure localization).

For the dense snow slab, the hardening and softening is modeled by expanding and shrinking the yield surface which is performed by varying p_0 . We assume the hardening and softening only depend on the volumetric plastic deformation $\epsilon_P^V = \log(\det(\mathbf{F}_P))$. We follow the derivation from [OP04] and use the following hardening law:

$$p_0 = K \sinh(\xi \max(-\epsilon_P^V, 0)), \quad (57)$$

where ξ is the hardening factor and K is the material bulk modulus. When the plastic deformation is compressive ($\dot{\epsilon}_P^V < 0$), p_0 will increase, causing the yield surface to grow in size. Snow will consequently receive more elastic responses resisting compression. When the plastic volume is increased ($\dot{\epsilon}_P^V > 0$), the yield surface shrinks to the original size and allows the snow to fracture in tension. This hardening law is represented in Fig. 5b (in black).

Classical hardening/softening laws such as the one described above for the dense snow slab (Eq. 57) fail in reproducing the collapse of porous cohesive materials under com-



Figure 6: MPM simulation of remote avalanche triggering (the trigger is a snowman at the bottom of the slope) and subsequent flow of the avalanche [GGT⁺18].

pression. This is shown in Figs 5c and 5d (black lines) in which p significantly increases after reaching the yield surface and q slightly decreases before increasing. Hence, for the porous weak layer, we propose a modified softening law which describes cohesion and volume loss under compressive stresses. This new softening law involves looking at the volumetric plastic strain rate $\dot{\epsilon}_P^V$. We introduce the anticrack plastic strain η which is related to ϵ_P^V as follows:

$$\dot{\eta} = \begin{cases} \alpha |\dot{\epsilon}_P^V|, & \text{if } t \leq t_c \\ \dot{\epsilon}_P^V, & \text{if } t > t_c \end{cases} \quad (58)$$

where α is a softening factor which controls the fracture energy dissipated during collapse and t_c is the time corresponding to complete softening, i.e. $\epsilon_P^V = 0$ and $p_0 = 0$ (state (2*)) in Fig. 5). Our new softening law for the weak layer is obtained by replacing ϵ_P^P by η in Eq. 57 (the discretization is shown in the Methods section). Hence, when stresses in the weak layer reach the yield surface, the introduction of the norm of $\dot{\epsilon}_P^V$ in Eq. 58 will lead to softening (through a decrease in p_0) even under compression for which $\dot{\epsilon}_P^V < 0$. The yield surface thus shrinks until it corresponds to a point at the origin of the $p - q$ space. In addition, cohesion is removed by setting $\beta = 0$ when $\epsilon_P^V = 0$ which ensures continuity. After reaching this point, the yield surface is free to expand according to the classical hardening law (Eq. 57), leading to volume reduction (collapse) due to the weight of the slab (blue arrows in Fig. 5b) and then a purely frictional/compaction behavior. Our softening rule reproduces bond breaking in the weak layer and subsequent grain rearrangement leading to volumetric collapse due to the compressive weight of the slab [vHJ05]. In contrast to classical hardening laws, our new formulation induces a strain-softening behavior even under macroscopic uniaxial compression, as shown in Figs 5c and 5d. The observed mechanical behavior is very similar to that reported in discrete element simulations of porous cohesive gran-

ular materials [GLTT17] and follows the following sequence of mechanical regimes: elastic regime, failure, drop in pressure and shear stress (strain softening), plastic consolidation corresponding to the volumetric collapse and, finally, dense packing regime corresponding to the jamming transition. This typical post-peak behavior was also observed in laboratory experiments of snow failure [Rei11, RS13] as well as during the propagation of compaction bands in confined compression of snow [BBL⁺17]. Physically, this behavior is related to the fact that even under a macroscopic compressive loading mode, the solid matrix of porous cohesive materials is mostly under tension (bending) and shear [GLTT17].

We show in Fig. 6 that the combination of these two models (weak layer and slab) could reproduce, for the first time, a very complex and puzzling process in geosciences, namely the remote triggering and flow of a snow slab avalanche. In this example, the slope is initially metastable. The weight of a snowman located at the bottom of the slope (on the flat) initiates a failure within the buried weak snow layer which then propagates across the slope as a mixed-mode anticrack, leading to the failure and detachment of the slab (see [GGT⁺18] and [GvHG⁺19] for more details). The model is also able to reproduce the dynamics of the avalanche (see also § 5.3 and [LSJG20]).

5 Applications of MPM for Snow and Avalanche Mechanics

5.1 Microstructure-based snow modeling

The mechanical behavior of snow depends on its microstructure. Snow microstructures can be experimentally imaged by X-ray micro-computed tomography. Considering snow as a porous two-phase (solid ice and voids) medium, we can simulate the mechanical response of snow under imposed loading, see Fig. 7. This necessitates

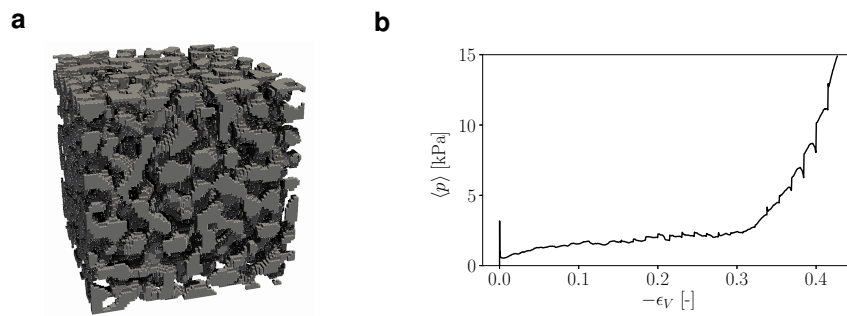


Figure 7: Microstructure-based simulations. **a** Discretized microstructure. **b** Stress-strain curve from uniaxial confined compression.

choosing accurate models for the solid ice behavior. In the present case, ice is modeled using a Drucker-Prager constitutive model with cohesion softening based on the amount of deviatoric plastic deformation. Under loading, we observe a classical stress-strain curve (Figure 7b), i.e., i) an elastic phase followed by ii) strain softening, iii) volumetric collapse and finally iv) densification. The analysis of simulations performed for different loading conditions can help define an homogenized microstructure-based constitutive snow model.

5.2 Anticrack propagation in snow slab avalanche release

The Propagation Saw Test (PST) is one of the most advanced field experiments to analyze the release process of snow slab avalanches [vHGB⁺16]. As illustrated by

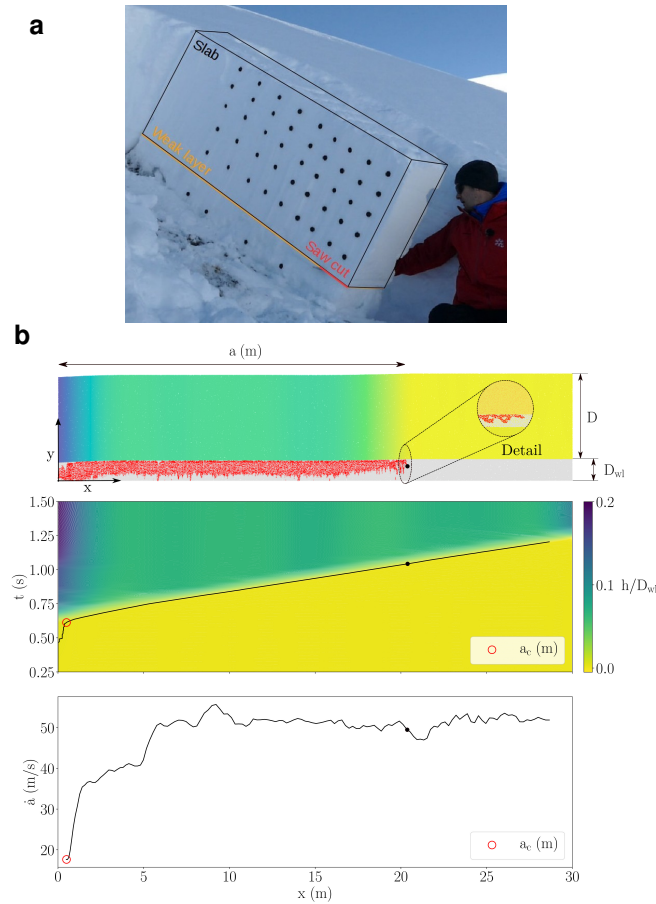


Figure 8: **a** Field experiment of a Propagation Saw Test (reprinted from [RSRvH19]). **b** MPM simulation of a Propagation Saw Test, (top) snapshot of the simulation state, (middle) space-time representation of the anticrack propagation, (bottom) crack propagation speed evolution.

Fig. 8a, the PST consists of isolating a snowpack column and cutting with a snow saw through a buried weak snow layer. The initiated crack may propagate dynamically once a critical length a_c is reached. The propagation mechanism may be self-sustained even on low angle terrain due to the volumetric collapse of the weak layer (crack under compression = anticrack) and thus potential energy released by the slab.

Simulation of such a process is challenging using classical numerical methods because of mesh interpenetration induced by the anticrack. Yet, dynamic anticrack propagation can be simulated numerically using MPM and appropriate constitutive laws for both the slab and the weak layer [GGT⁺18]. Fig. 8b shows the outcomes of a PST simulation where a_c corresponds to the critical crack length, h corresponds to the collapse height and $\dot{a}$ corresponds to the crack propagation speed. For crack lengths above ~ 5 m, the crack propagation speed becomes almost constant around 50 m/s.

5.3 Snow avalanches in different flow regimes

Here, we show the capability of MPM and of the general snow constitutive model (no weak layer) to simulate avalanche dynamics. Fig. 9 demonstrates the distinct profiles of four simulated snow avalanches. The bed surface in the four cases consists of an inclined slope, a connecting arc zone, and a horizontal deposition region.

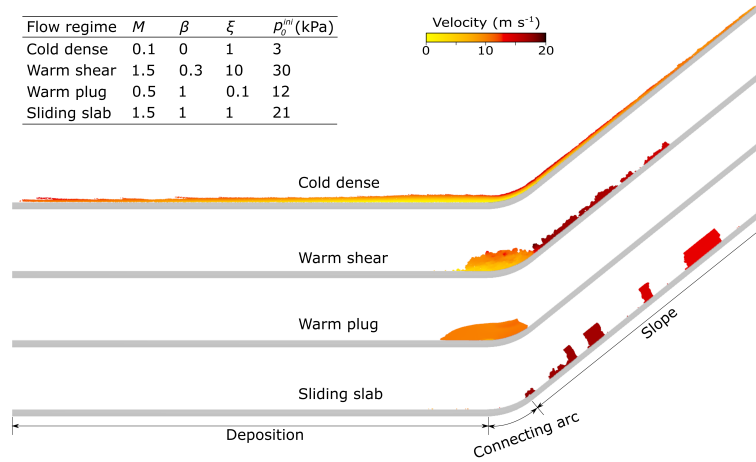


Figure 9: Distinct profiles of four flows in different flow regimes.

With the implementation of different snow properties in the MPM simulations, a wide range of flow regimes of snow avalanches from fluid-like flow to solid-like sliding slab has been identified. From top to bottom in Fig. 9, the first flow behaves as a fluid or a dry cohesionless granular flow, agreeing with the cold dense regime observed in reality. The second flow demonstrates a fluctuated free surface and a discontinuous tail, due to the occurrence of a granulation process. In practice, snow granules are

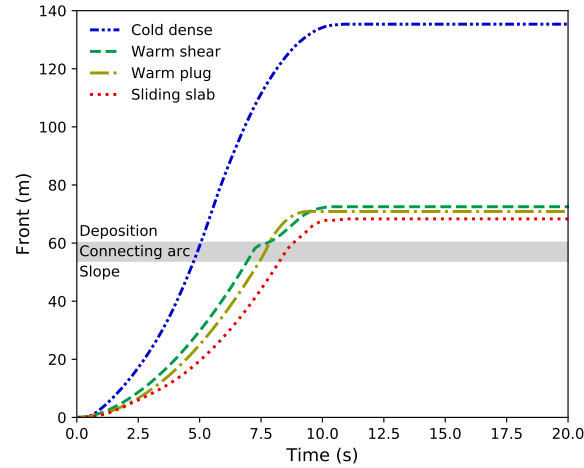


Figure 10: Front evolution of four flows in different flow regimes.

formed in avalanches in warm shear regime. The third flow displays ductile behavior, and slides down the slope and reaches the horizontal deposition zone with no significant deformation and no cracks. These characteristics are consistent with the snow avalanches in warm plug regime. The fourth flow in Fig. 9 shows rigid and brittle features as clear cracks and broken pieces are observed, which commonly occur in snow avalanches in sliding slab regime.

The front evolution of the four flows is presented in Fig. 10. The gray band in Fig. 10 shows the region where a flow front enters the connecting arc zone, below and above which the flow front is on the slope and in the horizontal deposition area, respectively. When the flows are on the slope, the front of the cold dense flow is the fastest (low value of M), followed by the warm shear and warm plug flows, and the sliding slab is the slowest. In the warm shear flow, discrete granules form a discontinuous flow front. The final front position of the four flows show a consistent relation as that obtained when they are on the slope. More information can be found in [LSJG20].

References

- [ASB13] Keita Abe, Kenichi Soga, and Samila Bandara. Material point method for coupled hydromechanical problems. *Journal of Geotechnical and Geoenvironmental Engineering*, 140(3):04013033, 2013.
- [BBL⁺17] TW Barraclough, JR Blackford, S Liebenstein, S Sandfeld, TJ Stratford, G Weinländer, and M Zaiser. Propagating compaction bands in confined compression of snow: Experiment and modelling. *Nature Physics*, 2017.

- [BBS00] SG Bardenhagen, JU Brackbill, and Deborah Sulsky. The material-point method for granular materials. *Computer Methods in Applied Mechanics and Engineering*, 187(3-4):529–541, 2000.
- [BFL16] Samila Bandara, Alessio Ferrari, and Lyesse Laloui. Modelling landslides in unsaturated slopes subjected to rainfall infiltration using material point method. *International Journal for Numerical and Analytical Methods in Geomechanics*, 40(9):1358–1380, 2016.
- [BW08] J. Bonet and R. D. Wood. *Nonlinear Continuum Mechanics for Finite Element Analysis*. Cambridge University Press, 2nd edition, 2008.
- [CSM15] Chaman Chandel, Praveen K Srivastava, and P Mahajan. Determination of failure envelope for faceted snow through numerical simulations. *Cold Regions Science and Technology*, 116:56–64, 2015.
- [DBD16] Gilles Daviet and Florence Bertails-Descoubes. A semi-implicit material point method for the continuum simulation of granular materials. *ACM Transactions on Graphics (TOG)*, 35(4):102, 2016.
- [EYZ20] Margarita Eglit, Alexander Yakubenko, and Julia Zayko. A review of russian snow avalanche models—from analytical solutions to novel 3d models. *Geosciences*, 10(2):77, 2020.
- [FLG04] J Failletaz, F Louchet, and J.R Grasso. Two-threshold model for scaling laws of noninteracting snow avalanches. *Physical Review Letters*, 93(20):208001, 2004.
- [FZ07] B Fyffe and M Zaiser. Interplay of basal shear fracture and slab rupture in slab avalanche release. *Cold Regions Science and Technology*, 49:26–38, 2007.
- [GCEN13] J. Gaume, G. Chambon, N. Eckert, and M. Naaim. Influence of weak-layer heterogeneity on snow slab avalanche release: Application to the evaluation of avalanche release depths. *Journal of Glaciology*, 59(215):423–437, 2013.
- [GGT⁺18] J Gaume, T Gast, J Teran, A van Herwijnen, and C Jiang. Dynamic anticrack propagation in snow. *Nature Communications*, 9(1):3047, 2018.
- [GJ08] Dave Gauthier and Bruce Jamieson. Evaluation of a prototype field test for fracture and failure propagation propensity in weak snowpack layers. *Cold Regions Science and Technology*, 51(2):87–97, 2008.
- [GLTT17] J. Gaume, H. Löwe, S Tan, and L. Tsang. Scaling laws for the mechanics of loose and cohesive granular materials based on baxter’s sticky hard spheres. *Physical Review E*, 96(3):032914, 2017.
- [GR17] J. Gaume and B. Reuter. Assessing snow instability in skier-triggered snow slab avalanches by combining failure initiation and crack propagation. *Cold Regions Science and Technology*, 114:6–15, 2017.

- [GS08] O. Gonzalez and A. M. Stuart. *A First Course in Continuum Mechanics*. Cambridge Texts in Applied Mathematics. Cambridge University Press, 2008.
- [GSvH⁺14] J. Gaume, J. Schweizer, A. van Herwijnen, G. Chambon, B. Reuter, N. Eckert, and M. Naaim. Evaluation of slope stability with respect to snowpack spatial variability. *Journal of Geophysical Research: Earth Surface*, 119(9):1783–1789, 2014.
- [GvHC⁺15] J. Gaume, A. van Herwijnen, G. Chambon, K. Birkeland, and J. Schweizer. Modeling of crack propagation in weak snowpack layers using the discrete element method. *The Cryosphere*, 9:1915–1932, 2015.
- [GvHC⁺17] J. Gaume, A. van Herwijnen, G. Chambon, N. Wever, and J. Schweizer. Snow fracture in relation to slab avalanche release: critical state for the onset of crack propagation. *The Cryosphere*, 11:217–228, 2017.
- [GvHG⁺19] Johan Gaume, Alec van Herwijnen, Ted Gast, Joseph Teran, and Chenfanfu Jiang. Investigating the release and flow of snow avalanches at the slope-scale using a unified model based on the material point method. *Cold Regions Science and Technology*, 168:102847, 2019.
- [Hag17] Pascal Hagenmuller. Microstructure-based finite element modeling of snow failure envelope. In *Geophysical Research Abstracts*, volume 19, page 4459, 2017.
- [HCN15] P. Hagenmuller, G Chambon, and M Naaim. Microstructure-based modeling of snow mechanics: a discrete element approach. *The Cryosphere*, 9(5)(1969-1982), 2015.
- [HGZ08] J Heierli, P Gumbsch, and M. Zaiser. Anticrack nucleation as triggering mechanism for snow slab avalanches. *Science*, 321:240–243, 2008.
- [JSS⁺15] C. Jiang, C. Schroeder, A. Selle, J. Teran, and A. Stomakhin. The affine particle-in-cell method. *ACM Trans Graph*, 34(4):51:1–51:10, 2015.
- [JST⁺16] C. Jiang, C. Schroeder, J. Teran, A. Stomakhin, and A. Selle. The material point method for simulating continuum materials. In *ACM SIGGRAPH 2016 Course*, pages 24:1–24:52, 2016.
- [KGP⁺16] Gergely Klár, Theodore Gast, Andre Pradhana, Chuyuan Fu, Craig Schroeder, Chenfanfu Jiang, and Joseph Teran. Drucker-prager elastoplasticity for sand animation. *ACM Transactions on Graphics (TOG)*, 35(4):103, 2016.
- [KS14] Berna Köchle and Martin Schneebeli. Three-dimensional microstructure and numerical calculation of elastic properties of alpine snow with a focus on weak layers. *Journal of Glaciology*, 60(222):705–713, 2014.

- [LSJG20] Xingyue Li, Betty Sovilla, Chenfanfu Jiang, and Johan Gaume. The mechanical origin of snow avalanche dynamics and flow regime transitions. *The Cryosphere Discussions*, pages 1–25, 2020.
- [Mal69] L. E. Malvern. *Introduction to the Mechanics of Continuous Medium*. Prentice-Hall, Inc, 1969.
- [Mas13] C. M. Mast. *Modeling Landslide-induced Flow Interactions with Structures Using the Material Point Method*. PhD thesis, University of Washington, Seattle, 2013.
- [McC79] D.M. McClung. Shear fracture precipitated by strain softening as a mechanism of dry slab avalanche release. *Journal of Geophysical Research: Solid Earth*, 84(B7):3519–3526, 1979.
- [Mis13] R v Mises. Mechanik der festen körper im plastisch-deformablen zustand. *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, 1913:582–592, 1913.
- [MJ08] P Mahajan and S Joshi. Modeling of interfacial crack velocities in snow. *Cold Regions Science and Technology*, 51:98–111, 2008.
- [MKC10] P. Mahajan, R. Kalakuntla, and C. Chandel. Numerical simulation of failure in a layered thin snowpack under skier load. *Annals of Glaciology*, 51(54):169–175, 2010.
- [MLM96] Günther Meschke, Changhong Liu, and Herbert A Mang. Large strain finite-element analysis of snow. *Journal of Engineering Mechanics*, 122(7):591–602, 1996.
- [NDEC13] Mohamed Naaim, Yves Durand, Nicolas Eckert, and Guillaume Chambon. Dense avalanche friction coefficients: influence of physical properties of snow. *Journal of Glaciology*, 59(216):771–782, 2013.
- [NGL10] R. Narain, A. Golas, and M. Lin. Free-flowing granular materials with two-way solid coupling. *ACM Trans Graph*, 29(6):173:1–173:10, 2010.
- [OP04] M. Ortiz and A. Pandolfi. A variational cam-clay theory of plasticity. *Computer Methods in Applied Mechanics and Engineering*, 193(2729):2645 – 2666, 2004.
- [Par72] RHG Parry. *Stress-strain Behaviour of Soils*. GT Foulis, 1972.
- [PR73] A.C Palmer and J.R Rice. The growth of slip surfaces in the progressive failure of over-consolidated clay. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 332:527–548, 1973.
- [RB68] K. Roscoe and J. Burland. On the generalised stress-strain behaviour of wet clay. *Engineering Plasticity*, pages 535–609, 1968.
- [Rei11] I Reiweger. *Failure of a Layer of Buried Surface Hoar*. PhD thesis, ETH Zürich, 2011.

- [RGS15] I. Reiweger, J. Gaume, and J. Schweizer. A new mixed-mode failure criterion for weak snowpack layers. *Geophysical Research Letters*, 42(5):1427–1432, 2015.
- [RKHF18] Matthias Rauter, Andreas Kofler, Andreas Huber, and Wolfgang Fellin. fasavagehutterfoam 1.0: depth-integrated simulation of dense snow avalanches on natural terrain with openfoam. *Geoscientific Model Development*, 11(7):2923–2939, 2018.
- [RS10] I Reiweger and J Schweizer. Failure of a layer of buried surface hoar. *Geophysical Research Letters*, 37(24):L24501, 2010.
- [RS13] I Reiweger and J Schweizer. Weak layer fracture: facets and depth hoar. *The Cryosphere*, 7(5):1447–1453, 2013.
- [RSDH09] I Reiweger, J Schweizer, J Dual, and H.J Herrmann. Modelling snow failure with a fibre bundle model. *Journal of Glaciology*, 55(194):997–1002, 2009.
- [RSRvH19] Bettina Richter, Juerg Schweizer, Mathias Rotach, and Alec van Herwijnen. Validating modeled critical crack length for crack propagation in the snow cover model snowpack. *The Cryosphere*, 13:3353–3366, 12 2019.
- [SAY⁺15] Kenichi Soga, E Alonso, A Yerro, K Kumar, and S Bandara. Trends in large-deformation analysis of landslide mass movements with particular emphasis on the material point method. *Géotechnique*, 66(3):248–273, 2015.
- [SCM17] P. Srivastava, C. Chandel, and P Mahajan. Micromechanical modeling of elastic and strength properties of snow. In *SLAM3 - Slab Avalanche Multiscale Mechanical Modeling, 3-5 April 2017, Davos, Switzerland*, 2017.
- [SCMP16] Praveen K. Srivastava, Chaman Chandel, Puneet Mahajan, and Pankaj Pankaj. Prediction of anisotropic elastic properties of snow from its microstructure. *Cold Regions Science and Technology*, 125:85 – 100, 2016.
- [SGH⁺15] W Steinkogler, J Gaume, Löwe H, B Sovilla, and M Lehning. Granulation of snow: from tumbler experiments to discrete element simulations. *Journal of Geophysical Research: Earth Surface*, 120(6):1107–1126, 2015.
- [Sim92] J. C. Simo. Algorithms for static and dynamic multiplicative plasticity that preserve the classical return mapping schemes of the infinitesimal theory. *Computer Methods in Applied Mechanics and Engineering*, 99(1):61–112, 1992.

- [SM93] J. Simo and G. Meschke. A new class of algorithms for classical plasticity extended to finite strains. application to geomaterials. *Computational Mechanics*, 11(4):253–278, 1993.
- [SS07] Christian Sigrist and Jürg Schweizer. Critical energy release rates of weak snowpack layers determined in field experiments. *Geophysical Research Letters*, 34(L03502), 2007.
- [SSC⁺13] Alexey Stomakhin, Craig Schroeder, Lawrence Chai, Joseph Teran, and Andrew Selle. A material point method for snow simulation. *ACM Transactions on Graphics (TOG)*, 32(4):102, 2013.
- [SW68] A. Schofield and P. Wroth. *Critical State Soil Mechanics*. McGraw-Hill London, 1968.
- [SZS95] Deborah Sulsky, Shi-Jian Zhou, and Howard L Schreyer. Application of a particle-in-cell method to solid mechanics. *Computer Physics Communications*, 87(1-2):236–252, 1995.
- [TGK⁺17] Andre Pradhana Tampubolon, Theodore Gast, Gergely Klár, Chuyuan Fu, Joseph Teran, Chenfanfu Jiang, and Ken Museth. Multi-species simulation of porous sand and water mixtures. *ACM Transactions on Graphics (TOG)*, 36(4):105, 2017.
- [vHGB⁺16] Alec van Herwijnen, Johan Gaume, Edward H Bair, Benjamin Reuter, Karl W Birkeland, and Jürg Schweizer. Estimating the effective elastic modulus and specific fracture energy of snowpack layers from field experiments. *Journal of Glaciology*, 62(236):997–1007, 2016.
- [vHH09] A van Herwijnen and J. Heierli. Measurements of crack-face friction in collapsed weak snow layers. *Geophysical Research Letters*, 36, 2009. L23502.
- [vHJ05] A van Herwijnen and B Jamieson. High speed photography of fractures in weak snowpack layers. *Cold Regions Science and Technology*, 43(1-2):71–82, 2005.
- [vHSH10] A van Herwijnen, J Schweizer, and J Heierli. Measurement of the deformation field associated with fracture propagation in weak snowpack layers. *Journal of Geophysical Research: Earth Surface*, 115(F3), 2010.
- [VWH17] Philip J Vardon, Bin Wang, and Michael A Hicks. Slope failure simulations with mpm. *Journal of Hydrodynamics, Ser. B*, 29(3):445–451, 2017.
- [WGF15] A. Wautier, C. Geindreau, and F. Flin. Linking snow microstructure to its macroscopic elastic stiffness tensor: A numerical homogenization method and its application to 3-d images from x-ray tomography. *Geophysical Research Letters*, 42(19):8031–8041, 2015. 2015GL065227.

Implicit MPM and coupled MPM-FEM in geomechanics

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1 Introduction

Within the past two decades, mass movements hazards involving fast and large soil deformation have increased significantly in frequency and magnitude due to climate changes and global warming. During these extreme phenomena rocks, debris, and heavy materials can seriously damage and destroy landscape and infrastructures, causing devastating economic loss, and human casualties.

An essential step to be prepared to the catastrophic effect of these events is the capability to assess in an accurate way the interaction between the moving mass and the surrounding structures or landscape. Physical modeling with ad hoc scale model is not sufficient for this purpose due to its complexity, the difficulty for its scaling up to real life problems, its long execution time and unaffordable cost. The alternative is, therefore, numerical modeling.

While the Finite Element Method (FEM) is the standard and well established technique in engineering applications, unfortunately it shows some limitation when dealing with large deformation problems like those cited before and particle-based approaches could represent an effective solution to such drawbacks. The Material Point Method in particular, maintains most of the strong features of FEM, overcoming some of its shortcomings thanks to its hybrid nature.

While the computational analysis of landslide, debris flow or other mass movements has been mainly dominated by the development of advanced geomechanical constitutive models suited for different types of soil materials such as multi-phase unsaturated

soil model [SAY⁺15, AA10, Mas13], this study focuses more on the dynamic interaction of such masses with the installed protective structures.

In what follows, an implicit formulation of the Material Point Method (MPM) is implemented to model the dynamics of the mass movements considering finite strain assumption. In the present work, the soil is modeled as a non-associated elastoplastic constitutive law assuming Mohr-Coulomb yield criterion as specified by [CDA07] and implemented using Hencky or logarithmic strain assumption. Here, a monolithic coupling between soil and structural elements is considered; i.e. the linear system of equations of both soil and structure is solved at the same time. Furthermore, a staggered coupling scheme with traditional Finite Element Method (FEM) is proposed to simulate accurately and robustly the dynamic force and displacement coupling of soil-structure interaction (SSI).

All developments of the method are implemented within the *Kratos-Multiphysics* opensource framework [DRO10] and available under the BSD license (<https://github.com/KratosMultiphysics/Kratos/wiki>).

These notes are mostly based on the following documents and are not intended to be comprehensive of all details:

- Iaconeta, I. Larese, A., Rossi, R., Oñate, E. A stabilized, mixed, implicit Material Point Method for non-linear incompressible solid mechanics problems; Computational mechanics 175, 226-232,(2019)
- Iaconeta, I., Larese, A., Rossi, R., Guo, Z. Comparison of a Material Point Method and a Meshfree Galerkin Method for the simulation of cohesive-frictional materials, Materials, 10 , 1150, (2017)
- Chandra, B.; Singer, V.; Teschemacher, T.; Wuechner, R. and Larese, A. Nonconforming Dirichlet boundary conditions in Implicit Material Point Method by means of penalty augmentation Submitted to Acta Geotechnica, 2020
- Chandra, B.; Singer Veronika ; Bucher, P.; Larese, A.; Rossi, R. and Wuechner, R. A staggered Implicit MPM-FEM coupling strategy Submitted, 2020
- PhD Thesis: I. Iaconeta Discrete-continuum hybrid modelling of flowing and static regimes. Universidad Polit cnica de Catalunya, UPCBarcelonaTech, Spain. 29/11/2019
- MsC Thesis: B. Chandra, Soil structure interaction simulation using a coupled implicit material point- finite element method (2019) , Technical University of Munich (TUM), Germany;

The interested reader is strongly recommended to refer to the above documentation and relative literature for a detailed formulation.

1.1 MPM in short

Classical FEM models traditionally employ two different kinematic descriptions: Eulerian and Lagrangian frameworks. While a Lagrangian approach is a preferable choice when dealing with large deformation problems for its simplicity (absence of the convective term and “natural” tracking of the interface displacements), we have to

deal with the need of a frequent remeshing to ensure that the big distortion of the elements does not compromise the mesh quality. An alternative is to get rid of the mesh choosing either meshless approaches such as the Smoothed Particle Hydrodynamics (SPH) or hybrid approaches, such as the Material Point Method (MPM). The later uses a fixed background grid for the Lagrangian calculation with moving integration points (the material points MPs) that are storing all the historical variables [VSWN19].

In this study, a fully-implicit formulation of the Material Point Methods (MPM) is presented. Introduced by [SCS94, SZS95], as the extension of particle-in-cell (PIC) method [Har64], the MPM has gained a remarkably increasing popularity due to its capability in simulating solid mechanics problems which involve history-dependent materials and large deformations. The method stores the historically changing variables and the material information at the moving particles, the so-called material points (MP), and uses a constantly-reset background mesh to solve the linear system of equations. It combines the strengths of Eulerian and Lagrangian methods, with no need to remesh. MPM has been utilized in various civil engineering applications, mostly in the analysis of moving discontinuities and large deformation systems. With few notable exceptions [GW03, WVHC16], the majority of the MPM algorithms are written assuming an explicit scheme, in particular, for the simulation of mass movements and landslides [SAY⁺15, AA10, Mas13]. While explicit approach is generally favorable to simulate fast transient problems, the implicit formulation, is often more optimal to simulate cases when the rate of loading increment is slow, the rate of deformation is small, or when the driving force is solely gravity. On top of that, the stability of the method (for properly chosen dissipative methods) does not depend on the wave propagation speed within the media, and thus, allows the usage of a relatively larger time increment. This scheme can also be extremely advantageous to solve a multi-physics coupling problems such as the soil-structure interaction (SSI) being coupled with FEM or other implicit-based methods.

