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Energetical background of common approaches in geomechanics

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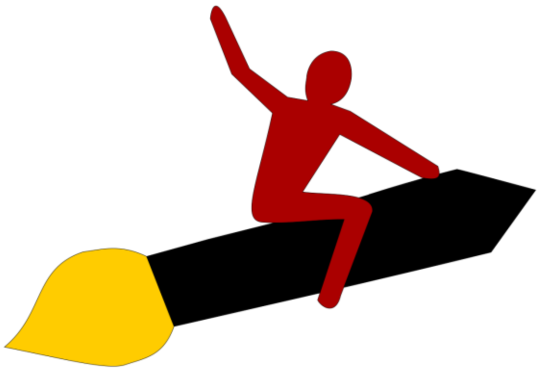
Outlook

- Derivation of balance equations and stress measures
- Localized deformation
- Elastoplasticity
- Anisotropy
- Coupling

Derivation of the balance equations

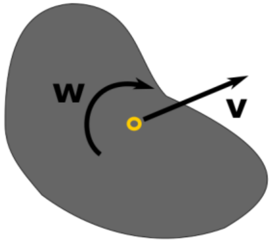
- *The laws of physics are invariant under a transformation between two coordinate frames moving at a constant velocity with respect to each other.*



Conserved quantities

$$\dot{\tilde{E}} = \dot{W}_F + \dot{W}_C - \dot{E}_{kin}$$

- W_F is the work of the forces
- W_C is the work of the couples
- E_{kin} is the kinetic energy



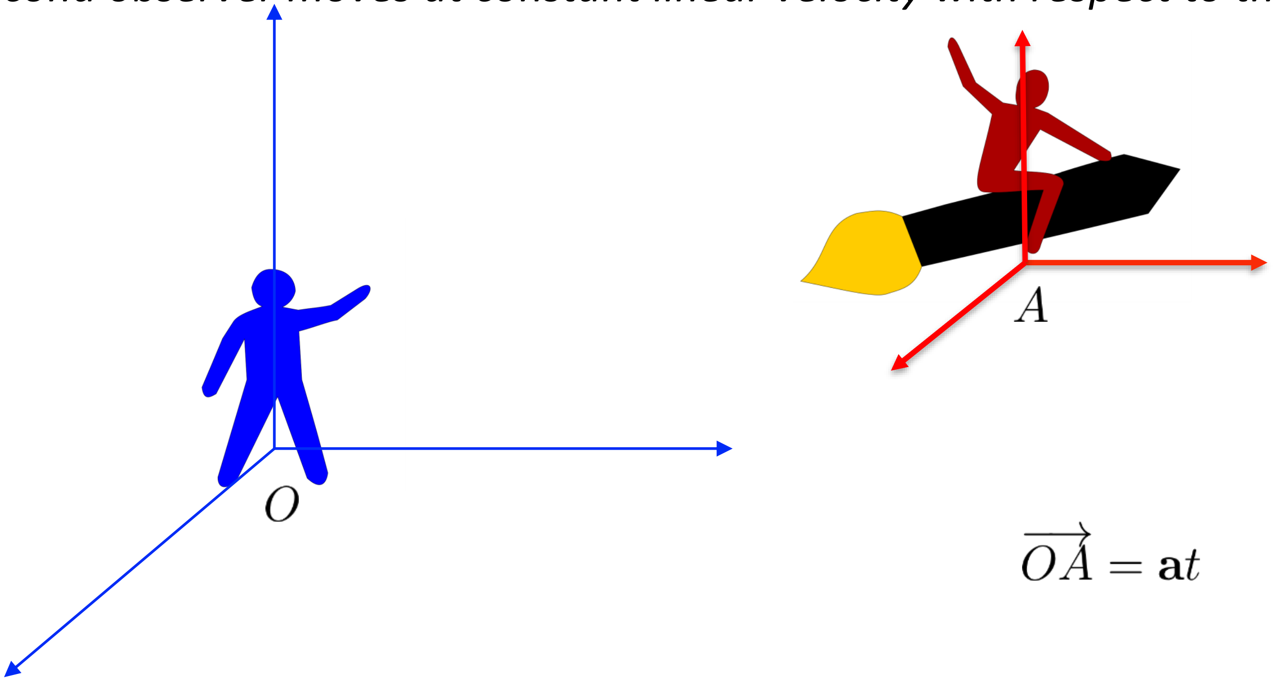
For a single, rigid object this means:

$$\dot{W}_F + \dot{W}_C = \mathbf{f} \cdot \mathbf{v} + \mathbf{m} \cdot \mathbf{w}$$

$$\dot{E}_{kin} = \frac{1}{2}\dot{m}\mathbf{v} \cdot \mathbf{v} + m\mathbf{v} \cdot \dot{\mathbf{v}} + \frac{1}{2}\mathbf{w}^T \underline{\dot{\boldsymbol{\theta}}}\mathbf{w} + \mathbf{w}^T \underline{\boldsymbol{\theta}}\dot{\mathbf{w}}$$

Galilean change of observer

- *A second observer moves at constant linear velocity with respect to the initial system*



$$\overrightarrow{OA} = \mathbf{a}t$$

Galilean change of observer

- *A second observer moves at constant linear velocity with respect to the initial system*

$$\underline{\boldsymbol{\theta}}' = \underline{\boldsymbol{\theta}} \quad \& \quad \mathbf{w}' = \mathbf{w} \quad \& \quad \mathbf{m}' = \mathbf{m} \quad \& \quad \mathbf{v}' = \mathbf{v} - \mathbf{a}$$

- Then it must hold that:

$$\left(\dot{W}_F + \dot{W}_C - \dot{E}_{kin}\right)_0 = \left(\dot{W}_F + \dot{W}_C - \dot{E}_{kin}\right)_a$$

$$\mathbf{f} \cdot \mathbf{v} \quad + \quad \mathbf{m} \cdot \mathbf{w} - \mathbf{f}' \cdot \mathbf{v}' - \mathbf{m} \cdot \mathbf{w} = \frac{1}{2}\dot{m}\mathbf{v} \cdot \mathbf{v} + m\mathbf{v} \cdot \dot{\mathbf{v}} +$$

$$+ \quad \frac{1}{2}\mathbf{w}^T\dot{\underline{\boldsymbol{\theta}}}\mathbf{w} + \mathbf{w}^T\underline{\boldsymbol{\theta}}\dot{\mathbf{w}} - \frac{1}{2}\dot{m}\mathbf{v}' \cdot \mathbf{v}' - m\mathbf{v}' \cdot \dot{\mathbf{v}}' - \frac{1}{2}\mathbf{w}^T\dot{\underline{\boldsymbol{\theta}}}\mathbf{w} - \mathbf{w}^T\underline{\boldsymbol{\theta}}\dot{\mathbf{w}} \Rightarrow$$

$$\boxed{\mathbf{f}' \cdot \mathbf{a}} = \boxed{(\mathbf{f}' - \mathbf{f}) \cdot \mathbf{v}} + \boxed{\dot{m}\mathbf{a} \cdot \mathbf{v} + m\mathbf{a} \cdot \dot{\mathbf{v}}} - \boxed{\frac{1}{2}\dot{m}\mathbf{a} \cdot \mathbf{a}}$$

Galilean change of observer

- Since a is arbitrarily selected,

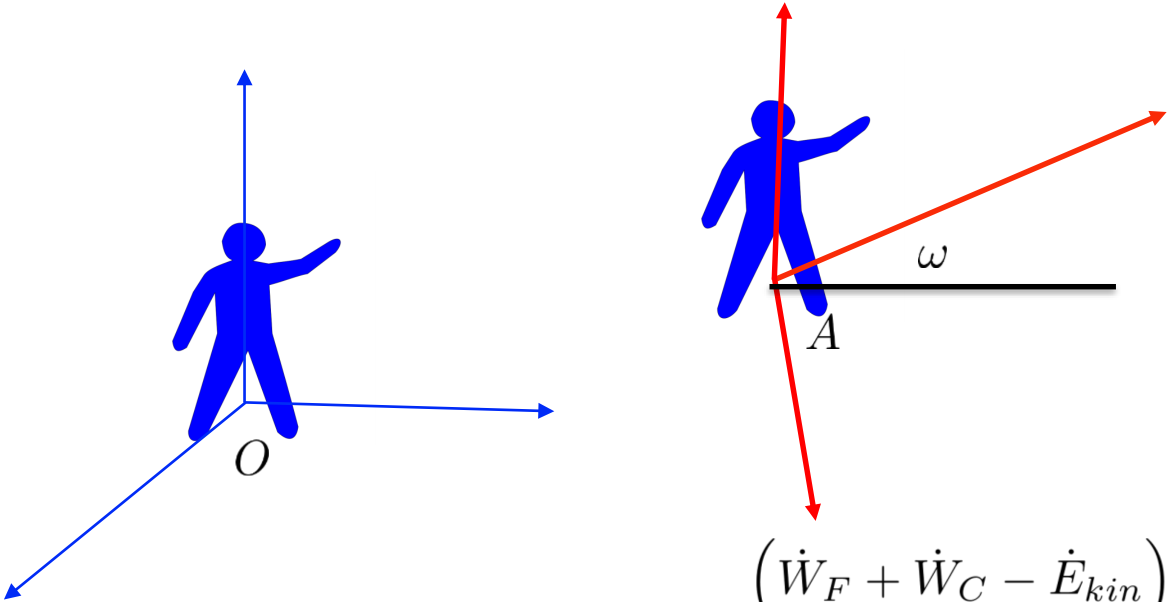
$$\mathbf{f}' \cdot \mathbf{a} = (\mathbf{f}' - \mathbf{f}) \cdot \mathbf{v} + \dot{m}\mathbf{a} \cdot \mathbf{v} + m\mathbf{a} \cdot \dot{\mathbf{v}} - \frac{1}{2}\dot{m}\mathbf{a} \cdot \mathbf{a}$$

- means that the following holds:

- Force transformation rule $\mathbf{f}' = \mathbf{f}$
- Mass balance $\dot{m} = 0$
- Momentum balance $\mathbf{f} = \dot{m}\mathbf{v} + m\dot{\mathbf{v}}$

Leibniz change of observer

- *A second observer moves at constant angular velocity with respect to the initial system*



$$\boldsymbol{\omega} = \dot{\mathbf{o}}t$$

$$\left(\dot{W}_F + \dot{W}_C - \dot{E}_{kin}\right)_0 = \left(\dot{W}_F + \dot{W}_C - \dot{E}_{kin}\right)_o$$

Leibniz change of observer

- *A second observer moves at constant angular velocity with respect to the initial system*

$$
\begin{aligned}
\dot{E}'_{kin} &= \frac{1}{2}\dot{m}\left[\underline{\dot{\mathbf{O}}}^T\mathbf{x}+\underline{\mathbf{O}}^T\mathbf{v}\right]^T\left[\underline{\dot{\mathbf{O}}}^T\mathbf{x}+\underline{\mathbf{O}}^T\mathbf{v}\right]+\\
&+\ m\left[\underline{\dot{\mathbf{O}}}^T\mathbf{x}+\underline{\mathbf{O}}^T\mathbf{v}\right]^T\left[\underline{\dot{\mathbf{O}}}^T\ \underline{\mathbf{W}}^T\mathbf{x}+2\underline{\dot{\mathbf{O}}}^T\mathbf{v}+\underline{\mathbf{O}}^T\dot{\mathbf{v}}\right]+\\
&+\ \frac{1}{2}\left[\mathbf{w}^T-\mathbf{b}^T\right]\underline{\mathbf{O}}\ \underline{\dot{\boldsymbol{\theta}}'}\ \underline{\mathbf{O}}^T\left[\mathbf{w}-\mathbf{b}\right]+\\
&+\ \frac{1}{2}\left[\mathbf{w}^T-\mathbf{b}^T\right]\underline{\mathbf{O}}\ \underline{\boldsymbol{\theta}'}\left[\underline{\dot{\mathbf{O}}}^T\left(\mathbf{w}-\mathbf{b}\right)+\underline{\mathbf{O}}^T\dot{\mathbf{w}}\right]+\\
&+\ \frac{1}{2}\left[\left(\mathbf{w}^T-\mathbf{b}^T\right)\underline{\dot{\mathbf{O}}}+\dot{\mathbf{w}}^T\underline{\mathbf{O}}\right]\ \underline{\boldsymbol{\theta}'}\ \underline{\mathbf{O}}^T\left[\mathbf{w}-\mathbf{b}\right]
\end{aligned}
$$

where ***O*** is a rotation tensor.

