Numerical modeling of granular materials for plant biorefinery

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Funding:
INRAE (TRANSFORM department) and University of Montpellier (I2S doctoral school)

Duration:
3 years, Starting Date: 1st October 2021

Required skills:
Master in physics, mechanics or applied mathematics with strong interest in computational mechanics and numerical modeling. The candidate is expected to work in a multidisciplinary research context.

Location:
The PhD candidate will work on the sites of the La Gaillarde (INRAE) and Saint-Priest campuses (both depending on the University of Montpellier).

Keywords:
Granular Materials, Computational mechanics, Fragmentation, Biorefinery, Discrete Element Method, Fracture Mechanics, Image Analysis

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Summary

Agricultural and forestry plant residues are available sources of carbon, but require fragmentation/ separation operations to extract ultrafine powders with targeted properties. This plant-based dry biorefinery is a promising alternative to oil, particularly for energy and materials applications. IATE laboratory hosts the INRAE national plant fractionation platform and is developing, in collaboration with LMGC laboratory, unique numerical models for granular materials composed of breakable particles. A major challenge is to understand how the microstructure and interactions in plant tissues influence the size, composition and shapes of the fragments. In this thesis, we will associate a massively parallel peridynamic model for the propagation of the fracture across the histological structures of plants (µm scale), and a Discrete Element approach for grain fragmentation (process scale). The ultimate goal is to elucidate the deconstruction mechanisms and develop bottom-up models accounting for both mechanical and physicochemical interactions.

Challenges and Context

Plants are a source of renewable product traditionally exploited in many sectors of human activity: food, pharmaceuticals, chemistry, construction, heating, etc. However, the variety of their composition and histological structures makes them difficult to exploit in advanced applications where high product quality matters. IATE laboratory has acquired internationally recognized expertise in the transformation processes and their adaptation to the complexity and variability of biomass [1]. These developments have made possible various applications for bio-based composites [2], 3D printing filaments [3], biofuels [4], solid fuels [5]... This concerns in particular the development of a "dry" biorefinery [6] where the material is dissociated using different technologies, mainly mechanical (cutting, fragmentation, grinding...), and then sorted using innovative techniques such as electrostatic sorting. Unlike conventional biorefineries, which have similarities with oil, dry-process biorefineries directly exploit the reactivity of powders without the need for water, additives or degradation agents and reducing energy losses by filtration, drying or cracking operations.

A fundamental issue is to understand how energy is transmitted from the scale of the milling process to the scale of the material, and how it dissociates the plant tissues. The numerical approaches (Discrete Elements Method, Peridynamics) jointly developed for several years between LMGC and IATE are able to push forward experimental approaches by integrating small-scale inhomogeneities and providing scenarios for a better understanding of the experimental data.

In this context, the goal of the PhD thesis will be to develop a multi-scale numerical modeling approach to investigate the mechanisms of fragmentation from the scale of plant tissue dissociation up to the process scale. The proposed bottom-up models will proceed from the mechanical and physicochemical interactions at the scale of the relevant constituents (cell walls, envelopes, organs...) [7] to simulate and model single particle fracture that will then allow simulating a large number of particles at the process scale. In the longer term, a major challenge is to lay the foundations of a virtual biorefinery approach with the aim of predicting fragmentation behavior for various plant biomasses.

State of the art

The milling process involves inhomogeneities at three scales: 1) At the scale of a collection of particles (the granular material), the microstructure is characterized by a highly disordered contact network that evolves by the action of collisions and non-affine displacements of the grains. The contact forces and grain velocities show a broad distribution, long-distance correlations and anomalous fluctuations. The energy injected at the process scale is therefore dissipated at intermediate scales down to the grain scale; 2) At the grain scale, the cracks initiated at the contacts and their propagation depend not only on the nature of the material but also on the effects of the shape, surface roughness and size of the grains. 3) At the level of the constituent tissue of the material, the statistical distribution of the phases and their mechanical properties play a crucial role, with micro-cracks appearing in the weak layers (cell walls, interface between phases...) which then coalesce into macro-cracks.

A realistic treatment of these inhomogeneities at different scales is now within reach by means of novel numerical methods that can incorporate the phases and their mechanical and physicochemical interactions at small scales to simulate the dynamics and evolution of the system by temporal integration of the equations of motion. Owing to computational power, methods such as XFEM Finite Elements, Cohesive Zones, Lattice Element Method and Peridynamics are able to incorporate tissue inhomogeneities and structural elements to predict failure modes whereas Discrete Element Methods (DEM) accurately reproduce granular dynamics.