2 Formulation

2.1 Governing equations

Let us consider the body $\mathcal{B}$ which occupies a region Ω of the 3D Euclidean space $\mathcal{E}$ with a regular boundary $\partial\Omega$ in its reference configuration. A deformation of $\mathcal{B}$ is defined by a one-to-one mapping

$$\varphi : \Omega \rightarrow \mathcal{E} \quad (1)$$

that maps each point $\boldsymbol{p}$ of the body $\mathcal{B}$ into a spatial point $\boldsymbol{x}$

$$\boldsymbol{x} = \varphi(\boldsymbol{p}) \quad (2)$$

which represents the location of $\boldsymbol{p}$ in the deformed configuration of $\mathcal{B}$. The region of $\mathcal{E}$ occupied by $\mathcal{B}$ in its deformed configuration is denoted as $\varphi(\Omega)$.

The problem is governed by mass and linear momentum balance equations

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0 \quad \text{in } \varphi(\Omega) \quad (3a)$$

$$\rho \mathbf{a} - \nabla \cdot \boldsymbol{\sigma} = \rho \mathbf{b} \quad \text{in } \varphi(\Omega) \quad (3b)$$

where ρ is the mass density, $\mathbf{a}$ is the acceleration, $\mathbf{v}$ is the velocity, $\boldsymbol{\sigma}$ is the symmetric Cauchy stress tensor and $\mathbf{b}$ is the body force. Acceleration and velocity are, by definition, the material derivatives of the velocity, $\mathbf{v}$, and the displacement, $\mathbf{u}$, respectively. For a compressible material the conservation of mass is satisfied by

$$\rho = \frac{\rho_0}{\det(\mathbf{F})} \quad (4)$$

where ρ_0 is the density in the undeformed configuration and $\det(\mathbf{F})$ is the determinant of the total deformation gradient $\mathbf{F} := d\mathbf{x}/d\mathbf{X}$ with $\mathbf{x}$ and $\mathbf{X}$ representing the current and initial position, respectively. Equation 4 holds at any point, and in particular at the sampling points where the equation is written, e.g. the material points. Thermal effects are not considered in the present work, so the energy balance is considered implicitly fulfilled.

The balance equations are solved numerically in a three-dimensional region $\Omega \subseteq \mathcal{R}^3$, in the time range $t \in [0, T]$, given the following boundary conditions on the Dirichlet ($\varphi(\partial\Omega_D)$) and Neumann boundaries ($\varphi(\partial\Omega_N)$), respectively

$$\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \varphi(\partial\Omega_D) \quad (5a)$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \varphi(\partial\Omega_N) \quad (5b)$$

where $\mathbf{n}$ is the unit outward normal.

In order to fully define the Boundary Value Problem (BVP) a proper constitutive model defining the stress strain relation is needed. Since the formulation proposed is not influenced by the choice of the constitutive law, we will not describe the possible elasto-plastic models available in detail. Nevertheless, the interested reader can refer to [Iac19] for further details on the material laws.

2.2 Weak form

In this section, the weak form is derived. Following the formulation explained in [Wri06, Wri08], a displacement-based finite element procedure.

Let the displacement space $\mathcal{V} \in [\mathbf{H}^1(\mathcal{B})]^d$ be the space of vector functions whose components and their first derivatives are square-integrable, the integral form of the problem is

$$\int_{\varphi(\Omega)} (\nabla \cdot \boldsymbol{\sigma}) \cdot \mathbf{w} dv + \int_{\varphi(\Omega)} \rho (\mathbf{b} - \mathbf{a}) \cdot \mathbf{w} dv - \int_{\varphi(\partial\Omega_N)} (\boldsymbol{\sigma} \cdot \mathbf{n} - \bar{\mathbf{t}}) \cdot \mathbf{w} da = 0, \quad \forall \mathbf{w} \in \mathcal{V} \quad (6)$$

where $\mathbf{w}$ is an arbitrary test function, such that $\mathbf{w} = \{\mathbf{w} \in \mathcal{V} \mid \mathbf{w} = \mathbf{0} \text{ on } \varphi(\partial\Omega_D)\}$, dv is the differential volume and da the differential boundary surface. By integrating by parts, applying the divergence theorem and considering the symmetry of the stress tensor, the following expression is obtained

$$\int_{\varphi(\Omega)} \boldsymbol{\sigma} : (\nabla^S \mathbf{w}) dv - \int_{\varphi(\Omega)} \rho (\mathbf{b} - \mathbf{a}) \cdot \mathbf{w} dv - \int_{\varphi(\partial\Omega_N)} \bar{\mathbf{t}} \cdot \mathbf{w} da = 0 \quad (7)$$

Under the assumption that the stress tensor is a function of the current strain only

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\epsilon}) \quad (8)$$

the problem is reduced to find a kinematically admissible field $\mathbf{u}$ that satisfies

$$G(\mathbf{u}, \mathbf{w}) = 0 \quad \forall \mathbf{w} \in \mathcal{V} \quad (9)$$

where G is the virtual work functional defined as

$$G(\mathbf{u}, \mathbf{w}) = \int_{\varphi(\Omega)} \boldsymbol{\sigma} : (\nabla^S \mathbf{w}) dv - \int_{\varphi(\Omega)} \rho (\mathbf{b} - \mathbf{a}) \cdot \mathbf{w} dv - \int_{\varphi(\partial\Omega_N)} \bar{\mathbf{t}} \cdot \mathbf{w} da \quad (10)$$

2.3 Linearisation of the spatial weak formulation

In this work the BVP is characterized by both geometrical and material non-linearity. When a non-linear BVP is considered, the discretisation of the weak form results in a system of non-linear equations. A linearisation is, therefore, needed for the solution of such a system. The Newton-Raphson's iterative procedure is used. This uses directional derivatives to linearise the non-linear equations. The virtual work functional of Equation 10 is linearised with respect to the unknown $\mathbf{u}$, using an arbitrary argument $\mathbf{u}^*$, which is chosen to be the last known equilibrium configuration.

The linearised problem is to find $\delta\mathbf{u}$ such that

$$L(\delta\mathbf{u}, \mathbf{w}) \simeq G(\mathbf{u}^*, \mathbf{w}) + DG(\mathbf{u}^*, \mathbf{w})[\delta\mathbf{u}] = 0, \quad \forall \mathbf{w} \in \mathcal{V} \quad (11)$$

where L is the linearised virtual work function and

$$DG(\mathbf{u}^*, \mathbf{w})[\delta\mathbf{u}] = \left. \frac{d}{d\gamma} \right|_{\gamma=0} G(\mathbf{u}^* + \gamma\delta\mathbf{u}, \mathbf{w}) \quad (12)$$

is the directional derivative of G at $\mathbf{u}^*$ in the direction of $\delta\mathbf{u}$, given by

$$\begin{aligned} DG(\mathbf{u}^*, \mathbf{w})[\delta\mathbf{u}] &= \left. \frac{d}{d\gamma} \right|_{\gamma=0} \int_{\varphi(\Omega)} [\boldsymbol{\sigma}(\boldsymbol{\epsilon}(\gamma)) : (\nabla^S \mathbf{w}) - \rho (\mathbf{b} - \mathbf{a}) \cdot \mathbf{w}] dv + \\ &\quad - \left. \frac{d}{d\gamma} \right|_{\gamma=0} \int_{\varphi(\partial\Omega_N)} \bar{\mathbf{t}} \cdot \mathbf{w} da \end{aligned} \quad (13)$$

Under the assumption of conservative external loads, only the terms related to the internal and inertial forces are dependent on the deformation. Using the following definitions

$$\boldsymbol{\epsilon}(\gamma) = \nabla^S(\mathbf{u}^* + \gamma \delta \mathbf{u}) = \boldsymbol{\epsilon}^* + \gamma \nabla^S(\delta \mathbf{u}) \quad (14)$$

where $\boldsymbol{\epsilon}^* = \nabla^S(\mathbf{u}^*)$ is the strain field at $\mathbf{u}^*$ and $\mathbf{u}(\gamma) = \mathbf{u}^* + \gamma \delta \mathbf{u}$, the directional derivative $DG(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}]$ reduces to

$$\begin{aligned} DG(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] &= \left. \frac{d}{d\gamma} \right|_{\gamma=0} \left(\int_{\varphi(\Omega)} [\boldsymbol{\sigma}(\boldsymbol{\epsilon}(\gamma)) : (\nabla^S \mathbf{w}) + \rho \mathbf{a}(\mathbf{u}(\gamma)) \cdot \mathbf{w}] dv \right) \\ &= DG^{static}(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] + DG^{dynamic}(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] \end{aligned} \quad (15)$$

which can be split in a static and dynamic contribution.

Under the assumption of finite strains and adopting an Updated Lagrangian kinematic framework, the expression of the directional derivative (Equation 15) should be derived in spatial form. A common way to do that consists in linearising the material weak form and in doing a push-forward operation to recover the spatial form [Wri06]. Therefore, the linearisation of the weak form derived with respect to the initial configuration reads:

$$\begin{aligned} DG(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] &= \int_{\Omega} \nabla_X \delta \mathbf{u} \mathbf{S} \cdot \nabla_X \mathbf{w} dV \\ &\quad + \int_{\Omega} \left[(\mathbf{F}^T \nabla_x^S \mathbf{w} \mathbf{F}) : \mathbb{C}(\mathbf{F}^T \nabla_x^S \delta \mathbf{u} \mathbf{F}) \right] dV \\ &\quad + \int_{\Omega} \rho_0 \frac{d\mathbf{a}}{d\mathbf{u}} \cdot \mathbf{w}[\delta \mathbf{u}] dV \end{aligned} \quad (16)$$

where ∇_X and ∇_x are the material and spatial gradient operator, respectively, $\mathbf{S}$ is the Second Piola Kirchhoff stress tensor, $\mathbb{C}$ is the fourth order incremental constitutive tensor and dV is the differential volume element in the underformed configuration. The linearisation of the weak form with respect to the current configuration can be derived by pushing-forward the linearisation of Equation 16. The first term can be directly written in terms of the Kirchhoff stress $\boldsymbol{\tau} = \mathbf{F} \mathbf{S} \mathbf{F}^T$ as

$$\nabla_X \delta \mathbf{u} \mathbf{S} \cdot \nabla_X \mathbf{w} = \nabla_X \delta \mathbf{u} \mathbf{F}^{-1} \boldsymbol{\tau} \mathbf{F}^{-T} \cdot \nabla_X \mathbf{w} \quad (17)$$

and using this standard identity $\nabla_x a = \nabla_X a \mathbf{F}^{-1}$, Equation 17 can be written as

$$\nabla_X \delta \mathbf{u} \mathbf{S} \cdot \nabla_X \mathbf{w} = \nabla_x \delta \mathbf{u} \boldsymbol{\tau} \cdot \nabla_x \mathbf{w} \quad (18)$$

The second integral of Equation 16 can be re-written as:

$$\int_{\Omega} \nabla_x^S \mathbf{w} : \hat{\mathbb{C}} [\nabla_x^S \delta \mathbf{u}] dV \quad (19)$$

adopting the transformation of the fourth order incremental constitutive tensor $\mathbb{C}$ in Voigt notation [Wri06]:

$$\hat{\mathbb{C}}_{iklm} = F_{iA} F_{lC} F_{mD} F_{kB} \mathbb{C}_{ABCD} \quad (20)$$

where lowercase indexes are referred to the incremental constitutive tensor relative to the Kirchhoff stress, while uppercase indexes to the incremental constitutive tensor relative to the Second Piola Kirchhoff stress.

With these transformations, the linearisation of the static contribution at the current configuration is

$$DG^{static}(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] = \int_{\Omega} \nabla_x \delta \mathbf{u} \boldsymbol{\tau} \cdot \nabla_x \mathbf{w} + \nabla_x^S \mathbf{w} : \widehat{\mathbb{C}}[\nabla_x^S \delta \mathbf{u}] dV \quad (21)$$

Considering the definition of the determinant of the deformation gradient: $\det(\mathbf{F}) = J = \frac{dv}{dV}$, the following relations hold

$$\boldsymbol{\sigma} = \frac{1}{J} \boldsymbol{\tau} \quad (22)$$

$$\overline{\widehat{\mathbb{C}}} = \frac{1}{J} \widehat{\mathbb{C}} \quad (23)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are the Cauchy and Kirchhoff stress tensor, respectively, and $\overline{\widehat{\mathbb{C}}}$ is the incremental constitutive tensor relative to the Cauchy stress. Equation 16 can now be re-written in the current configuration as

$$DG(\mathbf{u}^*, \mathbf{w})[\delta \mathbf{u}] = \int_{\varphi(\Omega)} \left(\nabla_x \delta \mathbf{u} \boldsymbol{\sigma} \cdot \nabla_x \mathbf{w} + \nabla_x^S \mathbf{w} : \overline{\widehat{\mathbb{C}}}[\nabla_x^S \delta \mathbf{u}] + \rho \frac{d\mathbf{a}}{d\mathbf{u}} \cdot \mathbf{w}[\delta \mathbf{u}] \right) dv \quad (24)$$

Equation 24 represents the linearisation of the spatial weak formulation, also known as the Updated Lagrangian formulation, since the deformation state $\mathbf{u}^*$ is continuously updated during the non-linear incremental solution procedure, e.g. the Newton Raphson's method.

2.3.1 Spatial Discretisation

Let $\mathcal{V}_h$ be a finite element space to approximate $\mathcal{V}$. The problem is now finding $\mathbf{u}_h \in \mathcal{V}_h$ such that

$$DG(\mathbf{u}_h^*, \mathbf{w}_h)[\delta \mathbf{u}_h] = -G(\mathbf{u}_h^*, \mathbf{w}_h), \quad \forall \mathbf{w}_h \in \mathcal{V}_h \quad (25)$$

or using Equation 24

$$\begin{aligned} \int_{\varphi(\Omega)} \left\{ \nabla_x \delta \mathbf{u}_h \boldsymbol{\sigma} \cdot \nabla_x \mathbf{w}_h + \nabla_x^S \mathbf{w}_h : \overline{\widehat{\mathbb{C}}}[\nabla_x^S \delta \mathbf{u}_h] + \rho \frac{d\mathbf{a}_h}{d\mathbf{u}_h} \cdot \mathbf{w}_h[\delta \mathbf{u}_h] \right\} dv = \\ - \left(\int_{\varphi(\Omega)} \boldsymbol{\sigma} : (\nabla^S \mathbf{w}_h) dv - \int_{\varphi(\Omega)} \rho (\mathbf{b} - \mathbf{a}_h) \cdot \mathbf{w}_h dv - \int_{\varphi(\partial\Omega_N)} \bar{\mathbf{t}} \cdot \mathbf{w}_h da \right) \end{aligned} \quad (26)$$

Let us assume to discretise the continuum body $\mathcal{B}$ by a set of n_p material points and to assign a finite volume of the body Ω_p to each of those material points. Thus, the geometrical representation ($\mathcal{B}_h$) of $\mathcal{B}$ reads

$$\mathcal{B} \approx \mathcal{B}_h = \bigcup_{p=1}^{n_p} \Omega_p \quad (27)$$

and with this approximation the integrals of the weak form can be written as

$$\int_{\mathcal{B}} (...)dV \approx \int_{\mathcal{B}_h} (...)dV = \bigcup_{p=1}^{n_p} \int_{\Omega_p} (...)d\Omega_p \quad (28)$$

For the computation of the linearised system of equations, an integration is necessary over the volume occupied by each material point Ω_p . By using the spatial discretisation defined in Equation 27, the linearised system of equations (see Equation 26) is rewritten as

$$\begin{aligned} & \bigcup_{p=1}^{n_p} \int_{\Omega_p} \left(\left\{ \nabla_x \delta \mathbf{u}_h \boldsymbol{\sigma} \cdot \nabla_x \mathbf{w}_h + \nabla^S \mathbf{w}_h : \bar{\mathbb{C}}[\nabla^S \delta \mathbf{u}_h] + \rho \frac{d\mathbf{a}_h}{d\mathbf{u}_h} \cdot \mathbf{w}_h [\delta \mathbf{u}_h] \right\} \right) d\Omega_p \\ &= - \bigcup_{p=1}^{n_p} \left(\int_{\Omega_p} (\boldsymbol{\sigma} : (\nabla^S \mathbf{w}_h) - \rho (\mathbf{b} - \mathbf{a}_h)) d\Omega_p - \int_{\partial\Omega_{N_p}} \bar{\mathbf{t}} \cdot \mathbf{w}_h da_p \right) \end{aligned} \quad (29)$$

and by exploiting the finite element approximation with particle integration the final discretised form is obtained

$$\begin{aligned} & \bigcup_{p=1}^{n_p} \sum_{I=1}^n \sum_{K=1}^n \mathbf{w}_I^T \left((\nabla_x N_I)^T \boldsymbol{\sigma} (\nabla_x N_K) \mathbf{I} + \mathbf{B}_I^T \mathbf{D} \mathbf{B}_K + \frac{N_I \rho N_K}{\beta \Delta t^2} \mathbf{I} \right) V_p \delta \mathbf{u}_K \\ &= - \bigcup_{p=1}^{n_p} \sum_{I=1}^n \mathbf{w}_I^T \left(\mathbf{B}_I \boldsymbol{\sigma} - \rho \mathbf{b} N_I + \sum_{K=1}^n N_I \rho N_K \mathbf{a}_K \right) V_p - \bigcup_{l=1}^{n_l} \sum_{I=1}^{n_m} \mathbf{w}_I^T N_I \bar{\mathbf{t}} A_l \end{aligned} \quad (30)$$

where I and K are the indexes of the finite element's nodes, $\nabla_x N_I$ is the spatial gradient of the shape function evaluated at node I , $\mathbf{D}$ is the matrix form of the incremental constitutive tensor $\bar{\mathbb{C}}$, V_p is the volume relative to a single material point, A_l is the surface and $\mathbf{B}_I$ is the deformation matrix relative to node I , expressed here for a 2D

problem as:

$$\mathbf{B}_I = \begin{bmatrix} \frac{\partial N_I}{\partial x} & 0 \\ 0 & \frac{\partial N_I}{\partial y} \\ \frac{\partial N_I}{\partial y} & \frac{\partial N_I}{\partial x} \end{bmatrix} \quad (31)$$

The left hand side of Equation 30 is given by three addends multiplied by the increment of the unknowns. The first one is commonly known as the *geometric* stiffness matrix

$$\mathbf{K}_{IK}^G = (\nabla_x N_I)^T \boldsymbol{\sigma} (\nabla_x N_K) \mathbf{I} V_p \quad (32)$$

while the second term is known as the *material* stiffness matrix

$$\mathbf{K}_{IK}^M = \mathbf{B}_I^T \mathbf{D} \mathbf{B}_K V_p \quad (33)$$

and their sum represents the static contribution to the tangent stiffness matrix

$$\mathbf{K}_{IK}^{static} = \mathbf{K}_{IK}^G + \mathbf{K}_{IK}^M \quad (34)$$

The *dynamic* component is given by

$$\mathbf{K}_{IK}^{dynamic} = \frac{N_I \rho N_K}{\beta \Delta t^2} \mathbf{I} V_p \quad (35)$$

Finally the tangent stiffness matrix is given by

$$\mathbf{K}_{IK}^{tan} = \mathbf{K}_{IK}^{static} + \mathbf{K}_{IK}^{dynamic} \quad (36)$$

and represents the submatrix relative to one node of the discretisation with dimension $[n_{dof} \times n_{dof}]$, where n_{dof} is the number of degrees of freedom of a single node. This matrix can be considered as the Jacobian matrix of the right hand side of Equation 30, i.e., the residual $\mathbf{R}_I$. Equation 30 can be rewritten in compact form as

$$\mathbf{K}_{IK}^{tan} \delta \mathbf{u}_K = -\mathbf{R}_I. \quad (37)$$

2.4 Irreducible vs mixed formulation. Some words

In these notes only the classical irreducible formulation has been derived. It is well known that overly stiff numerical solutions appear when Poisson's ratio ν tends to 0.5 or when plastic flow is constrained by the volume conservation condition. In these cases, the standard Galerkin displacement-based formulation ($\mathbf{u}$ formulation) fails [ZTZ13] due to the inability to evaluate the correct strain field.

In the literature, many possible solutions can be found. For instance, the *Mixed Enhanced Element* for small deformation problems [SR90]. The B-bar methods [Hug80] and the classical incompatible modes formulation [TBW76] fall under this theory. .

Alternative procedures suitable for geometrically non-linear regimes, are given by the F-BAR method [dSNPDO96], the non-linear B-bar method [MOS90] and the family of enhanced elements [SA92]. Though the good performance of all the aforementioned methods, none of such techniques is, however, suitable for application on simplicial meshes [RS95, OBHC15].

Among the successful strategies, it is worth mentioning the group of the *Mixed Variational Methods*. A application of a mixed displacement-pressure ($\mathbf{u}$ - p) method to MPM. It is worth mentioning that the treatment of the incompressibility constraint is relatively new in the context of the Material Point Method (MPM). Most MPM formulations deal with compressible materials, avoiding the issues arising from the imposition of the incompressibility constraint. However, some procedures for the treatment of locking issues can be found in the recent literature.

3 MPM formulation

The Material Point Method (MPM)[SCS94, SZS95] is a particle-based method, whose origin goes back to the paper of [Har64], where the particle-in-cell method (PIC), a technique for the solution of fluid flow problems, was proposed for the first time. Some decades after, the PIC method was redefined within the solid mechanics framework, and after that, it was known to the computational community with the name of Material Point Method. MPM combines a Lagrangian description of the body under analysis, which is represented by a set of particles, the so-called *material points*, with the use of a computational mesh, named *background grid*, as can be observed in Figure 1.

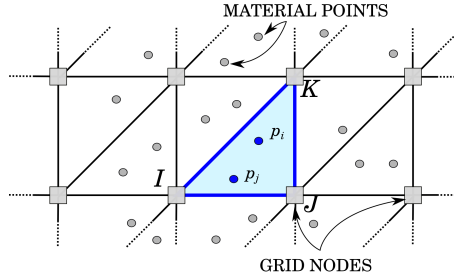


Figure 1: *MPM*. The shape functions on the material point p_i are evaluated using FE shape function of element I-J-K.

This distinctive feature allows to track the deformation of the body and retrieve the history-dependent material information at each time instant of the simulation, without committing mapping information errors, typical of methods which make use of remeshing techniques. This makes the method particularly attractive for the solution of problems, characterized by very large deformations and by the use of complex constitutive laws [Wie04, SS15]. For instance, the method has been extensively used for

geotechnical problems [ZA11, YAP15, SS15] for its capabilities in tracking extremely large deformation while preserving material properties of the material points.

In the key works of Sulsky and co-workers [SCS94, SZS95], the MPM has been applied for the first time in the solid mechanics framework. Even if through the original MPM it was possible to solve complex problems involving, for instance, contact [HZMH11], interaction between different materials [YSS00, HXQ⁺09] and the use of history-dependent material laws [SCS94], it was observed that the first version of MPM suffers from some intrinsic shortcomings. Indeed, due to the use of piece-wise linear shape functions, the latter are only locally defined and their gradients are discontinuous. This implies that a material point on the cell boundary would not be covered by the local shape functions defined within the respective cells around the particle. This would produce a noise in the numerical solution, which is called *cell-crossing error*. Recently, many improvements to the original MPM have been provided to alleviate the cell-crossing noise and to have a more efficient and algorithmically straightforward evaluation of grid node integrals in the weak formulation. The Generalized Interpolation Material Point method (GIMP) [BK04] represents the first attempt to provide an improved version of the original MPM. The essence of this method is based on the definition of a characteristic function $\chi_p(x)$ which has to satisfy the partition of unity criterion, i.e., $\sum_p \chi_p(x) = 1$

The particle characteristic function defines the spatial volume occupied by the particle V_p as

$$V_p = \int_{\Omega_p \cap \Omega} \chi_p(x) dV \quad (38)$$

where Ω_p and Ω are the current particle domain and the current domain occupied by the continuum, respectively. Moreover, since a material property $f(x)$ can be approximated by its particle value f_p as

$$f(x) = \sum_p f_p \chi_p(x) \quad (39)$$

$\chi_p(x)$ acts as a smoothing of the particle properties and it determines the smoothness of the spatial variation. The full version of GIMP requires integration over the current support of $\chi_p(x)$, which deforms and rotates according to the deformation of the background grid. To do that, a tracking of the particle shape is mandatory, but in a multi-dimensional problem this could be very difficult to accomplish. Thus, an alternative version of the GIMP is represented by the uniform GIMP (uGIMP), where shear deformation and rotation of the particles are neglected. The uGIMP assumes that the sizes of particles are fixed during the material deformation. In this way, the particle characteristic function, whose support may overlap or leave gaps for very large deformation, is no longer able to satisfy the partition of unity criterion, and, thus, the ability of computing rigid body motion is lost. Therefore, the uGIMP is unable to completely eliminate the *cell-crossing error*.

In the attempt to improve the issues left by the GIMP, the Convected Particle Domain Interpolation technique (CPDI) [SBB11] is proposed. In the CPDI the particle has an initial parallelogram shape and a constant deformation gradient is assumed over the particle domain. This technique is a first-order accurate approximation of the particle domain Ω_p . Even if in the CPDI a more accurate approximation of Ω_p is obtained, the issues of overlaps and gaps are not overcome. Only with the second-order Convected Particle Domain Interpolation (CPDI2) [SBG13], an enhanced CPDI, which provides a second-order approximation of the particle domain, these issues are totally corrected. It is also worth mentioning the Dual Domain Material Point Method (DDMPM) [ZMG11], an alternative technique which is able to definitely eliminate the *cell-crossing error*. Unlike the GIMP or CPDI, the DDMPM does not make use of particle characteristic functions and the issue of tracking the particle domain through the whole simulation is avoided. The essence of this technique relies on the use of modified gradient of the shape function, defined as follows

$$\widehat{\nabla N_I}(\mathbf{x}) = \alpha(\mathbf{x})\nabla N_I(\mathbf{x}) + (1 - \alpha(\mathbf{x}))\widehat{\nabla N_I}(\mathbf{x}) \quad (40)$$

where $\nabla N_I(\mathbf{x})$ is the gradient of the shape function evaluated as in the original MPM, $\widehat{\nabla N_I}(\mathbf{x})$ is the gradient from the node-based calculation as used in FLIP (FLuid-Implicit Particle)[BKR88].

Most MPM codes make use of explicit time integration, due to the ease of the formulation and implementation [SCS94, BBS00, WG08]. Explicit methods are preferable to solve transient problems, such as impact or blast, where high frequencies are excited in the system [SZS95, ZSM06, HZMH11]. However, when only the low-frequency motion is of interest, the adoption of an implicit time scheme may reduce the computational cost in comparison to the employment of an explicit time scheme [ZCL16]. Some implicit versions of MPM can be found in the literature. For instance, Guilkey [GW03] exploits the similarities between MPM and FEM in an implicit solution strategy. Beuth [BWV11] proposes an implicit MPM formulation for quasi-static problems using high order elements and a special integration procedure for partially filled boundary elements. Sanchez [SSSW15] presented an implicit MPM for quasi-static problems using a Jacobian free algorithm and in [CCA17] a GIMP method is used together with an implicit formulation.

It is observed that in the small deformation range the MPM has a lower accuracy and efficiency than a Lagrangian FEM. Nevertheless, the FEM procedure shows its advantageous use only in a narrow range of strain magnitude, established by a critical deformed configuration for which the element quality is seriously compromised, which may cause a drastic deterioration of accuracy or even the end of the computation. In this regard, it is evident that MPM finds its natural field of application in large deformation problems. However, it is important to highlight that an extra computational cost is expected in MPM compared to FEM. This is due to additional steps in the MPM algorithmic procedure, in order to be able to track the kinematic and historical variables through the deformation process, and to a number of *material points* higher than the number of Gauss points normally employed in a FEM simulation.

The MPM is characterized by some features which make this technique able to overcome all the typical disadvantages of other particle methods. MPM does not employ any kind of remeshing procedure, the calculation is performed always at a local level, allowing an easy adaptation of the code to parallel computation and a good conservation of the properties. A conservation of the mass is also guaranteed during the whole simulation time, as the total mass is distributed between the material points representing the volume of the entire continuum under study. A remapping of the state variables is avoided and the employment of complex time dependent constitutive laws can be used without committing any mapping error. In addition, since this technique is a grid-based method all the issues, related to the meshless methods, such as, lack of interpolation consistency and difficulties in enforcing the Essential Boundary conditions are (partially) avoided. Last but not least, MPM is a technique defined in the continuum mechanics framework, thus, it can be easily applied to real scale problems at an acceptable computational cost.

3.1 MPM Algorithm

Traditionally, the MPM is made of three different phases [SZS95], as graphically represented in Figure 2 and below described:

- a) *Initialization phase (Fig.2(a))*: at the beginning of the time step the connectivity is defined for each material points and the initial conditions on the FE grid nodes are created by means of a projection of material points information obtained at the previous time step t_n ;
- b) *UL-FEM calculation phase (Fig.2(b))*: the local elemental matrix, the left-hand-side (*lhs*) and the local elemental force vector, the right-hand-side (*rhs*) are evaluated in the current configuration; the global matrix *LHS* and the global vector *RHS* are obtained by assembling the local contributions of each material point, as in a classical FEM approach, and, finally, the solution system is iteratively solved. During the iterative procedure, the nodes are allowed to move, accordingly to the nodal solution, and the material points do not change their local position within the geometrical element until the solution has reached convergence;
- c) *Convective phase (Fig.2(c))*: the nodal information at time t_{n+1} are interpolated back to the material points. The position of the material points is updated and the undeformed FE grid is recovered.

Many features of the MPM are features of the Finite Element Method [SCS94]. Indeed, phase *b* coincides with the calculation step of a standard non-linear FE code, while phases *a* and *c* are peculiar of the MPM. At the beginning of each time step (t_n), during phase *a*, the degrees of freedom and the variables on the nodes of the fixed mesh are defined gathering the information from the material points (Figure 2(a)).

For the sake of clarity, hereinafter, p and I subscripts are used to refer to variables at-

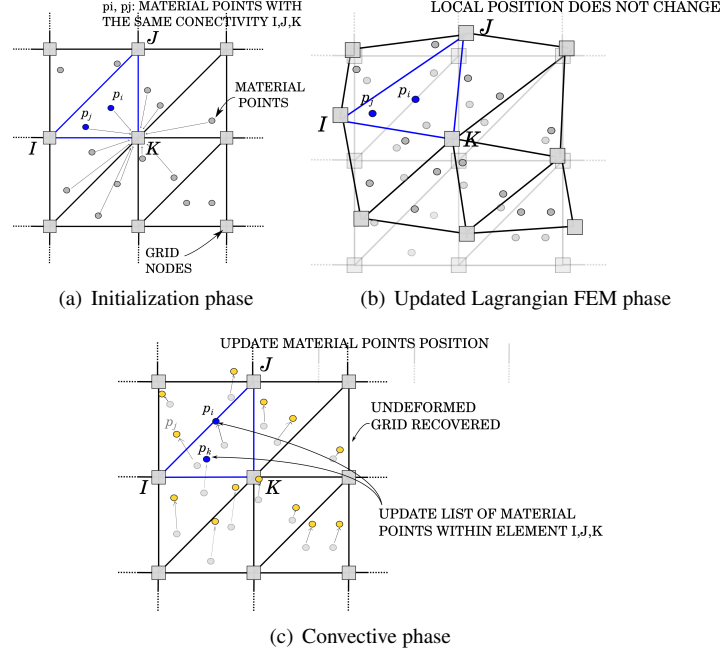


Figure 2: MPM phases.

tributed to material points and computational nodes, respectively, while n superscript refers to the time instance in which the variable is defined. The momentum $\mathbf{q}_p$ and inertia $\mathbf{f}_p$ on the material points, which are expressed as functions of mass m_p , velocity $\mathbf{v}_p$ and acceleration $\mathbf{a}_p$

$$\mathbf{q}_p^n := \mathbf{v}_p^n m_p \quad (41)$$

$$\mathbf{f}_p^n := \mathbf{a}_p^n m_p \quad (42)$$

are projected on the background grid by evaluating in a first step, the global values of mass m_I , momentum $\mathbf{q}_I$ and inertia $\mathbf{f}_I$ on node I as described in Algorithm 1.