Leibniz change of observer

- The previous equation yields the already known mass balance and
- The couple transformation rule

$$\mathbf{m}' = \mathbf{m}$$

- the angular inertia tensor balance

$$\dot{\underline{\boldsymbol{\theta}}} = \underline{\mathbf{W}\boldsymbol{\theta}} + \underline{\boldsymbol{\theta}\mathbf{W}}$$

- and the angular momentum balance

$$\mathbf{m} = \dot{\underline{\boldsymbol{\theta}}}\mathbf{w} + \underline{\boldsymbol{\theta}}\dot{\mathbf{w}}$$

- where $\underline{\mathbf{W}}$ is the rotational velocity tensor corresponding to the vector **w**.

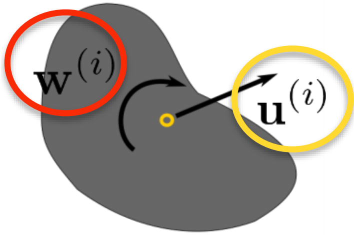
Micromechanical stress tensors – two particles in contact

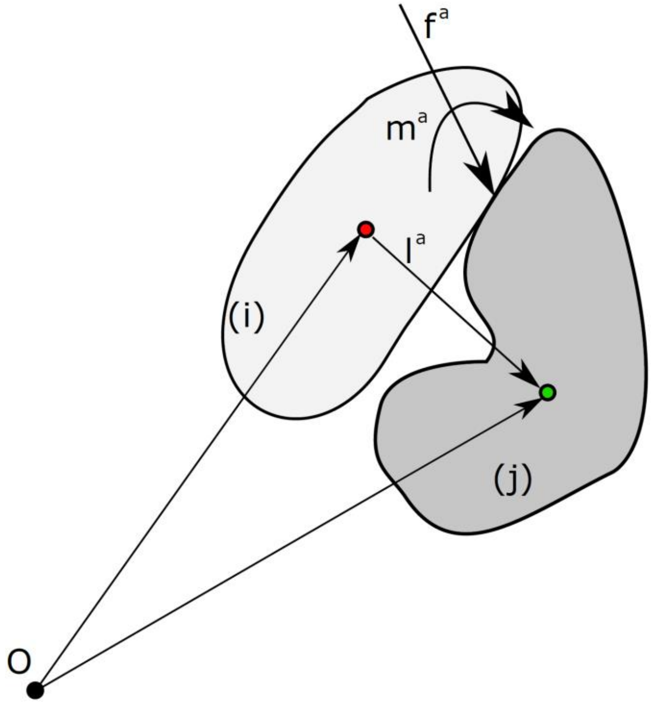
- Consider the depicted grains and their contact.
- The relative displacement at the contact is:

$$\mathbf{u}^{(i,j)} = \mathbf{u}^{(i,a)} - \mathbf{u}^{(j,a)}$$

- with

$$\mathbf{u}^{(i,a)} = \mathbf{u}^{(i)} + \mathbf{w}^{(i)} \times \left(\mathbf{x}^{(a)} - \mathbf{x}^{(i)}\right)$$





Micromechanical stress tensors

- *The same principle can be applied to assemblies of rigid particles, such as granular media*

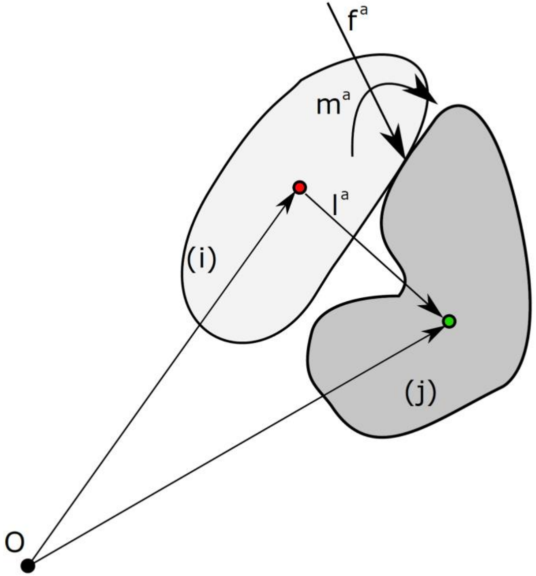
Assumption:

- The displacement and rotation rates are affine:

$$\mathbf{u}^{(i)} = \mathbf{u}^{O} + \nabla \mathbf{u}^{O} \cdot \mathbf{x}^{(i)}$$

$$\mathbf{w}^{(i)} = \mathbf{w}^{O} + \nabla \mathbf{w}^{O} \cdot \mathbf{x}^{(i)}$$

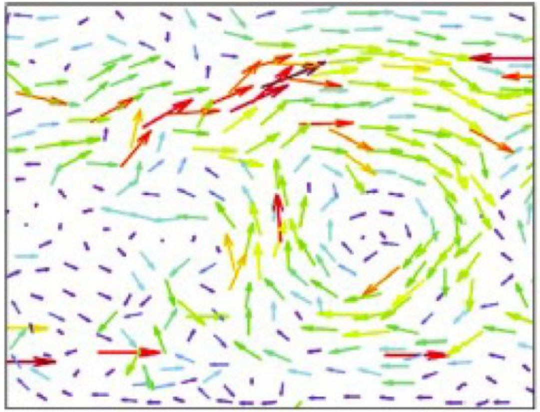
- meaning that



$$P_{int} = \sum_{a \in \mathcal{C}} \left((\mathbf{f}^a \otimes \mathbf{l}^a) : \left(\nabla \mathbf{v}^O - \underline{\mathbf{W}}^O \right) \right) + \sum_{a \in \mathcal{C}} \left((\mathbf{f}^a \times \mathbf{l}^a) \otimes (\mathbf{x}^a - \mathbf{x}^O) : \nabla \mathbf{w}^O \right) + \sum_{a \in \mathcal{C}} \left(\mathbf{m}^a \otimes \mathbf{l}^a : \nabla \mathbf{w}^O \right)$$

Affinity of displacements and rotations

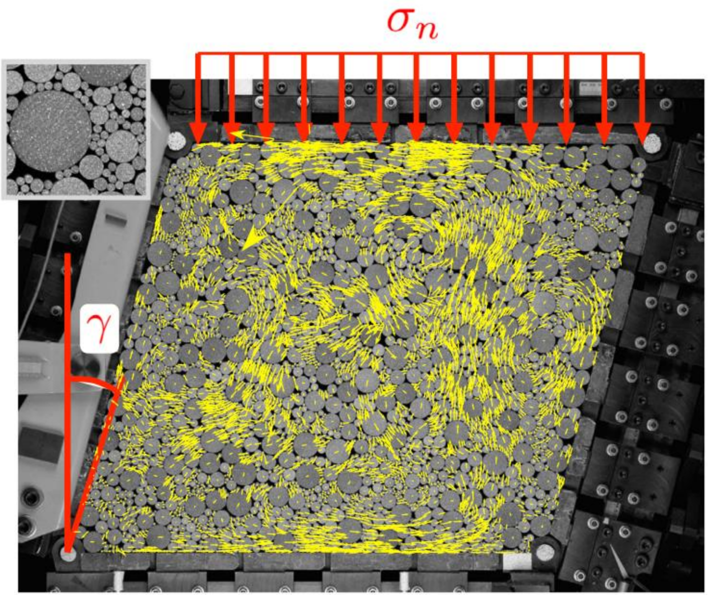
DEM Simulation Velocities



Miller et al. (2013)

Experiment

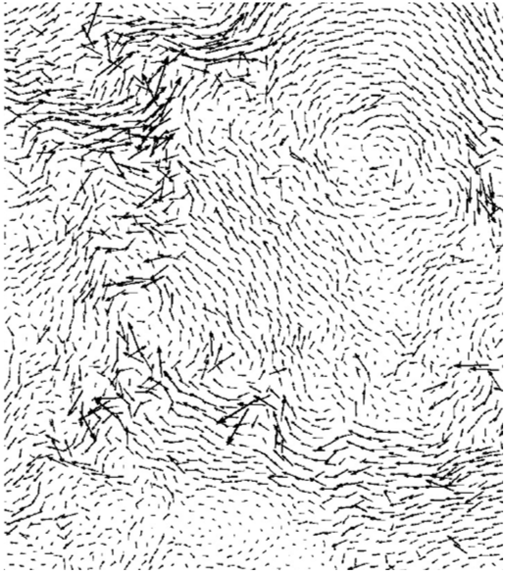
Displacement Fluctuations



Combe et al. (2015)

DEM Simulation

Velocity Fluctuations



Radjai and Roux (2002)

Micromechanical stress tensors

Assumption: $\bar{P}_{int} = V\left(\underline{\boldsymbol{\sigma}} : \underline{\dot{\boldsymbol{\Gamma}}} + \underline{\boldsymbol{\mu}} : \underline{\dot{\boldsymbol{\kappa}}}\right)$

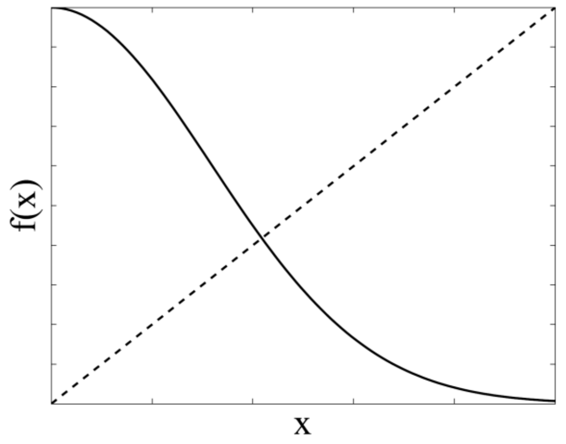
- meaning that

$$\underline{\boldsymbol{\sigma}} = \frac{1}{V}\sum_{a\in\mathcal{C}} \mathbf{f}^a \otimes \mathbf{l}^a \qquad \underline{\boldsymbol{\mu}} = \frac{1}{V}\sum_{a\in\mathcal{C}} (\mathbf{m}^a \otimes \mathbf{l}^a) + \frac{1}{V}\sum_{a\in\mathcal{C}} ((\mathbf{f}^a \times \mathbf{l}^a) \otimes \mathbf{x}^a)$$

