Institute of
Continuum Mechanics

Leibniz
University
Hannover

Seventh Meeting
UNILATERAL PROBLEMS IN
STRUCTURAL ANALYSIS

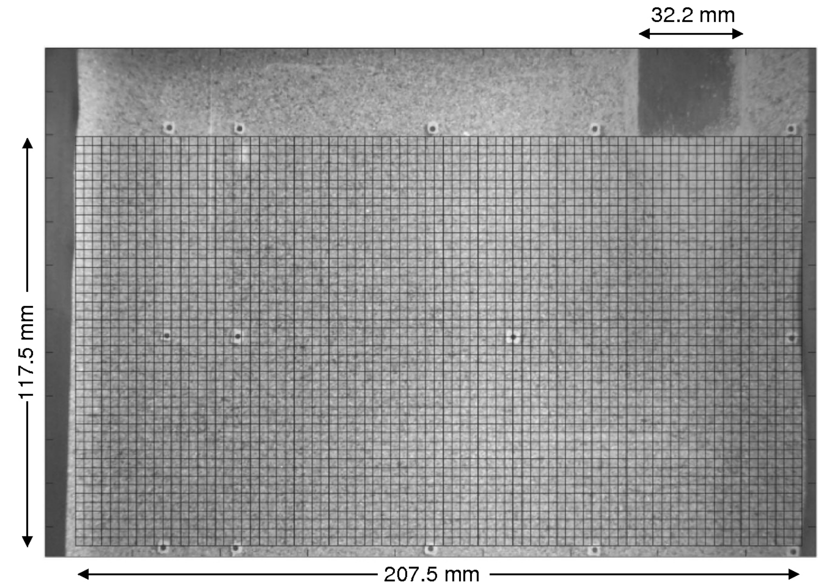
June 17-19 2010
Palmanova, Italy

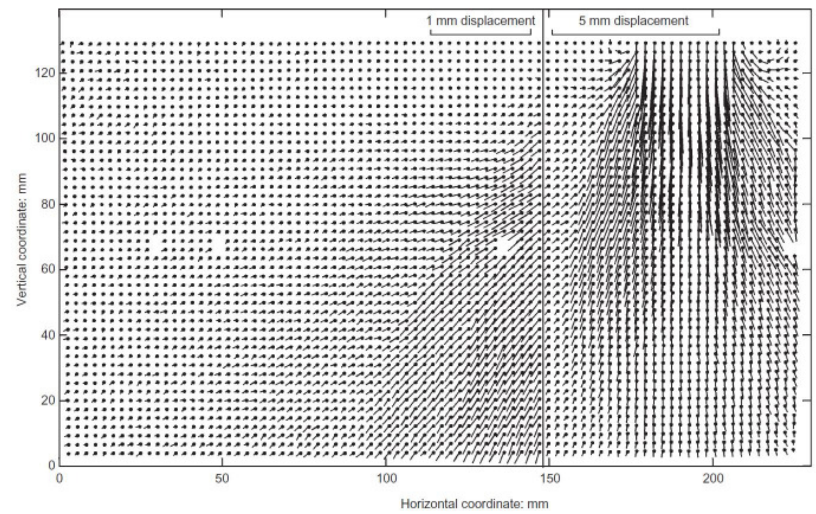
Multiscale Modeling of Non-Cohesive Granular Materials

Christian Wellmann, Peter Wriggers

motivation

- complex material behavior
- phenomenological approach
  - assume continuum
  - elasto-plastic constitutive equation
- drawbacks
  - numerous parameters
  - stability, accuracy and technical issues for large deformations
- multi-scale model
  - particle model for “hot-spot” regions
  - continuum model elsewhere
- requires coupling at interface
- fit continuum model to homogenized particle behavior





pictures from [*White & Bolton*, 2004]

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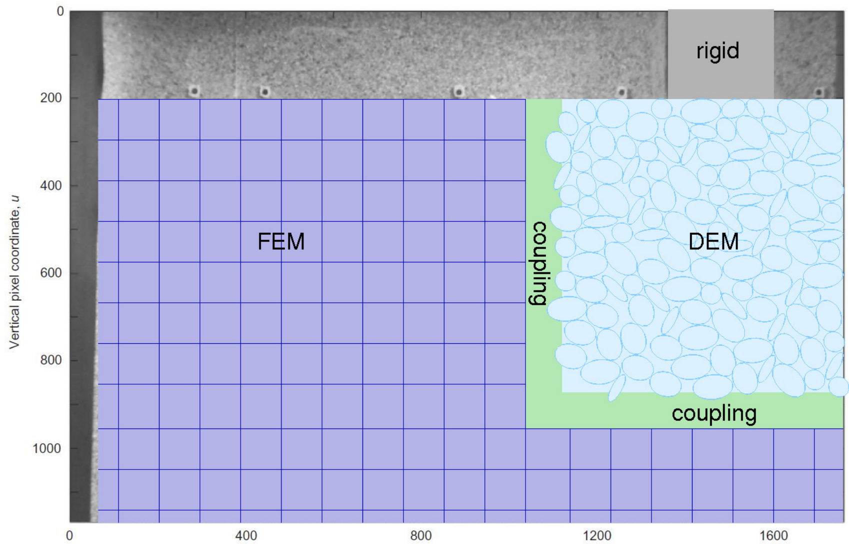
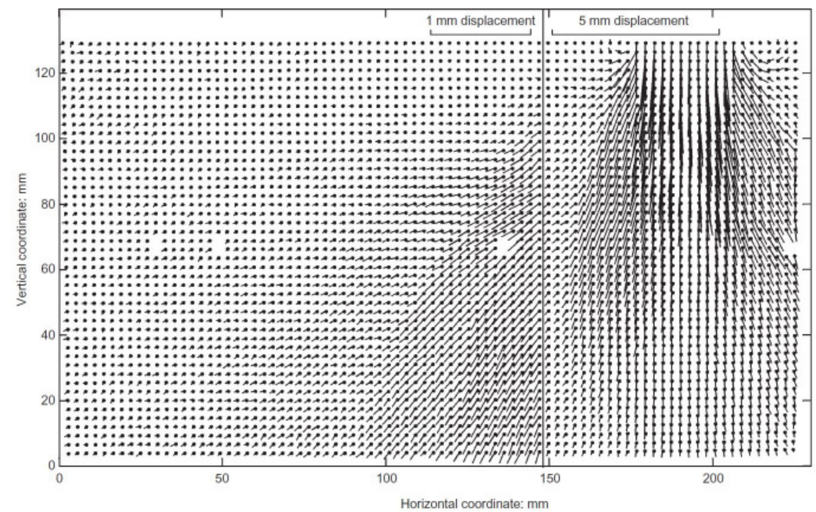
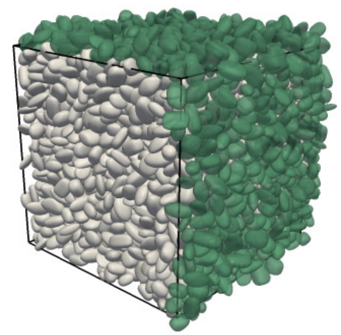