Once m_I , $\mathbf{q}_I$ and $\mathbf{f}_I$ are obtained, it is possible to compute the values of nodal velocity $\tilde{\mathbf{v}}_I^n$ and nodal acceleration $\tilde{\mathbf{a}}_I^n$ of the previous time step as

$$\tilde{\mathbf{v}}_I^n = \frac{\mathbf{q}_I^n}{m_I} \quad (43)$$

$$\tilde{\mathbf{a}}_I^n = \frac{\mathbf{f}_I^n}{m_I} \quad (44)$$

It is worth mentioning that, the initial nodal conditions are evaluated at each time step using material point information in order to have initial values even on grid elements empty at the previous time step ($t_{n-1} - t_n$).

The MPM makes use of a predictor/corrector procedure, based on the Newmark integration scheme. The prediction of the nodal displacement, velocity and acceleration reads

$${}^{it+1}\Delta\mathbf{u}_I^{n+1} = 0.0 \quad (45)$$

$${}^{it+1}\mathbf{v}_I^{n+1} = \frac{\lambda}{\zeta\Delta t} [{}^{it+1}\Delta\mathbf{u}_I^{n+1}] - \left(\frac{\lambda}{\zeta} - 1\right) \tilde{\mathbf{v}}_I^n - \frac{\Delta t}{2} \left(\frac{\lambda}{\zeta} - 2\right) \tilde{\mathbf{a}}_I^n \quad (46)$$

$${}^{it+1}\mathbf{a}_I^{n+1} = \frac{1}{\zeta\Delta t^2} [{}^{it+1}\Delta\mathbf{u}_I^{n+1}] - \frac{1}{\zeta\Delta t} \tilde{\mathbf{v}}_I^n - \left(\frac{1}{2\zeta} - 1\right) \tilde{\mathbf{a}}_I^n \quad (47)$$

where the upper-left side index it indicates the iteration counter, while the upper-right index n the time step. λ and ζ are the Newmark's coefficients equal to 0.5 and 0.25, respectively.

Once the nodal velocity and acceleration are predicted (Equations 45-47), the system of linearised governing equations is formulated, as in classic FEM, and the local matrix $\mathbf{K}^{tan}$ and the residual $\mathbf{R}_I$ are evaluated and assembled, respectively (phase b , Figure 2(b)).

The solution in terms of increment of nodal displacement is found iteratively solving the residual-based system. Once the solution ${}^{it+1}\delta\mathbf{u}_I^{n+1}$ is obtained, a correction of the nodal increment of displacement is performed

$${}^{it+1}\Delta\mathbf{u}_I^{n+1} = {}^{it}\Delta\mathbf{u}_I^{n+1} + {}^{it+1}\delta\mathbf{u}_I^{n+1} \quad (48)$$

Velocity and acceleration are corrected according to Equations 46 and 47, respectively. This procedure has to be repeated until convergence is reached.

Unlike a FEM code, the nodal information is available only during the calculation of a time step: at the beginning of each time step a reset of all the nodal information is performed and the accumulated displacement information is deleted. The computational mesh is allowed to deform only during the iterative procedure of a time step, avoiding the typical element tangling of a standard FEM. When convergence is achieved, the position of the nodes is restored to the original one (phase c , Figure 2(c)). Before restoring the undeformed configuration of the FE grid, the solution in terms of nodal displacement, velocity and acceleration is interpolated on the material points, as

$$\Delta\mathbf{u}_p^{n+1} = \sum_{n=1}^{n_n} N_I(\xi_p, \eta_p) \Delta\mathbf{u}_I^{n+1} \quad (49)$$

$$\mathbf{a}_p^{n+1} = \sum_{n=1}^{n_n} N_I(\xi_p, \eta_p) \mathbf{a}_I^{n+1} \quad (50)$$

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \frac{1}{2}\Delta t (\mathbf{a}_p^n + \mathbf{a}_p^{n+1}) \quad (51)$$

where n_n is the total number of nodes per geometrical element, (ξ_p, η_p) are the local coordinates of material point p and $N_I(\xi_p, \eta_p)$ is the shape function evaluated at the position of the material point p , relative to node I .

Finally the current position of the material points is updated as

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta \mathbf{u}_p^{n+1} \quad (52)$$

The details of the MPM algorithm are presented in Algorithm 1.

4 Coupled problems using MPM

Soil-structure interaction (SSI) is important to be studied in the design of various civil engineering structures, such as dams, foundations of skyscrapers, tunnels, and other underground structures. Most of these structures involve direct contact and interaction with the ground, especially in combination with external loads such as wind or earthquakes, the motion of the structure is inherently depending on the grounds motion. The accurate understanding of soil characteristics, geomechanical loads exerted onto the structures, and soil bearing capacity provides important information for the structural design and safety assessment.

The theory and study of SSI within the field of soil mechanics and geotechnical engineering was initiated back in the early 20th century by [Rei36] about vibrational foundations, and since then, has been continuously developed align with the establishment of modern seismic design codes [MG00]. To date, SSI has been widely utilized to predict structural and soil responses, not only during an earthquake but also with respect to other ground-borne vibrations elicited by other sources, such as fast-moving trains. Although a lot of research has been done in this thriving field, with sometimes very impressive results, some of the key issues have not been answered yet in a satisfying way, and thus, making the comprehensive study of SSI remains a challenge [Kau10, LWCZ11]. When superstructures, foundations, and topographic and geological conditions become complicated, e.g. by involving other non-linear effects, such as partial lift-off and multi-phase soil properties, producing a mathematical solution can be extremely difficult. In order to solve such complex SSI problems, numerical simulations may be employed, to investigate the fundamental physics involved in the complex interaction between soil and structures, as analytical solutions are impossible to obtain and laboratory experiments are limited in scope and scale. Recently, particle methods have been utilized extensively to study the SSI phenomena, particularly in the vicinity of problems involving large deformation soil. Discrete approaches, such as the discrete element method (DEM), has been applied to simulate interactions between granular soil flows with rigid or flexible structures [OFdSN⁺04], e.g. by

Algorithm 1 MPM algorithm.Material DATA: E, ν, ρ Initial data on material points: $m_p, \mathbf{x}_p^n, \Delta t, \mathbf{u}_p^n, \mathbf{v}_p^n, \mathbf{a}_p^n, \mathbf{F}_p^n = \sum_I \frac{\partial N_I}{\partial \mathbf{x}_I^0} \cdot \mathbf{x}_I^n$ and

$$\Delta \mathbf{F}_p = \sum_I \frac{\partial N_I}{\partial \mathbf{x}_I^n} \cdot \mathbf{x}_I^{n+1}$$

Initial data on nodes: **NONE - everything is discarded during initialization phase**OUTPUT of calculations: $\Delta \mathbf{u}_I^{n+1}, \sigma_p^{n+1}$ **1. INITIALIZATION PHASE**

- Clear nodal info and recover undeformed grid configuration
- Calculation of initial nodal conditions.
 - (a) for $p = 1:N_p$
 - * Calculation of nodal data
 - $\mathbf{q}_I^n = \sum_p N_I m_p \mathbf{v}_p^n$
 - $\mathbf{f}_I^n = \sum_p N_I m_p \mathbf{a}_p^n$
 - $m_I^n = \sum_p N_I m_p$
 - (b) for $I = 1:N_I$
 - * $\tilde{\mathbf{v}}_I^n = \frac{\mathbf{q}_I^n}{m_I^n}$
 - * $\tilde{\mathbf{a}}_I^n = \frac{\mathbf{f}_I^n}{m_I^n}$
- Newmark method: PREDICTOR. Evaluation of $^{it+1}\Delta \mathbf{u}_I^{n+1}, ^{it+1}\mathbf{v}_I^{n+1}$ and $^{it+1}\mathbf{a}_I^{n+1}$ using Equations (45)–(47)

2. UL-FEM PHASE

- for $p = 1:N_p$
 - (a) Evaluation of local residual (rhs)
 - (b) Evaluation of local Jacobian matrix of residual (lhs)
 - (c) Assemble rhs and lhs to the global vector RHS and global matrix LHS
- Solving system ($\Delta \mathbf{u}_I^{n+1}$)
- Newmark method: CORRECTOR (Equations (46)–(48))
- Check convergence
 - (a) NOT converged: go to Step 2
 - (b) Converged: go to Step 3

3. CONVECTIVE PHASE

- Update the kinematics on the material points by means of an interpolation of nodal information (Equations (49)–(52))
- Save the stress σ_p^{n+1} , strain ϵ_p^{n+1} and total deformation gradient $\mathbf{F}_p^{n+1}$ on material points (the latter by $\mathbf{F}_p^{n+1} = \Delta \mathbf{F}_p \cdot \mathbf{F}_p^n$)

coupling with FEM [TMC13, LROI12, SILO16]. Meanwhile, within the continuum-based approaches, the Smoothed Particle Hydrodynamics (SPH) [BFSO08, AA14] and the Particle Finite Element Method (PFEM) [OCI⁺11, MCAG16] are the two most popular methods for the simulations of complex coupled problems, including the analysis involving the interaction of fluids, soil/rocks, and structures. Within the MPM, the studies for SSI between landslides or avalanches with obstacles and protection structures have been discussed by [MMHAM11, MAMMH14, CBVS16], assuming an explicit formulation. The analysis, furthermore, extended by [CLI⁺19] to the implicit MPM incorporating finite strain assumption and a prediction-correction scheme. The particle methods, including the MPM, allow more accurate and realistic simulations of large deformation in soil, as the traditional FEM will inherently suffer from mesh entanglement and distortion issues.

4.1 MPM-MPM coupling (the "natural" way)

The monolithic SSI approach solves the governing equations for both the soil and the structure simultaneously, within a single solver. This approach produces a larger and more complex tangent matrix, which could be non-symmetric and may require suitable preconditioning to invert. As a result, the monolithic SSI problem will converge as fine as the approximation of the tangent matrix allows, resulting in a very robust solver if it can be done effectively. Disregarding frictional contact MPM-MPM monolithic coupling strategy is naturally present in MPM. In fact MPM simulates multi-materials automatically since no slip, no penetration contact is inherent in MPM. Each material point has its own constitutive law and maps its data to the nodes independently of the other material points in the same elements. Let us make a simple conceptual example looking at Figure 3. We have two materials, the orange (the structure) and the green one (the soil). Each material point is of either the orange or the green material (i.e. with its own constitutive law). There are elements of the background grid which contains only green material points or orange material points, but there are also elements which contains both. These are the interface elements. Let us consider the classical solution system $K\Delta u = -R$ where K is the stiffness matrix, Δu the increment of the unknown calculated in a Newton-Raphson scheme and R is the residual of the governing equations and using the subscripts s , st and Γ for the soil nodes, the structure and the interface nodes, respectively. Setting up the global solution system (in a FEM fashion), we will obtain

$$\begin{pmatrix} K_s & K_{s\Gamma} & 0 \\ K_{\Gamma s} & K_\Gamma & K_{\Gamma st} \\ 0 & K_{st\Gamma} & K_{st} \end{pmatrix} \begin{pmatrix} \Delta u_s \\ \Delta u_\Gamma \\ \Delta u_{st} \end{pmatrix} = - \begin{pmatrix} R_s \\ R_\Gamma \\ R_{st} \end{pmatrix} \quad (53)$$

Nevertheless, often frictional contact plays a relevant role and cannot be omitted. The reader is recommended to see [VSWN19] for a comprehensive literature overview of MPM-MPM monolithic algorithms availables.

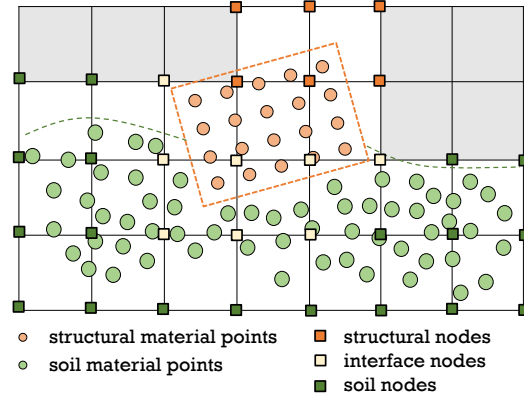


Figure 3: Monolithic coupling in MPM. The concept.

4.2 MPM-FEM coupling, a staggered approach

A staggered, or partitioned, coupling strategy intends to solve a coupled problem, defined by two fields or subsystems, which are represented by a certain mathematical model, with possible different discretization, formulations, and algorithms. The partitioned approach can be: *one-way* and *two-way* coupling. The one-way coupling methods provide a possibility to reduce the computational effort by only passing the coupling variables from one system to another (and not vice versa) at every calculation step. On the other hand, the two-way coupling approach transfers the coupling variables back to the first subsystem as an additional "feedback step". In other words the two systems are mutually influenced by each other. The two-way coupling schemes are further divided into weakly and strongly coupled approaches, where the convergence at the interface between the coupled systems is, respectively, neglected or considered. The different approaches are illustrated in the following Figure 4.

4.2.1 Boundary conditions on non matching meshes

Having to deal with bodies that move and deform over a fixed mesh, we often need to impose boundary conditions on a surface or line which does not match with the background grid (Figure 5).

This common issue is even more important in the case of coupled problems. In this case, in fact, the accurate imposition of the coupling variables on the shared interface is crucial during the whole simulation. This open issue is a well known problem in the community of unfitted methods for Computational Fluid Dynamics (CFD) [CB09, UGF14, MSW18, WSMW18, ZLR19]. The MPM community proposed several alternative solutions to this problem: one possibility is to move the background fixed mesh according to the material displacements and deformation [aK13, WCA⁺17, CBVS16].

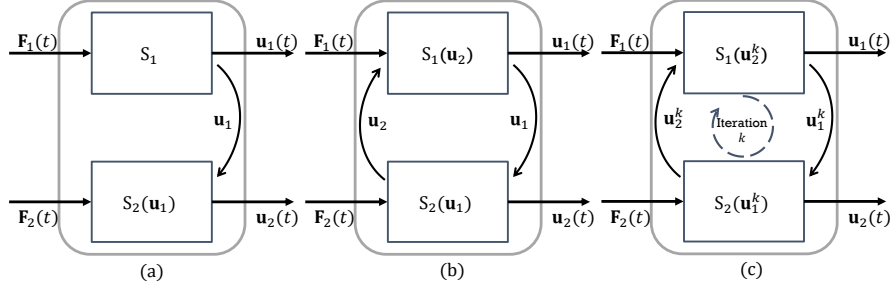


Figure 4: Staggered coupling strategy for two subsystems S_1 and S_2 : (a) one-way coupling, (b) two-way "weak" coupling, and (c) two-way "strong" coupling.

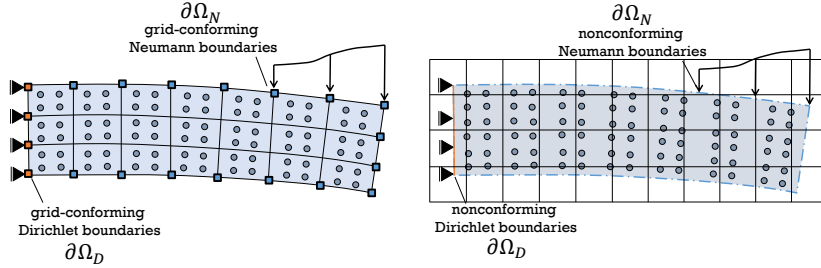


Figure 5: Grid conforming(a) and non conforming (b) boundaries (source [CST⁺20]).

While this approach ensures that the interface is always matching with the background grid, its accuracy strongly depends on the shape of the boundary and on its deformation and it generates numerical noise due to the cell-crossing instabilities [GBC⁺17]. An alternative is to impose the boundary condition directly on the particles either creating a layer of mass-less particles or using the boundary particles of the given body [Beu12]. The problem in this case is that the boundary conditions are not applied on the boundary but on a "band" [Beu12], [aK13].

Mast et al. [MMHAM11] proposed a dual-grid approach. They introduce an additional grid which follows the geometry of the material boundary. Unfortunately this approach seems to be problematic even for simple 1D problems, since it is sensitive to different boundary cell size and location [BCC⁺19].

An interesting alternative is represented by the use of a boundary detection algorithm using the Proximity Field Method (PFM). However, the PFM approach is computationally expensive, highly mesh dependent, and its accuracy, at the moment, is still questionable [RVHA17].

Finally, Bing and coworkers have proposed a more general way to track the evolution of physical boundary by utilizing a cubic B-spline interpolation method [Bin17, CCA⁺18, BCC⁺19]. The integration of surface traction for Neumann boundary can be done directly along the B-spline surface by incorporating Gauss quadrature. The B-spline surface can also be combined with a Dirichlet boundary imposition using the Implicit Boundary Method (IBM) inherited from FEM [BK08, KBPG08, KPB08, ZK17]. IBM has been proven to be suitable for imposing homogeneous and non-homogeneous Dirichlet boundary conditions for 2D quasi-static linear-elastic problems in MPM with structured quadrilateral elements [Bin17, CCA⁺18, BCC⁺19]. Yet, so far, implementation for 3D cases, with unstructured background mesh, and for nonlinear dynamic problems involving elasto-plastic materials are not yet presented.

We conclude presenting a last alternative, which is the one we developed in Kratos Multiphysics. We use a penalty approach for the imposition of Dirichlet boundary conditions. Penalty formulation is widely used by the FEM community to impose constraint conditions [BZ73], as well as in isogeometric B-Rep analysis (IBRA) [BAP⁺15, TBO⁺18] to couple boundary conditions between patches. Penalty has also been used in meshfree methods [ZA98, AZ00, FMH04] and other continuum based methods, such as in the CutFEM [BCH⁺15] and the finite cell methods (FCM) [SRZ⁺12]. The adaption of the penalty method to MPM is briefly presented in what follows. The reader is recommended to consult [CST⁺20] for more details.

The penalty augmentation is adopted using boundary particles, which can be fixed or can move not only according to the material deformation, but also following prescribed field values, independently from the deformation.

Let us assume two coupling boundary edges Γ_1 and Γ_2 , which can be discretized by using any methods, e.g. as surface meshes, B-spline surfaces, or even as particles. Each of the boundary edge contains a corresponding displacement field $\mathbf{u}_1 = \mathbf{u}_1(\mathbf{x}_1)$ and $\mathbf{u}_2 = \mathbf{u}_2(\mathbf{x}_2)$, respectively. We can therefore define the following virtual work statement:

$$\begin{aligned} \delta W^{\text{penalty}} &= \beta \int_{\Gamma_1} (\mathbf{u}_1 - \mathbf{u}_2) \cdot (\delta \mathbf{u}_1 - \delta \mathbf{u}_2) d\Gamma_1, \\ &= \beta \int_{\Gamma_2} (\mathbf{u}_2 - \mathbf{u}_1) \cdot (\delta \mathbf{u}_2 - \delta \mathbf{u}_1) d\Gamma_2, \end{aligned} \quad (54)$$

where β is the user-defined penalty factor. Here, $\delta W^{\text{penalty}}$ corresponds to the coupling between the displacement (i.e the position) of two coupling surfaces, written in a weak sense.

The modified system of equations can be written as:

$$(\mathbf{K}^{\text{tan}} + \mathbf{K}^{\text{penalty}}) \Delta \mathbf{u} = -(\mathbf{R} + \mathbf{R}^{\text{penalty}}), \quad (55)$$

where $\mathbf{K}^{\text{tan}}$ and $\mathbf{R}$ are the regular local tangent stiffness matrix and residual vector. The additional penalty terms in the system matrix is given as:

$$\mathbf{K}^{\text{penalty}} = \beta \int_{\Gamma_D} \mathbf{H}^T \cdot \mathbf{H} d\Gamma_D, \quad (56)$$

while the additional residual term is:

$$\begin{aligned}
 \mathbf{R}^{\text{penalty}} &= \beta \int_{\Gamma_D} \mathbf{H}^T \cdot (\mathbf{u} - \bar{\mathbf{u}}) \, d\Gamma_D \\
 &= \left[\beta \int_{\Gamma_D} \mathbf{H}^T \cdot \mathbf{H} \, d\Gamma_D \right] (\mathbf{u}_I - \bar{\mathbf{u}}_I) \\
 &= \mathbf{K}^{\text{penalty}} (\mathbf{u}_I - \bar{\mathbf{u}}_I)
 \end{aligned} \tag{57}$$

with matrix $\mathbf{H}$ is defined as follow:

$$\mathbf{H} = \begin{bmatrix} N_1 & 0 & 0 & \cdots & N_{nel} & 0 & 0 \\ 0 & N_1 & 0 & \cdots & 0 & N_{nel} & 0 \\ 0 & 0 & N_1 & \cdots & 0 & 0 & N_{nel} \end{bmatrix}. \tag{58}$$

Here, the subscript *nel* denotes the number of nodes for each element.

4.3 Granular flow impacting on an obstacle

4.3.1 The model

A two-dimensional numerical simulation to analyze the soil-structure interaction coupling schemes is presented. A granular column collapse is impacting on a structural obstacle with a purpose to block the soil run-out as illustrated in figure 6. In the present study, two types of materials are considered; one is a concrete-like structure, which will be referred as 'stiff' from here on, with a linear-elastic behaviour, and the other is a 'flexible' hyper-elastic rubber-like material assuming a neo-Hookean model. In order to check the simulation performance, a measurement point "A" is selected to measure the structural displacement upon the soil impact. The material data used to simulate the structural obstacle is specified in table 1, while the soil model is considered to be the same material as in table 2.

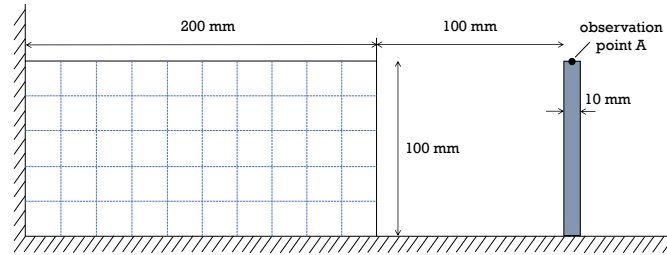


Figure 6: Granular flow simulations with an obstacle: Initial geometry.

4.3.2 Monolithic Coupling by Implicit MPM

A mesh sensitivity analysis is carried out to understand how the mesh refinement affects the obtained coupling results. The SSI simulation is first conducted in a mono-

Table 1: Granular flow simulations with an obstacle: Material data of the structure.

Case	Material type	Density [kg/m ³]	Young's Mod [MPa]	Poisson's Ratio
a)	Concrete-like (stiff)	2550	3×10^4	0.3
b)	Rubber-like (flexible)	1100	1	0.0

Table 2: Granular flow validation: Material data.

Material density [kg/m ³]	Young's modulus [kPa]	Poisson's ratio	Angle of internal friction °	Cohesion	Dilatancy angle °
2650	840	0.3	19.8	0.0	0.0

lithic way by using solely the implicit MPM-MPM. Here, three mesh sizes are tested: $h = 5, 2.5, 2$ mm for the two structural cases, with 3 MP/cell are assumed in each simulation. The details of the simulation setup are listed in details in table 3.

Table 3: Granular flow simulations with an obstacle: Mesh and material point setup for convergence studies.

Case No	MP/cell	Mesh size [m]	MPs	Cells	Nodes	Time step
1	3	0.005	5040	7200	4611	2×10^{-4}
2	3	0.0025	20160	28800	18101	2.5×10^{-5}
3*	3	0.002	31500	45150	28252	2×10^{-5}

* Default case

Figure 7 and 8 present the mesh convergence analysis in the monolithic coupling. Here, the horizontal displacement at point "A" is compared for both the stiff (case a) and the flexible (case b) structure. As the displacement of the stiff structures is significantly small (figure 7), i.e. in the order of 10^{-7} , it is hard to compare them and recognize the tendency. However, if we focus at the later end of the plot, where the vibrations almost reach their steady state, approximately at $t = 1.0$ s, we can see the slight increasing pattern from the three different discretizations. Meanwhile, the displacement results of the flexible structures (figure 8) clearly showed a very good increasing tendency as the meshes are refined, and according to the results, the highest amplitude of the displacement may converge at some value around 0.008. One more thing which can be noticed while comparing the two figures are the comparisons of the magnitude of both displacement results. Since the stiff structure's Young's modulus is around 10^4 times larger than the flexible one, the order of the response displacements obtained is 10^{-4} times smaller than the flexible one. These provided us a good assurance that the constitutive laws are formulated well. All in all, by seeing

these results, it can be verified that our monolithic coupling formulation is able to reach a converging tendency upon mesh refinement.

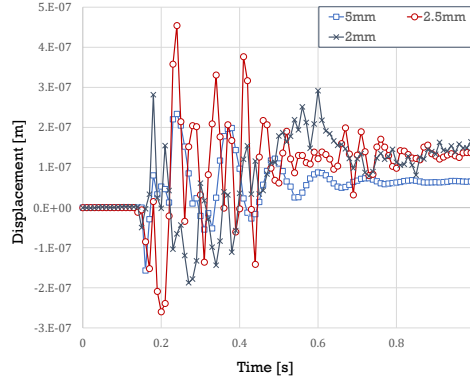


Figure 7: Granular flow simulations with an obstacle: Displacement of stiff structure (case a) at observation point "A" for three different mesh sizes assuming monolithic coupling.

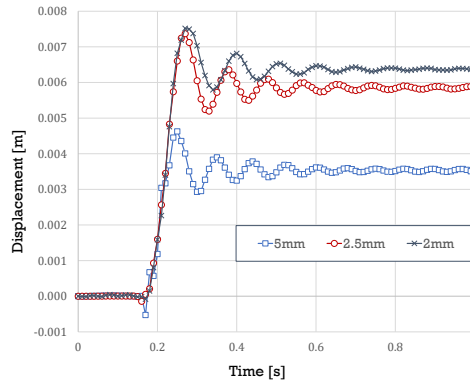


Figure 8: Granular flow simulations with an obstacle: Displacement of flexible structure (case b) at observation point "A" for three different mesh sizes assuming monolithic coupling.

Next, the following figure 9 and 10 present the final deformed configuration and the Cauchy stress measured at $t = 1.0$ s for the default case ($h = 0.002$ m). As can be noticed the earlier figure, the deformation of the more flexible structure is clearly seen and larger than the stiffer structure. Moreover, the Cauchy stress profile along the lateral direction shows a physical and realistic bending stress profile.

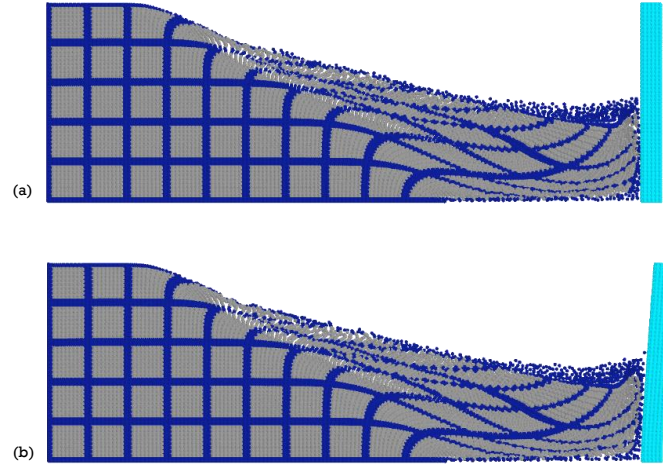


Figure 9: Granular flow simulations with an obstacle: Deformed configuration at $t = 1.0$ s of the monolithic SSI tests with (a) stiff and (b) flexible structure.

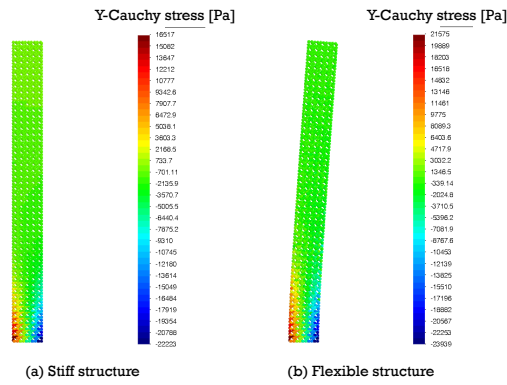


Figure 10: Granular flow simulations with an obstacle: Stress profile of the structure at final configuration $t = 1.0$ s: (a) stiff and (b) flexible structure.

The monolithic SSI coupling by using the implicit MPM shows a very good mesh convergence as the background grids are refined. It is also very robust as the equilibrium of forces and kinematic continuity are directly satisfied after the linear system of equation for soil and structure are solved simultaneously. However, the "natural" monolithic formulation directly assumes a sticking contact at the soil and structural

interface, as the kinematic variables at the interface material points are interpolated by the same nodal variables by using the same shape functions. The sticking contact, here, may result in a stiffer deformation of the structure, as when it moves away from the soil, the soil will exert a pulling force to the structure by means of the sticking contact condition. This, furthermore, causes a numerical damping effect to the structure as it vibrates, which can be noticed clearly from the vibration pattern showed by figure 8.

4.3.3 Staggered Coupling Using Coupled MPM-FEM

Using the staggered coupling of MPM with FEM a similar model is constructed by using the nonconforming fixed boundaries and SSI interface by means of penalty methods. The initial geometry for the staggered MPM-FEM coupling can be seen in figure 11. In this validation, only the flexible structure, case b in table 1, will be considered since the displacement of this structure is significantly larger than the stiffer one, and therefore, it is able to validate the performance of the implemented inhomogeneous Dirichlet imposition along the structural boundaries better. Moreover, we only perform tests with $h = 0.005, 0.0025$ m, as the deformation differences of the $h = 0.0025$ m and $h = 0.002$ m cases are not that significant as shown by the monolithic case.

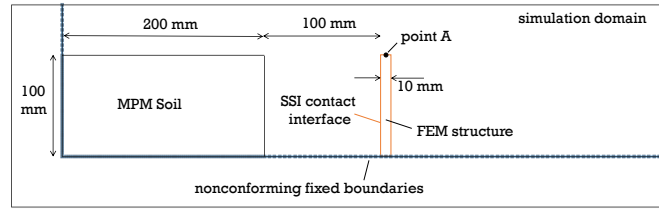


Figure 11: Granular flow simulations with an obstacle: Initial geometry for staggered MPM-FEM coupling.

The staggered coupling simulations are performed considering a strongly coupled formulation, where a series of iteration is performed to reach a certain convergence of Dirichlet and Neumann conditions at the soil-structure interface. For the MPM simulations, structured triangular meshes are used to generate particles, as such that the initial arrangement is the same with the monolithic case with $MP/cell = 3$. Meanwhile, unstructured triangular background grids are used to perform the MPM computations. As can be seen from figure 11, a nonconforming fixed boundary is assumed to impose the left and bottom walls. Here, we assume the penalty factor $\omega = 10^{11}$. The reason that the nonconforming boundaries are preferred here, instead of the fixed grid-conforming boundaries, is mainly because the bottom wall is intersecting with another penalty-based imposition, which is the SSI interface (marked by orange lines in figure 11).

Table 4 listed all the simulation setups including the chosen penalty factors for the

Table 4: Granular flow simulations with an obstacle: MPM and FEM mesh arrangement.