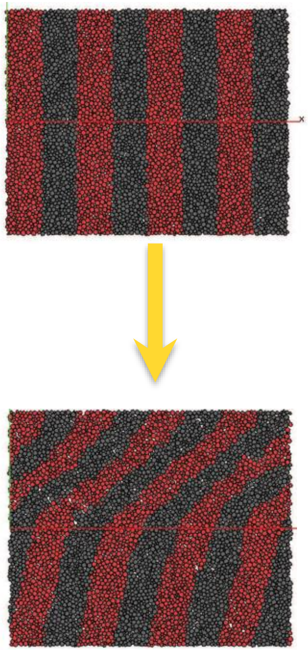
- alternatively

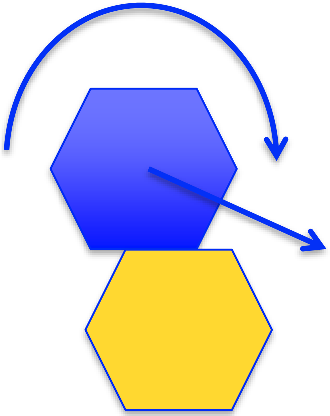
$$\underline{\boldsymbol{\mu}}' = \frac{1}{V}\sum_{a\in\mathcal{C}} (\mathbf{m}^a \otimes \mathbf{l}^a) + \frac{1}{V}\sum_{a\in\mathcal{C}} ((\mathbf{f}^a \times \mathbf{l}^a) \otimes \mathbf{l}^a)$$

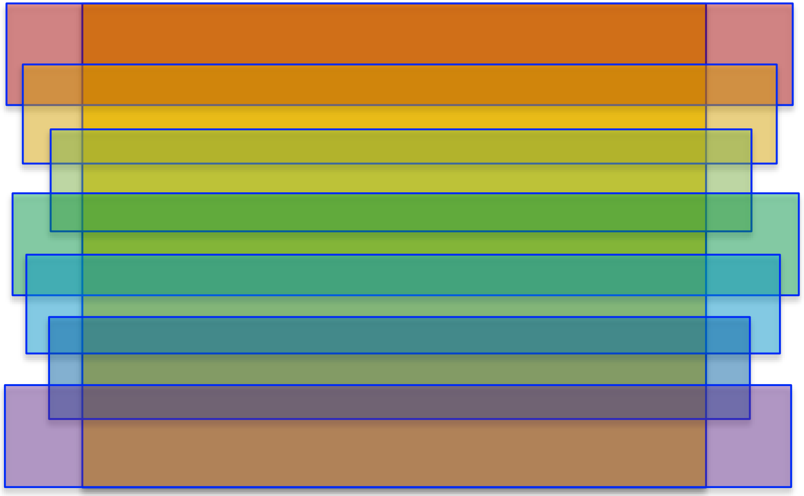
Tordesillas and Walsh (2002)



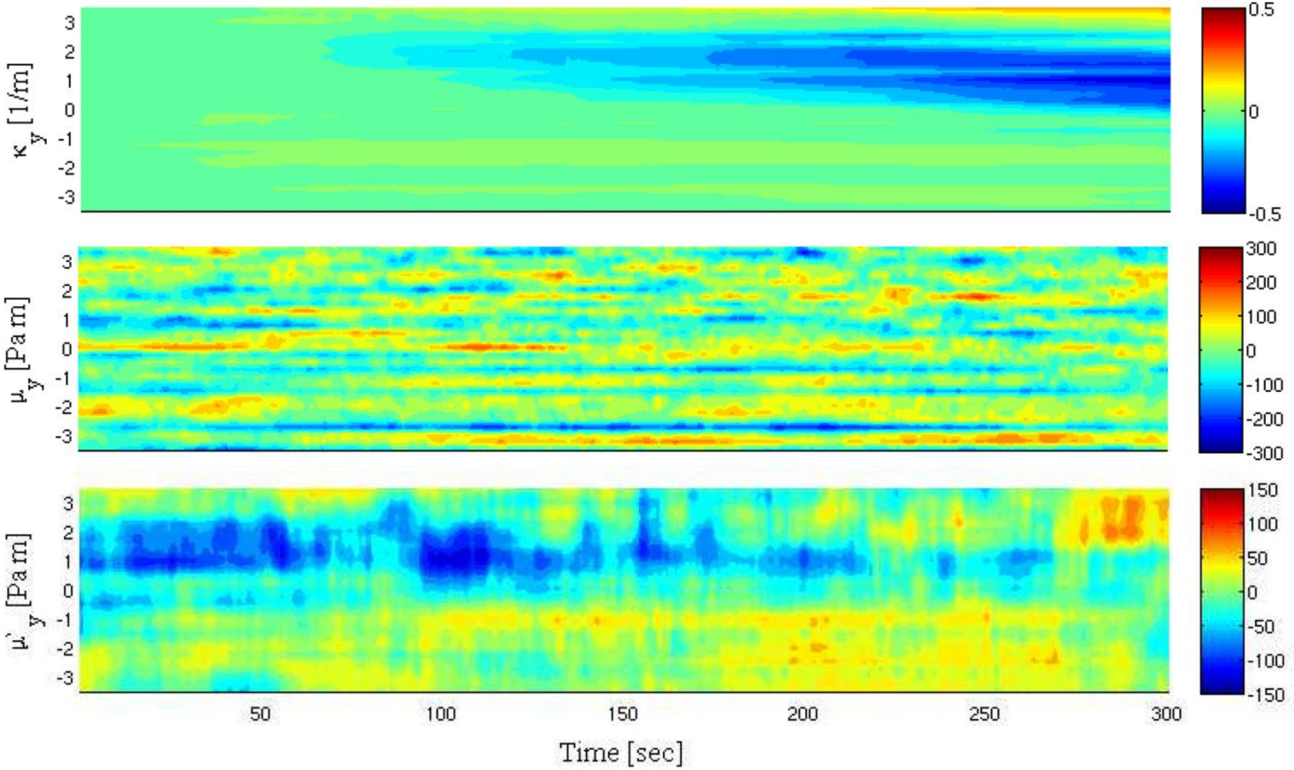
Comparison of different formulations

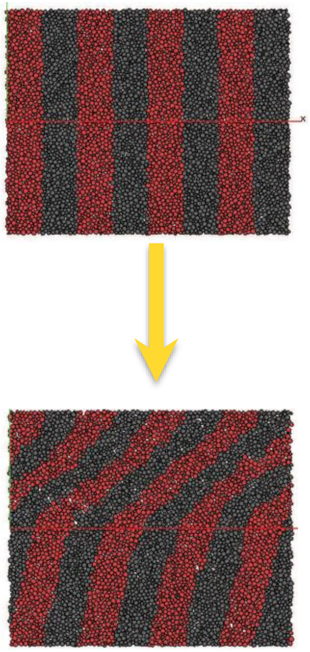






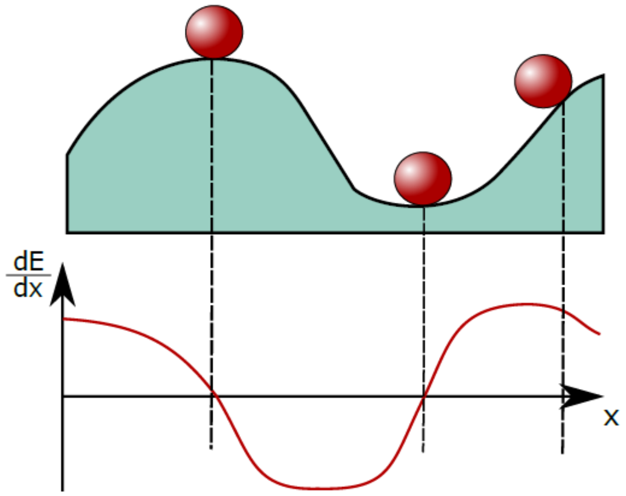
Comparison of different formulations





Stability – potential energy characteristics

- A force field exists
- To move something in the force field, work must be done
- The force field is conservative
- The force field itself does negative work when another force is moving something against it
- It is recoverable energy



Minimum potential energy -> Stable equilibrium

Stability – Equivalence of virtual work and balance equation

- The solution coincides with the one of the virtual work method
- The balance equations read

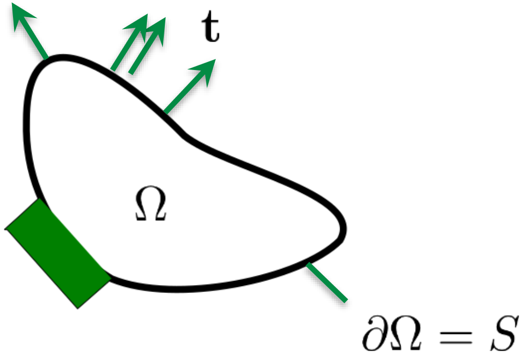
$$\sigma_{ij,j} + f_i = 0 \Leftrightarrow \left(\sigma_{ij,j} + f_i\right) u_i^* = 0 \Leftrightarrow$$

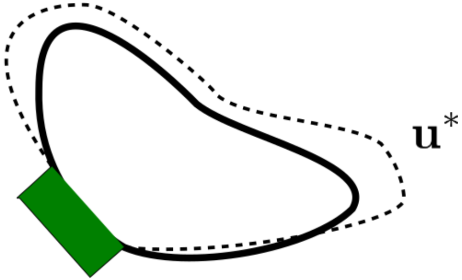
$$\left(\sigma_{ij} u_i^*\right)_{,j} - \sigma_{ij} u_{i,j}^* + f_i u_i^* = 0 \Leftrightarrow$$

$$\sigma_{ij}\epsilon_{ij}^* = \left(\sigma_{ij} u_i^*\right)_{,j} + f_i u_i^*$$

- Integrating over the domain and using the divergence theorem

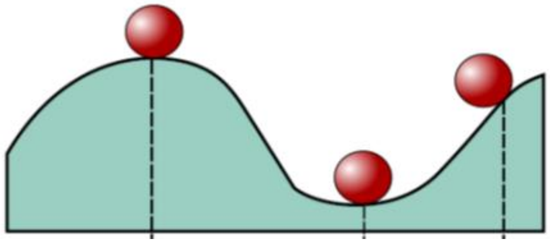
$$\int_\Omega \sigma_{ij}\epsilon_{ij}^* \mathrm{d}\omega = \int_\omega f_i u_i^* \mathrm{d}\omega + \int_S t_i u_i^* \mathrm{d}s$$

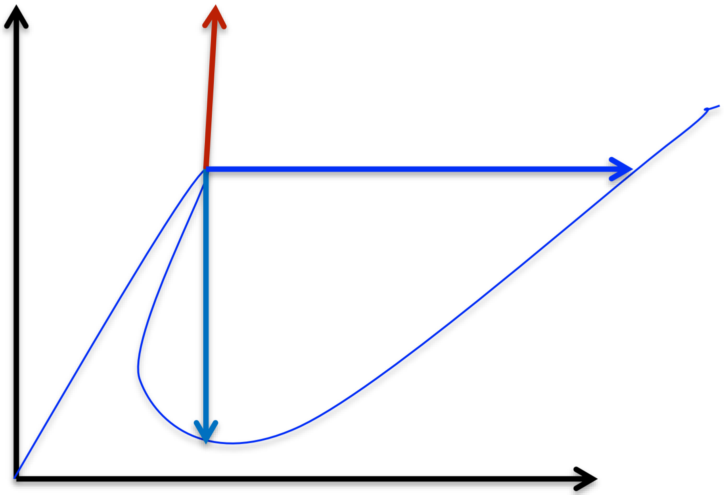




Stability – Mathematically?