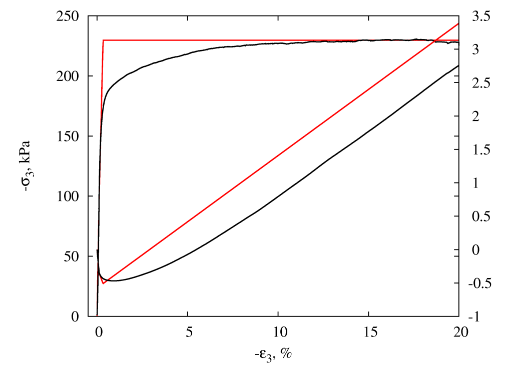
pictures from [*White & Bolton*, 2004]

outline

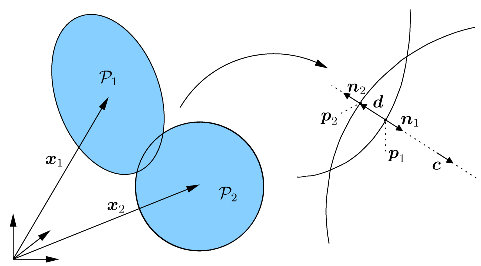
homogenization



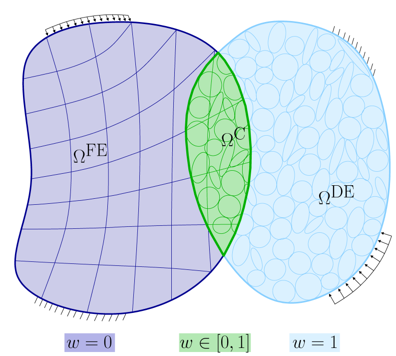
fit elasto-plastic parameters



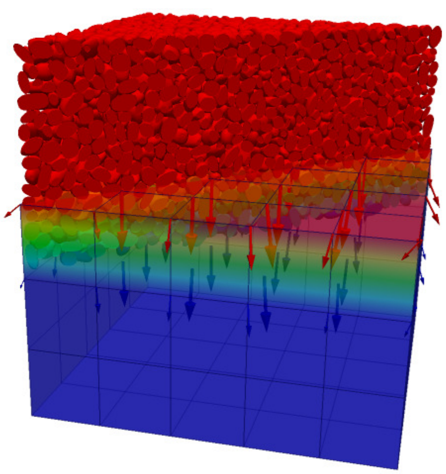
discrete element model



DE-FE coupling scheme



numerical examples



discrete element method

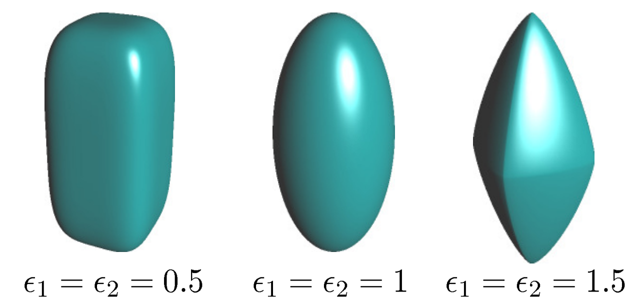
- dry non-cohesive frictional granular material
- individual grains are modeled as rigid bodies
- superquadric geometry [*Barr*, 1981]

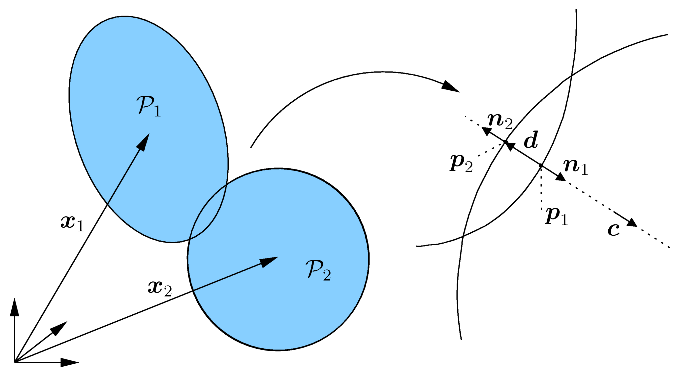
$$F(\boldsymbol{x}) = \left(\left| \frac{x_1}{r_1} \right|^{\frac{2}{\epsilon_1}} + \left| \frac{x_2}{r_2} \right|^{\frac{2}{\epsilon_1}} \right)^{\frac{\epsilon_1}{\epsilon_2}} + \left| \frac{x_3}{r_3} \right|^{\frac{2}{\epsilon_2}} = 1$$

- arbitrary aspect ratios & angularity
- contact:
  - admit small overlap
  - Hertz-Mindlin contact theory
  - Coulomb friction
- explicit time integration