Case No	Mesh size [m]	Implicit MPM			FEM		Time Step
		MPs	Cells	Penalty	Elements	Nodes	
1	0.005	4800	12,094	2×10^8	121	63	2×10^{-4}
2	0.0025	19200	24,573	3.8×10^9	401	205	2.5×10^{-5}

SSI coupling interface. Here, the value of the interface penalty factors can be chosen differently than the one used to impose the left and bottom walls. These interface penalty factors will be used to impose the structural displacement in the MPM system, and to approximate the contact forces which will be sent back to the FEM as external loads. The value of these penalty factors should be initially calibrated to eliminate interpenetration of the particles to the SSI interface, and as can be noticed from table 4, the value for different mesh resolution is generally different to each other, though showing the same tendency to the increase or decrease of resolution. However, if the value is set too high, the contact force may be over-estimated, which may lead to local element inversion in the FEM system or cause further stability issue in the MPM-FEM coupling loop. Moreover, as the approximated penalty forces are often over-estimated at the first coupling iteration, a relaxation method based on the multi-vector update quasi-Newton (MVQN) approach [BKR14] is assumed in this case. Last but not least, for the strong coupling iteration settings, the maximum coupling iteration is set to be 20, and both of the absolute and relative tolerances are set to be 10^{-5} .

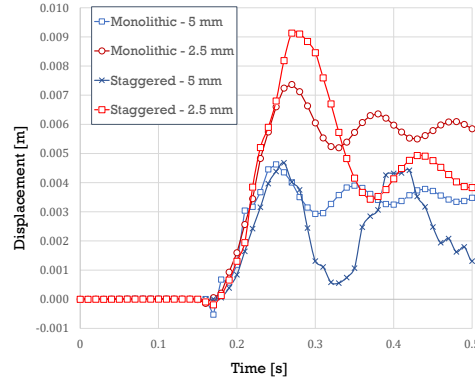


Figure 12: Granular flow simulations with an obstacle: Comparison of displacement of flexible structure at point "A" upon impact between the monolithic and staggered SSI coupling.

Figure 12 shows the comparisons of lateral displacement obtained at the observation

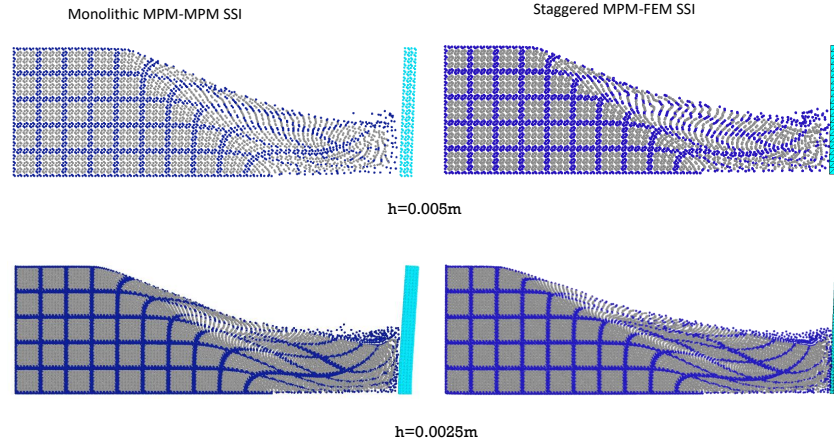


Figure 13: Granular flow simulations with an obstacle: Comparisons of deformed configuration at $t = 0.5$ s between the monolithic MPM-MPM and staggered MPM-FEM SSI tests: (left) monolithic , (right) staggered, (upper) $h = 0.005$ m, (lower) $h = 0.0025$ m

point A for the monolithic and staggered SSI coupling, while figure 13 shows the deformed configuration at $t = 0.5$. In general, the staggered simulations are showing a good tendency and physical deformation, as can be compared with the results of monolithic cases. There are, however, two consideration that it is worth making.

First, the displacement of the staggered simulations, in particular for $h = 0.0025$ m, reaches a higher peak than the monolithic counterpart, even though at the latter end of the simulation the displacement shows a lower tendency. Moreover, the staggered SSI displacements also vibrate with higher amplitude and longer period. These differences are mostly caused by the different "contact" conditions assumed. The monolithic approach, by default, considers a non-slip and sticking contact, where pulling forces are also exerted from soil to structure and vice versa when the separation between them occurs. This assumption is, as expected, non-physical. The staggered approach, on the contrary, assumes an appropriate contact condition, i.e. the coupling is skipped when the gap computed shows a positive value, which indicates separation. The soil and the structure are free to separate from each other. This is one of the main reasons why the staggered simulations show a higher peak during impact.

Secondly, notice that the aforementioned different contact assumptions between the monolithic and staggered approaches may lead to a different deformed configuration as shown by figure 13. There, notice two important differences:

1. The staggered simulations (pictures on the left) show a closer gap between the soil and the structure, than the monolithic results (pictures on the right);

2. At the upper-left region of each picture, the staggered simulations are able to mobilize more mass than the monolithic simulations with the same mesh size.

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References

- [AA10] S. Andersen and L. Andersen. Modelling of landslides with the material point method. *Computational Geosciences*, 14(1):137–147, 2010.
- [AA14] Abdelraheem M Aly and Mitsuteru Asai. Incompressible smoothed particle hydrodynamics simulations of fluid-structure interaction on free surface flows. *International Journal of Fluid Mechanics Research*, 41(6), 2014.
- [aK13] Issam KJ al Kafaji. *Formulation of a dynamic material point method (MPM) for geomechanical problems*. PhD thesis, University of Stuttgart, 2013.
- [AZ00] SN Atluri and T-L Zhu. The meshless local Petrov-Galerkin (MLPG) approach for solving problems in elasto-statics. *Computational Mechanics*, 25(2-3):169–179, 2000.
- [BAP⁺15] M Breitenberger, A Apostolatos, B Philipp, R Wüchner, and K-U Bletzinger. Analysis in computer aided design: Nonlinear isogeometric b-rep analysis of shell structures. *Computer Methods in Applied Mechanics and Engineering*, 284:401–457, 2015.
- [BBS00] S.G. Bardenhagen, J.U. Brackbill, and D. Sulsky. The material-point method for granular materials. *Computer Methods in Applied Mechanics and Engineering*, 187(3-4):529–541, 2000.
- [BCC⁺19] Y Bing, M Cortis, TJ Charlton, WM Coombs, and CE Augarde. B-spline based boundary conditions in the material point method. *Computers & Structures*, 212:257–274, 2019.
- [BCH⁺15] Erik Burman, Susanne Claus, Peter Hansbo, Mats G Larson, and André Massing. CutFEM: discretizing geometry and partial differential equations. *International Journal for Numerical Methods in Engineering*, 104(7):472–501, 2015.

- [Beu12] Lars Beuth. *Formulation and application of a quasi-static material point method*. PhD thesis, University of Stuttgart, 2012.
- [BFSO08] H. H. Bui, R. Fukagawa, K. Sako, and S. Ohno. Lagrangian mesh-free particles method (sph) for large deformation and failure flows of geomaterial using elastic-plastic soil constitutive model. *International Journal for Numerical and Analytical Methods in Geomechanics*, 32(12):1537–1570, 2008.
- [Bin17] Yun Bing. *B-spline based boundary method for the material point method*. PhD thesis, Durham University, 2017.
- [BK04] S.G. Bardenhagen and E.M. Kober. The generalized interpolation material point method. *CMES - Computer Modeling in Engineering and Sciences*, 5(6):477–495, 2004.
- [BK08] Ravi K Burla and Ashok V Kumar. Implicit boundary method for analysis using uniform B-spline basis and structured grid. *International journal for numerical methods in engineering*, 76(13):1993–2028, 2008.
- [BKR88] J.U. Brackbill, D.B. Kothe, and H.M. Ruppel. Flip: A low-dissipation, particle-in-cell method for fluid flow. *Computer Physics Communications*, 48(1):25 – 38, 1988.
- [BKR14] Alfred EJ Bogaers, Schalk Kok, B Dayanand Reddy, and Thierry Franz. Quasi-newton methods for implicit black-box fsi coupling. *Computer Methods in Applied Mechanics and Engineering*, 279:113–132, 2014.
- [BWV11] L. Beuth, Z. Wiecewski, and P.A. Vermeer. Solution of quasi-static large-strain problems by the material point method. *International Journal for Numerical and Analytical Methods in Geomechanics*, 35(13):1451–1465, 2011.
- [BZ73] Ivo Babuška and Miloš Zlámal. Nonconforming elements in the finite element method with penalty. *SIAM Journal on Numerical Analysis*, 10(5):863–875, 1973.
- [CB09] R. Codina and J. Baiges. Approximate imposition of boundary conditions in immersed boundary methods. *International Journal for Numerical Methods in Engineering*, 80(11):1379–1405, 2009.
- [CBVS16] Francesca Ceccato, Lars Beuth, Pieter A Vermeer, and Paolo Simonini. Two-phase material point method applied to the study of cone penetration. *Computers and Geotechnics*, 80:440–452, 2016.
- [CCA17] Tim Charlton, William Coombs, and Charles Augarde. igimp: An implicit generalised interpolation material point method for large deformations. *Computers & Structures*, 190:108–125, 10 2017.

- [CCA⁺18] Michael Cortis, William Coombs, Charles Augarde, Michael Brown, Andrew Brennan, and Scott Robinson. Imposition of essential boundary conditions in the material point method. *International Journal for Numerical Methods in Engineering*, 113(1):130–152, 2018.
- [CDA07] Johan Clausen, Lars Damkilde, and Lars Andersen. An efficient return algorithm for non-associated plasticity with linear yield criteria in principal stress space. *Computers & Structures*, 85(23-24):1795–1807, 2007.
- [CLI⁺19] Bodhinanda Chandra, Antonia Larese, Ilaria Iaconeta, Riccardo Rossi, and Roland Wüchner. Soil-structure interaction simulation of landslides impacting a structure using an implicit material point method. *Proceedings of the 2nd International Conference on the Material Point Method for Modelling Soil-Water-Structure Interaction*, Cambridge, UK, pages 72–78, 2019.
- [CST⁺20] Bodhinanda Chandra, Veronika Singer, Tobias Teschemacher, Roland Wuechner, and Antonia Larese. Nonconforming Dirichlet boundary conditions in Implicit Material Point Method by means of penalty augmentation. *Submitted to Acta Geotechnica*, 2020.
- [DRO10] P. Dadvand, R. Rossi, and E. Oñate. An object-oriented environment for developing finite element codes for multi-disciplinary applications. *Archives of Computational Methods in Engineering*, 17:253–297, 2010.
- [dSNPDO96] E.A. de Souza Neto, D. Perič, M. Dutko, and D.R.J. Owen. Design of simple low order finite elements for large strain analysis of nearly incompressible solids. *International Journal of Solids and Structures*, 33(20):3277 – 3296, 1996.
- [FMH04] Sonia Fernández-Méndez and Antonio Huerta. Imposing essential boundary conditions in mesh-free methods. *Computer Methods in Applied Mechanics and Engineering*, 193(12-14):1257–1275, 2004.
- [GBC⁺17] Vahid Galavi, Lars Beuth, Bruno Zuada Coelho, Faraz S Tehrani, Paul Hölscher, and Frits Van Tol. Numerical simulation of pile installation in saturated sand using material point method. *Procedia Engineering*, 175:72–79, 2017.
- [GW03] J. E. Guilkey and J. A. Weiss. Implicit time integration for the material point method: Quantitative and algorithmic comparisons with the finite element method. *International Journal for Numerical Methods in Engineering*, 57(9):1323–1338, 2003.
- [Har64] FH Harlow. The particle-in-cell computing method for fluid dynamics. *Methods for Computational Physics*, 3:319–343, 1964.

- [Hug80] Thomas J. R. Hughes. Generalization of selective integration procedures to anisotropic and nonlinear media. *International Journal for Numerical Methods in Engineering*, 15(9):1413–1418, 1980.
- [HXQ⁺09] Patrick Hu, Liping Xue, Kun Qu, Kan Ni, and Martin Brenner. *Unified Solver for Modeling and Simulation of Nonlinear Aeroelasticity and Fluid-Structure Interactions*. 2009.
- [HZMH11] P. Huang, X. Zhang, S. Ma, and X. Huang. Contact algorithms for the material point method in impact and penetration simulation. *International Journal for Numerical Methods in Engineering*, 85(4):498–517, 2011.
- [Iac19] I. Iaconeta. *A Discrete-continuum hybrid modelling of flowing and static regimes*. 2019.
- [Kau10] Eduardo Kausel. Early history of soil–structure interaction. *Soil Dynamics and Earthquake Engineering*, 30(9):822–832, 2010.
- [KBPG08] Ashok V Kumar, Ravi Burla, Sanjeev Padmanabhan, and Linxia Gu. Finite element analysis using nonconforming mesh. *Journal of Computing and Information Science in Engineering*, 8(3):031005, 2008.
- [KPB08] Ashok V Kumar, Sanjeev Padmanabhan, and Ravi Burla. Implicit boundary method for finite element analysis using non-conforming mesh or grid. *International Journal for Numerical Methods in Engineering*, 74(9):1421–1447, 2008.
- [LROI12] A. Larese, R. Rossi, E. Oñate, and S.R. Idelsohn. A coupled PFEM-Eulerian approach for the solution of porous FSI problems. *Computational Mechanics*, 50 (6):805–819, 2012.
- [LWCZ11] Menglin Lou, Huaifeng Wang, Xi Chen, and Yongmei Zhai. Structure–soil–structure interaction: Literature review. *Soil Dynamics and Earthquake Engineering*, 31(12):1724–1731, 2011.
- [MAMMH14] Carter M. Mast, Pedro Arduino, Gregory R. Miller, and Peter Mackenzie-Helnwein. Avalanche and landslide simulation using the material point method: flow dynamics and force interaction with structures. *Computational Geosciences*, pages 817–830, 2014.
- [Mas13] Carter M. Mast. *Modeling Landslide-Induced Flow Interactions with Structures using the Material Point Method*. PhD thesis, University of Washington, 2013.
- [MCAG16] Lluís Monforte, Josep Maria Carbonell, Marcos Arroyo, and Antonio Gens. Performance of mixed formulations for the particle finite element method in soil mechanics problems. *Computational Particle Mechanics*, pages 1–16, 2016.

- [MG00] George Mylonakis and George Gazetas. Seismic soil-structure interaction: beneficial or detrimental? *Journal of Earthquake Engineering*, 4(3):277–301, 2000.
- [MMHAM11] Carter M Mast, Peter Mackenzie-Helnwein, Pedro Arduino, and Gregory R Miller. Landslide and debris flow-induced static and dynamic loads on protective structures. In *Multiscale and Multiphysics Processes in Geomechanics*, pages 169–172. Springer, 2011.
- [MOS90] B. Moran, M. Ortiz, and C. F. Shih. Formulation of implicit finite element methods for multiplicative finite deformation plasticity. *International Journal for Numerical Methods in Engineering*, 29(3):483–514, 1990.
- [MSW18] A. Massing, B. Schott, and W.A. Wall. A stabilized Nitsche cut finite element method for the Oseen problem. *Computer Methods in Applied Mechanics and Engineering*, 328:262–300, 2018.
- [OBHC15] A. Ortiz-Bernardin, J.S. Hale, and C.J. Cyron. Volume-averaged nodal projection method for nearly-incompressible elasticity using meshfree and bubble basis functions. *Comput. Methods Appl. Mech. Engrg*, 285:427–451, 2015.
- [OCI⁺11] E. Oñate, M.A. Celigueta, S.R. Idelsohn, F. Salazar, and B. Suarez. Possibilities of the particle finite element method for fluid-soil-structure interaction problems. *Journal of Computational Mechanics*, 48:307–318, 2011.
- [OFdSN⁺04] DRJ Owen, YT Feng, EA de Souza Neto, MG Cottrell, F Wang, FM Andrade Pires, and J Yu. The modelling of multi-fracturing solids and particulate media. *International Journal for Numerical Methods in Engineering*, 60(1):317–339, 2004.
- [Rei36] Erich Reissner. Stationäre, axialsymmetrische, durch eine schüttelnde masse erregte schwingungen eines homogenen elastischen halbraumes. *Archive of Applied Mechanics*, 7(6):381–396, 1936.
- [RS95] B.D. Reddy and J.C. Simo. Stability and convergence of a class of enhanced strain methods. *SIAM Journal on Numerical Analysis*, 32:1705–1728, 1995.
- [RVHA17] Guido Remmerswaal, PJ Vardon, MA Hicks, and JL Gonzalez Acosta. Development and implementation of moving boundary conditions in the Material Point Method. *ALERT Geomaterials*, page 28, 2017.
- [SA92] J. C. Simo and F. Armero. Geometrically non-linear enhanced strain mixed methods and the method of incompatible modes. *International Journal for Numerical Methods in Engineering*, 33(7):1413–1449, 1992.

- [SAY⁺15] Kenichi Soga, E. Alonso, Alba Yerro, K. Kumar, and Samila Bandara. Trends in large-deformation analysis of landslide mass movements with particular emphasis on the material point method. *Geotechnique*, 66:1–26, 11 2015.
- [SBB11] A. Sadeghirad, R. Brannon, and J. Burghardt. A convected particle domain interpolation technique to extend applicability of the material point method for problems involving massive deformations. *Int. J. Numer. Meth. Eng.*, 86(12):1435–1456, 2011.
- [SBG13] A. Sadeghirad, R.M. Brannon, and J.E. Guilkey. Second-order convected particle domain interpolation (cpdi2) with enrichment for weak discontinuities at material interfaces. *International Journal for Numerical Methods in Engineering*, 95(11):928–952, 2013.
- [SCS94] D. Sulsky, Z. Chen, and H.L. Schreyer. A particle method for history-dependent materials. *Computer Methods in Applied Mechanics and Engineering*, 118(1-2):179–196, 1994.
- [SILO16] F. Salazar, J. Irazabal, A. Larese, and E. Oñate. Numerical modelling of landslide-generated waves with the particle finite element method (PFEM) and a non-Newtonian flow model. *International Journal for Numerical and Analytical Methods in Geomechanics*, 40:809–926, 2016.
- [SR90] J. C. Simo and M. S. Rifai. A class of mixed assumed strain methods and the method of incompatible modes. *International Journal for Numerical Methods in Engineering*, 29(8):1595–1638, 1990.
- [SRZ⁺12] Dominik Schillinger, Martin Ruess, Nils Zander, Yuri Bazilevs, Alexander Düster, and Ernst Rank. Small and large deformation analysis with the p- and B-spline versions of the Finite Cell Method. *Computational Mechanics*, 50(4):445–478, 2012.
- [SS15] WT Sołowski and SW Sloan. Evaluation of material point method for use in geotechnics. *International Journal for Numerical and Analytical Methods in Geomechanics*, 39(7):685–701, 2015.
- [SSSW15] J. Sanchez, H. Schreyer, D. Sulsky, and P. Wallstedt. Solving quasi-static equations with the material-point method. *International Journal for Numerical Methods in Engineering*, 103(1):60–78, 2015.
- [SZS95] Deborah Sulsky, Shi-Jian Zhou, and Howard L. Schreyer. Application of a particle-in-cell method to solid mechanics. *Computer Physics Communications*, 87(1-2):236–252, 1995.
- [TBO⁺18] Tobias Teschemacher, AM Bauer, Thomas Oberbichler, Micheal Breitenberger, Riccardo Rossi, Roland Wüchner, and K-U Bletzinger. Realization of cad-integrated shell simulation based on isogeometric b-

- rep analysis. *Advanced Modeling and Simulation in Engineering Sciences*, 5(1):19, 2018.
- [TBW76] Robert L. Taylor, Peter J. Beresford, and Edward L. Wilson. A non-conforming element for stress analysis. *International Journal for Numerical Methods in Engineering*, 10(6):1211–1219, 1976.
- [TMC13] VDH Tran, MA Meguid, and LE Chouinard. A finite–discrete element framework for the 3d modeling of geogrid–soil interaction under pullout loading conditions. *Geotextiles and Geomembranes*, 37:1–9, 2013.
- [UGF14] J.M. Urquiza, A. Garon, and M.-I. Farinas. Weak imposition of the slip boundary condition on curved boundaries for stokes flow. *Journal of Computational Physics*, 256:748–767, 2014.
- [VSWN19] Alban de Vaucorbeil, Sina Sinaie, Jian-Ying Wu, and Vinh Phu Nguyen. *Advances in Applied Mechanics*, volume 53, chapter Material point method after 25 years: theory, implementation and applications. Elsevier, 1st edition, 10 2019.
- [WCA⁺17] Lei Wang, William M Coombs, Charles E Augarde, Michael Brown, Jonathan Knappett, Andrew Brennan, David Richards, and Anthony Blake. Modelling screwpile installation using the mpm. *Procedia Engineering*, 175:124–132, 2017.
- [WG08] P. C. Wallstedt and J. E. Guilkey. An evaluation of explicit time integration schemes for use with the generalized interpolation material point method. *Journal of Computational Physics*, 227(22):9628–9642, 2008.
- [Wie04] Z. Wieckowski. The material point method in large strain engineering problems. *Computer Methods in Applied Mechanics and Engineering*, 193(39-41):4417–4438, 2004.
- [Wri06] P. Wriggers. *Computational Contact Mechanics*. Springer, 2006.
- [Wri08] Peter Wriggers. *Nonlinear finite element methods*. Springer Science & Business Media, 2008.
- [WSMW18] M. Winter, B. Schott, A. Massing, and W.A. Wall. A Nitsche cut finite element method for the Oseen problem with general Navier boundary conditions. *Computer Methods in Applied Mechanics and Engineering*, 330:220–252, 2018.
- [WVHC16] B. Wang, P.J. Vardon, M.A. Hicks, and Z. Chen. Development of an implicit material point method for geotechnical applications. *Computers and Geotechnics*, 71:159 – 167, 2016.
- [YAP15] A. Yerro, E.E. Alonso, and N.M. Pinyol. The material point method for unsaturated soils. *Géotechnique*, 65(3):201–217, 2015.

- [YSS00] Allen R. York, Deborah Sulsky, and Howard L. Schreyer. Fluid-membrane interaction based on the material point method. *International Journal for Numerical Methods in Engineering*, 48(6):901–924, 2000.
- [ZA98] T. Zhu, , and S.N. Atluri. A modified collocation method and a penalty formulation for enforcing the essential boundary conditions in the element free galerkin method. *Computational Mech. Berlin*, 21:211 – 222, 1998.
- [ZA11] F. Zabala and E.E. Alonso. Progressive failure of aznalcóllar dam using the material point method. *Géotechnique*, 61(9):795–808, 2011.
- [ZCL16] Xiong Zhang, Zhen Chen, and Yan Liu. *The material point method: A continuum-based particle method for extreme loading cases*. Elsevier, 2016.
- [ZK17] Zhiyuan Zhang and Ashok V Kumar. Immersed boundary modal analysis and forced vibration simulation using step boundary method. *Finite Elements in Analysis and Design*, 126:1–12, 2017.
- [ZLR19] R. Zorrilla, A. Larese, and R. Rossi. A modified finite element formulation for the imposition of the slip boundary condition over embedded volumeless geometries. *Computer Methods in Applied Mechanics and Engineering*, 353 (15):123–157, 2019.
- [ZMG11] Duan Zhang, Xia Ma, and Paul Giguere. Material point method enhanced by modified gradient of shape function. *J. Comput. Physics*, 230:6379–6398, 07 2011.
- [ZSM06] X. Zhang, K. Y. Sze, and S. Ma. An explicit material point finite element method for hyper-velocity impact. *International Journal for Numerical Methods in Engineering*, 66(4):689–706, 2006.
- [ZTZ13] O.C. Zienkiewicz, R.L. Taylor, and J.Z. Zhu, editors. *The Finite Element Method: Its Basis and Fundamentals*. Butterworth-Heinemann, Oxford, seventh edition edition, 2013.

Upscaling lattice Boltzmann and discrete element simulations for porous media

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The purpose of this lecture note is to provide a brief overview of the state-of-the-art multiscale techniques that utilize the lattice Boltzmann for flow simulations and the discrete element simulations for simulating the granular system fully saturated with pore fluid. We will review the basics of discrete element and lattice Boltzmann methods, the different options for multiscale coupling, and the recent research trend for more accurate and fast predictions for the multiscale modeling of porous media.

1 Introduction

From the bone remodeling to the failure of landslides, the micro-mechanical coupling between the solid skeleton and the pore fluid plays an important role to the macroscopic mechanical outcomes. While there are numerous works dedicated to model the interaction of the solid and fluid constituents at the representative element volume scale where continuum models are valid, the recent advancement of computational resource has made it possible to replicate the coupling mechanisms of the pore fluid and solid at the macroscopic scales. This lecture note provides a brief overview of the theoretical framework and numerical treatment that enables the linkage between the microscopic particle-fluid interactions and the macroscopic responses of the mixture continua.

The rest of this lecture note is organized in 4 sections. We begin this lecture note with a brief review of the discrete element method for the granular materials and the lattice Boltzmann method for the pore fluid flow. We then present the multiscale techniques used to upscale the homogenized constitutive responses inferred from the representative elementary volume to the bulk and interface effective media. Each section ends with numerical examples used to verify the implementations and demonstrate the proper usages of the mathematical models.

As for notations and symbols, bold-faced letters denote tensors; the symbol $\cdot$ denotes a single contraction of adjacent indices of two tensors (e.g. $\mathbf{a} \cdot \mathbf{b} = a_i b_i$ or $\mathbf{c} \cdot \mathbf{d} = c_{ij} d_{jk}$); the symbol $:$ denotes a double contraction of adjacent indices of a tensor of rank two or higher (e.g. $\mathbf{C} : \boldsymbol{\epsilon}^e = C_{ijkl} \epsilon_{kl}^e$); the symbol $\otimes$ denotes a juxtaposition of two vectors (e.g. $\mathbf{a} \otimes \mathbf{b} = a_i b_j$) or two symmetric second-order tensors (e.g. $(\boldsymbol{\alpha} \otimes \boldsymbol{\beta})_{ijkl} = \alpha_{ij} \beta_{kl}$). Moreover, $(\boldsymbol{\alpha} \oplus \boldsymbol{\beta})_{ijkl} = \alpha_{jl} \beta_{ik}$ and $(\boldsymbol{\alpha} \ominus \boldsymbol{\beta})_{ijkl} = \alpha_{il} \beta_{jk}$. We also define identity tensors $(\mathbf{I})_{ij} = \delta_{ij}$, $(\mathbf{I}^4)_{ijkl} = \delta_{ik} \delta_{jl}$, and $(\mathbf{I}_{\text{sym}}^4)_{ijkl} = \frac{1}{2}(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{kj})$, where δ_{ij} is the Kronecker delta. As for sign conventions, unless specify otherwise, we consider the direction of the tensile stress and dilative pressure as positive.

2 Discrete element method for solid skeleton

To obtain effective stress measure from the DEM, we constitute a microscopic problem in which the macroscopic deformation measure is recast as the boundary condition for the unit problem. The unit cell problem is used to replace the macroscopic constitutive model that relates macroscopic strain measure and internal variables with the macroscopic effective stress measure. In the DEM model we employed, there is no microscopic internal variable introduced for the contact laws. Instead, path dependent behavior is mainly caused by the rearrangement of the grain contacts and the evolution of the force chain network topology.

In the unit cell DEM problem, the frame or walls of the particle assemblies are driven to move according to the macroscopic deformation measure via applying boundary traction or prescribing displacements on boundary particles [MDZ10, GZ14]. The contact forces are computed for each particle and the equations of motion are integrated by an explicit time integrator [CS79]. In quasi-static problems, to achieve static equilibrium of the particle assemblies, a dynamic relaxation scheme is employed.

Consider two rigid spheres p and q with radii R_p and R_q modeling a particle pair in contact inside a granular assembly. Let $\mathbf{y}_p$ and $\mathbf{y}_q$ denote the position vectors of their centers in a global coordinate system, while their orientations are represented by unit orientation quaternions $\mathbf{q}_p$ and $\mathbf{q}_q$ [ŠCC⁺10]. The relative velocity $\dot{\mathbf{d}}_t$ of the contact point $\mathbf{y}_c$ depends on the rate of change of the position vectors $\dot{\mathbf{y}}_p$ and $\dot{\mathbf{y}}_q$ and the rate of change of the particle orientations $\mathbf{w}_p$ and $\mathbf{w}_q$, i.e.,

$$\dot{\mathbf{d}}_t = \dot{\mathbf{y}}_q - \dot{\mathbf{y}}_p - \mathbf{w}_q \times (\mathbf{y}_c - \mathbf{y}_q) - \mathbf{w}_p \times (\mathbf{y}_c - \mathbf{y}_p) \quad (1)$$

Assuming that the contact areas of all particle pairs are infinitesimal and neglecting the gravitational force, and we also don't consider torques/couples at contacts due to rolling and torsion in the numerical examples in this paper, the

equations of motion for the translational and rotational degrees of freedom of particle p reads,

$$\begin{cases} m_p \ddot{\mathbf{y}}_p = \mathbf{f}_p = \sum_c^{n_c} \mathbf{f}_p^c \\ I_p \dot{\mathbf{w}}_p = \mathbf{t}_p = \sum_c^{n_c} (\mathbf{y}_c - \mathbf{y}_p) \times \mathbf{f}_p^c \end{cases} \quad (2)$$

with the mass m_p and moment of inertia I_p of the sphere p , $\mathbf{f}_p$ the sum of n_c contact forces $\mathbf{f}_p^c$ and $\mathbf{t}_p$ the sum of n_c contact torques due to tangential forces.

In YADE, following the form of Cundall's global damping [CS79], artificial numerical damping forces and torques are applied on each particle to reduce the total force and total torque that increases kinematic energy, while introducing damping to all eigen-frequencies [ŠCC⁺10]. The damping force $\mathbf{f}_p^{\text{damp}}$ on particle p is a function of the total contact force $\mathbf{f}_p$, the particle velocity $\dot{\mathbf{y}}_p$ and a dimensionless damping coefficient λ_{damp} (which we set to be 0.2 for all numerical examples presented in this paper). The damping torque $\mathbf{t}_p^{\text{damp}}$ on the rotational degree of freedom is constructed in a similar way, i.e.,

$$\begin{cases} \mathbf{f}_p^{\text{damp}} = -\lambda_{\text{damp}} \mathbf{f}_p \text{sgn}(\mathbf{f}_p \cdot \dot{\mathbf{y}}_p) \\ \mathbf{t}_p^{\text{damp}} = -\lambda_{\text{damp}} \mathbf{t}_p \text{sgn}(\mathbf{t}_p \cdot \dot{\mathbf{w}}_p) \end{cases} \quad (3)$$

Finally, (2) is integrated with a central difference scheme. Consider the incremental update from time step t to time step $t + \Delta t$ and let $(\mathbf{y}_p)_{t-\Delta t}$, $(\mathbf{y}_p)_t$, $(\mathbf{y}_p)_{t+\Delta t}$ denote the translational degrees of freedom for the p -th particle in three consecutive time steps. The explicit central difference scheme that updates $(\mathbf{y}_p)_{t+\Delta t}$ reads,

$$(\mathbf{y}_p)_{t+\Delta t} = \frac{1}{m_p} (\mathbf{f}_p + \mathbf{f}_p^{\text{damp}})_t \Delta t^2 + 2(\mathbf{y}_p)_t - (\mathbf{y}_p)_{t-\Delta t} \quad (4)$$

For updating the orientation of the p -th particle $(\mathbf{q}_p)_{t+\Delta t}$, the explicit central difference scheme leads to the angular velocity at time $t + \frac{\Delta t}{2}$ [ŠCC⁺10],

$$(\mathbf{w}_p)_{t+\frac{\Delta t}{2}} = (\mathbf{w}_p)_{t-\frac{\Delta t}{2}} + \Delta t (\dot{\mathbf{w}}_p)_t = (\mathbf{w}_p)_{t-\frac{\Delta t}{2}} + \Delta t \frac{1}{I_p} (\mathbf{t}_p + \mathbf{t}_p^{\text{damp}})_t \quad (5)$$

The Euler axis and angle of the rotation quaternion $\Delta \mathbf{q}_p$ are represented by a unit vector and the magnitude of the rotation $\Delta t (\mathbf{w}_p)_{t+\frac{\Delta t}{2}}$, respectively, i.e.,

$$\begin{cases} (\Delta \mathbf{q}_p)_u = \widehat{(\mathbf{w}_p)_{t+\frac{\Delta t}{2}}} \\ (\Delta \mathbf{q}_p)_\theta = |\Delta t (\mathbf{w}_p)_{t+\frac{\Delta t}{2}}| \end{cases} \quad (6)$$

The rotation quaternion $(q_p)_{t+\Delta t}$ is then updated by combining two rotation quaternions together, i.e.,

$$(q_p)_{t+\Delta t} = \Delta q_p (q_p)_t \quad (7)$$

Note that the multiplication of quaternions is not commutative. Following the update of particle positions and orientations, the contact forces, moment are updated and the energy balance is checked. The static equilibrium is achieved when the particle velocity becomes sufficiently small. In YADE, this is indicated by the magnitude of the kinetic energy and the unbalanced force index (cf. [Ng06]).