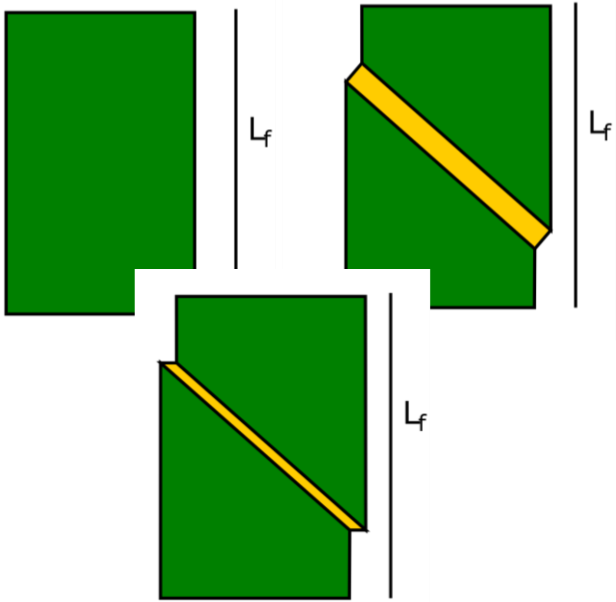
- A problem is well posed when
  - There is a solution
  - The solution is unique
  - The solution's behavior changes continuously with the initial conditions
- Deviations lead to numerical instability
- This has nothing to do with energy

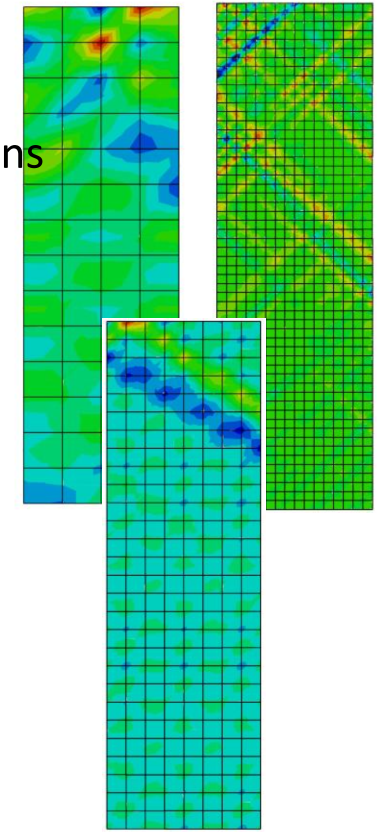


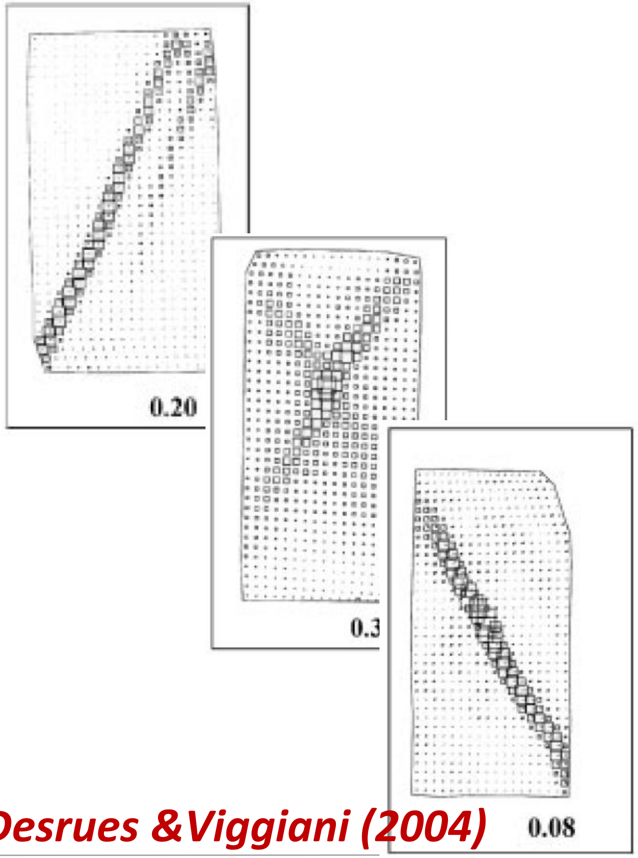


Strain localization

- More than one possible solutions



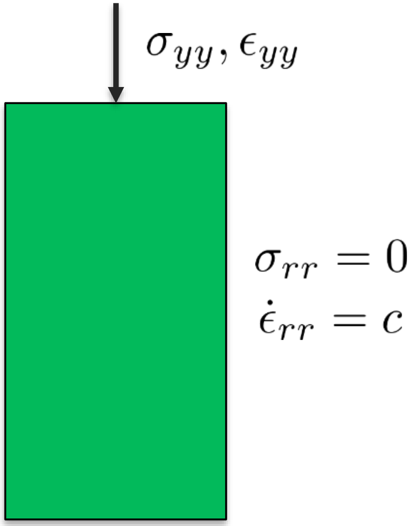


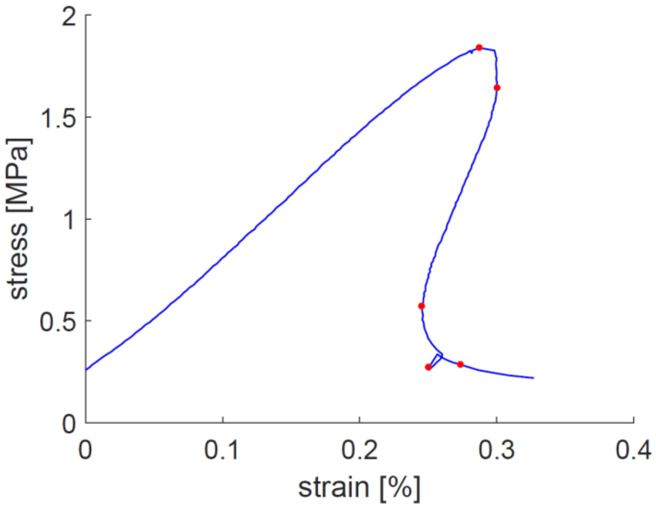


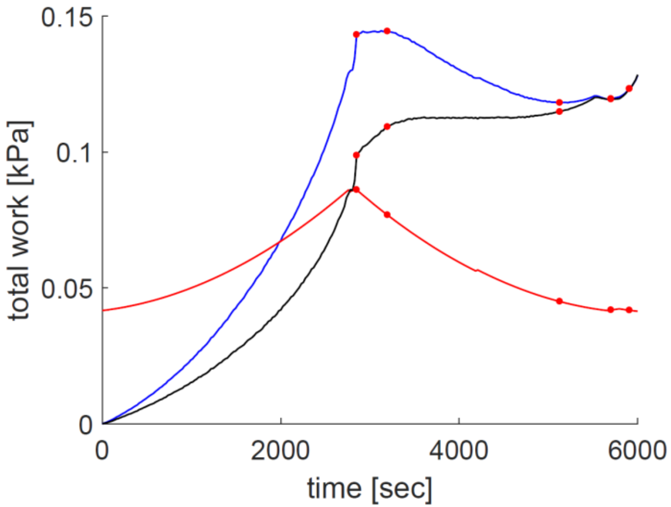
Desrues &Viggiani (2004)

And the energy?

- A simple example: uniaxial test with radial strain rate control







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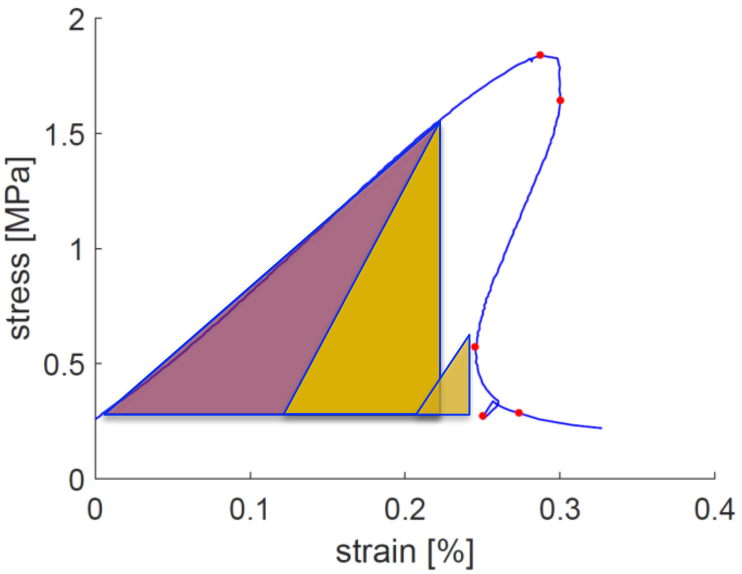
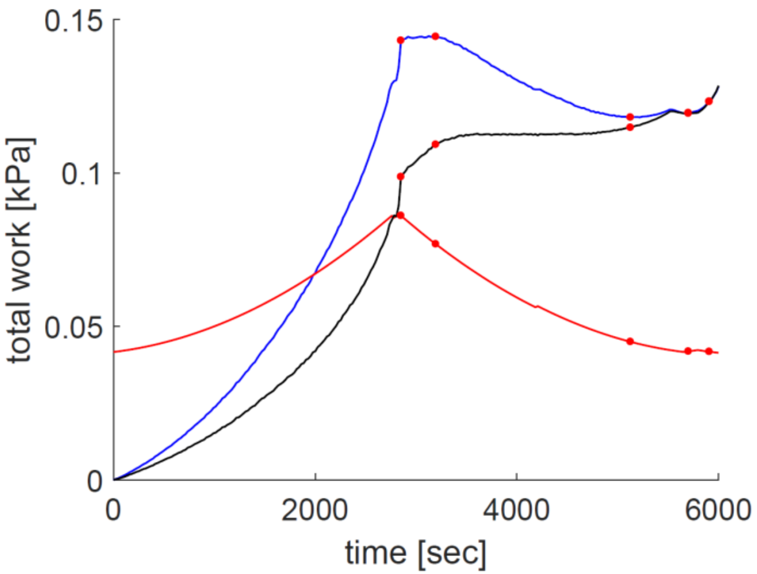
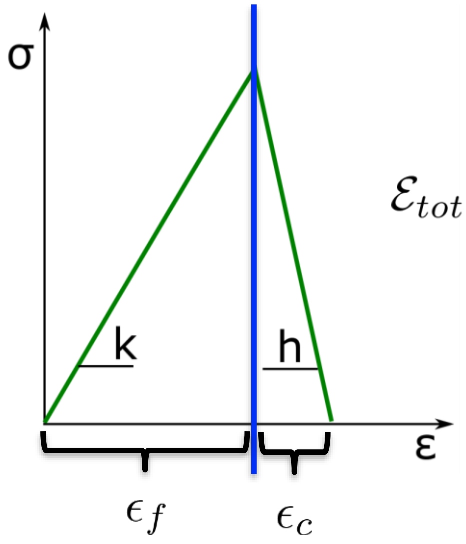


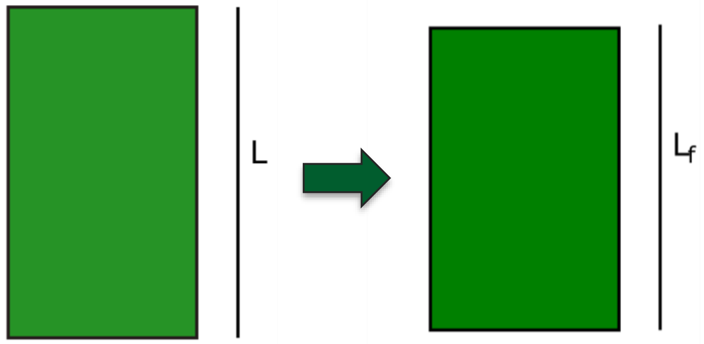


Strain localization – Thought example in 1D

- Consider the constitutive response of the material point to be the one shown here.