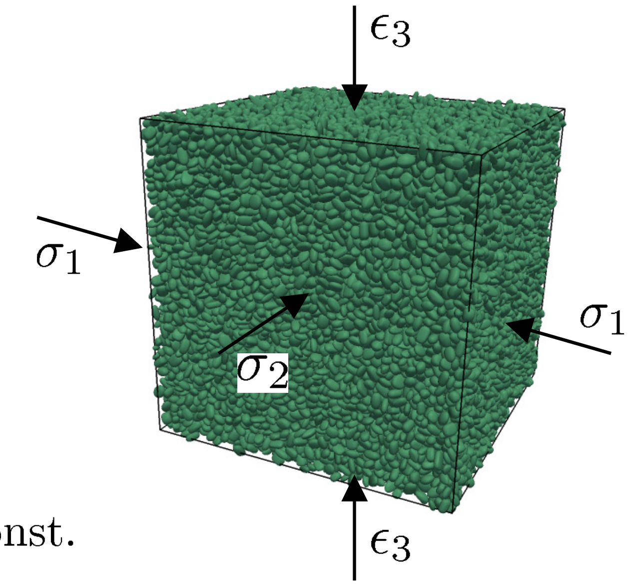
$$\begin{aligned} m\,\ddot{\boldsymbol{x}} &= \boldsymbol{f}^{\text{res}} \\ \boldsymbol{I}\cdot\dot{\boldsymbol{\omega}} + \boldsymbol{\omega}\times\boldsymbol{I}\cdot\boldsymbol{\omega} &= \boldsymbol{m}^{\text{res}} \end{aligned}$$

$r_1 = r_2 = r_3/2$



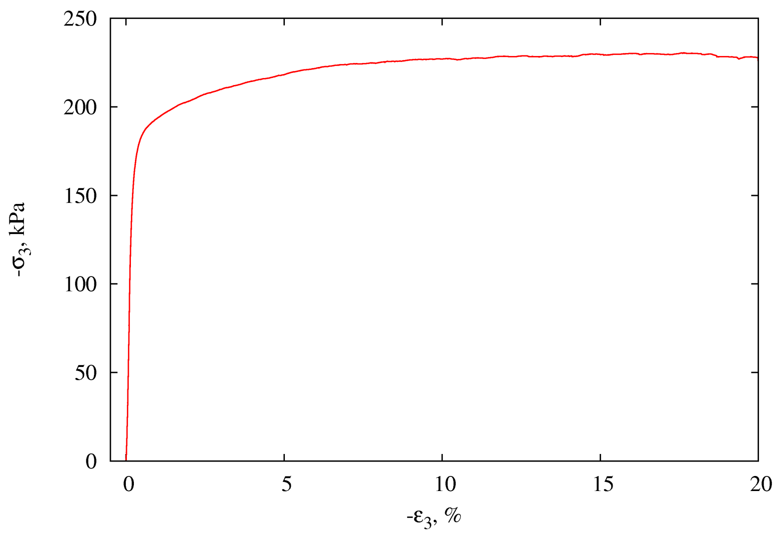


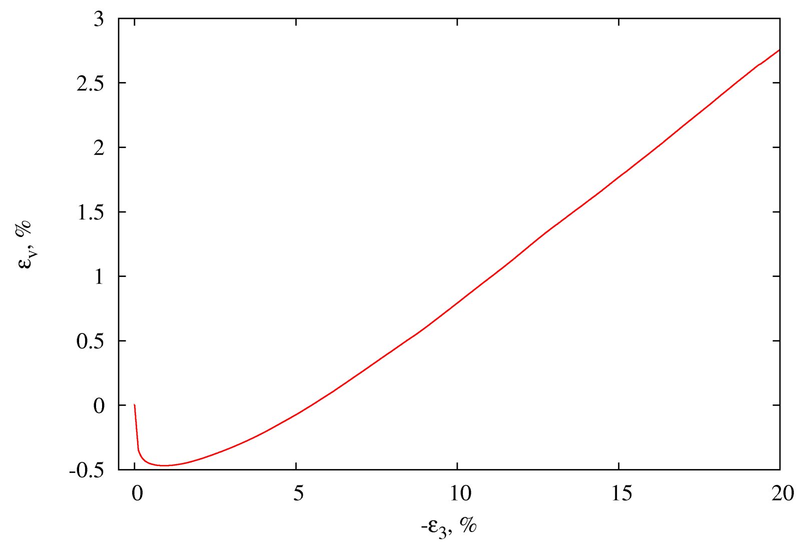
homogenization



- random periodic unit cell
- DEM parameters adapted to Leighton Buzzard Sand fraction B
  - size: 0.6 – 1.18 mm
  - E=50 GPa, ν=0.2
  - friction [*Rowe*, 1962], [*Ishibashi*, 1994]: μ=0.24
- triaxial test with adaptive dimension control:

$$\sigma_1 = \sigma_2 = \text{const.}$$
$$\dot{\epsilon}_3 = \text{const.}$$

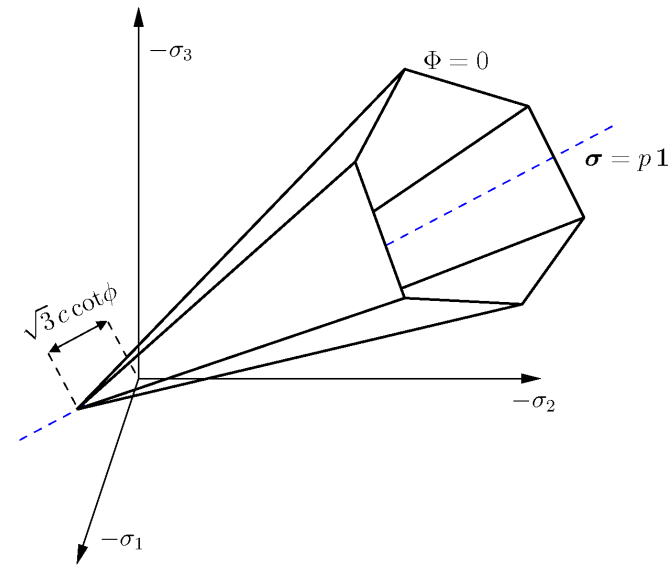


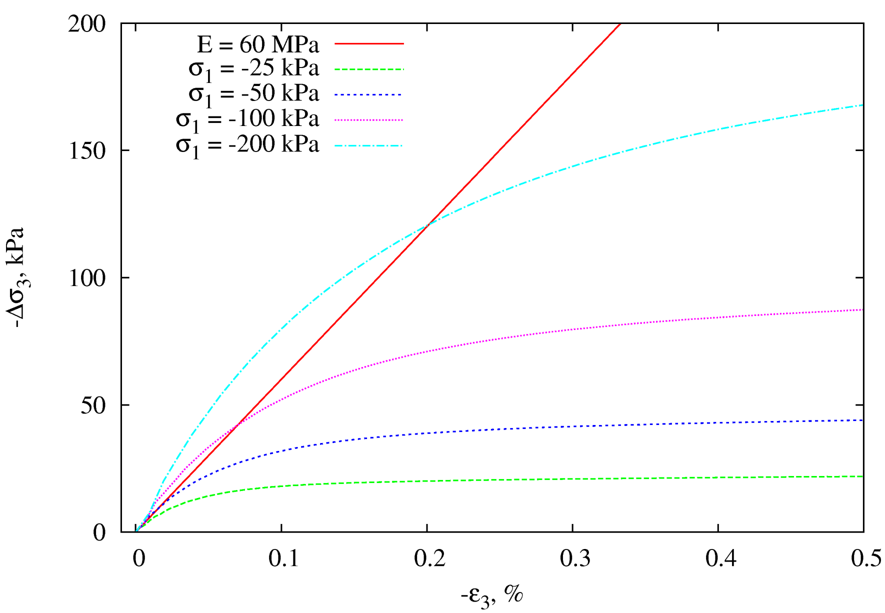


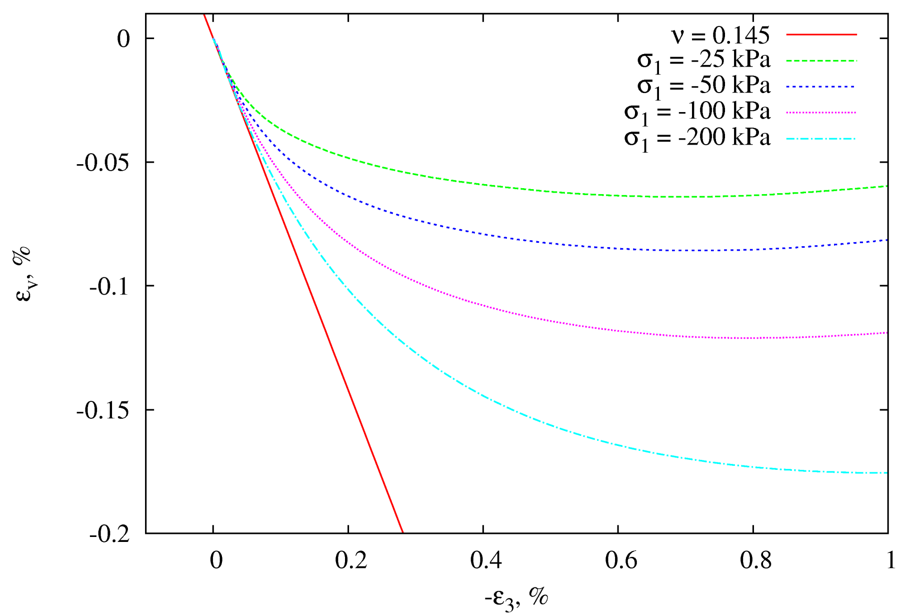
fitting of constitutive equation

- non-associative Mohr-Coulomb

$$\epsilon = \epsilon^e + \epsilon^p$$
$$\sigma = 2\,G\,\epsilon^e_{\mathrm{dev}} + K\,\epsilon^e_V\,\mathbf{1}$$
$$\Phi = \sigma_1 - \sigma_3 + (\sigma_1 + \sigma_3)\,\sin\varphi + 2\,c\,\cos\varphi$$
$$\Psi = \sigma_1 - \sigma_3 + (\sigma_1 + \sigma_3)\,\sin\psi + 2\,c\,\cos\psi$$
$$\Rightarrow G,\ K,\ \varphi,\ \psi,\ (c)$$







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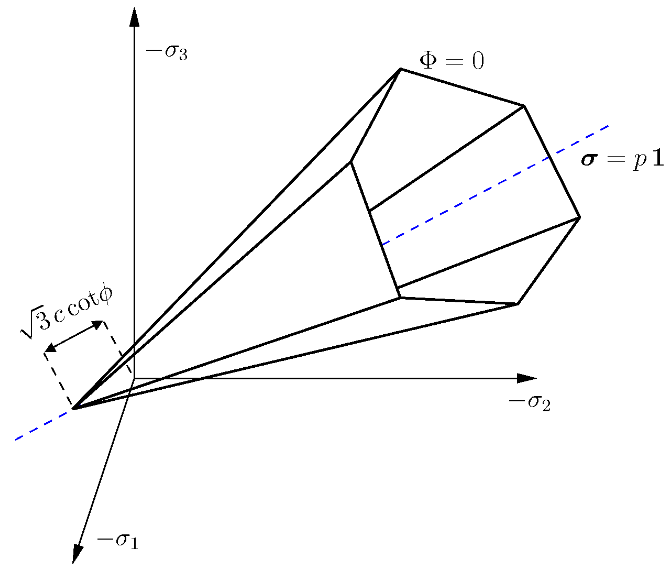
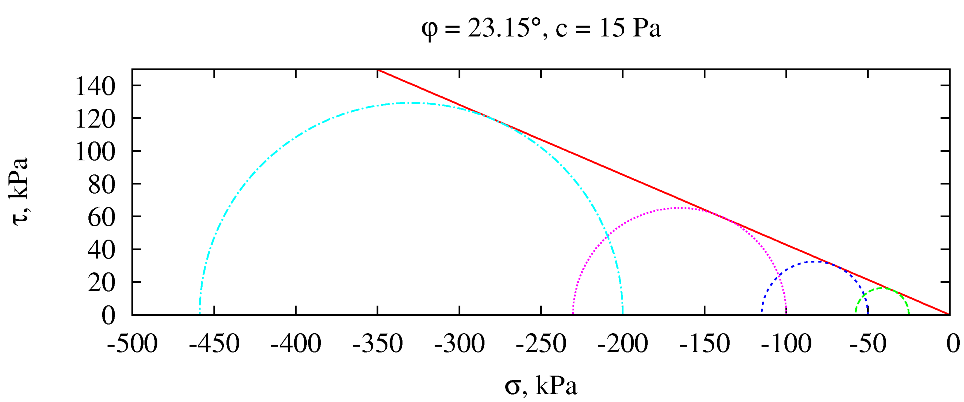
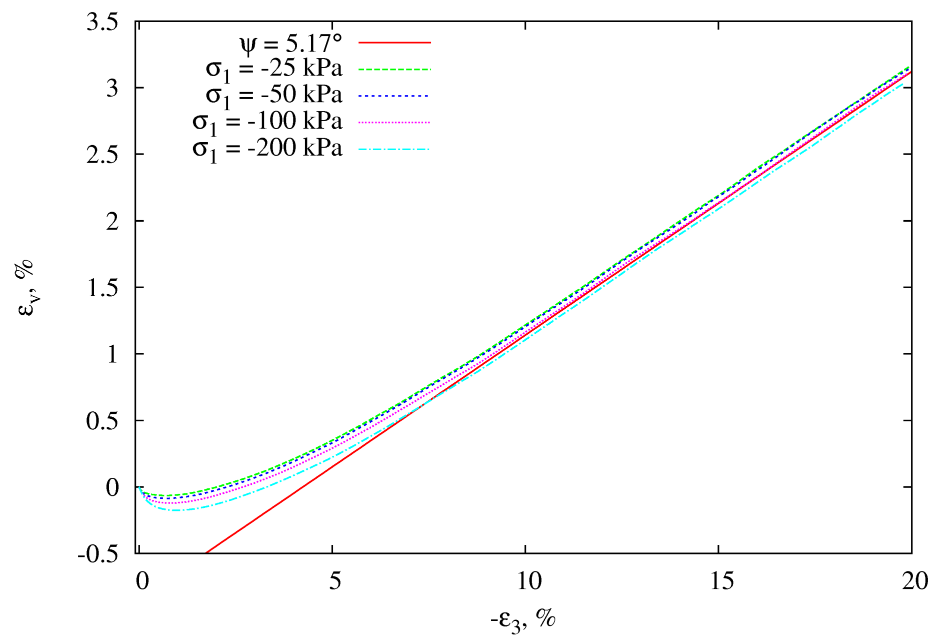