In the actual numerical simulations, we employ a simple contact law model that can be decomposed into the normal and tangential components, $(f_p^c)^n$ and $(f_p^c)^t$ i.e.,

$$\sum_c f_p^c = \sum_c ((f_p^c)^n + (f_p^c)^t) \quad (8)$$

The normal contact force between a particle pair p and q is nonzero if and only if the particles are in contact, i.e.,

$$(f_p^c)^n = (f_p^c)^n \mathbf{n} = \begin{cases} -k_n d_n \mathbf{n} & \text{if } d_n \leq 0 \\ 0 & \text{if } d_n > 0 \end{cases} ; d_n = \sqrt{(\mathbf{y}_p - \mathbf{y}_q) \cdot (\mathbf{y}_p - \mathbf{y}_q)} - R_p - R_q \quad (9)$$

where $\mathbf{n}$ is the contact normal vector, d_n is the overlapped length. Furthermore, the normal stiffness k_n of the grain contact is related to the radii (R_p and R_q) and Young's modulus of the particle E^g , i.e.,

$$k_n = 2 \frac{E^g R_p R_q}{R_p + R_q} \quad (10)$$

Meanwhile, the tangential force $(f_p^c)^t$ depends on the shear stiffness k_t and the relative tangential displacement, but is also capped by the Coulomb's frictional force. As shown in [CCB14], the rate form of the tangential constitutive law reads,

$$\dot{(f_p^c)}^t = \begin{cases} -k_t \dot{\mathbf{d}}_t & \text{if } ||k_t \dot{\mathbf{d}}_t|| \leq |(f_p^c)^n| \tan(\beta) \\ 0 & \text{if } ||k_t \dot{\mathbf{d}}_t|| > |(f_p^c)^n| \tan(\beta) \end{cases} ; k_t = A k_n \quad (11)$$

where c is the cohesion, A is a dimensionless material parameter, β is the friction angle.

Notice that the proposed multiscale coupling model is not limited to the DEM model with this particular set of constitutive laws.

RVE generation

The granular assemblies used in this study is obtained using the RVE generation engine available in an open source DEM software YADE [KD09]. In particular, we use the isotropic-compression method first introduced in [CS79]. For completeness, we briefly outline the procedure below:

1. First, a cell box with its six faces serving as the periodic boundaries is prepared. Spheres with defined particle size distribution are then randomly inserted into the box. Initially, these inserted particles are not allowed to overlap.
2. Material parameters of particles such as the contact stiffness, density and friction angle are then assigned to the particle. At this point, the assigned inter-particle friction coefficient is set to an artificial value to manipulate the amount of particle sliding and achieve the desired porosity. A large value of friction angle will yield a loosely packed RVE, and the value is set to a very low value when a dense packing is desired.
3. The unit cell is latter subjected to isotropic compression with prescribed confining pressure. The loading is carried out by an implemented engine which is capable of controlling either the Cauchy stress or the velocity gradient of the RVE. This process terminates when the entire RVE achieves static equilibrium.
4. Finally, the real values of friction coefficient are re-assigned to all particles and the RVE is now ready for future simulations.

If frictionless rigid walls are used as the RVE driving boundary, they are simply generated in the first step to replace the periodic box. As pointed out by [JKL03], the isotropic compression method is very efficient in generating dense granular assemblies. However, it is hard to maintain uniformity for loose specimens.

2.1 Numerical Example: successive sample reduction test for boundary condition sensitivity

The size of the unit cell (and therefore number of particles in the RVE) determines whether the apparent responses homogenized from microstructures of RVE could give converged coarse-scale effective properties. The size of the unit cell must be sufficiently large such that the apparent responses are insensitive to the imposed boundary condition [WLW08] and that it contains statistically enough mechanisms for the deformation processes. To ensure that the size of the unit cell is sufficiently large to be an RVE, we conduct a series of numerical experiments to empirically determine the representative element size. Following the ideas of successive sample tests discussed in [ZW01, WBF06, SAR11], we first create a large assembly composed of 979

equal-size spherical particles and obtain the local equilibrium state under a 100 kPa isotropic compression. Then we successively reduce the size of the cubic sampling window and obtain four other granular assemblies with 619, 413, 311 and 75 particles. Four of these assemblies are shown in in Fig. 1. Each RVE is then brought to equilibrium state under confining pressure of 100 kPa. To analyze whether the granular assembly is homogeneous, we also plot the Rose diagram of the contact normal orientation and show them in Fig. 1. We observed that the the contact normals are distributed quite evenly in all assemblies, except the smallest one with 75 particles. This result is consistent with the finding on 2D granular assemblies reported in [GZ14] in which a granular assembly consisting of too few particles tends to exhibit more anisotropic responses. Nevertheless, the contact normal distribution also indicates that a few hundreds of particles may be enough to generate a dense assembly with a statistically homogeneous fabric.

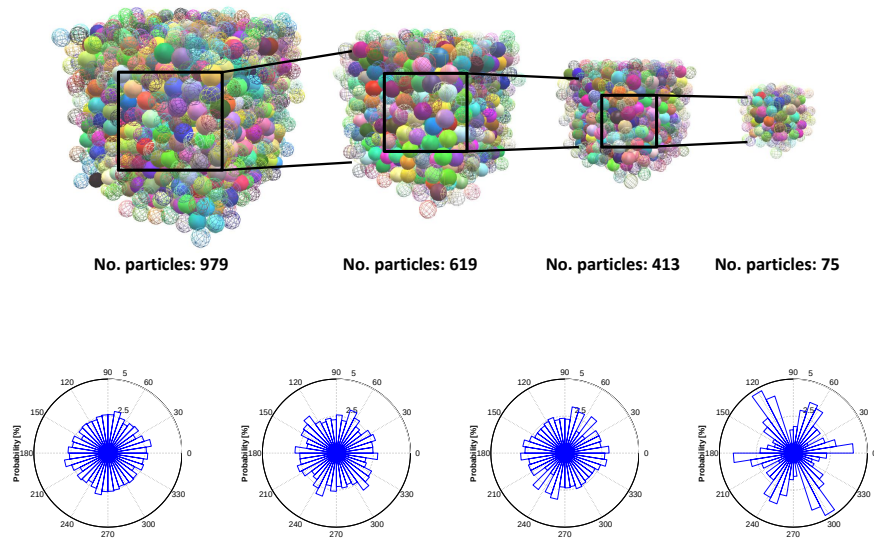


Figure 1: Four different sizes of granular assemblies used in the RVE study (UPPER) and the corresponding Rose diagram for contact normal orientation (LOWER).

All five numerical specimens are then subjected to triaxial loading until 20% axial strain. Previous studies have established that the boundary conditions driving the frame or surrounding wall of the unit cell may affect the macroscopic behavior. This sensitivity to the boundary condition is more severe

when the unit cell is smaller than the RVE size, but less important when the unit cell contains enough particles [ZW01, MD04, WBF06, WLW08, MDZ10, GZ14]. In particular, [MDZ10] has conducted systematic study to compare various constraints which transform periodic, linear displacement (zero rotation) and uniform stress to particle assemblies and found that all three satisfy a priori the Hill-Mandel condition. The study in [MDZ10] demonstrates that the linear displacement constraint produces the stiffest homogenized responses, the uniform stress constraint leads to the softest homogenized responses, while the periodic constraint leads to the intermediate response which is considered the optimal choice in [MD04]. In this study, we conduct numerical experiments for two types of boundary conditions, i.e. periodic boundary and frictionless rigid walls that impose linear displacement and zero rotation. The shear stress responses and porosity paths of triaxial compression tests on different size of RVEs are shown in Fig. 2.

3 Lattice Boltzmann method for fluid flow

A multi-scale lattice Boltzmann/Finite element method is used to extract geometrical features and permeability from the granular assemblies. This hybrid method was originally proposed in [WBF06] to estimate permeability of Castlegate Sandstone. Sun et al 2011a [SAR11] improved the accuracy and computation efficiency of this method by incorporating geometrical analysis in permeability calculations. The key to this improvement is partitioning the entire grain assembly into unit cells where pore-scale lattice Boltzmann simulations are conducted in the **connected** pores of each unit cell. Since discretized voxel images may contain isolated pore if the resolution is insufficient, this method is used to ensure that discretization does not alter connectivity of the pores.

The lattice Boltzmann method we used is a single-relaxation time BGK model [ZH97], which solves a discretized Boltzmann equation by simulating the evolution of particle distribution that propagates and collides locally among lattice nodes. The evolution of particle distribution function f_i in direction e_i is updated in each time step through the following equation,

$$f_i(\mathbf{x} + \mathbf{e}_i, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)) \quad (12)$$

where f^{eq} is a truncated equilibrium distribution defined as,

$$f_i^{eq} = w_i \rho \left(1 + \frac{3\mathbf{e}_i \cdot \mathbf{v}}{c_s^2} + \frac{9(\mathbf{e}_i \cdot \mathbf{v})^2}{c_s^4} - \frac{\mathbf{v} \cdot \mathbf{v}}{2c_s^2} \right) \quad (13)$$

τ is a parameter related to the dynamic fluid viscosity ν , as shown in the Chapman-Enskog equation (cf. [Suc01]),

$$\nu = \Delta t c_s^2 \left(\tau - \frac{1}{2} \right) \quad (14)$$

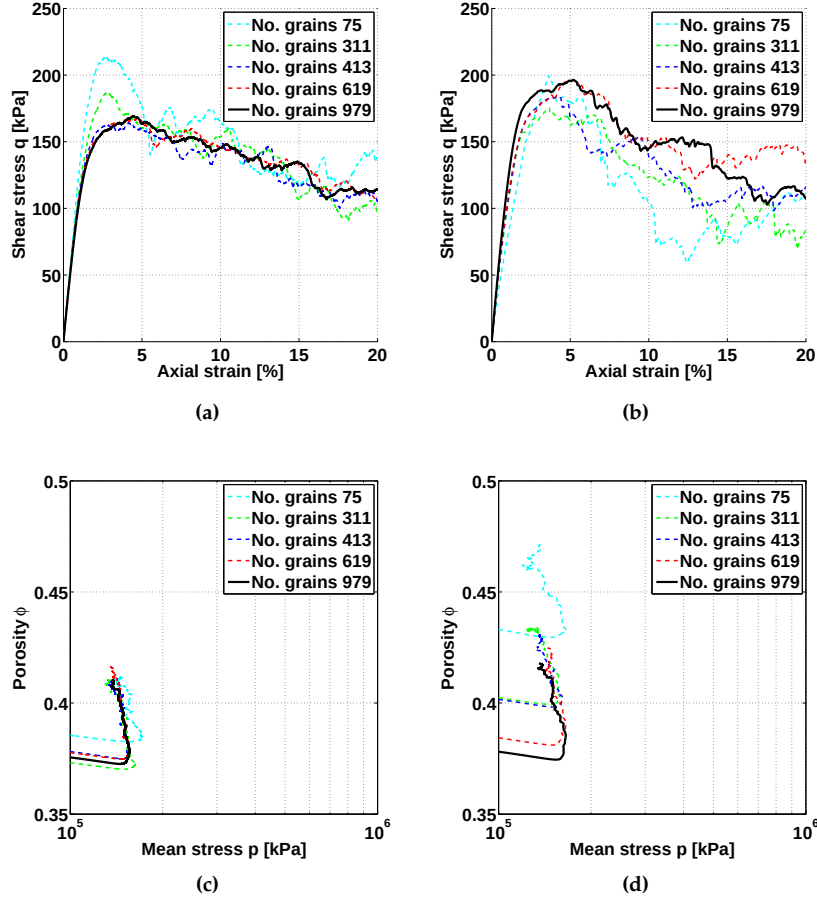


Figure 2: Shear stress response and porosity path of triaxial compression tests on different size of RVEs. (a)(c) RVE driven by periodic boundaries; (b)(d) RVE driven by frictionless rigid walls

where c_s is the constant speed of sound. ρ and v are the macroscopic density and velocity. They are determined from the evolution of the particle distribution, i.e.,

$$\rho = \sum_{i=1}^N f_i ; \quad v = \frac{1}{\rho} \sum_{i=1}^N f_i e_i \quad (15)$$

The effective permeability of a porous medium can be measured by applying a pore pressure gradient along a basis direction and determining the resultant fluid filtration velocity from a pore-scale hydrodynamics simulation. Then,

the effective permeability tensor is obtained according to,

$$k_{ij} = -\frac{\mu^v}{(\nabla^x p)_j} \frac{1}{V_\Omega} \int_\Omega v_i(\mathbf{x}) d\Omega \quad (16)$$

where μ^v is the kinematic viscosity of the fluid occupying the spatial domain of the porous medium Ω . To implement this procedure, we first assume that the effective permeability tensor k_{ij} is symmetric and positive definite. We then determine the diagonal components of the effective permeability tensor k_{ii} by three hydrodynamics simulations. In each simulation, we impose a pressure gradient on two opposite faces orthogonal to an axis $\mathbf{e}_i$ and no-slip boundary conditions on the four sides parallel to $\mathbf{e}_i$ where $\mathbf{e}_i$ denotes an orthogonal axis of a Cartesian system.

3.1 Numerical example 1: occluded porosity and its impact on homogenized permeability

In many situations, particularly in natural porous materials, occluded porosity occupies a significant portion of the pore space. Failure to identify occluded porosity can cause dramatic errors in multiscale modes. Typical situations where significant occluded porosity is expected to play a role include the migration of pore-fill cement into pore space, pore closure in limestones due to CO₂ sequestration, and the formation of compaction bands [SARE11].

To illustrate this point, let us consider a two dimensional LB simulation of the sample depicted in Figure 3. In this example, our objective is to obtain the vertical global permeability of a sample, discretized using a $30\ u \times 40\ u$ lattice (u =lattice unit), using three different techniques. In the first technique, LB simulations are conducted on the entire sample, without any domain decomposition. This is equivalent to a direct numerical simulation and is interpreted here as the ‘true’ solution. The second technique uses domain decomposition (sample is split into four parts along the vertical direction) and uses occluded space detection, keeping only connected porosity active. The third technique uses domain decomposition but does not distinguish between connected and occluded porosity. Global permeabilities for the partitioned samples are obtained from the local estimates by [BBM87],

$$k = \frac{\sum_{i=1}^n L_i}{\sum_{i=1}^n L_i / k_i} \quad (17)$$

where k_i are the local values of permeability in each layer of thickness L_i , and $n = 4$ denotes the number of unit cells (layers).

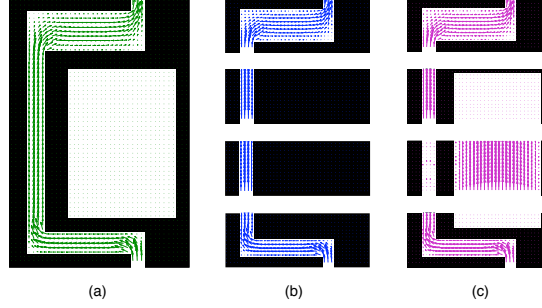


Figure 3: Velocity profiles of lattice Boltzmann simulations on (a) unpartitioned domain ($k = 0.015 u^2$), (b) partitioned domain with identified and deactivated occluded porosity ($k = 0.013 u^2$), and (c) partitioned domain without any special treatment for occluded porosity ($k = 0.0078 u^2$). Where u =lattice unit.

Results for the LB calculations are summarized in Table 1. It should be highlighted that the relative error induced by the third procedure with partition but no special treatment of occluded porosity yielded an error four times greater than that of the partitioned method that takes into account occluded porosity. It can be seen from Table 1 that the main sources of error come from the mistreatment of occluded porosities in the central partitions. The mistreatment of occluded porosity is not only the source of errors in the estimation of permeability, but it leads to longer calculations as occluded porosity is assigned active lattices. Hence, not accounting for occluded porosity may lead to inaccuracies and inefficiencies.

Case	1	2	3
Number of Unit Cell(s)	1	4	4
Occluded Pore Identified?	No	Yes	No
Local Permeability, u^2 (top)	N/A	0.011	0.011
Local Permeability, u^2 (2nd top)	N/A	0.015	0.0029
Local Permeability, u^2 (2nd bottom)	N/A	0.015	0.45
Local Permeability, u^2 (bottom)	N/A	0.014	0.014
Global Permeability, u^2	0.015	0.013	0.0078
Relative Error	0	12 %	48 %

Table 1: Global and local permeabilities obtained from LB simulation scenarios.

3.2 Numerical Example 2: Verification against periodic simple cubic (SC) lattice

Simple cubic (SC) cells can be formed by placing the centroid of eight identical spheres at the corners of a cube of equal dimensions. When the spheres are making point contact, it is often called SC bead pack [SSD95]. In this packing, the total porosity is simply $\phi^f = 1 - \pi/6$ and the geometrical tortuosity is simply unity, as the shortest flow path is one directly through the center of the cell. Furthermore, as in other simple packings, all porosity is connected.

Unlike micro-structural attributes, permeability of SC packings cannot be directly obtained using analytical techniques. Instead, numerical procedures are often employed. The closest analytical solutions are furnished by bounds, such as the lower bound obtained by Dormieux and co-workers [DKU06] where pore spaces are ordered in the sense of inclusions and the permeability of a cylinder with cross-section made up by four circles examined. Since the cylindrical pore space is a subset of that of the SC cell, the permeability of the cylindrical pore space serves as a lower bound for that of the SC cell. The lower bound can be expressed in dimensionless form as $k \geq 4.84 \times 10^{-3} R^2$, where R is the radius of the spheres in the SC cell. Naturally, the permeability tensor in the SC cell is isotropic. Additionally, Zick and Homsy [ZH82] have analyzed the permeability of the SC bead pack by reducing the Navier-Stokes equation to a set of Fredholm integral equations. They found $k = 5.04 \times 10^{-3} R^2$.

Next, we calculate the effective permeability of the SC bead pack. Our first task is to correctly identify the connected porosity in the sample. The pore geometry is discretized in the usual way using a lattice mesh. The resolution of the lattice, clearly affects the results of the computations. The center of the pore space is selected as the first active lattice and porosity is determined using the region-growing algorithm. Figure 4 shows the estimate of porosity as a function of the lattice resolution. Once the voxel length is smaller than $R/50$, the numerical solution closely captures the exact solution $(1 - \pi/6)$.

Using a resolution of $R/50$, the resultant level set function and the shortest flow path are illustrated in Figure 5. As shown in the figure, in this simple example the geometrical tortuosity is unity and Dijkstra's algorithm is able to obtain this result without any issues. Finally, turning our attention to the effective permeability calculation, we obtain an estimate using lattice Boltzmann at the aforementioned lattice resolution. In addition, we carried out a three dimensional Navier-Stokes finite element simulation to examine the reproducibility of the permeability calculation. The FE model is composed of 8937 tetrahedral Crouzeix-Raviart elements with non-periodic side walls and prescribed pressures on the top and bottom faces of the cubic domain. The FE model was solved using an open-source differential solver called FEniCS [LMW12].

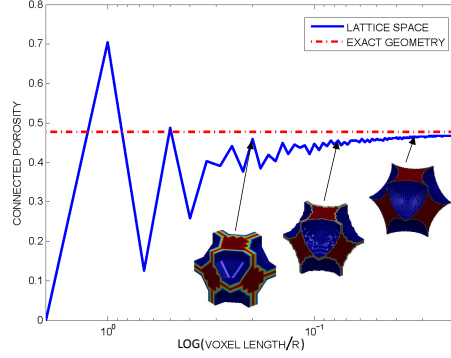


Figure 4: Connected porosity as a function of voxel length in a SC bead packing.

Figure 6 illustrates the results of the LB and FE simulations. The permeability using LB and FE is estimated to be $4.64 \times 10^{-3} R^2$ and $4.89 \times 10^{-3} R^2$, respectively. Since both methods are inherently different, and since the calculations are close to the previous values of permeability estimated for SC packings, we consider the 5.1% difference in solutions acceptable. We therefore conclude that the proposed framework to estimate permeability based on level sets and lattice Boltzmann is accurate.

4 Multiscale homogenization for bulk porous media

In this section, we describe the homogenization theory we adopt to establish the DEM-mixed-FEM coupling model for fully saturated porous media. Previous work for dry granular materials, such as [MD04, MDZ10, NCDD11, GZ14], has demonstrated that a hierarchical discrete-continuum coupling model can be established by using grain-scale simulations to provide Gauss point stress update for finite element simulations in a fully implicit scheme. Nevertheless, the extension of this idea for partially or fully saturated porous media has not been explored, to the best knowledge of the authors.

In this work, we hypothesize that the pore-fluid flow inside the pores is in the laminar regime and is dominated by viscous forces such that Darcy's law is valid at the representative elementary volume level [SARE11, SAR11, SKR13]. Provided that this assumption is valid, we define the pore pressure field only at the macroscopic level and neglect local fluctuation of the pore pressure at the pore- and grain-scale.

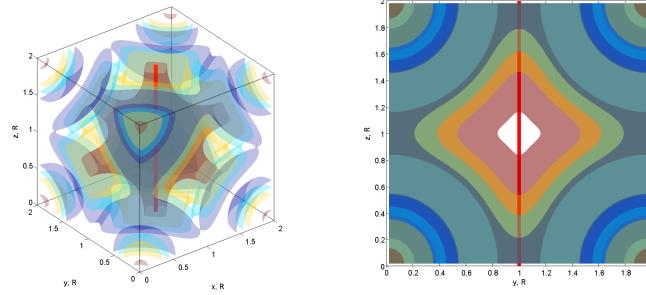


Figure 5: Level set function $\phi(x, y, z)$ (represented by the 3D color contour) and the corresponding shortest flow path (represented by the red straight line) as determined by Dijkstra's algorithm.

On the other hand, we abandon the usage of macroscopic constitutive law to replicate the constitutive responses of the solid constituent. Instead, we apply the effective stress principle [TTE⁺43, GSP09, GMS13] and thus allow the change of the macroscopic effective stress as a direct consequence of the compression, deformation and shear resistance of the solid constituent inferred from grain-scale simulations. As a result, the effective stress can be obtained from homogenizing the forces and branch vectors of the force network formed by the solid particles or aggregates, while the total stress becomes a partition of the homogenized effective stress from the microscopic granular assemblies, and the pore pressure from the macroscopic mixture continuum.

4.1 Dual-scale effective stress principle

In this study, we make assumptions that (1) a separation of scale exists and that (2) a representative volume element (RVE) can be clearly defined. Strictly speaking, the assumption (2) is true if the unit cell has a periodic microstructure or when the volume is sufficiently large such that it possesses statistically homogeneous and ergodic properties [GAS07].

With the aforementioned assumptions in mind, we consider a homogenized macroscopic solid skeleton continuum $\mathcal{B}^s \subset \mathbb{R}^3$ whose displacement field is C^0 continuous. Each position of the macroscopic solid body in the reference configuration, i.e., $\mathbf{X} = \mathbf{X}^s \in \mathcal{B}_0^s$, is associated with a micro-structure of the RVE size. Let us denote the trajectories of the macroscopic solid skeleton and the fluid constituent in the saturated two-phase porous medium from the reference configuration to the current solid configuration as,

$$\mathbf{x} = \boldsymbol{\varphi}^s(\mathbf{X}, t) ; \mathbf{x} = \boldsymbol{\varphi}^f(\mathbf{X}^f, t) \quad (18)$$

Unless the porous medium is locally undrained, the solid and fluid constituents are not bundled to move along the same trajectory, i.e., $\boldsymbol{\varphi}^s(\cdot, t) \neq$

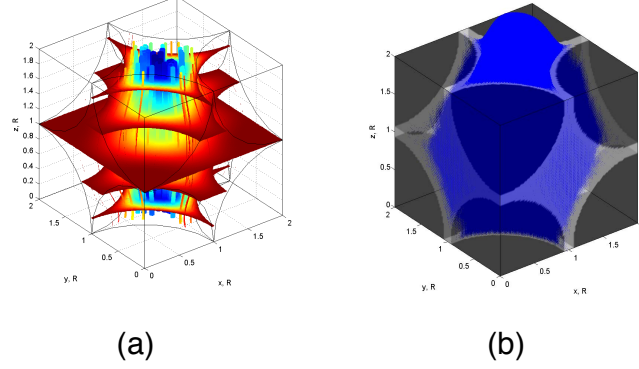


Figure 6: (a) Streamline of the simple cubic lattice computed via Stokes finite element model ($k = 4.89 \times 10^{-3} R^2$). (b) Velocity profile of the simple cubic lattice obtained via lattice Boltzmann simulation conducted on connected pore space ($k = 4.64 \times 10^{-3} R^2$).

$\varphi^f(\cdot, t)$. If we choose to follow the macroscopic solid skeleton trajectory to formulate the macroscopic balance principles, then the control volumes are attached to solid skeleton only, and the pore fluid motion is described by relative movement between the fluid constituent and the solid matrix, as shown in Fig. 7. The deformation gradient of the macroscopic solid constituent F can therefore be written as,

$$F = \frac{\partial \varphi(X^s, t)}{\partial X^s} = \frac{\partial \varphi(X, t)}{\partial X} = \frac{\partial x}{\partial X} \quad (19)$$

in which we omit the superscript s when quantities are referred to solid phase. Now, following [MD04], we associate each point in the current configuration x with an aggregate of N particles inside the representative volume $\mathcal{V}$. Furthermore, we introduce a local coordinate system for the RVE in which the position vector $y \in \mathbb{R}^3$ becomes $\mathbf{0}$ at the geometric centroid of the RVE. The locations of the centroids of the N particles expressed using the local coordinate system read, i.e.,

$$y_p \in \mathcal{V}, \quad p = 1, 2, \dots, N. \quad (20)$$

where y_p is the local position vector of the center of the p -th particle in the microstructure and $x + y_p$ is the same position expressed in the macroscopic current coordinate system. Particles inside the RVE may make contacts to each other. The local position vector of each contact between each particle-pair y_c can be written as,

$$y_c \in \mathcal{V}, \quad c = 1, 2, \dots, N_c. \quad (21)$$

Both the positions of the particles y_p and that of the contacts y_c are governed by contact law and the equilibrium equations. Previous works, such as

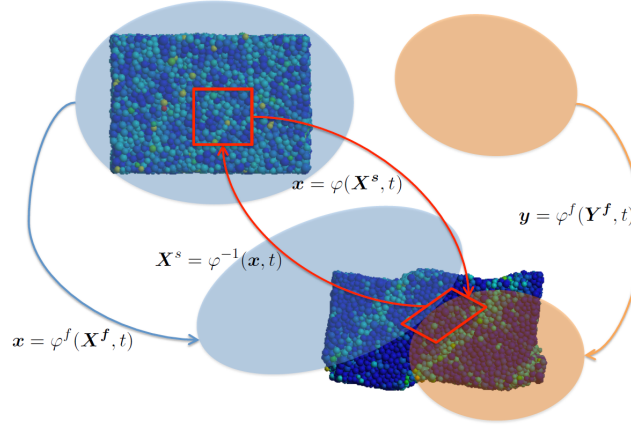


Figure 7: Trajectories of the solid and fluid constituents $\varphi^s = \varphi$ and φ^f . The motion φ conserves all the mass of the solid constituent, while the fluid may enter or leave the body of the solid constituent. Figure reproduced from [SOS13]

[CVW04, ESZ05, HC11, GTSMW13, RRL14, CLCC14], have found success in explicitly modeling the pore-scale grain-fluid interaction. Nevertheless, such grain-fluid interaction simulations do impose a very high computational demand due to the fact that the fluid flow typically requires at least an order more of degree of freedoms to resolve the flow in the void space among particles. However, for seepage flow that is within the laminar regime where Darcy's law applies, the new insight obtained from the costly simulations will be limited. As a result, this discrete-continuum coupling model does not explicitly model the pore-scale solid-fluid interaction. Instead, we rely on the hypothesis that effective stress principle is valid for the specific boundary value problems we considered. In particular, we make the following assumptions:

- The void space is always fully saturated with one type of fluid and there is no capillary effect that leads to apparent cohesion of the solid skeleton.
- The flow in the void space remains Darcian at the macroscopic level.
- All particles in the granular assemblies are in contact with the neighboring particles.
- Fluidization, suffusion and erosion do not occur.
- Grain crushing does not occur.

- There is no mass exchange between the fluid and solid constituents.

As a result, we may express the total macroscopic Cauchy stress as a function of homogenized Cauchy effective stress inferred from DEM and the macroscopic pore pressure obtained from the mixed finite element, i.e.

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \langle \boldsymbol{\sigma}'(\mathbf{x}, t) \rangle_{\text{RVE}} - B(\mathbf{x}, t) p^f(\mathbf{x}, t) \mathbf{I} \quad (22)$$

where

$$\langle \boldsymbol{\sigma}'(\mathbf{x}, t) \rangle_{\text{RVE}} = \frac{1}{2V_{\text{RVE}}} \sum_c^{N_c} (\mathbf{f}^c \otimes \mathbf{l}^c + \mathbf{l}^c \otimes \mathbf{f}^c) \quad (23)$$

$\mathbf{f}^c$ is the contact force and $\mathbf{l}^c$ is the branch vector, the vector that connects the centroids of two grains forming the contact [CMNN81, Bag96, SKR13], at the grain contact $\mathbf{x} + \mathbf{y}_c \in \mathbb{R}^3$. V_{RVE} is the volume of the RVE and N_c is the total number of particles in the RVE. Meanwhile, the Biot's coefficient B reads,

$$B(\mathbf{x}, t) = 1 - \frac{K_T^{\text{DEM}}(\mathbf{x}, t)}{K_s} \quad (24)$$

with $K_T^{\text{DEM}}(\mathbf{x}, t)$ and K_s being the effective tangential bulk modulus of the solid matrix inferred from DEM, and the bulk modulus of the solid grain respectively [NB71, SWZP86]. Notice that, in the geotechnical engineering and geomechanics literature, such as [Ng06, KRMK14], it is common to impose incompressible volumetric constraint on dry DEM assembly to simulate undrained condition at meso-scale. This treatment can be considered as a special case of (24) when the bulk modulus of the solid grain is significantly higher than that of the skeleton such that the Biot's coefficient is approximately equal to one.

4.2 Micro-macro-transition for solid skeleton

In this study, we consider the class of two-phase porous media of which the solid skeleton is composed of particles. These particles can be cohesion-less or cohesive, but the assemblies they formed are assumed to be of particulate nature and hence suitable for DEM simulations. [CS79].

In our implementation, the DEM simulations are conducted via YADE (Yet Another Dynamic Engine [ŠCC⁺10]), an open source code base for discontinua. These grain-scale DEM simulations are used as a replacement to the macroscopic constitutive laws that relate strain measure with effective stress measure for each RVE associated with a Gauss point in the macroscopic mixed finite element. In particular, a velocity gradient is prescribed to move the frame of the unit cell and the DEM will seek for the static equilibrium state via dynamics relaxation method. After static equilibrium is achieved, the internal forces and branch vectors are used to compute the homogenized effective Cauchy stress via the micro-macro transition theory [MD04, MDZ10, WLW08].