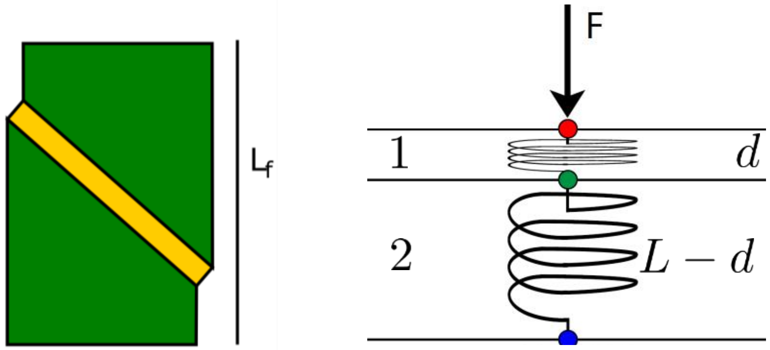
$$\mathcal{E}_{tot} = \frac{1}{2}\sigma_f \epsilon_f + \frac{1}{2}\sigma_f \epsilon_c$$



$$\epsilon_f + \epsilon_c = \frac{L - L_f}{L}$$

Strain localization – Thought experiment in 1D

- Assume a shear band forms with a width of d. Two springs in series can be viewed as the mechanical equivalent.



$$\sigma = \sigma_1 + \sigma_2$$

$$\epsilon = \frac{\epsilon_1 d + \epsilon_2 (L-d)}{L}$$

- The mechanical response for each spring is

$$\sigma_1 = k\epsilon_1 - (k+h) < \epsilon_1 - \epsilon_f >$$

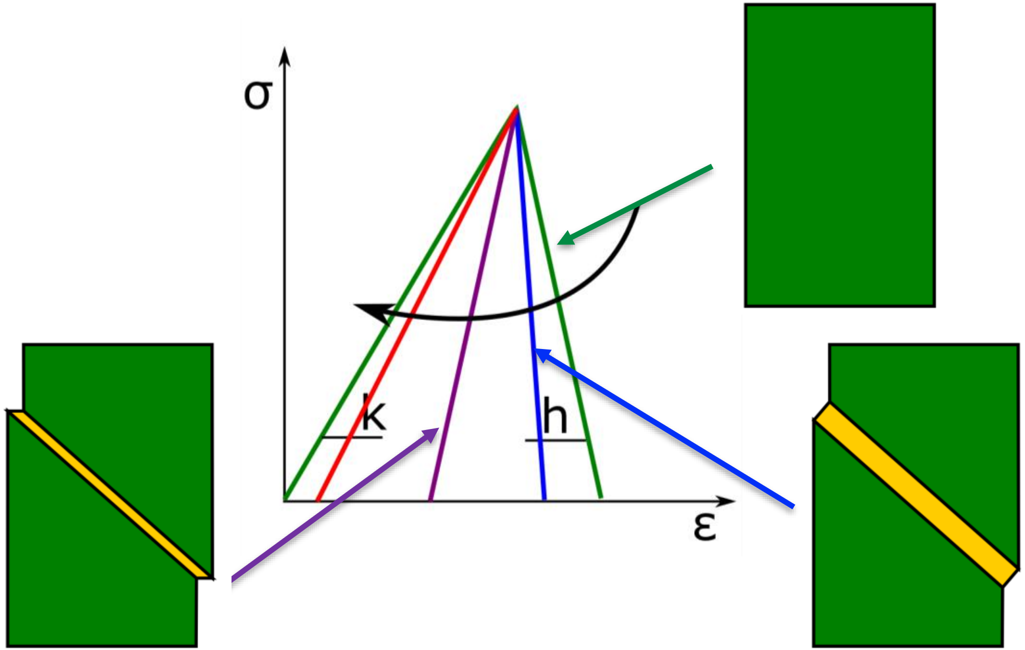
$$\sigma_2 = k\epsilon_2$$

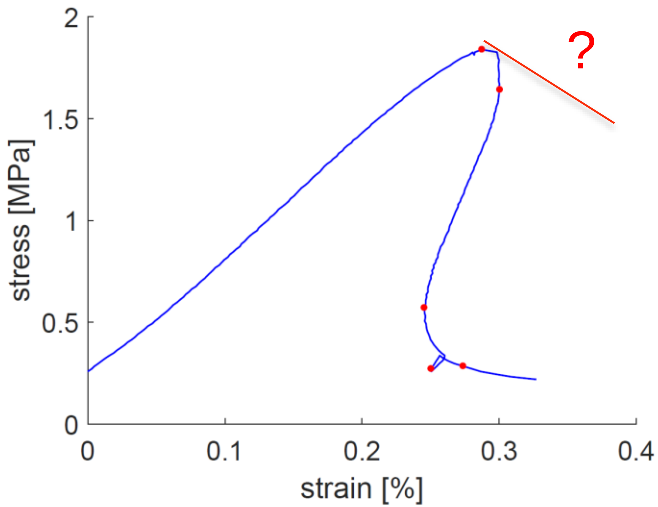
- The stress becomes zero when $\epsilon_1 = \epsilon_f + \epsilon_c$
- Meaning that it becomes zero at

$$\epsilon = (\epsilon_f + \epsilon_c)\,\frac{d}{L}$$

Strain localization – Thought experiment in 1D

- For different (decreasing) values of d:

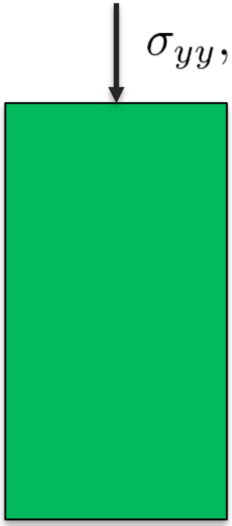




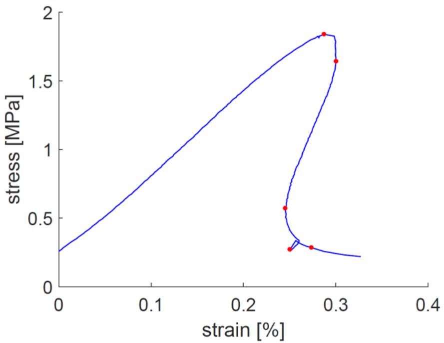
Controllability is another thing:

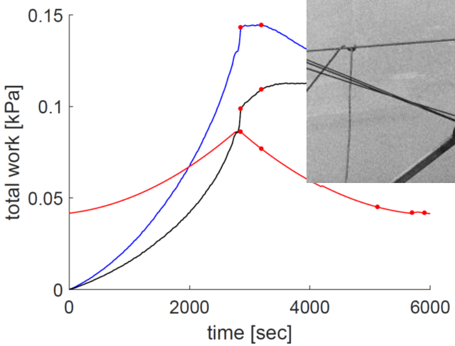
- A simple example: uniaxial test with radial strain rate control

$\sigma_{yy}, \epsilon_{yy}$



$$\sigma_{rr} = 0$$
$$\dot{\epsilon}_{rr} = c$$





Elasto-plasticity

- It is assumed that deformations are reversible (elastic) within a limited domain

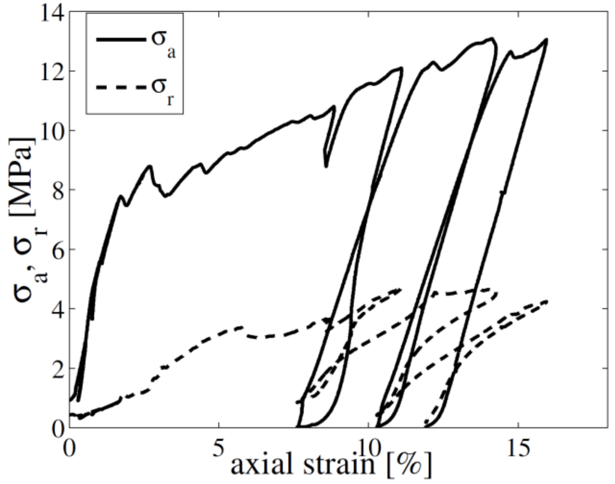
$$f(\underline{\boldsymbol{\sigma}}) < 0$$

- Strain rates are decomposed into reversible and irreversible:

$$\dot{\epsilon}_{ij} = \dot{\epsilon}^{e}_{ij} + \dot{\epsilon}^{p}_{ij}$$

- To solve the problem, the direction of the plastic strain increment is required. It is assumed that

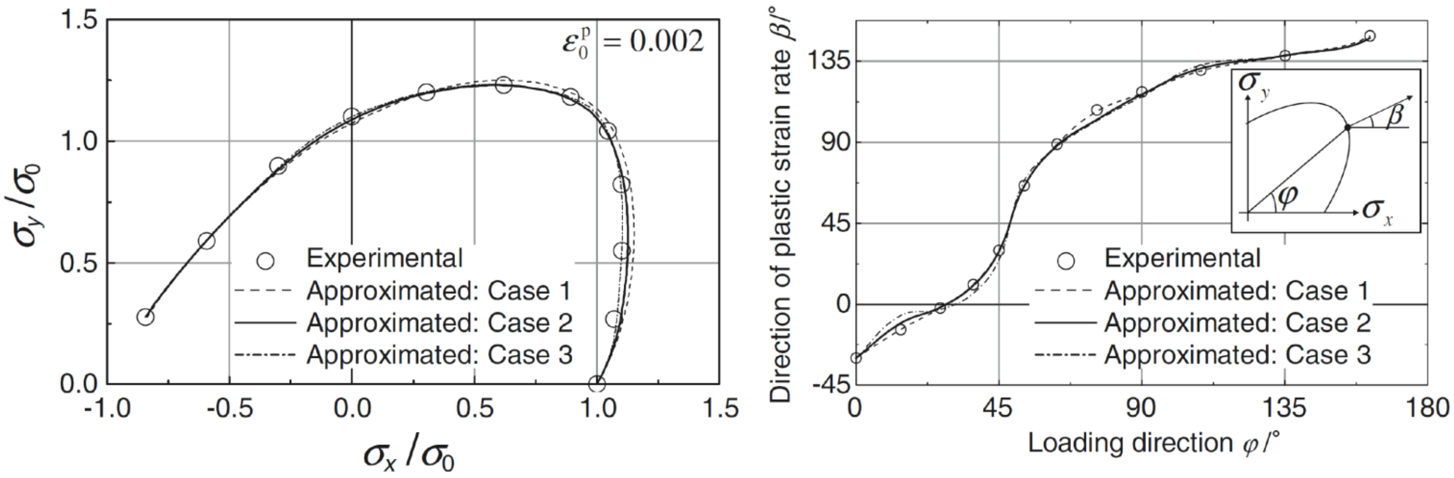
$$\dot{\epsilon}^{pl}_{ij} = \dot{\lambda}\frac{\partial g}{\partial \sigma_{ij}}$$



Castellanza et al. (2009)

Associativity

- The flow rule reads: $$\dot{\epsilon}_{ij}^{pl} = \dot{\lambda}\frac{\partial f}{\partial \sigma_{ij}}$$



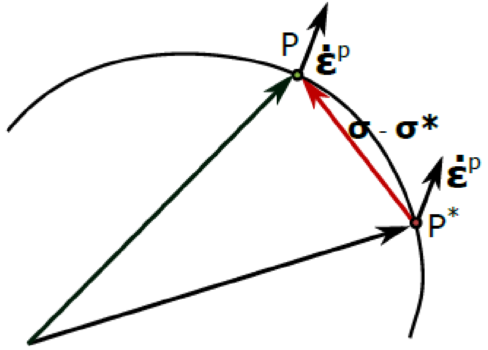
Ishiki et al. (2011)

Convexity &associativity

- **Assumption**: The stress state is such, that the dissipation rate is maximum (Hill 1948)
- For normality, the dissipation rate is maximum with respect to the stress, if the yield surface is convex.

$$\dot{W}_p = \left(\sigma_{ij} - \sigma^*_{ij}\right) \dot{\epsilon}^p_{ij} \geq 0$$

- which would mean that
  - the flow rule is associative
  - the yield surface is convex
- The underlying assumption is that the body tries to minimize its internal energy as fast as possible.