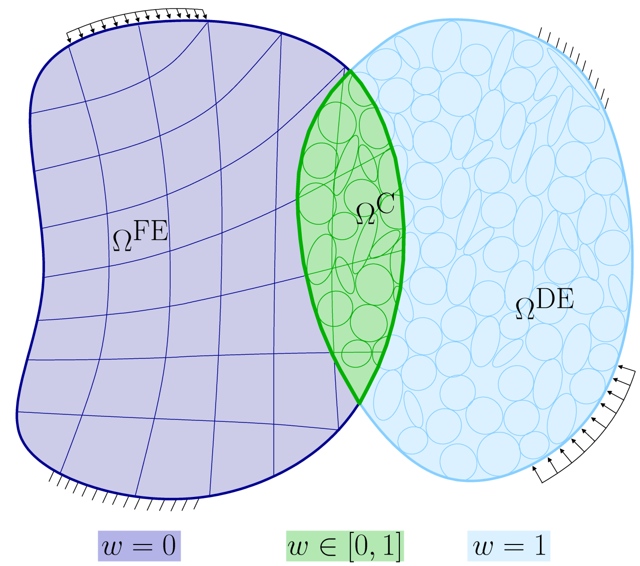


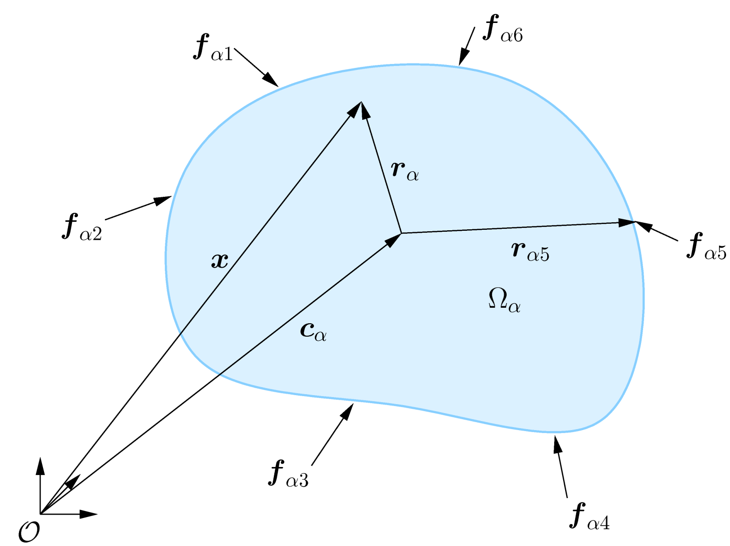
coupling discrete & finite element method

- use Arlequin method [*Ben Dhia*, 1998]
  - both models overlap in coupling domain Ω^{C}
  - introduce weight factor to interpolate virtual work

$$
\begin{aligned}
\delta W &= \delta W^{\mathrm{FE}} + \delta W^{\mathrm{DE}} \quad \text{with} \\
\delta W^{\mathrm{FE}} &= \int_{\Omega^{\mathrm{FE}}} (1-w)\,\boldsymbol{\sigma} : \delta \boldsymbol{\epsilon}\, \mathrm{d}\Omega + \int_{\Omega^{\mathrm{FE}}} (1-w)\,\rho\,(\ddot{\boldsymbol{x}} - \boldsymbol{b}) \cdot \delta \boldsymbol{u}\, \mathrm{d}\Omega - \\
&\quad \int_{\Gamma^{\mathrm{FE}}} (1-w)\,\boldsymbol{t} \cdot \delta \boldsymbol{u}\, \mathrm{d}\Gamma \\
\delta W^{\mathrm{DE}} &= \sum_{\alpha=1}^{n_p} \delta W_\alpha \\
&= \sum_{\alpha=1}^{n_p} \left[\int_{\Omega_\alpha} w\,\rho\,(\ddot{\boldsymbol{x}} - \boldsymbol{b}) \cdot \delta \boldsymbol{u}_\alpha\, \mathrm{d}\Omega - \sum_{\beta=1}^{n_\alpha} w_{\alpha\beta}\, \boldsymbol{f}_{\alpha\beta} \cdot \delta \boldsymbol{u}_\alpha \right]
\end{aligned}
$$