At the tissue scale, we will consider Peridynamics, which is based on the integral formulation of continuum mechanics (rather than differential equations). In this method, mechanical properties are deduced from non-local interactions between mass points. The main benefits are its natural handling of discontinuities at crack tips as well as its ability to incorporate internal structures and inhomogeneous mechanical properties without cumbersome remeshing procedures. Recently, we have developed a Bond-Based Peridynamics (BBP) method [8] that integrates the elastic behavior

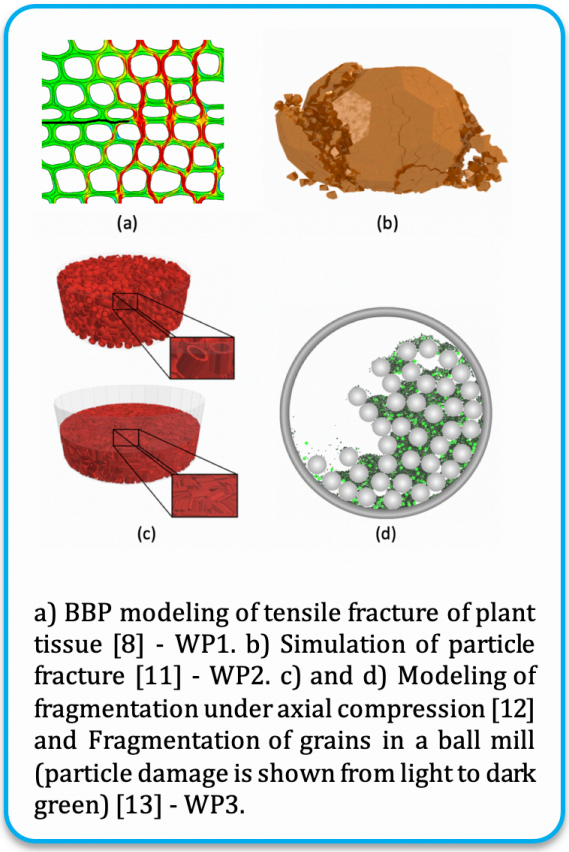
and fracture of the different phases and interfaces at the component level. It has been successfully applied to model disordered granular [8] and cellular [9] microstructures. Image analysis algorithms have also been developed to identify the evolution of damage, fragments and crack paths. The computational code and post-processing operations are parallelized via Message Passing Interface (MPI).

This method is, however, insufficient for the analysis of the grinding behavior, which involves also the complex transport of mass and momentum across a disordered granular microstructure that evolves as a result of particle fragmentation. Finally, the DEM, which has been developed to simulate the rheology of assemblies of a large number of particles, will be used on the basis of the fracture properties of a single particle in order to simulate the fragmentation process as a function of the operational and boundary conditions. In addition, the rheology of granular materials can only be addressed by considering the possibility of collisions, contacts and friction between particles. We will rely on a DEM code that we have developed for the simulation of non-spherical particles [11-12]. The LMGC and UMR IATE Laboratory have acquired internationally recognized expertise in this field. Major developments have been made to take into account the shape of the particles, the presence of interstitial fluids and the deformability of the grains. The association of BBP and DEM provides a unique and original bottom-up framework to address the fragmentation process of plant residues.

Thesis work

A coupled method involving crack propagation at different scales will be implemented. It will rely on BBP to describe the behavior of the different constituent of plants and on DEM to simulate any particle shape. The simulation parameters will be calibrated from plant histological structures already characterized at IATE (wheat straw, miscanthus, rice husk, pine bark, etc.) and from small-scale measurements carried out in previous studies.

Parametric studies will be carried out in which the effects of the different material parameters and the process geometry on the fragmentation dynamics will be analyzed. The results will be used to characterize the dissociation and dissipation modes by different mechanisms (rupture, friction, inelastic collisions) to understand the parameters that control energy efficiency. The physical mechanisms at the origin of the fragmentation of these plants will be specified. Dissociation kinetics will be characterized in relation to the dynamics of the force chains in the mill. Phenomena influencing grinding will be considered, such as the effects of humidity, van der Waals interactions for the finest particles, or entanglement for fibres.



a) BBP modeling of tensile fracture of plant tissue [8] - WP1. b) Simulation of particle fracture [11] - WP2. c) and d) Modeling of fragmentation under axial compression [12] and Fragmentation of grains in a ball mill (particle damage is shown from light to dark green) [13] - WP3.

Finally, this work requires developments in C/C++ language that can be carried out on the basis of software co-developed between the LMGC and IATE. Access to MESO@LR's HPC resources will allow parametric studies to be carried out on extended experimental designs. The figure illustrates the development of these axes based on studies previously carried out.

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