For completeness, we provide a brief overview of DEM, the procedure for generation of RVEs and the study on the size of RVEs in Appendix A,B and C.

The Hill-Mandel micro-heterogeneity condition demands that the power at the microscopic scale must be equal to the the rate of work done measured by the macroscopic effective stress and strain rate measures. For the solid constituent of the two-phase porous media, this condition can be expressed in terms of any power-conjugate effective stress and strain rate pair , such as $(\mathbf{P}', \dot{\mathbf{F}})$ and $(\mathbf{S}', \dot{\mathbf{E}})$ and $(\boldsymbol{\sigma}', \mathbf{D})$ [BA95, Arm99]. For instance, the condition can be written in terms of the effective stress and rate of deformation of the solid skeleton, i.e.,

$$\langle \boldsymbol{\sigma}' \rangle_{\text{RVE}} : \langle \mathbf{D} \rangle_{\text{RVE}} = \langle \boldsymbol{\sigma}' : \mathbf{D} \rangle_{\text{RVE}} \quad (25)$$

where $\mathbf{D}$ is the rate of deformation, i.e., the symmetric part of the velocity gradient tensor,

$$\langle \mathbf{D} \rangle_{\text{RVE}} = \frac{1}{2}(\langle \mathbf{L} \rangle_{\text{RVE}} + \langle \mathbf{L}^T \rangle_{\text{RVE}}) ; \mathbf{L} = \nabla^x \mathbf{v} \quad (26)$$

and $\langle \boldsymbol{\sigma}' \rangle_{\text{RVE}}$ is defined previously in (23). Previous studies, such as, [MD04, WLW08, MDZ10, Fis13], have established that the linear deformation, periodic, and uniform traction are three boundary conditions that satisfy the Hill-Mandel micro-heterogeneity condition. In our implementation, we apply the periodic boundary condition to obtain the effective stress measure, because the periodic boundary condition may yield responses that are softer than those obtained from the linear deformation BC but stiffer than those obtained from the uniform traction BC. In particular, the periodic boundary condition enforces two constraints: (1) the periodicity of the deformation, i.e.,

$$[[\mathbf{y}_b]] = \langle \mathbf{F} \rangle_{\text{RVE}} [[\mathbf{Y}_b]] \text{ and } [[\mathbf{R}_b]] = \mathbf{0} \quad (27)$$

where $[[\cdot]]$ denotes the jump across boundaries, $\mathbf{y}_b$ and $\mathbf{Y}_b$ represent the position vectors of the particles at the boundary of the reference and current configurations, $\mathbf{R}_b \in SO(3)$ represents the rotation tensor of particles at the boundary, and (2) the anti-periodicity of the force $\mathbf{f}_b$ and moment on the boundary of the RVE, i.e.,

$$[[\mathbf{f}_b]] = \mathbf{0} \text{ and } [[(\mathbf{y}_c - \mathbf{y}_b) \times \mathbf{f}_b]] = \mathbf{0} \quad (28)$$

In YADE, the DEM code we employed for grain-scale simulations, the deformation of an RVE is driven by a periodic cell box in which the macroscopic velocity gradient of the unit cell $\langle \mathbf{L} \rangle_{\text{RVE}}$ can both be measured and prescribed.

4.3 Multiscale hydro-mechanical model

The differential equations governing the isothermal saturated porous media in large deformation are derived based on the mixture theory, in which

solid matrix and pore fluid are treated together as a multiphase continuum [Pre82, BA95, Arm99, Cou04, SOS13, MNBT13]. The solid and fluid constituents may simultaneously occupy fractions of the volume of the same material point. The physical quantities of the mixture, such as density and total stress, are spatially homogenized from its components. For example, the averaged density of the fluid saturated soil mixture is defined as:

$$\rho = \rho^s + \rho^f = (1 - \phi)\rho_s + \phi\rho_f \quad (29)$$

where ρ^α is the partial mass density of the α constituent and ρ_α is the intrinsic mass density of the α constituent, with ϕ being the porosity.

4.3.1 Balance of linear momentum

For the balance of linear momentum law in finite strain, we adopt the total Lagrangian formulation and choose the total second Piola-Kirchhoff stress (PK2) $\mathbf{S}$ as the stress measure. The inertial effect is neglected. The equation takes the form:

$$\nabla^X \cdot (\mathbf{F}\mathbf{S}) + J(\rho^s + \rho^f)\mathbf{g} = \mathbf{0} \quad (30)$$

where the Jacobian $J = \det(\mathbf{F})$. The principle of effective stress postulates that the total Cauchy stress $\boldsymbol{\sigma}$ can be decomposed into an effective stress due to the solid skeleton deformation and an isotropic pore pressure (p^f) stress. The effective stress principle in terms of PK2 writes:

$$\mathbf{S} = \mathbf{S}'^{\text{DEM}} - J\mathbf{F}^{-1}B^{\text{DEM}}p^f\mathbf{I}\mathbf{F}^{-T} \quad (31)$$

where

$$\mathbf{S}'^{\text{DEM}} = J\mathbf{F}^{-1}\boldsymbol{\sigma}'^{\text{DEM}}\mathbf{F}^{-T} = J\mathbf{F}^{-1}\left(\frac{1}{V_{\text{RVE}}} \sum_i^{N_c} \mathbf{f} \otimes \mathbf{l}\right)\mathbf{F}^{-T} \quad (32)$$

Thus the balance of linear momentum becomes:

$$\nabla^X \cdot (\mathbf{F}\mathbf{S}'^{\text{DEM}} - J\mathbf{F}^{\text{DEM}}p^f\mathbf{F}^{-T}) + J(\rho^s + \rho^f)\mathbf{g} = \mathbf{0} \quad (33)$$

4.3.2 Balance of fluid mass

The simplified u-p formulation in finite strain requires another equation illustrating the balance of mass for pore fluid constituent:

$$\frac{D\rho^f}{Dt} = -\nabla^X \cdot (J\mathbf{F}^{-1}[\phi^{\text{DEM}}\rho_f(\mathbf{v}^f - \mathbf{v})]) \quad (34)$$

where $\frac{D[\cdot]}{Dt} = [\dot{\cdot}]$ is the material time derivative with respect to the velocity of solid skeleton $\mathbf{v}$.

We make isothermal and barotropic assumptions and suppose that $p^f \ll K_s$ and that $\frac{DB^{\text{DEM}}}{Dt} \sim 0$. After simplifications [SOS13], the balance of mass becomes:

$$\frac{B^{\text{DEM}}}{J} \frac{DJ}{Dt} + \frac{1}{M^{\text{DEM}}} \frac{Dp^f}{Dt} + \nabla^X \cdot \left(\frac{1}{\rho_f} (JF^{-1} [\phi^{\text{DEM}} \rho_f (\mathbf{v}^f - \mathbf{v})]) \right) = 0 \quad (35)$$

where

$$M^{\text{DEM}} = \frac{K_s K_f}{K_f (B^{\text{DEM}} - \phi^{\text{DEM}}) + K_s \phi^{\text{DEM}}} \quad (36)$$

is the Biot's modulus [NB71], with K_f being the bulk modulus of pore fluid.

In this paper, Darcy's constitutive law relating the relative flow and the pore pressure is employed, neglecting the inertial effect:

$$\mathbf{Q} = \mathbf{K}^{\text{DEM}} \cdot (-\nabla^X p^f + \rho_f \mathbf{F}^T \cdot \mathbf{g}) \quad (37)$$

where the pull-back permeability tensor $\mathbf{K}^{\text{DEM}}$ is defined as

$$\mathbf{K}^{\text{DEM}} = JF^{-1} \cdot \mathbf{k}^{\text{DEM}} \cdot F^T \quad (38)$$

Assume that the effective permeability tensor $\mathbf{k}^{\text{DEM}}$ is isotropic, i.e.,

$$\mathbf{k}^{\text{DEM}} = k^{\text{DEM}} \mathbf{I} \quad (39)$$

where k^{DEM} is the scalar effective permeability in unit of $\frac{m^2}{Pa \cdot s}$. It is updated from porosity of DEM RVEs according to the Kozeny-Carmen equation.

4.4 Numerical Example 1: Globally undrained shear test of dense and loose assemblies

For the second example we employ our multiscale scheme to perform shear tests on both dense and loose granular assemblies. The macroscopic geometry and boundary conditions are illustrated on a sample discretized by coarse mesh ($1 \times 5 \times 5$ in X,Y,Z directions) as Fig. 8. We also use a medium fine mesh ($1 \times 8 \times 8$) and a fine mesh ($1 \times 10 \times 10$) to investigate the mesh dependency issue of the proposed scheme. All results in this section are computed from the fine mesh model, if not specified. The nodes on the bottom boundary are fixed in all directions and those on the upper boundary are translated identically towards the positive y axis at a constant rate. They are maintained at a constant vertical stress $\sigma_z = 100kPa$ by a horizontal rigid layer (not shown). This constraint is imposed in the model by the Lagrange multiplier method. The lateral surfaces are constrained by frictionless rigid walls (not shown). All surfaces are impervious. The gravitational effect is not considered in this study. For coupled microscopic DEM models, periodic unit cells composed of uniform spheres are prepared by an isotropic compression engine in YADE

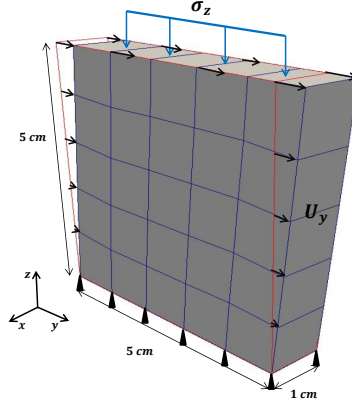


Figure 8: Geometry and boundary conditions for globally undrained shear test

up to $\sigma_{iso} = 100 \text{ kPa}$ with initial porosity of 0.375 and 0.427 for dense and loose assemblies respectively, and then are assigned identically to all the integration points of the FEM model before shearing.

The finite strain formulation is first adopted to study the hydro-mechanical coupling effect during the shearing of the dense and loose samples with undrained boundaries. The material parameters used in the simulations allowing hydraulic diffusion within the specimen are presented in Table 2. They are categorized into micromechanical material parameters used in DEM solver, poro and poro-plasticity parameters derived from DEM RVEs and macroscopic properties set in FEM. Note that the permeability k is updated with porosity of RVEs using the Kozeny-Carman relation during the simulation. To prevent local seepage of water within the samples, the permeability k is set to $0 \text{ m}^2 / (\text{Pa} \cdot \text{s})$.

Fig. 9 represents the global shear stress and volumetric strain behavior of shear simulations with and without local seepage of water. The strain-hardening behavior of undrained dense granular assemblies (left column) and strain-softening behavior of undrained loose granular assemblies (right column) are recovered [YIV98]. In both assemblies, when local seepage is prohibited, the shear stress immediately rises when the shearing begins and the saturated porous media behaves stiffer than the samples with local seepage. Note that the sudden drop in Fig. 9(b) is due to the unstable solid matrix of loosely confined DEM unit cell. The volumetric strain of the dense sample with seepage monotonically increases. This phenomenon is attributed to the

	Parameter	Value
Microscopic property in DEM	Solid grain normal stiffness k_n	$2.2 \times 10^6 \text{ N/m}$
	Solid grain tangential stiffness k_s	$1.9 \times 10^6 \text{ N/m}$
	Solid grain friction angle β	30°
	Solid grain bulk modulus K_s	0.33 GPa
Macroscopic property inferred from DEM	Porosity ϕ	dense: 0.375, loose: 0.427
	Biot's coefficient B	dense: 0.976, loose: 0.983
	Biot's Modulus M	dense: 180 Mpa, loose: 168 Mpa
Macroscopic property in FEM	Fluid bulk modulus K_f	0.1 GPa
	Initial permeability k	$1 \times 10^{-9} \text{ m}^2 / (\text{Pa} \cdot \text{s})$
	Solid density ρ_s	2700 kg/m^3
	Fluid density ρ_f	1000 kg/m^3

Table 2: Material parameters in globally undrained shear problem

rearrangement of solid matrix as the grains tend to rise over adjacent grains when they are driven by shear forces. In absence of local diffusion, the dense sample experiences a reduction of volume instead, suggesting that the compression of overall solid matrix predominates the above phenomenon. As for loose samples, however, the volumetric behavior is opposite. When local diffusion of water is prohibited, the pore collapse and densification of local regions within specimen could occur, resulting in a compression at early stage of shearing before the dilatancy phenomenon. The curve of no-local-seepage case shows that the dilatancy phenomenon prevails all along the shearing. In all cases, the volume changes are beneath 0.12%, confirming that the samples are indeed sheared under globally undrained condition.

We examine the mesh dependency by three aforementioned mesh densities adopted in simulations of dense assembly with local seepage. The effect is presented via plots of global $\sigma_{yz} - \gamma_{yz}$ and $\varepsilon_v - \gamma_{yz}$ responses as Fig. 10. For stress response, discrepancy between medium and fine meshes is not significant, but coarse mesh apparently yields stiffer solution after 2% shear strain and the maximum deviation is about 7.6% with respect to the fine mesh solution. The differences between ε_v curves are less significant and do not exceed 4% of the fine mesh solution. Thus, our choice of the fine mesh to conduct numerical experiments is acceptable.

We next display the difference between the finite-strain and small-strain multiscale schemes in simulations of dense granular sample in both local diffusion conditions in Fig. 11. According to the global shear responses, the small strain and finite strain yield consistent solutions within 2% shear strain. Then the discrepancy gradually emerges and the introduction of geometrical non-linearity renders the sample stiffer. This observation is the same as the conclusion in the previous Terzaghi's problem section. Finite strain solutions exhibit less volume changes in both cases. Moreover, geometrical non-linear term

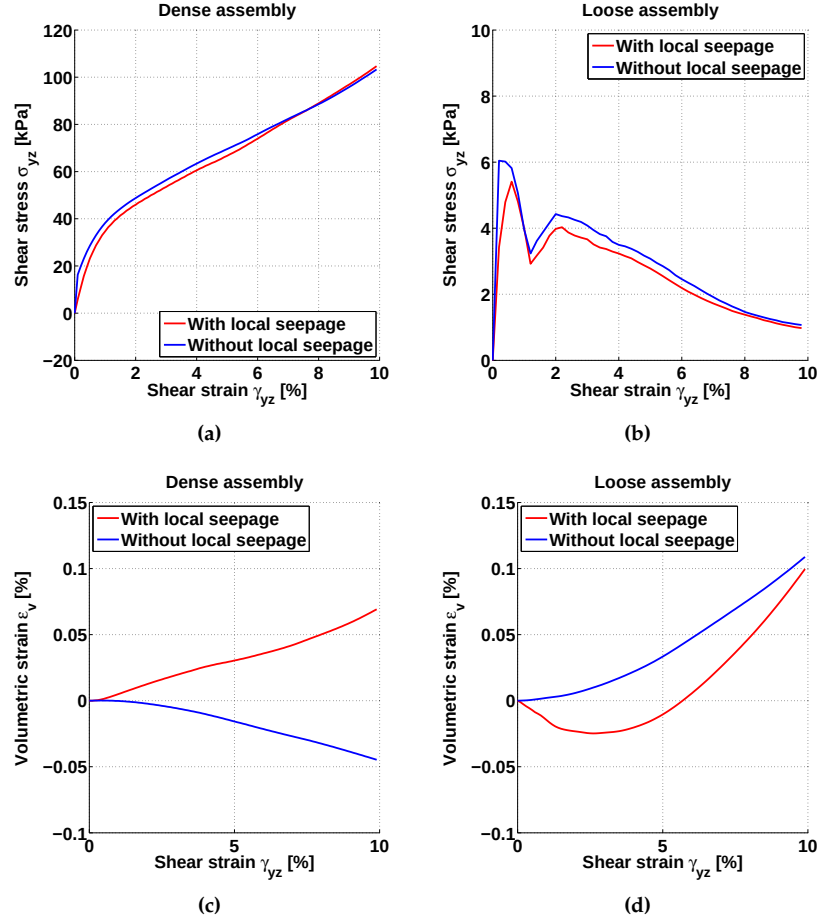


Figure 9: Comparison of global shear stress and volumetric strain behavior between globally undrained dense and loose assemblies with and without local diffusion

even alters the dilatancy behavior: the sample is computed to be compressed when no local seepage of water is allowed, while the small strain solution conserves the dilatant trend.

We also assess the local diffusion effect via color maps of pore pressure developed during the deformation, as shown in Fig. 12. The dense sample with local seepage has developed negative pore pressure and the pressure distribution is nearly uniform, since fluid flow could take place inside the specimen to dissipate pressure difference between neighboring pores. Without

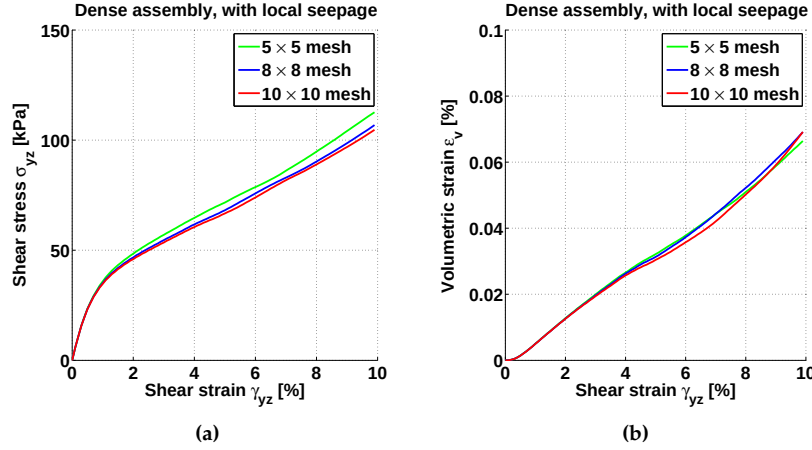


Figure 10: Comparison of global shear stress and global volumetric strain behavior between coarse mesh ($1 \times 5 \times 5$), medium mesh ($1 \times 8 \times 8$), fine mesh ($1 \times 10 \times 10$), finite strain formulation

local seepage of water, the pore pressure is concentrated to four corners of the sample, with the upper left and bottom right corners compressed (positive pressure) and the other two dilated (negative pressure). Furthermore, these corners have maximum pressure gradient $\|\nabla p^f\|$.

The multiscale nature of our method offers more insight into the local states of granular sample. With the granular material behavior homogenized from responses of RVEs, the grain displacements, the effective stress paths (shear stress $q = \sigma_1 - \sigma_3$ vs. effective mean stress $p' = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3}$) and the volumetric strain paths (ϵ_v vs. p') in each DEM unit cell are directly accessible. As an example, the local distribution of q at the end of shearing for globally undrained yet locally diffused dense sample (13) shows a concentration of shear stress in upper left and bottom right corners, while the corners correspondent to the other diagonal sustain comparably very little shear stress. The deformed configuration of spheres in three representative RVEs are colored according to the dimensionless displacement magnitude $\frac{\|u\|_2}{\text{initial size of unit cell}}$ compared to initial RVE configuration. We present stress paths of these three RVEs providing evidence that strain-softening (Fig. 14(a)), limited strain-softening (Fig. 14(b)) and strain-hardening (Fig. 14(c)) could locally occur in a dense sample which globally behaves in a strain-hardening manner. A critical state line $q = \eta p'$ is drawn for three stress paths and the value of slope η is identified as 1.16. η and the Mohr-Coulomb friction angle β' is computed to be 29.1° by the following

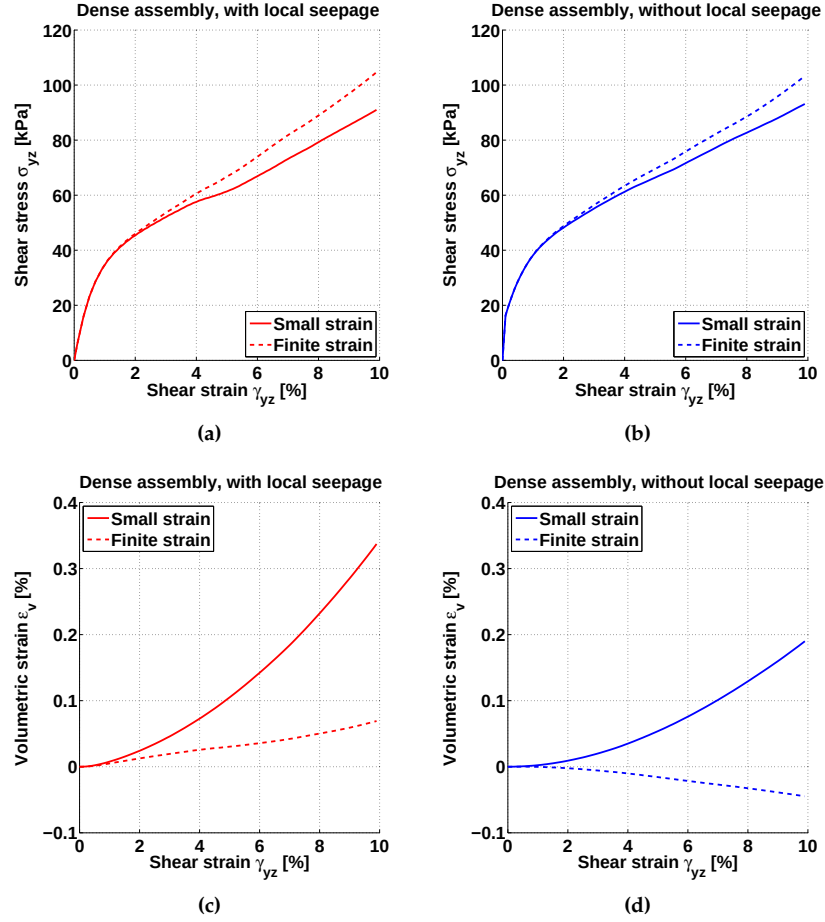


Figure 11: Comparison of global shear stress and global volumetric strain behavior between small strain and finite strain formulation. Left: globally undrained with local diffusion condition, Right: globally undrained but without local diffusion condition

relation for cohesionless soil [Woo90]:

$$\sin \beta' = \frac{3\eta}{6 + \eta} \quad (40)$$

, which is close to the inter-particle friction angle $\beta = 30^\circ$. Paths of ϵ_v further demonstrate that large local volume change up to 5.5% is possible even globally the sample is only dilated about 0.07%. According to these figures, the small strain and finite strain shear responses are almost identical. The stress

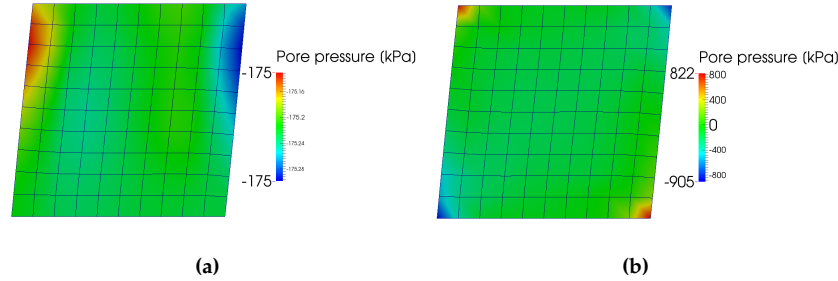


Figure 12: Comparison of pore pressure at 10% shear strain between (a) dense sample with local seepage and (b) dense sample without local seepage

path curves exhibit little difference. However, geometrical non-linearity has more significant effect on volumetric strain path. A major remark is that, inside the strain-softening spot as 14(d), the small strain solution has large fluctuation when the mean effective stress is very small, because DEM assemblies are highly unstable with nearly zero confining stress. On the contrary, finite strain scheme avoids this unstable regime and yield smooth solutions.

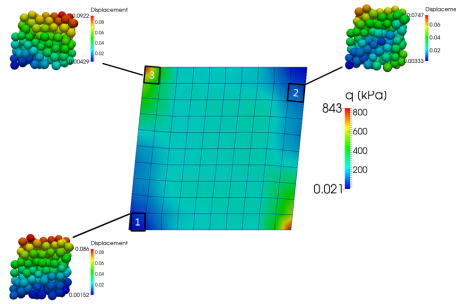


Figure 13: Spatial distribution of shear stress q at 10% shear strain for globally undrained dense sample allowing seepage within the specimen, attached with displacement magnitude of grains in unit cells (normalized by the initial cell size)

Lastly, we investigate the rate-dependent shearing behavior using the proposed coupling scheme. A faster shearing of saturated granular sample influences its mechanical response mainly by speeding up the solid matrix rearrangement and also by allowing less fluid diffusion inside the sample between loading steps. The former effect leads to swelling of the sample, while

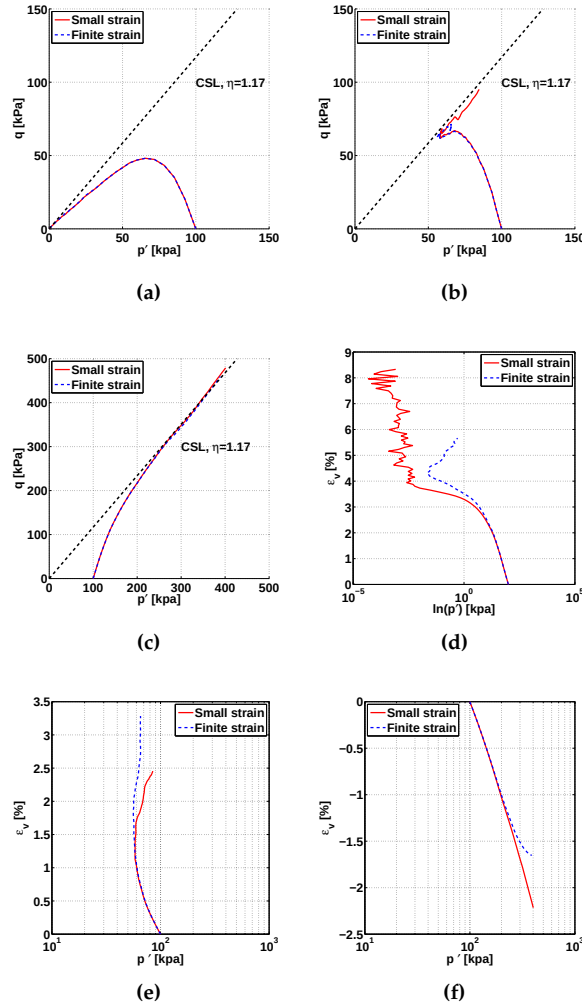


Figure 14: Shear stress vs. effective mean stress at different locations indexed as Fig. 13: (b) stress path at point 1 (c) stress path at point 2 (d) stress path at point 3; Volumetric strain vs. effective mean stress at different locations: (e) volume path at point 1 (f) volume path at point 2 (g) volume path at point 3

the latter renders the specimen more locally undrained. Fig.15 illustrates the combined effect of these two mechanisms on a dense sample with local seepage. The evolution of shear stress and volumetric strain with shearing rates of 0.1% and 0.5% per second are compared. When shearing is completed, shear stress sustained by the sample increases about 4.6% under higher shearing

rate. The rate effect on volumetric strain is more prominent, by the fact that the sample experiences more volume expansion of about 13.5% at the end.

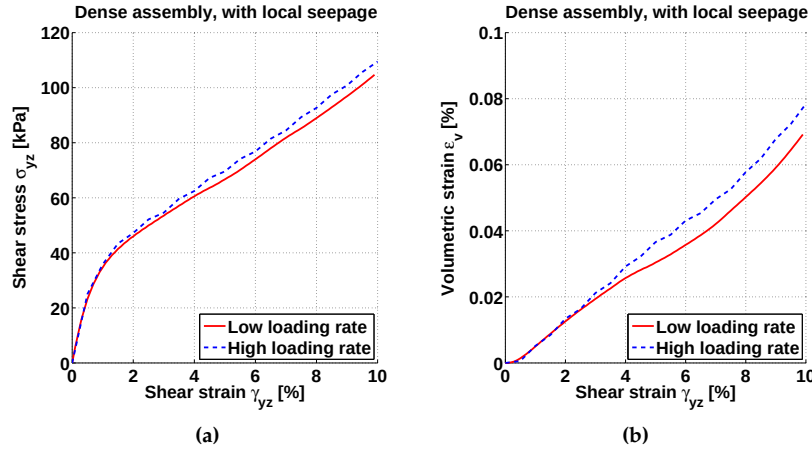


Figure 15: Comparison of global shear stress and global volumetric strain behavior between low loading rate (0.1% shear strain per second) and high loading rate (0.5% shear strain per second), finite strain formulation

4.5 Numerical Example 2: Globally drained triaxial compression test

The third example consists of the globally drained triaxial compression test on an isotropically consolidated cylindrical specimen. This example demonstrates the applicability of the proposed multiscale finite strain scheme on 3D problems. In this numerical example, we analyze (1) the difference between quarter-domain and full-domain simulations for material subjected to axial-symmetrical loading, (2) the consequence of the build-up of excess pore pressure due to a high loading rate and (3) the evolution of the fabric tensor inside and outside the shear band and the implications on the critical state of the materials. As a result, water is allowed to flow through the bottom and the top of the specimen. However, triaxial compression simulation is intentionally not conducted under a fully drained condition at a material point level. Instead, the rate dependence of the constitutive responses introduced via the hydro-mechanical coupling effect is studied to quantify what is the acceptable range of the prescribed loading rate that can prevent significant amount of excess pore pressure.

In addition, microscopic information such as the Biot's coefficient, Biot's modulus and micro-structure fabric are provided to highlight the advantage of the DEM-FEM coupled model. The convergence profile of this simulation is also

presented. In an experimental setting, the drained triaxial test is performed on a cylindrical water-saturated soil specimen, laterally enveloped by rubber membrane and drained through top and bottom surfaces. One of the idealized 3D numerical model constitutes only a quarter of the cylinder by assuming the rotational symmetry. The constant confining pressure is directly applied on the lateral surface, neglecting the effect of rubber membrane. The quasi-static compression is achieved by gradually increasing the axial strain ϵ_z at the rate of 0.05% per second. The lateral surface is impermeable and a no-flux boundary condition is imposed, while the pore water pressure on both top and bottom surfaces are constrained to be 0. Another simulation is triaxial compression of the full cylindrical domain. Similar confining pressure and pore pressure boundary conditions are applied. The middle point of the bottom surface is fixed to prohibit rigid body translation. The geometry, mesh and boundary conditions of the quarter-/full-domain simulations are illustrated in Fig. 16. The DEM assembly adopted in these simulations is identical to the dense sample in the previous section. The fluid bulk modulus in this example is 2.2 GPa.