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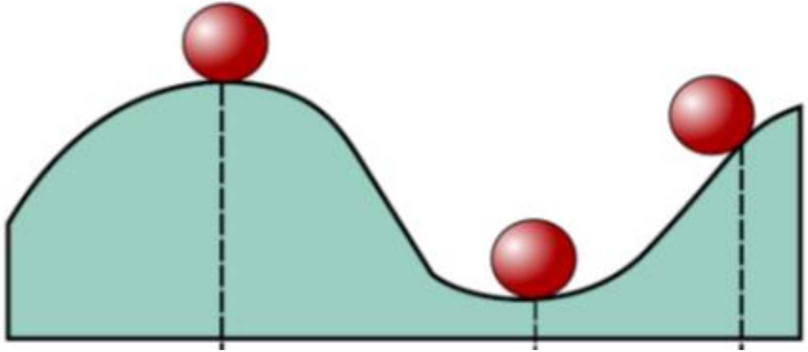
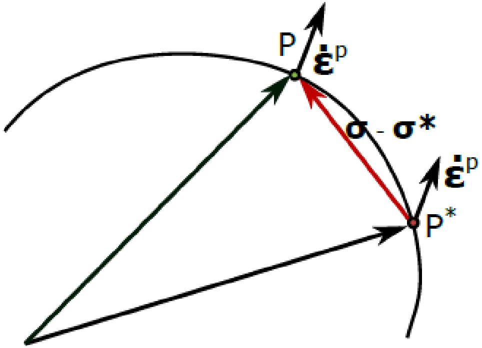
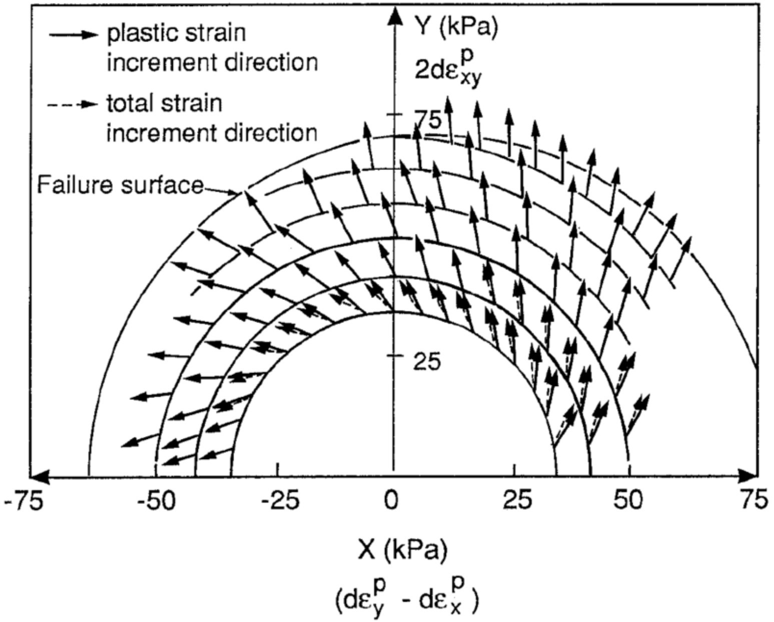
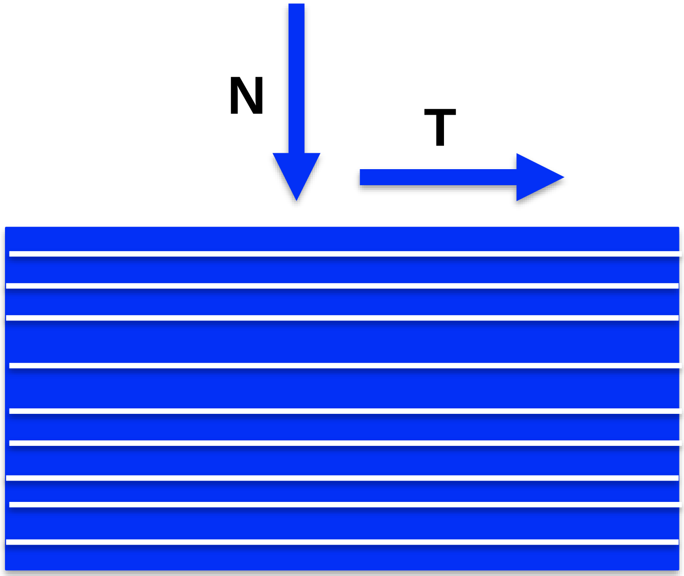




Non associativity



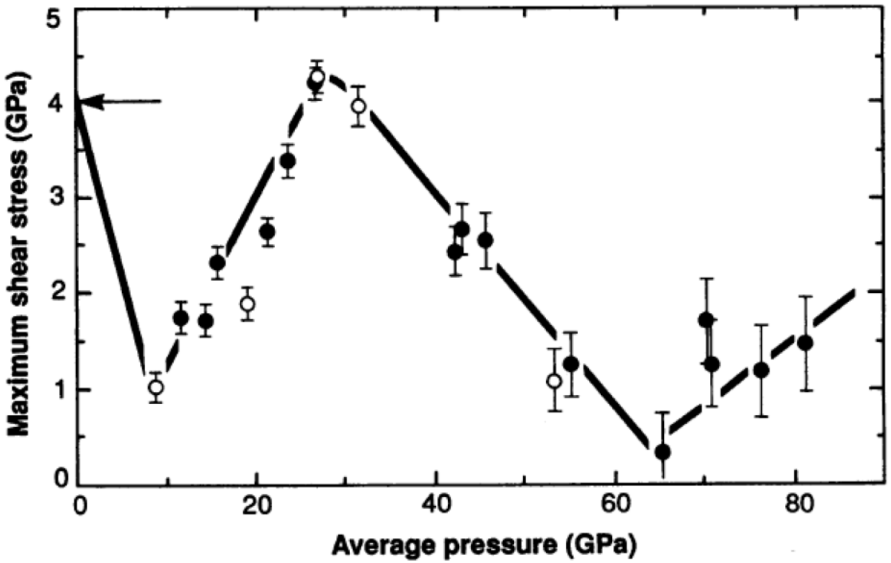
Gutierrez and Ishihara (2000)



No volumetric deformation

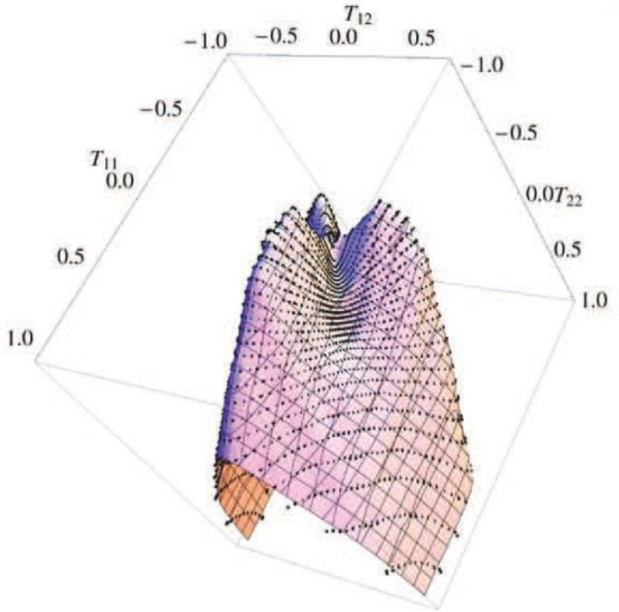
Non convexity?

Tests on fused silica glass



Meade and Jeanloz (1988)

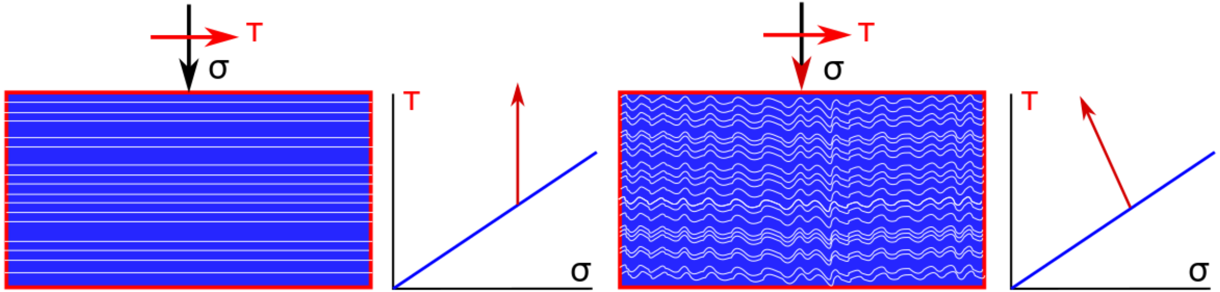
FEM on honeycombs



Glüge and Bucci (2017)

Limitations

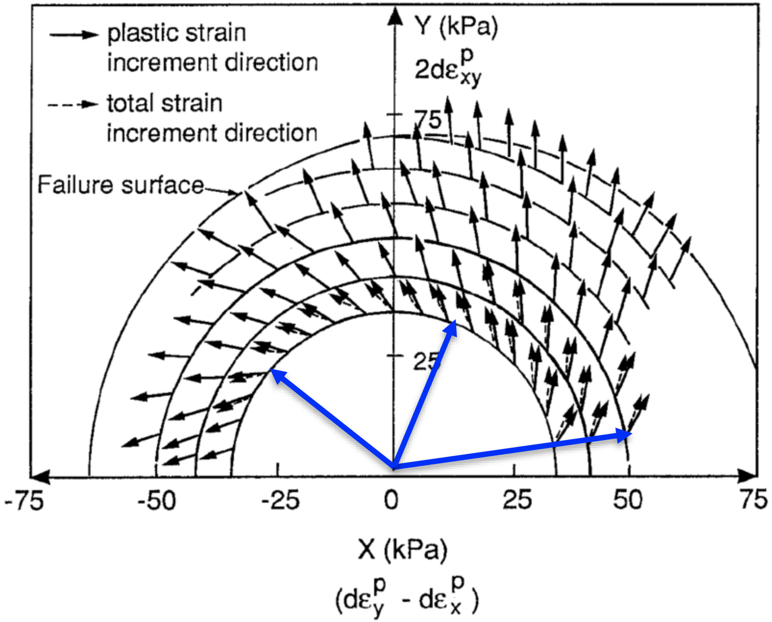
- The dissipation rate should always be non negative, or
- Dissipated energy along a closed loading path should be non-negative
- The angle between stress vector and plastic strain increment vector can never be more than 90°

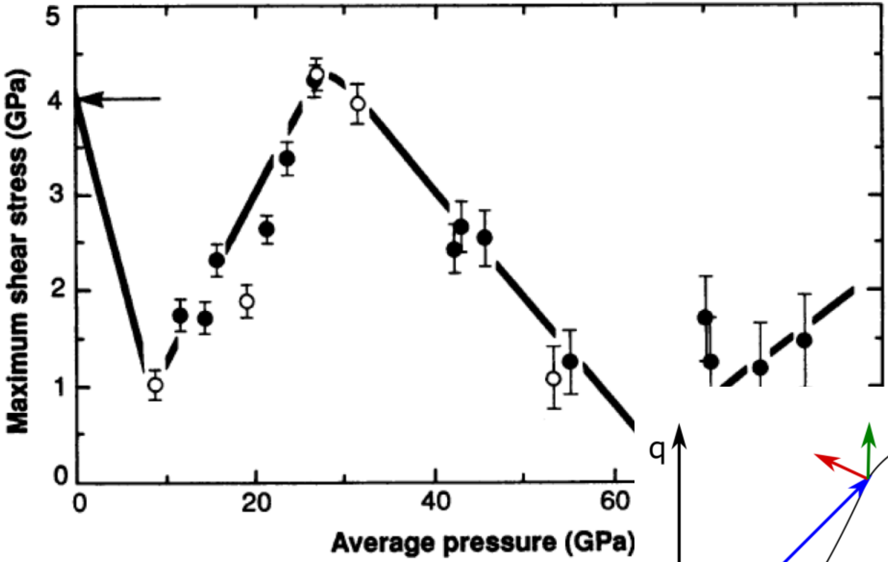


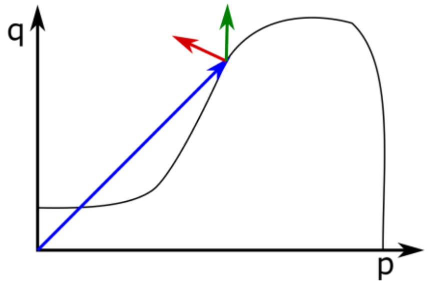
- Different types of constraints can determine the flow direction