- FE part: standard integration with additional weight factor





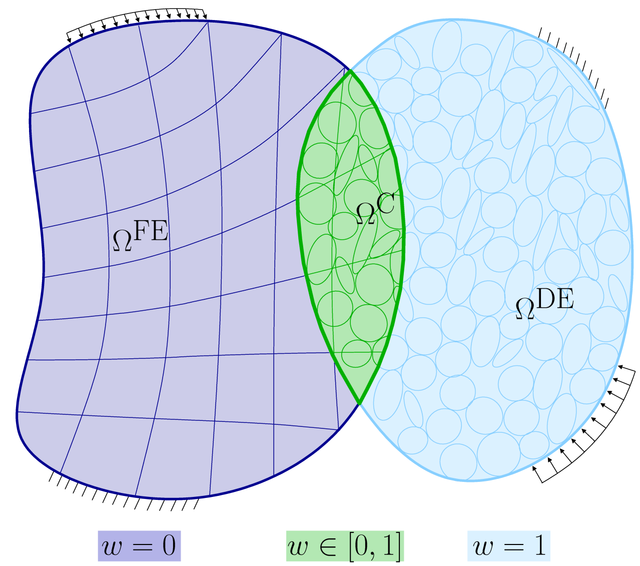
weighted virtual work of a rigid body

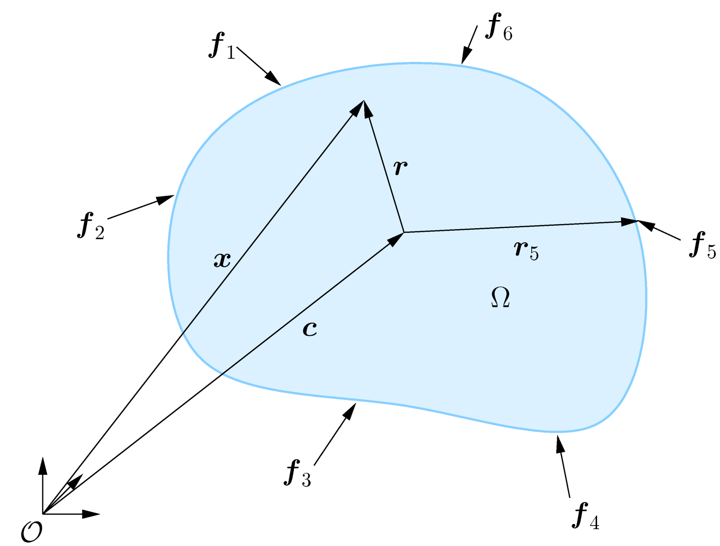
- $$\begin{aligned} \delta W &= \int_\Omega w\,\rho\,(\ddot{\boldsymbol{x}} - \boldsymbol{b}) \cdot \delta\boldsymbol{u}\,\mathrm{d}\Omega - \sum_{\beta=1}^{n} w_\beta\,\boldsymbol{f}_\beta \cdot \delta\boldsymbol{u} \\ \boldsymbol{x} &= \boldsymbol{c} + \boldsymbol{r} \Rightarrow \ddot{\boldsymbol{x}} = \ddot{\boldsymbol{c}} + \dot{\boldsymbol{\omega}} \times \boldsymbol{r} + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \boldsymbol{r}) \\ \delta\boldsymbol{u}(\boldsymbol{x}) &= \delta\boldsymbol{u}^0 + \delta\boldsymbol{\omega} \times \boldsymbol{r} \end{aligned}$$

- assuming w(**x**) smooth, continuous, monotonic

$$w(\boldsymbol{x}) \approx w(\boldsymbol{c}) + \mathrm{grad}\,w|_{\boldsymbol{c}} \cdot \boldsymbol{r} = w_c + w_c'\,\boldsymbol{n} \cdot \boldsymbol{r}, \quad \|\boldsymbol{n}\| = 1$$

- $$\begin{aligned} \delta W = {} & \left[w_c\,m\,(\ddot{\boldsymbol{c}} - \boldsymbol{b}) - \sum_{\beta=1}^{n} w_\beta\,\boldsymbol{f}_\beta \right] \cdot \delta\boldsymbol{u}^0 + \\ & \left[w_c\,(\boldsymbol{I} \cdot \dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \times \boldsymbol{I} \cdot \boldsymbol{\omega}) - \sum_{\beta=1}^{n} w_\beta\,\boldsymbol{r}_\beta \times \boldsymbol{f}_\beta \right] \cdot \delta\boldsymbol{\omega} + \\ & \underbrace{w_c'\,\boldsymbol{n} \cdot \int_\Omega \boldsymbol{r}\,\rho\,(\ddot{\boldsymbol{c}} + \dot{\boldsymbol{\omega}} \times \boldsymbol{r} + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \boldsymbol{r}) - \boldsymbol{b}) \cdot (\delta\boldsymbol{u}_0 + \delta\boldsymbol{\omega} \times \boldsymbol{r})\,\mathrm{d}\Omega}_{\text{negligible for } \Omega \ll \Omega^{\mathrm{C}}} \end{aligned}$$





kinematic constraints

- discrete -> continuous projection:

$$\Pi(\boldsymbol{u}_\alpha, \boldsymbol{u}_\beta, \ldots) = \boldsymbol{u}^{\mathrm{DE}}(\boldsymbol{x}) \quad \text{with} \quad \alpha, \beta, \ldots \in \mathcal{P}^{\mathrm{C}}$$

- L^2 penalty constraint term

$$C = \frac{\epsilon}{2} \int_{\Omega^{\mathrm{C}}} \|\boldsymbol{u}^{\mathrm{DE}}(\boldsymbol{x}) - \boldsymbol{u}^{\mathrm{FE}}(\boldsymbol{x})\|^2 \, d\Omega$$

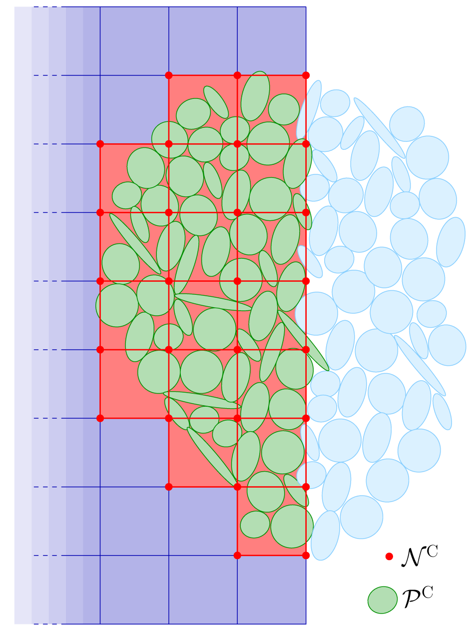
- projection via LSF using FE ansatz
  => split into coarse & fine scale [*Wagner & Liu*, 2003]