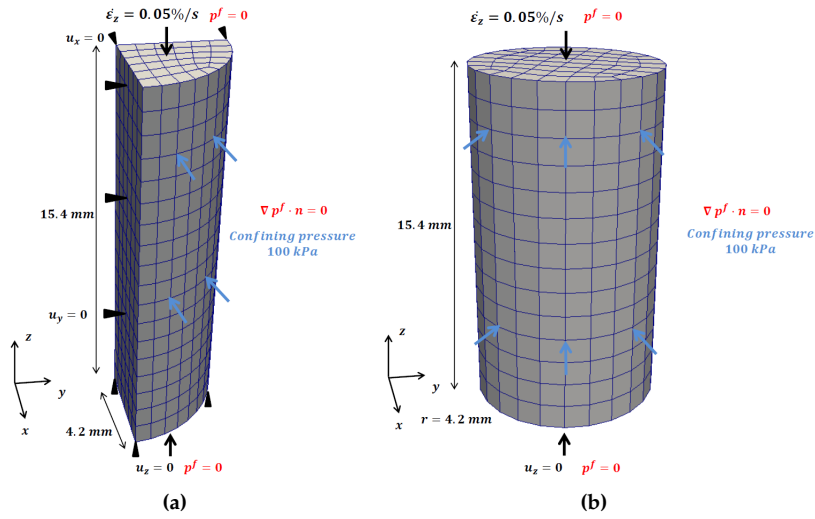


Figure 16: Geometry, mesh and boundary conditions for globally drained triaxial compression test. (a) Quarter-domain simulation. (b) Full-domain simulation

Fig. 17 compares the global shear stress and volumetric strain behavior from quarter-domain and full domain simulations. The shear stress curve obtained from full-domain simulation exhibits less peak stress and more significant softening than quarter-domain simulation. The volumetric strain curves,

however, only show notable difference after the axial strain approaches 7%. This discrepancy may be attributed to the strain localization in full-domain simulation, as shown by the distribution of deviatoric strain and porosity in Fig. 18. A dilatant shear band is developed inside the cylindrical specimen, while in the quarter-domain, the deformation is nearly homogeneous. This difference is more profound given the fact that the proposed model also incorporates the geometrical effect at the finite strain range. Results from this set of simulations show that the quarter-domain simulation is insufficient to capture the deformed configuration when bifurcation occurs. While the assumption of axial-symmetry is valid before the onset of strain localization, enforcing axial-symmetry via reduced domain and additional essential boundary condition may eliminate the bifurcation mode(s) that is not axial-symmetric.

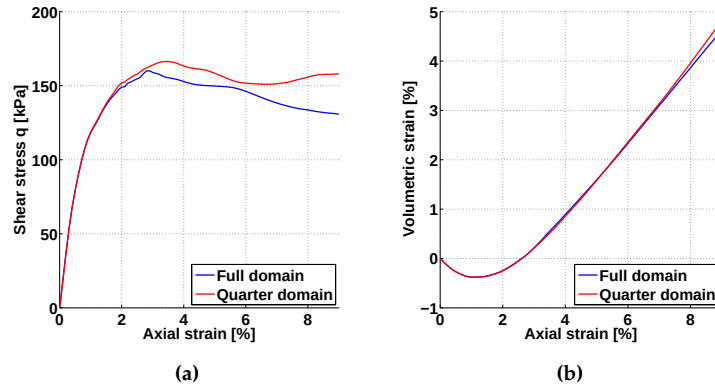


Figure 17: Global shear stress and volumetric strain behavior in globally drained triaxial compression test. Comparison of quarter-domain and full-domain simulations

An additional full-domain simulation is performed at a strain rate ten times slower: $\dot{\epsilon}_z = 0.005\%$ per second. The global shear stress and volumetric strain behavior are compared for the two loading rates in Fig. 19. The specimen under higher strain rate can sustain higher shear stress, but the strain rate has very little influence on volumetric strain behavior. The evolution of pore pressure at the center of the cylindrical specimen in two cases are also shown in Fig. 20. At a high strain rate, the pore water does not have time to fully diffuse through local pores and reach steady state. As a result, excess pore pressure builds up to about 5 kPa while the specimen shrinks. The pressure then decreases and becomes negative when the specimen dilates. In the low-strain-rate case, the magnitude of pore pressure is about five times smaller while the trend looks similar of the high-strain-rate counterpart.

One of the advantages of substituting macroscopic phenomenological consti-

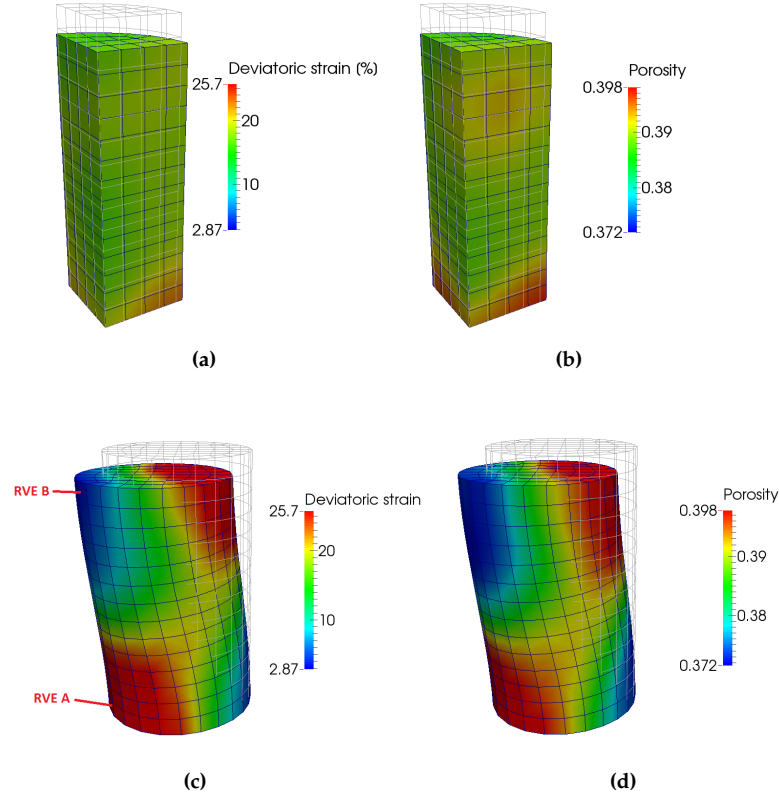


Figure 18: Distribution of deviatoric strain and porosity in globally drained triaxial compression test at 9% axial strain. Comparison of quarter-domain and full-domain simulations.

tutive model with DEM simulations for the poromechanics problem is that the macroscopic poro-elasticity properties, such as Biot's coefficient B , Biot's modulus M and effective permeability k could be inferred and updated from DEM at each Gauss point. As a result, the spatial variability of these poro-elasticity parameters triggered by material bifurcation or non-homogeneous loading can be properly captured. As an example, we monitor the evolution of these poro-elasticity parameters against axial strain ϵ_z for a RVE inside the shear band (RVE A, shown in Fig. 18(c)) and another RVE outside the shear band (RVE B, shown in Fig. 18(c)) in the $\dot{\epsilon}_z = 0.05\%$ -per-second, full-domain simulation (Fig. 21). The evolution of the Biot's coefficient B shown in Fig. 21(a) suggests that the effective bulk modulus of the solid skeleton (K_T^{DEM}) first increases and then decreases presumably due to the porosity changes in both RVEs A and B. The Biot's modulus M , which is related to the Biot's coeffi-

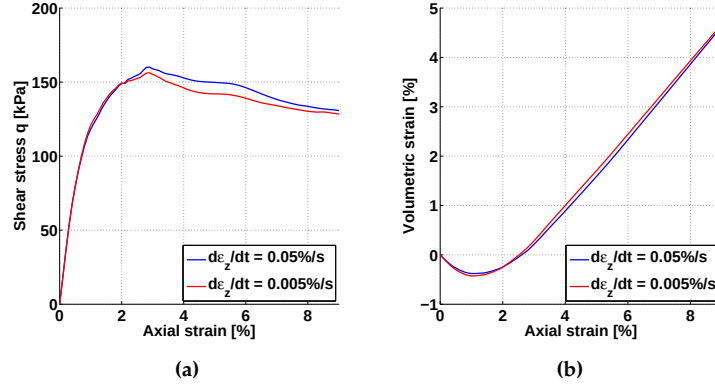


Figure 19: Global shear stress and volumetric strain behavior in globally drained triaxial compression test. Comparison of two loading rate.

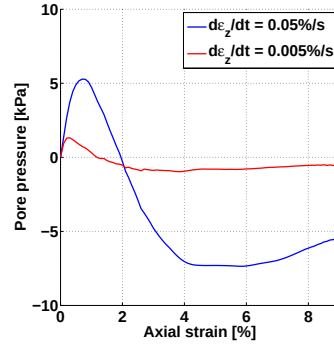


Figure 20: Evolution of pore pressure at the center of the cylindrical specimen during triaxial compression test subjected to two loading rate.

cient B and porosity ϕ , exhibits an initial reduction and largely increases after about $\varepsilon_z = 2\%$ for RVE A. For RVE B, M stays at a constant value. The effective permeability k also evolves with the porosity according to the Kozeny-Carmen relation.

Another advantage of the multiscale scheme is the accessibility to evolution of micro-structures during deformations. To demonstrate this, we perform a simple microstructural analysis in which the Anisotropic Critical State Theory (ACST) introduced by [LD12, ZG13, LD15] is adopted to analyze the fabric of the fluid-saturated granular assemblies at the finite strain range. The fabric anisotropy of two RVEs, one taken inside the shear band (RVE A) and another

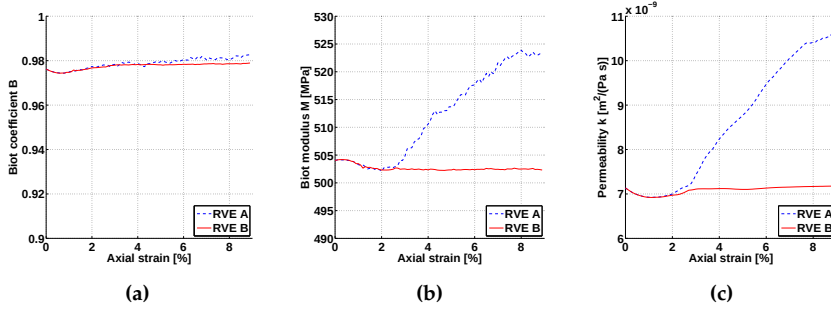


Figure 21: Evolution of (a) Biot's coefficient, (b) Biot's modulus and (c) effective permeability for RVE A (inside shear band, Fig. 18(c)) and RVE B (outside shear band, Fig. 18(c)).

one in the host matrix (RVE B) are analyzed and compared against each other. The fabric tensor G_{fabric} is contact-normal-based and is computed from a DEM RVE via [LD15]

$$G_{\text{fabric } ij} = \frac{1}{N_c} \sum_{c \in N_c} n_i^c n_j^c \quad (41)$$

where n^c is the unit vector of contact normal and N_c is the number of contacts inside the RVE. The tensor F_{fabric} characterizes the fabric anisotropy of the RVE and is written as [ZG13]

$$F_{\text{fabric } ij} = \frac{15}{2} (G_{\text{fabric } ij} - \frac{1}{3} \delta_{ij}) \quad (42)$$

where δ_{ij} is the Kronecker delta. Its norm F_{fabric} and direction n_F are defined by

$$F_{\text{fabric}} = F_{\text{fabric}} n_F, \quad F_{\text{fabric}} = \sqrt{F_{\text{fabric}} : F_{\text{fabric}}} \quad (43)$$

To analyze whether and how fabric evolves differently inside shear band and the host matrix, we compute the normalized fabric anisotropy variable (FAV) $A = n_F : n_s$ (a measure introduced in [LD12, ZG13] that quantifies the relative orientation of the tensor F_{fabric} and the deviatoric stress tensor s) for RVE A (inside shear band) and RVE B (outside shear band). The evolution of deviatoric stress q and porosity against axial strain ε_z are also monitored to measure how close the materials in the two RVEs reach the critical state according to the anisotropic critical state theory, i.e.,

$$\eta = \eta_c, \quad e = e_c = \hat{e}_c(p) \quad \text{and} \quad A = A_c = 1 \quad (44)$$

where η is the ratio between the effective mean pressure p' and the deviatoric stress q and e is the void ratio. $\eta_c, e_c = \hat{e}_c(p)$ and $A_c = 1$ are critical state values of the stress ratio, void ratio and fabric anisotropy variable (cf. [LD12, LD15]).

The results are summarized in Fig. 22. The stress-strain response shown in Fig. 22(a) indicates that RVE A becomes unstable after the peak shear stress and experiences significant dilation until the critical state indicated by the plateau in the porosity curve. The normalized FAV of RVE A rises to about 0.96 quickly upon subjected to the triaxial loading. Then, normalized FAV stay close to 1, which indicates that the fabric and stress directions in RVE A is nearly coaxial, as the RVE A approaches the critical state.

On the other hand, RVE B, which lies outside the shear band, experiences slightly more softening, but the dilatancy is much less than RVE A. The FAV curve of RVE B deviates from the curve of RVE A after axial strain of 2% and exhibits opposite trend that the fabric and stress directions loss coaxiality. This observation suggests that the critical states are not achieved simultaneously within an specimen that forms deformation band.

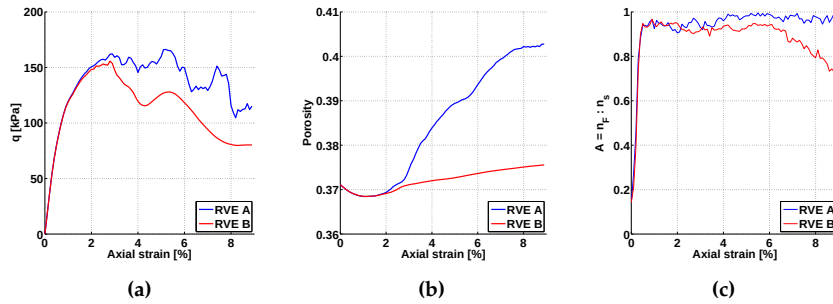


Figure 22: Evolution of (a) deviatoric stress q (b) porosity (c) $A = n_F : n_s$ (relative orientation between anisotropic fabric and deviatoric stress directions) during triaxial compression test ($\dot{\epsilon}_z = 0.05\%/s$) for RVE A (inside shear band, Fig. 18(c)) and RVE B (outside shear band, Fig. 18(c)).

To demonstrate the performance of the multiscale semi-implicit scheme, the convergence rate of the quarter-domain simulation is illustrated in Fig. 23 as an example. At different strain levels, the convergence curves show linear profiles in the logarithm-scale plot. The first step converges the fastest since the RVEs are linear elastic at $\epsilon_z = 0.1\%$.

The number of iterations required for convergence increases to 11 when the global shear stress reaches the peak (about $\epsilon_z = 2\%$). In the softening stage, the explicitly treated the elastic-plastic contribution K^{ep} to the material tangential stiffness becomes more significant. Therefore the convergence rate is further reduced and each time step requires about 20 iterations.

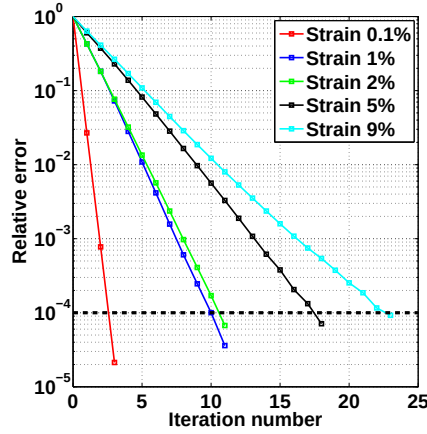


Figure 23: Convergence profiles of the triaxial compression test at different axial strain levels. The relative error is defined as $\frac{\|\Delta F^i\|}{\|\Delta F^{(i=0)}\|}$, where ΔF^i is the residual force at the iteration step i . The convergence is reached when the error falls below 10^{-4} .

5 Multiscale homogenization for embedded discontinuities

Here we present the procedure to obtain the hydro-mechanical constitutive updates for embedded strong discontinuity from microscale simulations on RVEs nested inside the material interfaces. The computational homogenization schemes of single-physics material layers have been explored in a number of previous studies [HRSS09, CKBG12, BKC⁺14, WS18]. For instance, [HRSS09] have introduced a procedure to generate an effective cohesive zone law for a single interface from microscale RVE. In those studies, FE^2 simulations with interface elements are used as the test bed. [CKBG12, BKC⁺14] establish a multi-scale approach for RVE (or Microstructural Volume Element as introduced in the literature) having localized zones and proposed a new generalized periodic boundary condition. The overall macro-homogeneous deformation is applied to the MVE and the stress and displacement jump are homogenized. The local equation to be solved is the consistency between the macro displacement jump and the homogenized displacement jump in the RVE, instead of the traction continuity equation. [TSH⁺14, TSP⁺16] proposed multiscale model at regular points (MMRp) and singular points (MMSp). It has been successfully used in enhanced strain finite element simulations [OCR⁺15]. In this study, the RVEs of discrete elements describe the underlying microstructures inside the discontinuity interface. Based on the effective

stress principle, the mechanical and hydraulic constitutive laws are obtained **separately** from two types microscale simulations, i.e. the grain-scale DEM simulation and the pore-scale LBM simulation, as explained in [SKR13] and [WS16]. In other words, the effective traction and the interfacial permeability (and hence the interfacial Darcy's velocity) are both obtained from the same deformed configuration. However, the deformed configuration is not obtained from LBM-DEM simulations but from DEM simulations that generate the admissible boundary conditions by assuming the validity of the effective stress principle. The major advantage of this approach is two-fold. First, the calculations of the interfacial permeability are much faster. This is due to the fact that the de-coupled permeability calculation can be conducted offline such that the trained and validated neural network can be used to replace the costly LB simulations). The second advantage is the simplicity. As the effective stress approach does not require the introduction of particle-scale hydro-mechanical force and any treatment to update the fluid-solid boundary at pore scale. Nevertheless, it should be noted that the validity of this split approach is designed for the case in which the effective stress principle is applicable for the dual-permeability system. In many situations that involve particle erosion [GTSMW15, TPF⁺17], soil liquefaction [ESA14], or solid-fluid mixture with non-Darcy flow or high Reynold's number, such a simplification may lead to significant errors. In such cases, one must derive the corresponding Hill-Mandel condition for the multi-physical poromechanics problems to obtain the admissible boundary conditions and apply them to the DEM-LBM model or use direct numerical simulation (DNS) to capture the multi-physical problems.

The homogenization procedure of mechanical constitutive law for interface is an extension of the approach described in [HRSS09] to particle assembly using the theory in [MD04, MDZ10]. Consider a domain at the continuum scale discretized by a finite element mesh with enhanced assumed strain or extended finite element to capture the displacement jump kinematics 24.

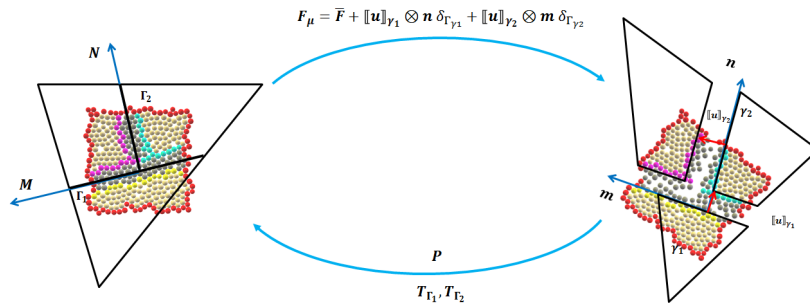


Figure 24: discrete element-informed interface constitutive responses.

At a material point across the interface, there exists a cubic sampled assem-

bly of discrete particles representing the granular material inside the strong discontinuity (Fig. 25). The body force is negligible at micro-scale. This RVE of domain Ω_μ and boundary $\partial\Omega_\mu$ has an initial height of h_μ^0 and is associated with a coordinate system with basis vectors $\mathbf{M}_\mu$ and $\mathbf{N}_\mu$. Choose the geometric center as the origin and place the RVE in alignment with the normal and tangential directions of the strong discontinuity Γ in the reference configuration ($\mathbf{N}_\mu = \mathbf{N}$, $\mathbf{M}_\mu = \mathbf{M}$). The current position $\mathbf{x}_\mu^c$ of a center of a particle is related to its position $\mathbf{X}_\mu^c$ in the reference configuration via the deformation map $\boldsymbol{\varphi}_\mu$. The local deformation gradient $\mathbf{F}_\mu = \frac{\delta \boldsymbol{\varphi}_\mu}{\delta \mathbf{X}_\mu^c}$. The volume average of $\mathbf{F}_\mu$ is given as:

$$\langle \mathbf{F}_\mu \rangle = \frac{1}{V_0} \int_{\Omega_\mu} \mathbf{F}_\mu d\Omega_\mu = \frac{1}{V_0} \sum_i^{N_{bound}} (\mathbf{x}_\mu^c)_i \otimes \mathbf{A}_i^c, \quad (45)$$

where V_0 is the initial volume of the RVE. $\mathbf{A}_i^c$ is the surface vector of $\partial\Omega_\mu$ associated with the particle i and N_{bound} is the number of particles on $\partial\Omega_\mu$. Assuming rigid particles, the motion of a particle material point can be decomposed to the motion of the particle center and the particle rotation, i.e.,

$$\mathbf{x}_\mu = \mathbf{x}_\mu^c + \mathbf{R}_\mu \cdot (\mathbf{X}_\mu - \mathbf{X}_\mu^c); \quad \mathbf{x}_\mu^c = \langle \mathbf{F}_\mu \rangle \cdot \mathbf{X}_\mu^c + \mathbf{w}_c, \quad (46)$$

where $\mathbf{w}_c$ is the particle center displacement fluctuation and $\mathbf{R}_\mu \in SO(3)$ describes the particle rotation.

The overall effective Piola stress is given by the volume average

$$\langle \mathbf{P}'_\mu \rangle = \frac{1}{V_0} \int_{\Omega_\mu} \mathbf{P}'_\mu d\Omega_\mu = \frac{1}{V_0} \sum_{cont}^{N_{cont}} \mathbf{f}_\mu^{cont} \otimes \mathbf{L}_\mu^{cont} = \frac{1}{V_0} \sum_i^{N_{bound}} (\mathbf{f}_\mu^{ext})_i \otimes (\mathbf{X}_\mu^c)_i, \quad (47)$$

where $\mathbf{f}_\mu^{cont}$ is the contact force at the grain contact $\mathbf{x}_\mu^{cont}$. $\mathbf{L}_\mu^{cont}$ is the initial branch vector, the vector that connects the centroids of two grains forming the contact. N_{cont} is the total number of particles contacts in the RVE. $(\mathbf{f}_\mu^{ext})_i$ is the external support force acting on the boundary particle i . The transition between the summation involving contact forces and the summation involving external support forces is ensured by the equilibrium of the RVE of particles.

The volume average of the virtual power in the RVE is given by

$$\langle \mathbf{P}'_\mu : \dot{\mathbf{F}}_\mu \rangle = \frac{1}{V_0} \int_{\Omega_\mu} \mathbf{P}'_\mu : \dot{\mathbf{F}}_\mu d\Omega_\mu = \frac{1}{V_0} \sum_i^{N_{bound}} (\mathbf{f}_\mu^{ext})_i \cdot (\dot{\mathbf{x}}_\mu^c)_i. \quad (48)$$

The Hill-Mandel micro-heterogeneity condition requires the volume average of the virtual power in the RVE to equal the virtual power done by the volume averages of power-conjugate stress and deformation measures:

$$\langle \mathbf{P}'_\mu : \dot{\mathbf{F}}_\mu \rangle = \langle \mathbf{P}'_\mu \rangle : \langle \dot{\mathbf{F}}_\mu \rangle. \quad (49)$$

Since the constitutive behavior of the RVE is homogenized to a traction-separation law on the interface, the Hill-Mandel condition is recast into the form involving power-conjugate effective traction and displacement jump measures

$$h_0 \langle \mathbf{P}'_\mu : \dot{\mathbf{F}}_\mu \rangle = \langle \mathbf{T}'_\Gamma \rangle \cdot \mathcal{L}_v \llbracket \mathbf{u} \rrbracket = \langle \mathcal{T}_\Gamma \rangle \cdot \llbracket \dot{\mathbf{u}} \rrbracket. \quad (50)$$

For the transition between the macro-scale kinematics of the strong discontinuity and the deformation of the micro-scale RVE, the volume average of deformation gradient is defined as

$$\langle \mathbf{F}_\mu \rangle = \mathbf{I} + \frac{1}{h_\mu^0} \llbracket \mathbf{u} \rrbracket \otimes \mathbf{N}. \quad (51)$$

The effective nominal traction $\langle \mathbf{T}'_\Gamma \rangle$ averaged in the RVE representing the interface is given by:

$$\langle \mathbf{T}'_\Gamma \rangle = \langle \mathbf{P}'_\mu \rangle \cdot \mathbf{N}. \quad (52)$$

Among the admissible boundary conditions fulfilling the Hill-Mandel micro-heterogeneity condition, we adopt the periodic boundary conditions, where for a pair of particles on opposite boundaries $\partial\mathcal{V}^+$ and $\partial\mathcal{V}^-$, the periodicity enforces the periodicity of fluctuations and rotations

$$\mathbf{w}_c^- = \mathbf{w}_c^+, \quad \mathbf{R}_\mu^- = \mathbf{R}_\mu^+, \quad (53)$$

and the anti-periodicity of support forces and couples

$$\mathbf{a}_c^- = -\mathbf{a}_c^+, \quad \mathbf{m}_c^- = -\mathbf{m}_c^+, \quad (54)$$

where $\mathbf{a}_c$ is the opposite of the resultant force on the boundary particle exerted by other particles, $\mathbf{m}_c$ is the opposite of the resultant couple about the center $\mathbf{X}_c$ on the boundary particle.

5.1 Offline incremental data-driven hydraulic responses for strong discontinuities

The homogenization procedure used to obtain the effective permeability from a microstructure RVE has been previously studied in [DOS06, OSDKL07, SAR11, SKR13]. Here we apply the same procedure to obtain the homogenized effective permeability of the embedded strong discontinuities. Assume that the separation of the spatial length scale is valid, one may use the Hill-Mandel lemma corresponding to Darcy's flow problem to determine the admissible boundary condition for the flow problems. Recall that the Hill-Mandel lemma requires that

$$\langle \nabla^x p_M \cdot \mathbf{q}_M \rangle_x = \langle \nabla^x p_M \rangle_x \cdot \langle \mathbf{q}_M \rangle_x \quad (55)$$

where $\langle \cdot \rangle_x$ is the spatial volume averaged operator.

As shown in [DOS06] and [OSDKL07], this can lead to a number of admissible boundary conditions. For instance, one may either prescribe flux or pore pressure gradient in two opposite faces of the RVEs. One interesting aspect found in previous works (cf. [DOS06, SAR11, SKR13, KSW15]) is that the choice of the boundary condition does not affect the effective permeability once the size of the RVE is sufficiently large. We follow the treatment in [dB17] and assume that there is no pore pressure jump across the interface, whereas discontinuous mass flux is admissible.

The effective permeability tensor of a RVE can be determined via inverse fluid flow problem performed on the deformed RVE subjected to prescribed loading paths. The Eulerian fluid flux vector $\mathbf{q}$ within the RVE is computed when subjected to Eulerian pressure gradient $\nabla^x p$, and the macro-pore effective permeability $\mathbf{k}_{\text{RVE}}^M$ is determined by Darcy's law

$$\mathbf{q}_M = -\frac{1}{\mu} \mathbf{k}_{\text{RVE}}^M \nabla^x p_M. \quad (56)$$

μ is the dynamic viscosity of the fluid. We assume that the normal and tangential directions of the interface are also the principal directions of the macro-pore effective permeability tensors. Thus, we need only two hydraulic simulations to determine the permeability values normal and tangential to the interface, denoted as k_n^M and k_m^M , respectively. Thus the permeability tensor is expressed as

$$\mathbf{k}_{\text{RVE}}^M = k_n^M \mathbf{n} \otimes \mathbf{n} + k_m^M \mathbf{m} \otimes \mathbf{m}, \quad (57)$$

where $\mathbf{n} = \bar{\mathbf{F}} \cdot \mathbf{N}$ and $\mathbf{m} = \bar{\mathbf{F}}^{-T} \cdot \mathbf{M}$. We choose the lattice Boltzmann (LB) method to solve the inverse fluid flow problem. For brevity, we omit the description of the LB method. Interested readers are referred to [SARE11, SKR13] and [KSW15] for details. The LB code used in this study is a C++ open source code called Palabos [DBBM10]. The procedure to obtain the two normal and tangential components is as follows. We first record the positions of all grains in the deformed microstructural assembly at different strain levels. As the size of each grain is known, the configuration of the pore space can be reconstructed and subsequently converted into binary images (cf. [SKR13]). Then, pore pressure difference is imposed on two opposite sides orthogonal to the flow direction and no-flow boundary conditions are applied on the four remaining side faces. This setting leads to a macroscopic pressure gradient. As the lattice Boltzmann flow simulation reaches steady state, the resultant fluid flow velocity is computed and the permeability value is derived via Darcy's law (Fig. 25). Fig. 28 illustrates an example computation of permeabilities from LBM. The RVE is subjected to various displacement loading paths with loading-unloading cycles. The evolution of normal and tangential permeabilities predicted by the neural network are presented and are compared to the empirical Kozeny-Carman equation.

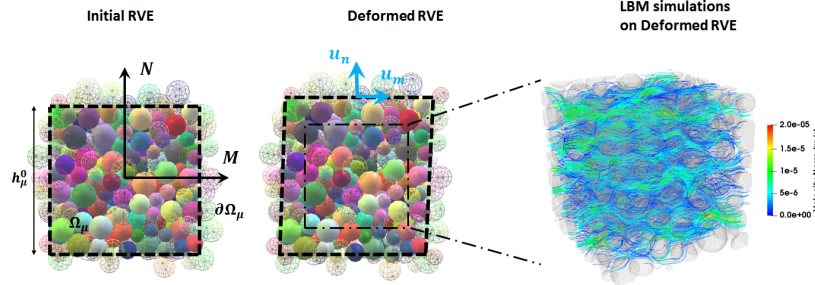


Figure 25: Initial and deformed configurations of the particle assembly representing the granular materials inside strong discontinuity. The effective permeabilities in the normal and tangential directions are determined by Lattice-Boltzmann simulations on representative volume of current particle assembly.

The numerical solutions of Stokes equations using Lattice-Boltzmann method yield accurate results, especially in the low Reynold number regime, but require significant computational resources to resolve the flow field at pore space. To achieve a reasonable accuracy, the number of degree of freedoms required to obtain the effective permeability is at least a few orders more than those used in discrete element simulations [SKR13]. Thus, querying the effective permeability tensor from LBM simulations from each RVE for all incremental steps during a multiscale simulation is computationally expensive. In this work, we resort to a deep learning approach to predict the effective permeability for each incremental step. The design, training, and testing of the LSTM network on path-dependent material constitutive laws are detailed in a separate and dedicated work (cf. [WS18]). For completeness, a brief overview is provided.

First, a database containing the prescribed displacement jump loading paths, porosity and associated computed permeabilities is established by running multiple LBM simulations on deformed discrete element RVEs. Then, a recurrent neural network consisting of Long-Short-Term-Memory (LSTM) layers (see Figure 26) is trained using the database generated by LBM simulations [HS97, WS17]. In a nutshell, the training process attempts to minimize an objective function by adjusting the weights of each neuron in the layers through a back-propagation process. The LSTM approach is different than the traditional feed-forward neural network proposed by [GPZHA98] and [LS02] in the sense that (1) the LSTM neuron (see Figure 27) has the capacity to use internal memory to process history and sequence and hence ideal for predictions for path-dependent materials, (2) the LSTM networks are designed to avoid a problem called vanishing or exploding gradient problems that may otherwise lead to issues during the training process.

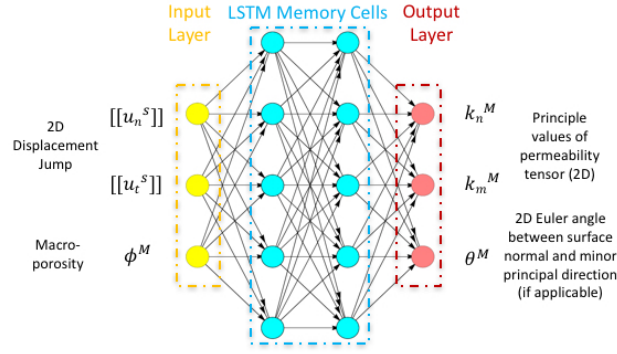


Figure 26: The recurrent neural network used to predict the permeability of the interface.