Limitations

Meade and Jeanloz (1988)





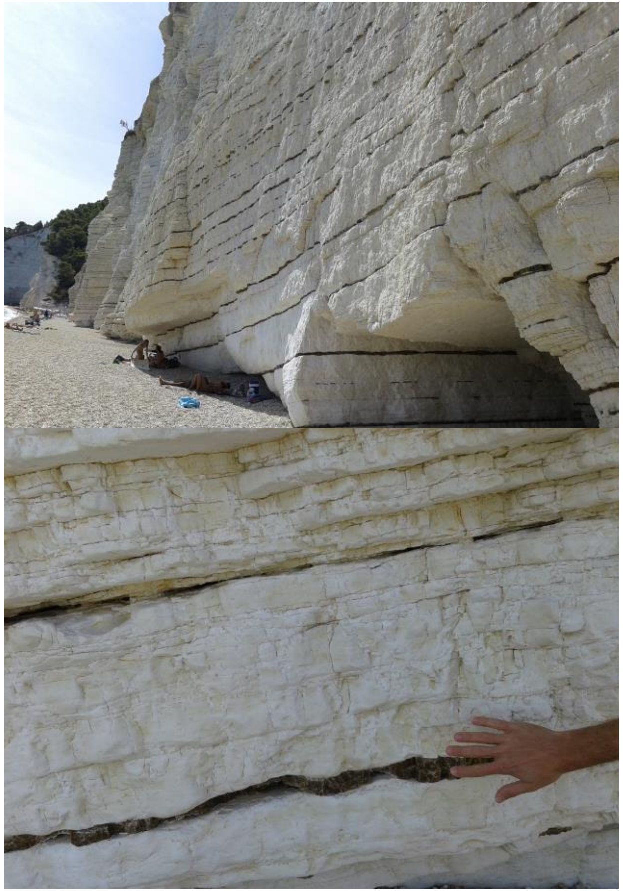


Gutierrez and Ishihara (2000)

Anisotropy

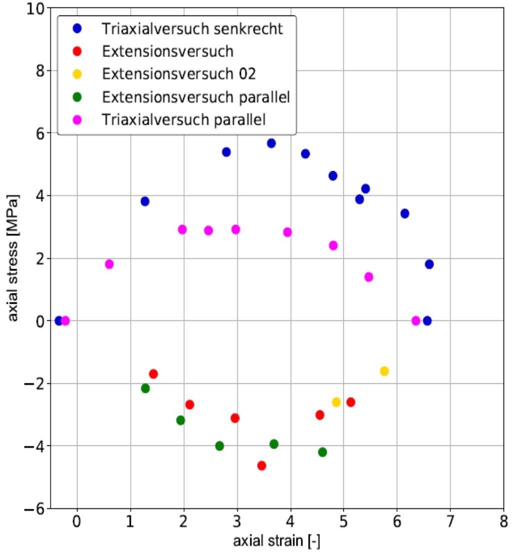
- Usually ignored because:
  - Usually not known
  - Experimentally hard/expensive to get
  - Already incorporated in the failure envelope from experimental data

- We will take a look at what this means for the elastic energy

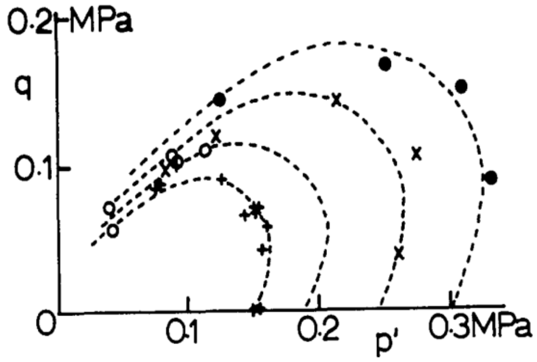


Anisotropy – Experimental observations

- For cohesive materials the yield locus is affected:



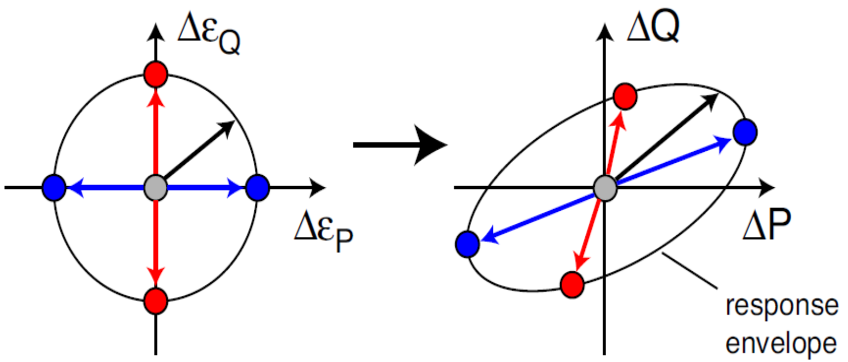
Courtesy of J. Leuthold

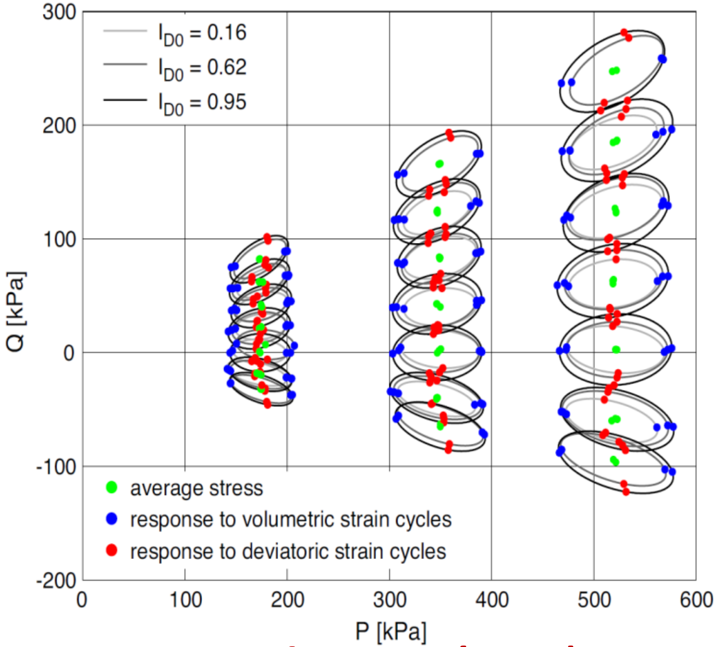


Muir Wood and Graham (1990)

Anisotropy – Experimental observations

- For granular materials the elastic response is affected:



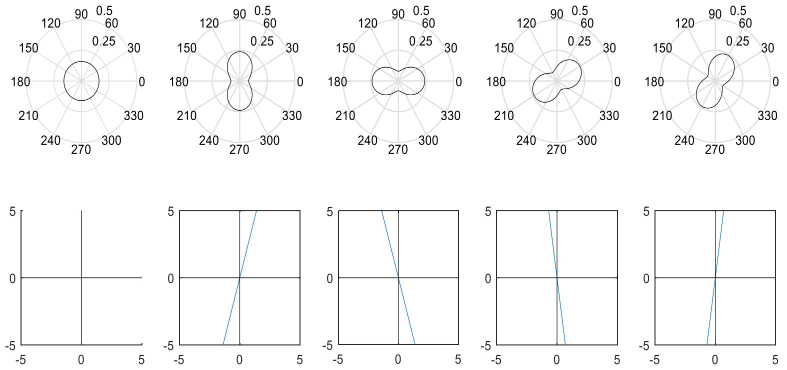


Wichtmann (2016)

Anisotropy

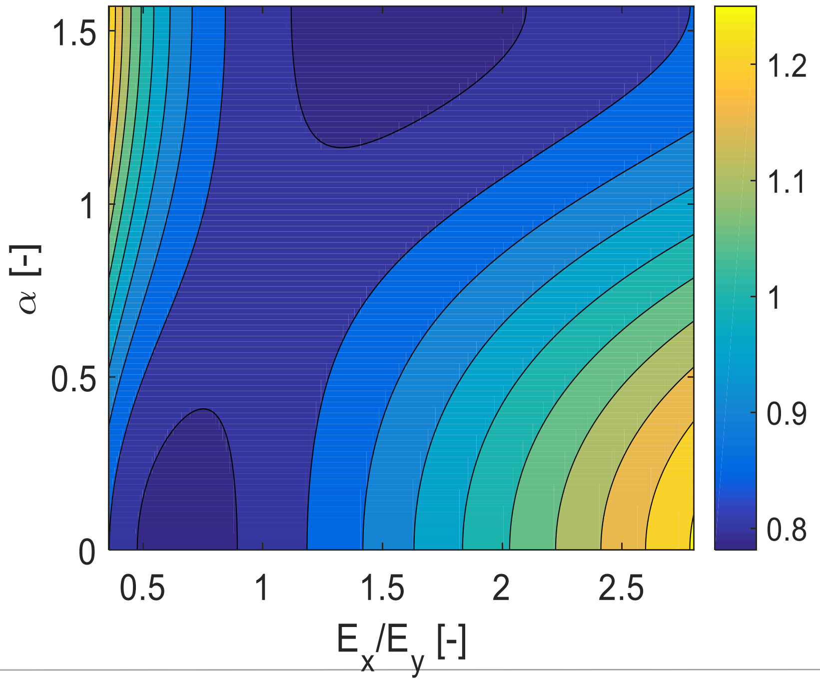
- To simplify matters, a 2-D elastic anisotropy is considered:

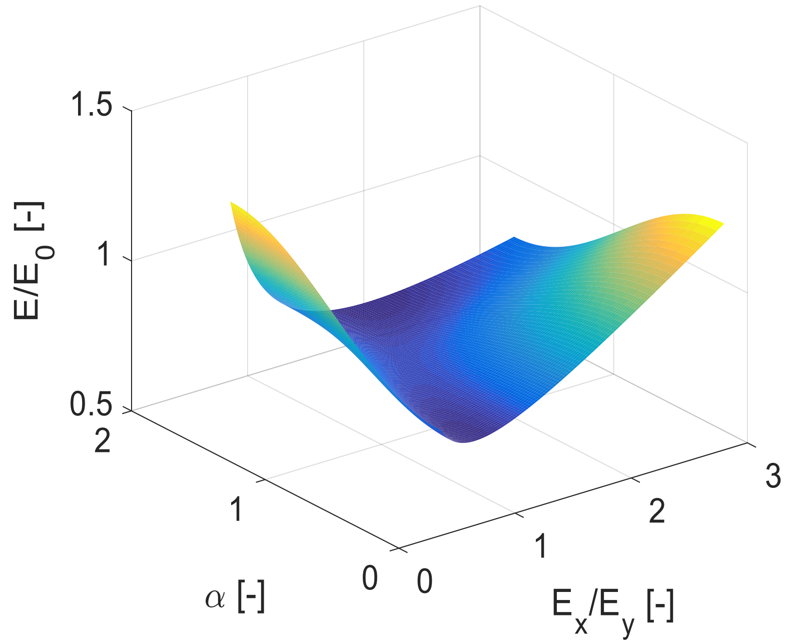
$$\begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{xy} \end{bmatrix} = \begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_y} & 0 \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_y} & 0 \\ 0 & 0 & \frac{1}{G_{xy}} \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix}$$