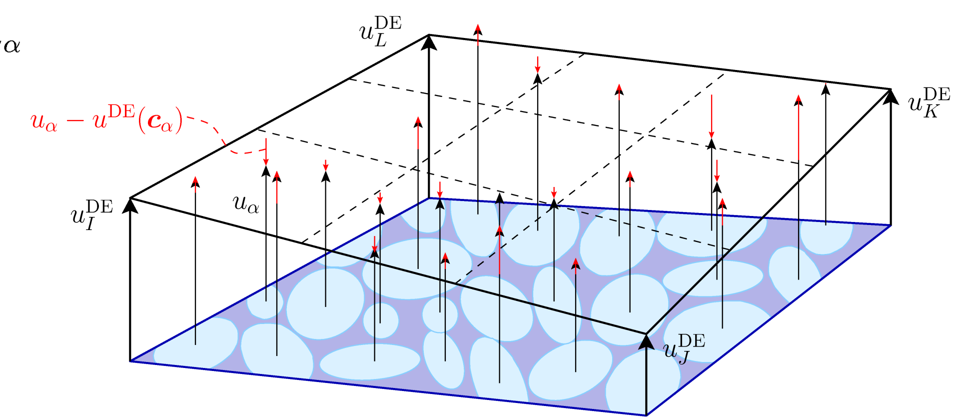
$$\boldsymbol{u}^{\mathrm{DE}}(\boldsymbol{x}) = \sum_{I \in \mathcal{N}^{\mathrm{C}}} N_I \, \boldsymbol{u}_I^{\mathrm{DE}}, \quad \min_{\boldsymbol{u}_I^{\mathrm{DE}}} \sum_{\alpha \in \mathcal{P}^{\mathrm{C}}} V_\alpha \, \|\boldsymbol{u}_\alpha - \boldsymbol{u}^{\mathrm{DE}}(\boldsymbol{c}_\alpha)\|^2$$

$$\Rightarrow \sum_{\alpha \in \mathcal{P}^{\mathrm{C}}} \sum_{J \in \mathcal{N}^{\mathrm{C}}} N_{I\alpha} \, V_\alpha \, N_{J\alpha} \, \boldsymbol{u}_J^{\mathrm{DE}} = \sum_{\alpha \in \mathcal{P}^{\mathrm{C}}} N_{I\alpha} \, V_\alpha \, \boldsymbol{u}_\alpha$$

$$\Rightarrow \underbrace{\underline{N} \, \underline{V} \, \underline{N}^T}_{\underline{A}} \, \underline{u}_c = \underline{N} \, \underline{V} \, \underline{u}_d$$

$$\underline{u}_c = \underbrace{\underline{A}^{-1} \, \underline{N} \, \underline{V}}_{\underline{\Pi}} \, \underline{u}_d \quad \text{with} \quad N_{I\alpha} = N_I(\boldsymbol{c}_\alpha)$$

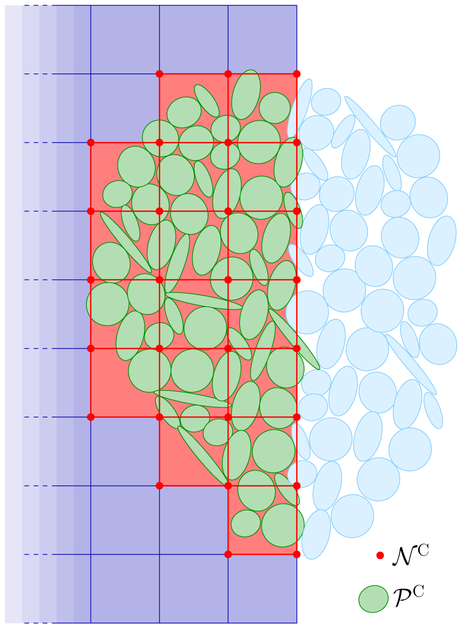




coupling forces

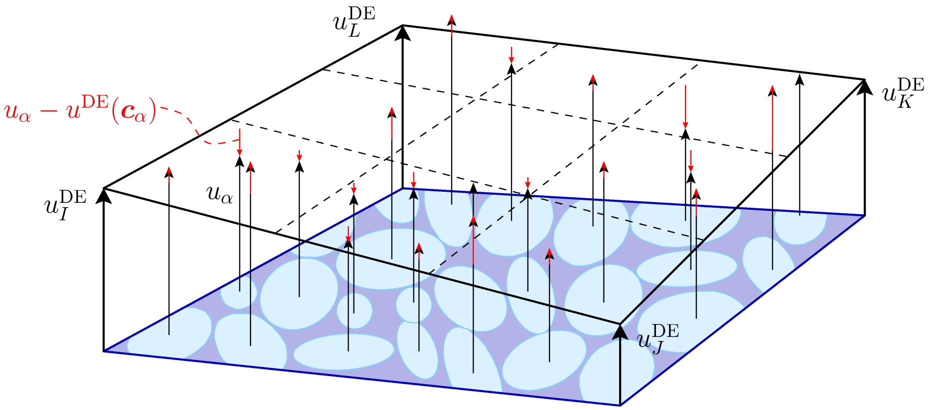
- variational formulation with penalty term

$$
\begin{aligned}
\delta W + \delta C &= 0 \quad \text{with} \\
\delta C &= \epsilon \int_{\Omega^C} \underbrace{\left(\boldsymbol{u}^{DE} - \boldsymbol{u}^{FE}\right)}_{\boldsymbol{r}} \cdot \left(\delta \boldsymbol{u}^{DE} - \delta \boldsymbol{u}^{FE}\right) \, d\Omega \\
&= \sum_{I \in \mathcal{N}^C} \delta \boldsymbol{r}_I \cdot \Big(\epsilon \sum_{J \in \mathcal{N}^C} \underbrace{\int_{\Omega^C} N_I \, N_J d\Omega}_{V_{IJ}} \, \boldsymbol{r}_J\Big) \\
&= \sum_{I \in \mathcal{N}^C} \delta \boldsymbol{r}_I \cdot \underbrace{\Big(\epsilon \sum_{J \in \mathcal{N}^C} V_{IJ} \, \boldsymbol{r}_J\Big)}_{\boldsymbol{f}_I^C}
\end{aligned}
$$