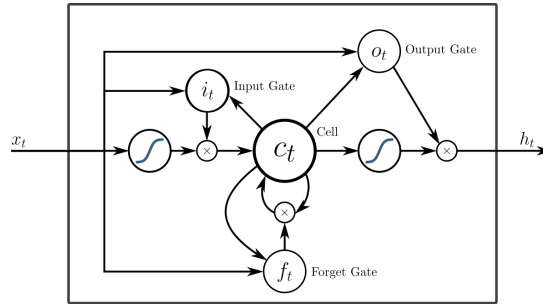


Figure 27: A LSTM block with input, output and forget gates.

Finally, in each incremental update of the multiscale strong discontinuity simulation, the updated effective permeability components are generated by propagating signals from the input layer of the recurrent neural network to the output layers. In this particular case, the current displacement jumps and porosity are used as the input and the principal values and the spectral directions of the effective permeability tensor are the output of the recurrent neural network. One important upshot of this approach is that the querying time is largely reduced, as the deep learning permeability model typically requires only few seconds to make predictions.

5.2 Numerical Example: Reactivation of faults

This example analyzes the slip of a pre-existing and formerly stable fault in saturated soil triggered by the injection of water at a nearby location. The idealized problem geometry and boundary conditions are shown in Fig. 29.

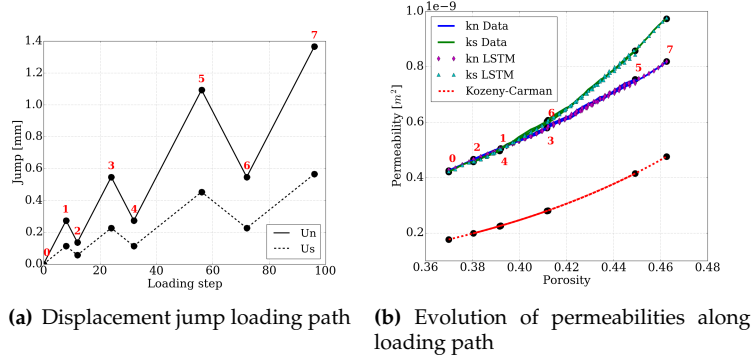


Figure 28: Example of permeability data generated from LBM simulations on RVEs undergoing loading-unloading sequences. (a) loading path of the normal U_n and tangential displacement jumps U_s . (b) Comparison between the normal k_n and tangential k_s permeability data from LBM simulations and the permeability components from predictions of LSTM neural network model.

The calculation from empirical Kozeny-Carman equation $k = \frac{d_{50}^2}{180} \frac{\phi^3}{(1-\phi)^2}$ ($d_{50} = 1mm$) is shown for comparison.

The dimensions of the 2D field of saturated porous media are 10 m x 10 m. The domain is constrained in the x-direction on the left boundary and in the y-direction on the bottom boundary. A foundation has been constructed on top of the domain, generating a uniform loading pressure of 10 MPa. A lateral confining pressure of 5 MPa is applied on the right boundary for the frictional porous media to sustain the vertical load. There exists a 45-degree fault under the foundation. The entire system is stable and has been in equilibrium for a long time since the construction of the foundation, thus the excess pore pressures in both fractures and host matrix are zero. The initial effective stress of the porous solid is hence

$$\sigma'_{\text{Init}} = \begin{bmatrix} -5 & 0 \\ 0 & -10 \end{bmatrix}_{xy} \text{ MPa}, \quad (58)$$

where the subscript xy refers to the coordinate system $\{x, y\}$ depicted in Fig. 29.

The DEM RVEs characterizing the traction-separation law of the fault are placed in alignment with the strong discontinuity. They must be in the initial stress state consistent to the macroscopic boundary conditions. From the initial stress state of the macro-scale problem (Eq. 58) and via a coordinate transformation ($\sigma^{mn} = R^T \cdot \sigma^{xy} \cdot R$), the initial stress tensor of the DEM as-

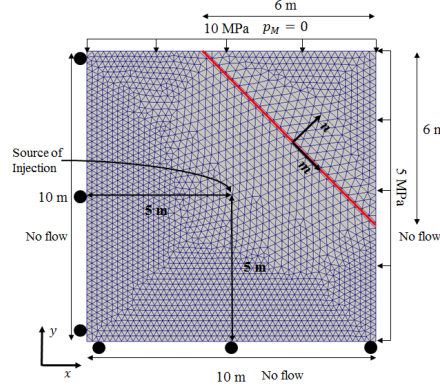


Figure 29: Geometry of fault reactivation problem and boundary conditions. Red line represents the pre-existing fault.

semblies is expressed as

$$\sigma'_{\text{InitRVE}} = \begin{bmatrix} -7.5 & 2.5 \\ 2.5 & -7.5 \end{bmatrix}_{mn} \text{ MPa}, \quad (59)$$

where the subscript mn refers to the rotated frame $\{m, n\}$ for the fault depicted in Fig. 29. The initial DEM RVEs in this stress state provide the correct amount of initial shear and normal tractions along the strong discontinuity.

In this example, the particle contact model for DEM is frictional and without cohesion. The normal and tangential permeabilities are obtained from machine learning models trained with LBM simulation data. The bulk material is idealized as isotropic hyperelastic material. The permeability tensors in macro- and micro-pores of the bulk are assumed isotropic and evolve according to the Kozeny-Carman equation. The material parameters used in the numerical example are summarized in [WS19].

Water is injected to the macropore space (pre-existing fractures) of the field through the source S located at the center of the domain. The macropore pressure is zero on the top surface and the other three surfaces are no-flow boundaries. There is no drainage boundary for micropore pressure. This flow boundary condition is to suppress spurious micropore pressure oscillations near the drainage boundary [CB15]. The prescribed time history of Darcy velocity at the source is shown in Fig. 30. The injection profile is composed of injection-pause cycles, in which water supply is provided for 40 hours under a constant rate of 0.02 m/s, followed by a pause for 10 hours before the next cycle of injection. From the simulation results, the time history of the pore pressure in both scales at the source S is presented in Fig. 30. Upon injection or pause, the macropore injection pressure jumps up or plunges immediately,

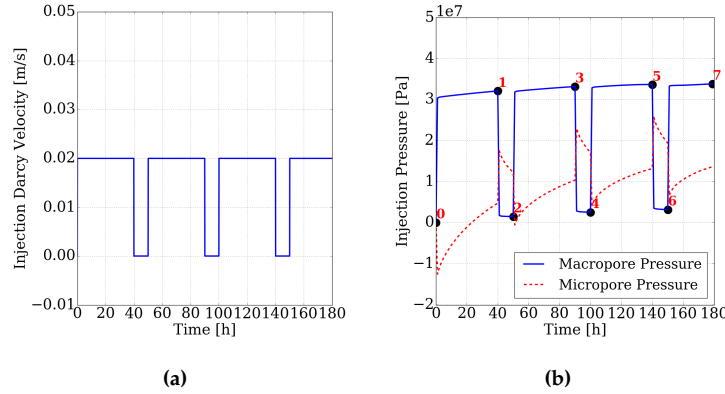


Figure 30: Water supply in the fault reactivation problem. (a) Time history of the prescribed injection velocity in macropore at the source point. (b) Computed responses of injection pressure in macropore and micropore at the source point. The numbers mark the sequence of injection-pause cycles.

while the micropore pressure at the injection point has the opposite behavior. This is caused by the low mass transfer permeability between the macropores and micropores. Then in the transient regime, when fluid gradually diffuses into the micropores by mass transfer, micropore pressure slowly approaches the macropore pressure. The two pressures will eventually be identical when the diffusion between pores reaches equilibrium.

The macropore and micropore pressure field at time 40 h, 100 h and 180 h are presented in Fig. 31. The pressure plume is initially of the shape of a circle and then expands as the increasing amount of water are being injected through the source. The pore pressure drops when the injection pauses, but the plume is still expanding, driven by the excess pore pressure that has not been entirely diffused. When the injection is resumed, the pore pressure rises again.

The presence of the fault with higher permeability disturbs the pressure plume. The fluid flows more quickly to the top surface through the channel inside the fault. As for the micropore pressure field, it has a similar but delayed evolution behavior, due to the time required for the fluid transfer between macropores and micropores. The difference between macropore and micropore pressure is due to the different permeability in macropores and micropores for the fluid to diffuse in the macro-scale field, and also the low transfer permeability between pores.

Due to the fully coupled nature of the problem, the mechanical responses of the porous solid, especially the displacement jump and traction at the strong discontinuity, strongly depend on how pore fluid diffuses inside the pore

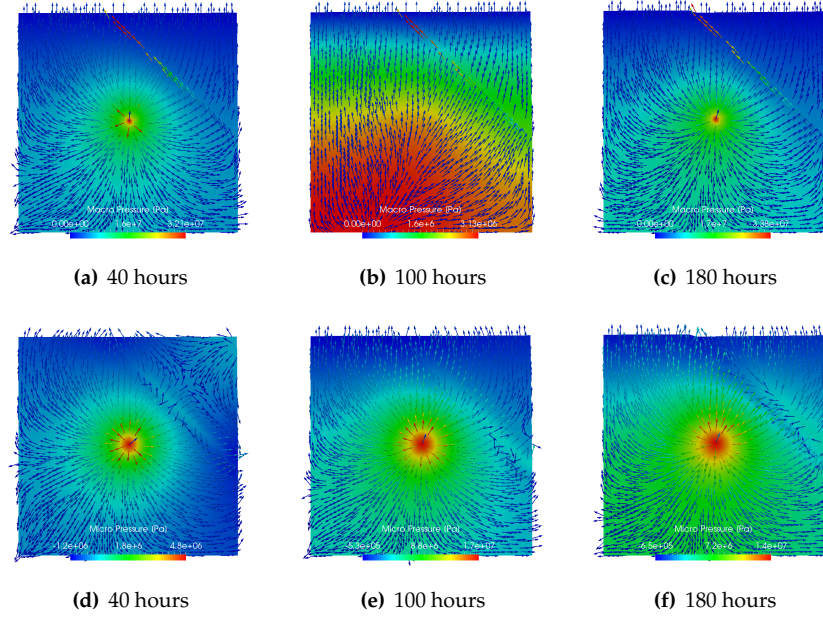


Figure 31: Evolution of macropore pressure (a-c) and micropore pressure (d-f) field. Arrows indicate the fluid flux vector field in macropores (a-c) and in micropores (d-f). The non-zero components normal to the impervious boundaries are due to the inaccuracy of the nodal projection of the flow vector field evaluated at quadrature points.

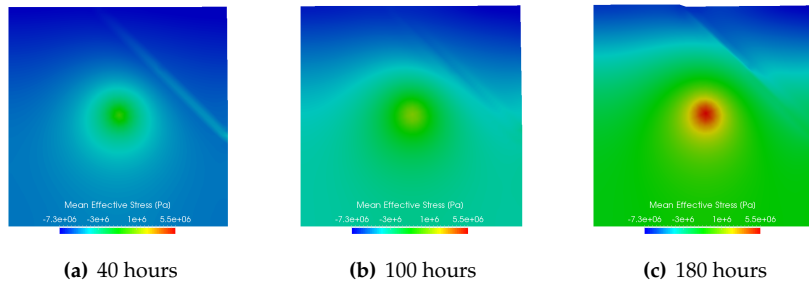


Figure 32: Evolution of the mean effective stress field in the macro-scale simulation.

space. The evolution of macro-scale mean effective stress field during the fluid injection cycles is shown in Fig. 32.

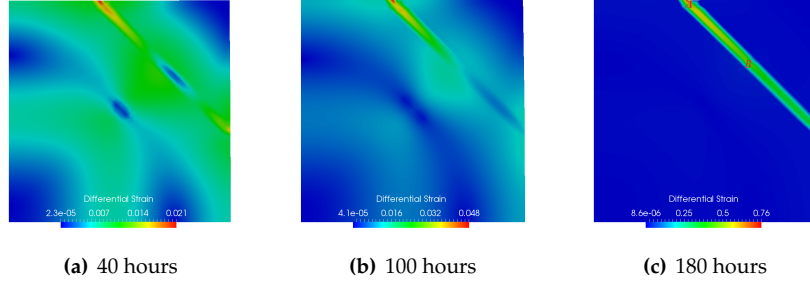


Figure 33: Evolution of the differential strain field in the macro-scale simulation.

The increase in the mean effective stress is due to the increase in excess pore pressure, in agreement to the effective stress principle. This results in a reduction in the normal compression traction. As the fault is frictional, this reduction in normal compression also reduce the shear strength and ultimately leads to the reactivation of the fault. The slip can be clearly observed from the changes in deviatoric strain field illustrated in 33. The deviatoric strain gradually increases and concentrates inside the fault zone.

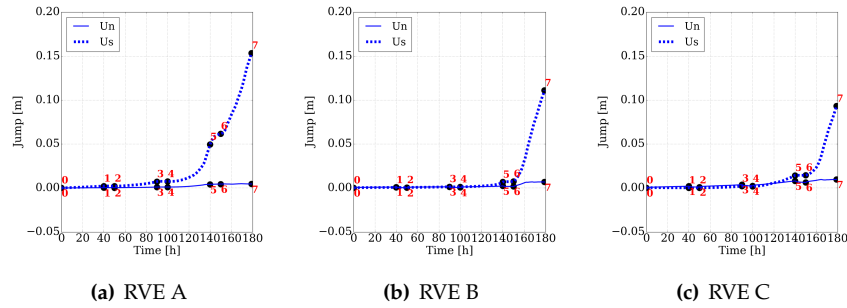
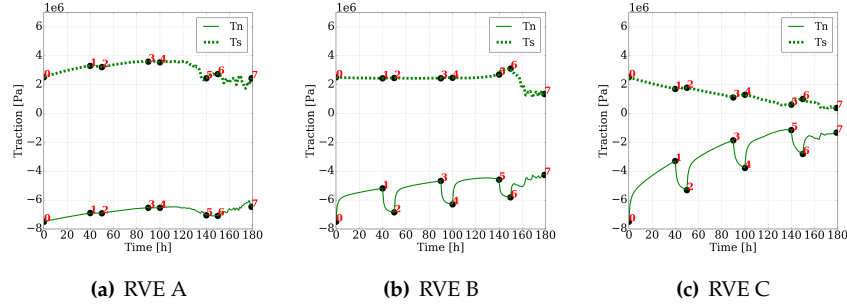


Figure 34: History of normal U_n and tangential U_s components of the displacement jump $[[u]]$ for local RVEs A, B and C (location shown in Fig. 33). The numbers mark the sequence of injection-pause cycles (Fig. 30).

This simulation result suggests the hazardous effect of injecting water to the underground, as a fast fluid flow may trigger the slip of a nearby pre-existing fault, leading to the failure of the foundation.

The Figures clearly illustrate the failure of the fault system by the opening and sliding of the local microstructures, caused by reductions in both normal and



The local responses to the fluid injection-pause cycles, including the spatial displacement jump, effective nominal traction and spatial macropore permeability, are illustrated in Fig. 34, Fig. 35 and 36 respectively for three locations A, B, C in the fault indicated in Fig. 33.

Figure 35: History of normal T_n and tangential T_s components of the effective nominal traction T' for local RVEs A, B and C (location shown in Fig. 33). The numbers mark the sequence of injection-pause cycles (Fig. 30).

tangential traction.

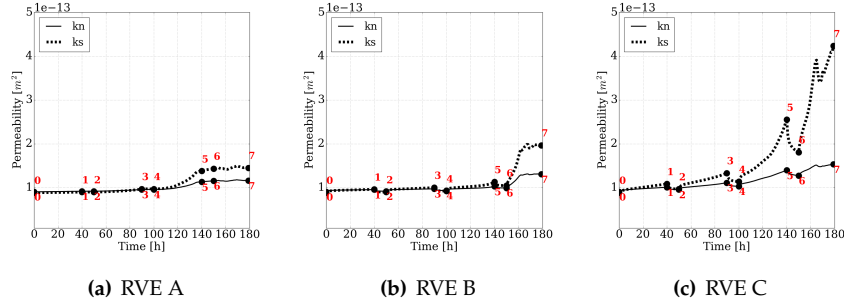


Figure 36: History of normal k_n and tangential k_s components of the macropore permeability k_{RVE} for local RVEs A, B and C (location shown in Fig. 33). The numbers mark the sequence of injection-pause cycles (Fig. 30).

These results demonstrate the capacity of our proposed multiscale model in capturing the complex mechanical and hydraulic behaviors of the interfacial materials. This is an improvement over the phenomenological traction-separation laws where idealized tensile and shear (linear or exponential) behavior is often adopted [PP11, BS18].

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References

- [Arm99] Francisco Armero. Formulation and finite element implementation of a multiplicative model of coupled poro-plasticity at finite strains under fully saturated conditions. *Computer methods in applied mechanics and engineering*, 171(3):205–241, 1999.
- [BA95] Ronaldo I Borja and Enrique Alarcón. A mathematical framework for finite strain elastoplastic consolidation part 1: Balance laws, variational formulation, and linearization. *Computer Methods in Applied Mechanics and Engineering*, 122(1):145–171, 1995.
- [Bag96] Katalin Bagi. Stress and strain in granular assemblies. *Mechanics of materials*, 22(3):165–177, 1996.
- [BBM87] Jacob Bear, Carol Braester, and Pascal C Menier. Effective and relative permeabilities of anisotropic porous media. *Transport in porous media*, 2(3):301–316, 1987.
- [BKC⁺14] Emanuela Bosco, VG Kouznetsova, EWC Coenen, MGD Geers, and Alberto Salvadori. A multiscale framework for localizing microstructures towards the onset of macroscopic discontinuity. *Computational Mechanics*, 54(2):299–319, 2014.
- [BS18] Eric C Bryant and WaiChing Sun. A mixed-mode phase field fracture model in anisotropic rocks with consistent kinematics. *Computer Methods in Applied Mechanics and Engineering*, 342:561–584, 2018.

- [CB15] Jinhyun Choo and Ronaldo I Borja. Stabilized mixed finite elements for deformable porous media with double porosity. *Computer Methods in Applied Mechanics and Engineering*, 293:131–154, 2015.
- [CCB14] Emanuele Catalano, Bruno Chareyre, and Eric Barthélemy. Pore-scale modeling of fluid-particles interaction and emerging poromechanical effects. *International Journal for Numerical and Analytical Methods in Geomechanics*, 38(1):51–71, 2014.
- [CKBG12] E WC Coenen, VG Kouznetsova, E Bosco, and M GD Geers. A multi-scale approach to bridge microscale damage and macroscale failure: a nested computational homogenization-localization framework. *International Journal of Fracture*, pages 1–22, 2012.
- [CLCC14] Xilin Cui, Jun Li, Andrew Chan, and David Chapman. Coupled dem–lbm simulation of internal fluidisation induced by a leaking pipe. *Powder Technology*, 254:299–306, 2014.
- [CMNN81] J Christoffersen, MM Mehrabadi, and S Nemat-Nasser. A micromechanical description of granular material behavior. *Journal of Applied Mechanics*, 48(2):339–344, 1981.
- [Cou04] Olivier Coussy. *Poromechanics*. John Wiley & Sons, 2004.
- [CS79] Peter A Cundall and Otto DL Strack. A discrete numerical model for granular assemblies. *Geotechnique*, 29(1):47–65, 1979.
- [CVW04] Jennifer Sinclair Curtis and Berend Van Wachem. Modeling particle-laden flows: A research outlook. *AIChE journal*, 50(11):2638–2645, 2004.
- [dB17] René de Borst. Fluid flow in fractured and fracturing porous media: A unified view. *Mechanics Research Communications*, 80:47–57, 2017.
- [DBBM10] Wim Degruyter, Alain Burgisser, Olivier Bachmann, and Orestis Malaspinas. Synchrotron x-ray microtomography and lattice boltzmann simulations of gas flow through volcanic pumices. *Geosphere*, 6(5):470–481, 2010.
- [DKU06] Luc Dormieux, Djimédo Kondo, and Franz-Josef Ulm. *Microporomechanics*. John Wiley & Sons, 2006.
- [DOS06] X Du and M Ostoj-Starzewski. On the size of representative volume element for darcy law in random media. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 462, pages 2949–2963. The Royal Society, 2006.

- [ESA14] Usama El Shamy and Yasser Abdelhamid. Modeling granular soils liquefaction using coupled lattice boltzmann method and discrete element method. *Soil Dynamics and Earthquake Engineering*, 67:119–132, 2014.
- [ESZ05] Usama El Shamy and Mourad Zeghal. Coupled continuum-discrete model for saturated granular soils. *Journal of engineering mechanics*, 131(4):413–426, 2005.
- [Fis13] Jacob Fish. *Practical multiscale modeling*. John Wiley & Sons, 2013.
- [GAS07] IM Gitman, H Askes, and LJ Sluys. Representative volume: existence and size determination. *Engineering fracture mechanics*, 74(16):2518–2534, 2007.
- [GMS13] William G Gray, Cass T Miller, and Bernhard A Schrefler. Averaging theory for description of environmental problems: What have we learned? *Advances in water resources*, 51:123–138, 2013.
- [GPZHA98] Jamshid Ghaboussi, David A Pecknold, Mingfu Zhang, and Rami M Haj-Ali. Autoprogressive training of neural network constitutive models. *International Journal for Numerical Methods in Engineering*, 42(1):105–126, 1998.
- [GSP09] William G Gray, Bernhard A Schrefler, and Francesco Pesavento. The solid phase stress tensor in porous media mechanics and the hill–mandel condition. *Journal of the Mechanics and Physics of Solids*, 57(3):539–554, 2009.
- [GTSMW13] SA Galindo-Torres, A Scheuermann, HB Mühlhaus, and DJ Williams. A micro-mechanical approach for the study of contact erosion. *Acta Geotechnica*, 10(3):357–368, 2013.
- [GTSMW15] SA Galindo-Torres, A Scheuermann, HB Mühlhaus, and DJ Williams. A micro-mechanical approach for the study of contact erosion. *Acta Geotechnica*, 10(3):357–368, 2015.
- [GZ14] Ning Guo and Jidong Zhao. A coupled fem/dem approach for hierarchical multiscale modelling of granular media. *International journal for numerical methods in engineering*, 99(11):789–818, 2014.
- [HC11] Yanhui Han and Peter A Cundall. Lattice boltzmann modeling of pore-scale fluid flow through idealized porous media. *International Journal for Numerical Methods in Fluids*, 67(11):1720–1734, 2011.
- [HRSS09] CB Hirschberger, S Ricker, P Steinmann, and N Sukumar. Computational multiscale modelling of heterogeneous material layers. *Engineering Fracture Mechanics*, 76(6):793–812, 2009.

- [HS97] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.
- [JKL03] MJ Jiang, JM Konrad, and S Leroueil. An efficient technique for generating homogeneous specimens for dem studies. *Computers and geotechnics*, 30(7):579–597, 2003.
- [KD09] J Kozicki and FV Donzé. Yade-open dem: an open-source software using a discrete element method to simulate granular material. *Engineering Computations*, 26(7):786–805, 2009.
- [KRMK14] Matthew R Kuhn, Hannah E Renken, Austin D Mixsell, and Steven L Kramer. Investigation of cyclic liquefaction with discrete element simulations. *Journal of Geotechnical and Geoenvironmental Engineering*, 140(12):04014075, 2014.
- [KSW15] Matthew R Kuhn, WaiChing Sun, and Qi Wang. Stress-induced anisotropy in granular materials: fabric, stiffness, and permeability. *Acta Geotechnica*, 10(4):399–419, 2015.
- [LD12] Xiang Song Li and Yannis F Dafalias. Anisotropic critical state theory: role of fabric. *Journal of Engineering Mechanics*, 138(3):263–275, 2012.
- [LD15] XS Li and YF Dafalias. Dissipation consistent fabric tensor definition from dem to continuum for granular media. *Journal of the Mechanics and Physics of Solids*, 78:141–153, 2015.
- [LMW12] Anders Logg, Kent-Andre Mardal, and Garth Wells. *Automated solution of differential equations by the finite element method: The FEniCS book*, volume 84. Springer Science & Business Media, 2012.
- [LS02] M Lefik and BA Schrefler. Artificial neural network for parameter identifications for an elasto-plastic model of superconducting cable under cyclic loading. *Computers & structures*, 80(22):1699–1713, 2002.
- [MD04] Christian Miehe and Joachim Dettmar. A framework for micro-macro transitions in periodic particle aggregates of granular materials. *Computer Methods in Applied Mechanics and Engineering*, 193(3):225–256, 2004.
- [MDZ10] C Miehe, J Dettmar, and D Zäh. Homogenization and two-scale simulations of granular materials for different microstructural constraints. *International Journal for Numerical Methods in Engineering*, 83(8-9):1206–1236, 2010.
- [MNBT13] Mario J Martinez, Pania Newell, Joseph E Bishop, and DZ Turner. Coupled multiphase flow and geomechanics model

- for analysis of joint reactivation during co₂ sequestration operations. *International Journal of Greenhouse Gas Control*, 17:148–160, 2013.
- [NB71] Amos Nur and JD Byerlee. An exact effective stress law for elastic deformation of rock with fluids. *Journal of Geophysical Research*, 76(26):6414–6419, 1971.
- [NCDD11] Michał Nitka, Gaël Combe, Cristian Dascalu, and Jacques Desrues. Two-scale modeling of granular materials: a dem-fem approach. *Granular Matter*, 13(3):277–281, 2011.
- [Ng06] Tang-Tat Ng. Input parameters of discrete element methods. *Journal of Engineering Mechanics*, 132(7):723–729, 2006.
- [OCR⁺15] J Oliver, M Caicedo, Emmanuel Roubin, Alfredo Edmundo Huepe, and JA Hernández. Continuum approach to computational multiscale modeling of propagating fracture. *Computer Methods in Applied Mechanics and Engineering*, 294:384–427, 2015.
- [OSDKL07] Martin Ostoja-Starzewski, X Du, ZF Khisaeva, and W Li. Comparisons of the size of the representative volume element in elastic, plastic, thermoelastic, and permeable random microstructures. *International Journal for Multiscale Computational Engineering*, 5(2), 2007.
- [PP11] Kyoungsoo Park and Glaucio H Paulino. Cohesive zone models: a critical review of traction-separation relationships across fracture surfaces. *Applied Mechanics Reviews*, 64(6):060802, 2011.
- [Pre82] J. H. Prevost. Nonlinear transient phenomena in saturated porous media. *Computer Methods in Applied Mechanics and Engineering*, 30(1):3 – 18, 1982.
- [RRL14] Martin Robinson, Marco Ramaioli, and Stefan Luding. Fluid-particle flow simulations using two-way-coupled mesoscale sph-dem and validation. *International journal of multiphase flow*, 59:121–134, 2014.
- [SAR11] WaiChing Sun, José E. Andrade, and John W. Rudnicki. Multi-scale method for characterization of porous microstructures and their impact on macroscopic effective permeability. *International Journal for Numerical Methods in Engineering*, 88(12):1260–1279, 2011.
- [SARE11] WaiChing Sun, José E Andrade, John W Rudnicki, and Peter Eichhubl. Connecting microstructural attributes and permeability from 3d tomographic images of in situ shear-enhanced compaction bands using multiscale computations. *Geophysical Research Letters*, 38(10), 2011.

- [ŠCC⁺10] V Šmilauer, E Catalano, B Chareyre, S Dorofeenko, J Duriez, A Gladky, J Kozicki, C Modenese, L Scholtès, L Sibille, et al. Yade documentation. *The Yade Project*. (<http://yade-dem.org/doc/>), 2010.
- [SKR13] WaiChing Sun, Matthew R. Kuhn, and John W. Rudnicki. A multiscale dem-lbm analysis on permeability evolutions inside a dilatant shear band. *Acta Geotechnica*, pages 1–16, 2013.
- [SOS13] WaiChing Sun, Jakob T. Ostien, and Andrew G. Salinger. A stabilized assumed deformation gradient finite element formulation for strongly coupled poromechanical simulations at finite strain. *International Journal for Numerical and Analytical Methods in Geomechanics*, 37(16):2755–2788, 2013.
- [SSD95] RB Saeger, LE Scriven, and HT Davis. Transport processes in periodic porous media. *Journal of Fluid Mechanics*, 299:1–15, 1995.
- [Suc01] Sauro Succi. *The lattice Boltzmann equation: for fluid dynamics and beyond*. Oxford university press, 2001.
- [SWZP86] B.R. Simon, J.S.-S. Wu, O.C. Zienkiewicz, and D.K. Paul. Evaluation of $u - w$ and $u - \pi$ finite element methods for the dynamic response of saturated porous media using one-dimensional models. *International Journal for Numerical and Analytical Methods in Geomechanics*, 10(5):461–482, 1986.
- [TPF⁺17] DK Tran, N Prime, F Froiio, Carlo Callari, and E Vincens. Numerical modelling of backward front propagation in piping erosion by dem-lbm coupling. *European Journal of Environmental and Civil Engineering*, 21(7-8):960–987, 2017.
- [TSH⁺14] Sebastian Toro, Pablo J Sánchez, Alfredo Edmundo Huespe, Sebastian Miguel Giusti, Pedro J Blanco, and RA Feijóo. A two-scale failure model for heterogeneous materials: numerical implementation based on the finite element method. *International Journal for Numerical Methods in Engineering*, 97(5):313–351, 2014.
- [TSP⁺16] Sebastian Toro, PJ Sánchez, JM Podestá, PJ Blanco, Alfredo Edmundo Huespe, and RA Feijóo. Cohesive surface model for fracture based on a two-scale formulation: computational implementation aspects. *Computational mechanics*, 58(4):549–585, 2016.
- [TTE⁺43] Karl Terzaghi, Karl Terzaghi, Civil Engineer, Austria Czechoslovakia, Karl Terzaghi, Ingénieur Civil, Autriche Tchécoslovaquie, and Etats Unis. *Theoretical soil mechanics*, volume 18. Wiley New York, 1943.
- [WBF06] Joshua A White, Ronaldo I Borja, and Joanne T Fredrich. Calculating the effective permeability of sandstone with multiscale

- lattice boltzmann/finite element simulations. *Acta Geotechnica*, 1(4):195–209, 2006.
- [WLW08] C Wellmann, C Lillie, and P Wriggers. Homogenization of granular material modeled by a three-dimensional discrete element method. *Computers and Geotechnics*, 35(3):394–405, 2008.
- [Woo90] David Muir Wood. *Soil behaviour and critical state soil mechanics*. Cambridge university press, 1990.
- [WS16] Kun Wang and WaiChing Sun. A semi-implicit discrete-continuum coupling method for porous media based on the effective stress principle at finite strain. *Computer Methods in Applied Mechanics and Engineering*, 304:546 – 583, 2016.
- [WS17] Kun Wang and WaiChing Sun. Data-driven discrete-continuum method for partially saturated micro-polar porous media. In *Poromechanics VI*, pages 571–578. 2017.
- [WS18] Kun Wang and WaiChing Sun. A multiscale multi-permeability poroplasticity model linked by recursive homogenizations and deep learning. *Computer Methods in Applied Mechanics and Engineering*, 334:337–380, 2018.
- [WS19] Kun Wang and WaiChing Sun. An updated lagrangian lbm–dem–fem coupling model for dual-permeability fissured porous media with embedded discontinuities. *Computer Methods in Applied Mechanics and Engineering*, 344:276–305, 2019.
- [YIV98] Mitsutoshi Yoshimine, Kenji Ishihara, and William Vargas. Effects of principal stress direction on intermediate principal stress on undrained shear behavior of sand. *Soils and Foundations*, 38(3):179–188, 1998.
- [ZG13] Jidong Zhao and Ning Guo. Unique critical state characteristics in granular media considering fabric anisotropy. *Géotechnique*, 63(8):695–704, 2013.
- [ZH82] AA Zick and GM Homsy. Stokes flow through periodic arrays of spheres. *Journal of fluid mechanics*, 115:13–26, 1982.
- [ZH97] Qisu Zou and Xiaoyi He. On pressure and velocity boundary conditions for the lattice boltzmann bgk model. *Physics of fluids*, 9(6):1591–1598, 1997.
- [ZW01] TI Zohdi and P Wriggers. Computational micro-macro material testing. *Archives of Computational Methods in Engineering*, 8(2):131–228, 2001.

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