Anisotropy

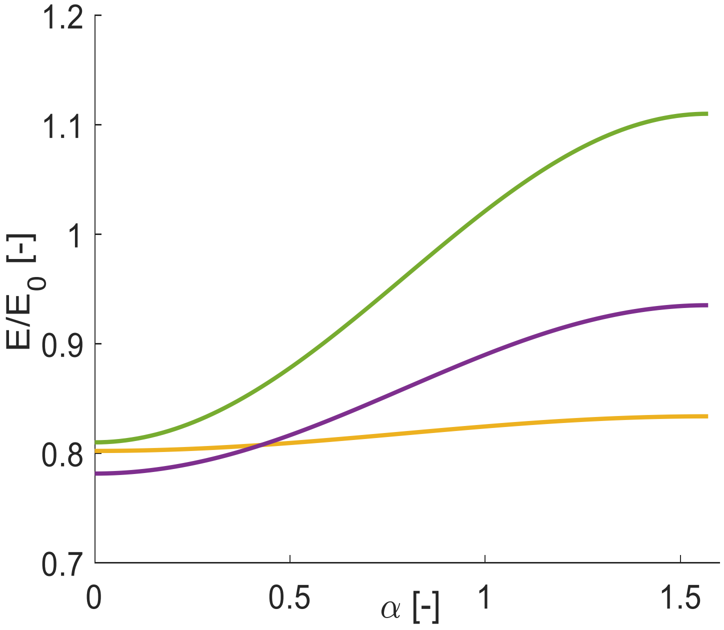
- The elastic energy depends on the relative angle and the degree of anisotropy:

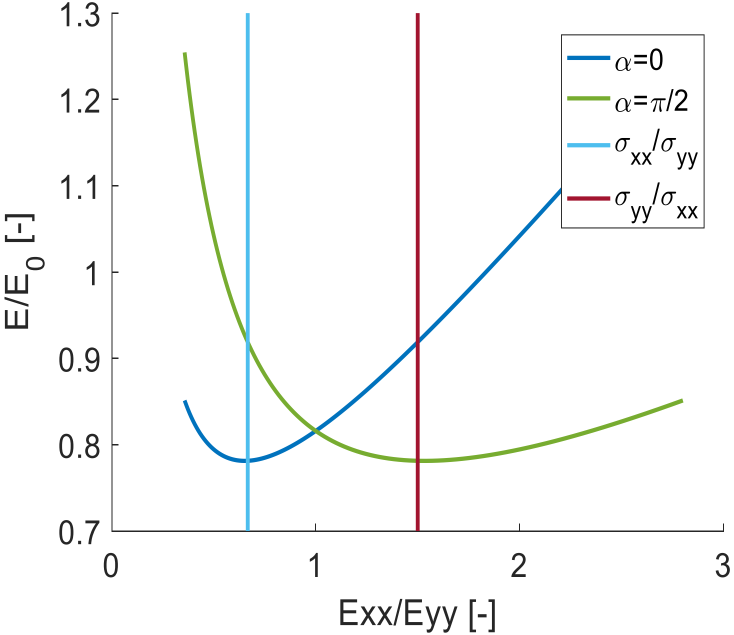




Anisotropy

- The minimum is found for coaxial tensors, when the stiffness ratio equals the stress ratio:





- In general granular media try to move in this direction

Implications for modelling

- Elastic strains are miscalculated
  - Elastic strain increments are usually much smaller than the plastic strain increments
- The elastic energy is overestimated
  - It is usually of no direct consequence to the results or application
- Energy ‘invested’ in changing the internal structure is neglected
  - This may affect coaxiality, but does not play a role for monotonic coaxial loading

Structure evolution: an example

- Work rate balance in general

$$\sigma_{ij}\dot{\epsilon}_{ij} = \dot{E}^{el} + D$$

- Ignoring the evolution of anisotropy

$$\sigma_{ij}\dot{\epsilon}_{ij} = \sigma_{ij}\dot{\epsilon}_{ij}^{el} + D \Rightarrow$$
$$D = \sigma_{ij}\dot{\epsilon}_{ij}^{pl}$$

- Considering the evolution of anisotropy

$$\sigma_{ij}\dot{\epsilon}_{ij} = \sigma_{ij}\dot{\epsilon}_{ij}^{el} + \frac{\partial E}{\partial \alpha}\dot{\alpha} + D \Rightarrow$$
$$D = \sigma_{ij}\dot{\epsilon}_{ij} - \sigma_{ij}\dot{\epsilon}_{ij}^{el} - \frac{\partial E}{\partial \alpha}\dot{\alpha}$$

Coupling: Thermoelasticity

- The heat equation reads

$$\rho c \frac{\partial T}{\partial t} - \nabla . (k \nabla T) = \dot{q}_v$$

  - where ρ is the density
  - c is the specific heat capacity
  - T is the temperature
  - k is the thermal conductivity
  - $\dot{q}_v$ is the volumetric heat source

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T$$

  - for constant conductivity and no volumetric source

- Temperature increase causes thermal expansion

$$\epsilon_T = -\alpha T$$

  - where α is the thermal expansion coefficient and compression is assumed positive

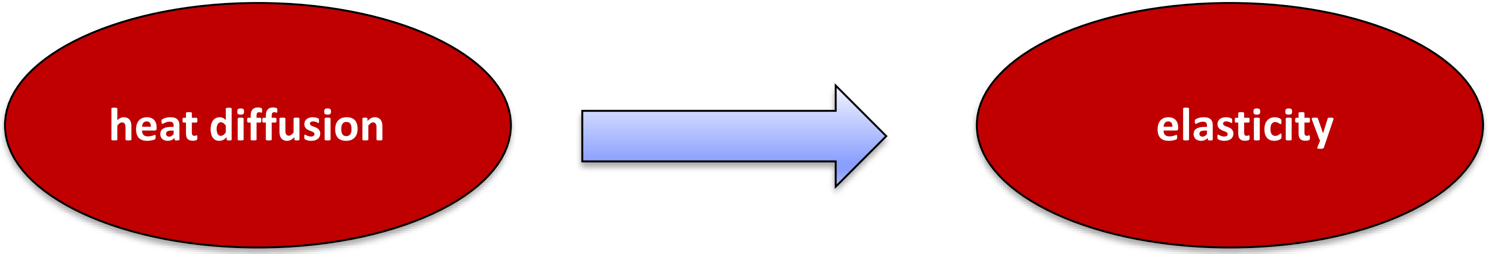
Thermoelasticity – one way coupling

- The heat diffusion is assumed uncoupled from the elastic response:

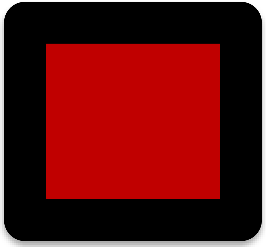
$$\rho c \frac{\partial T}{\partial t} - \nabla . \left(k \nabla T \right) = \dot{q}_v$$

- The elastic response depends on the (independently evaluated) temperature change

$$\boldsymbol{\sigma} = \underline{\mathbf{E}} \left(\boldsymbol{\epsilon} - \alpha T \mathbf{I} \right)$$



Thermoelasticity – a simple example



- Consider a small uniform volume.
- No boundary displacements are allowed.
- The temperature is increased from T_0 to T_1.
- The heat equation becomes

$$\rho c \frac{\partial T}{\partial t} - \nabla . \left(k \nabla T \right) = \dot{q}_v \Rightarrow \rho c \frac{\partial T}{\partial t} = \dot{q}_v \Rightarrow q_v = \rho c \left(T_1 - T_0 \right)$$

- meaning that the energy density stored due to the temperature change is

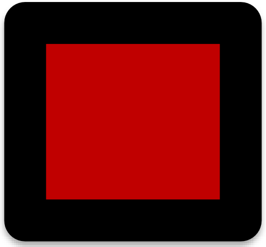
$$Q = \rho c \left(T_1 - T_0 \right)$$

- generated by the volumetric heat source

Thermoelasticity – a simple example

- The thermal expansion – since the material is constrained – causes an increase in mean pressure:

$$\boldsymbol{\sigma} = -\underline{\mathbf{E}}\left(\alpha(T_1 - T_0)\mathbf{I}\right)$$



- increasing the elastic energy stored to

$$E = \frac{1}{2}\boldsymbol{\sigma} \cdot \boldsymbol{\epsilon} = \frac{1}{2}K\alpha^2(T_1 - T_0)^2$$

$$Q = \rho c\left(T_1 - T_0\right)$$

- Where did this come from?

Thermoelasticity – coupled

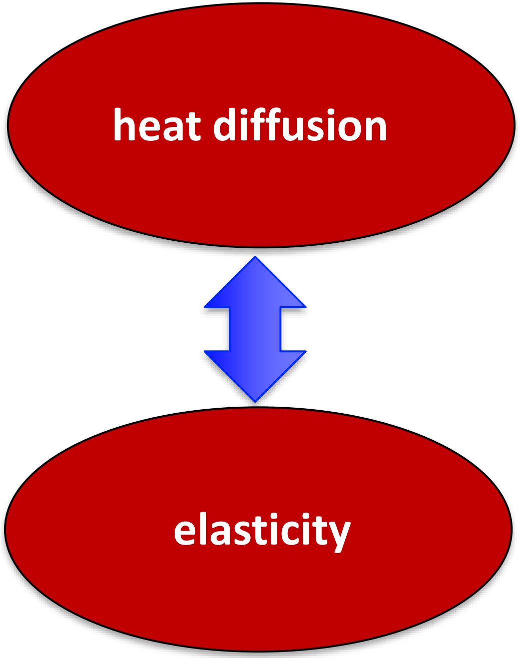
- The heat equation is derived from the energy balance and Fourier's law:

$$\Delta Q = Q_{in} - Q_{out} \qquad \overrightarrow{q} = -k\nabla T$$

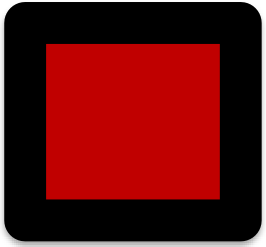
- If the internal energy does not depend only on temperature:

$$\rho c \frac{\partial T}{\partial t} + T_0 \alpha p - \nabla . (k \nabla T) = \dot{q}_v$$

- again under assumptions:
  - $(T_1 - T_0)/T_0 << 1$
  - All coefficients are independent of temperature and pressure



Thermoelasticity – a simple example



- How large is the discrepancy?

$$E = \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\epsilon} = \frac{1}{2}K\alpha^2(T_1 - T_0)^2$$

- Temperature increase of 100 ^{o}C results in a discrepancy of

Material	**K [MPa]**	**a [10^{-6}/K]**	**E [J/m^3]**
Aluminium	70000	23	18.51
Concrete	20000	12	1.44
Water	2200	69	5.24

- Volumetric compression by 10^{-6} results in elastic energy of 105, 30, 3.3 kJ/m^3 correspondingly

Closing remarks

- Take the time to find out the underlying assumptions
- Don’t use models outside their domain of validity
- Keep in mind where errors can arise and how big they can get
- Keep an eye on reality
- No model is perfect, small discrepancies for the sake of convenience can be acceptable