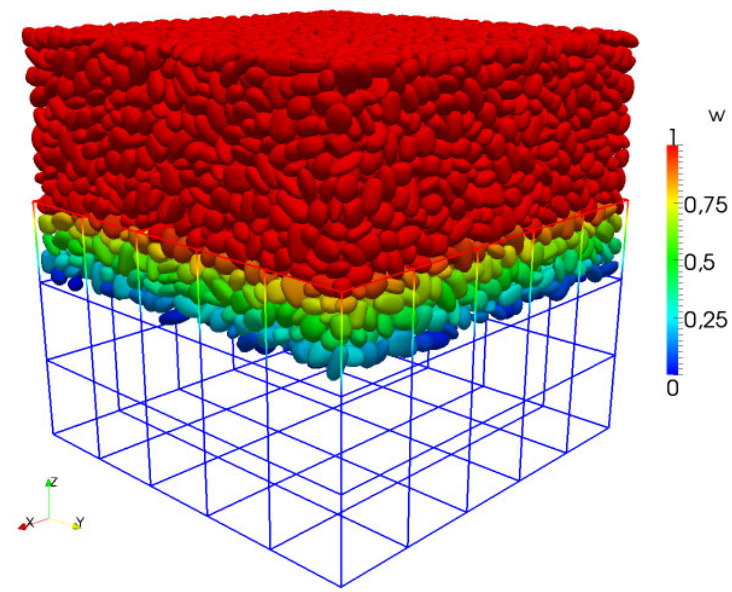


- the projection yields

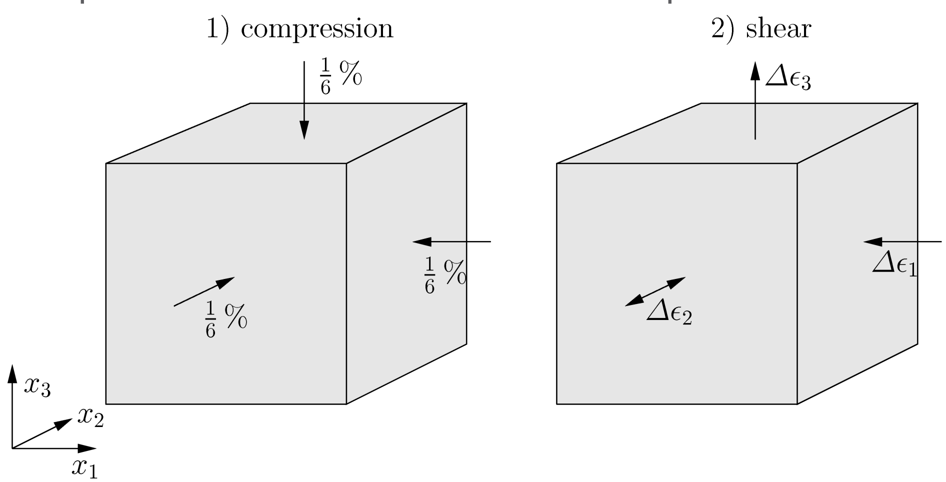
$$
\begin{aligned}
\delta \boldsymbol{u}_I^{DE} &= \sum_{\alpha \in \mathcal{P}^C} \Pi_{I\alpha} \, \delta \boldsymbol{u}_\alpha^0 \\
\Rightarrow \boldsymbol{f}_\alpha^C &= -\sum_{I \in \mathcal{N}^C} \Pi_{I\alpha} \, \boldsymbol{f}_I^C
\end{aligned}
$$



numerical example: triaxial test



- system:
  - Ω^{C} = 1 element layer
  - weight function defined on FE ansatz
  - trilinear hexahedral elements
  - full DE: ~ 14,000 particles
    coupled: ~ 8,000 particles
  - $\epsilon = 10^8\,\mathrm{Pa/mm}^2$
- loading:
  - 3 displacement controlled tests with two phases:

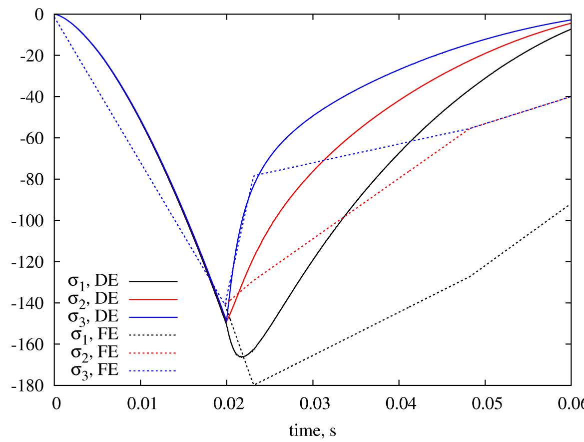


test	1	2	3
$\Delta\epsilon_V, \%$	$1/2$	0	$-1/2$
$\Delta\epsilon_1, \%$	-1	-1	-1
$\Delta\epsilon_2, \%$	$1/6$	0	$-1/6$
$\Delta\epsilon_3, \%$	$4/3$	1	$2/3$

results

full DE & FE

1



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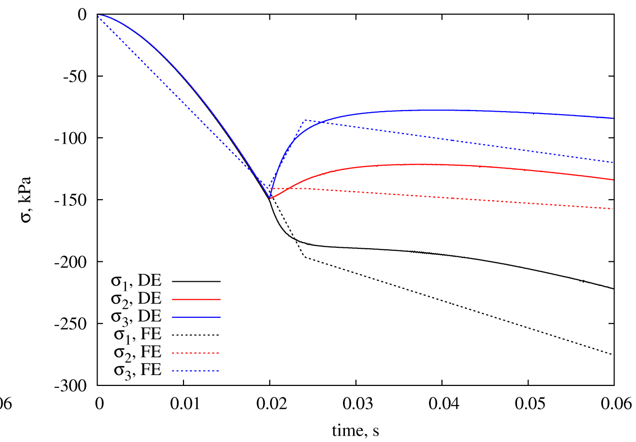
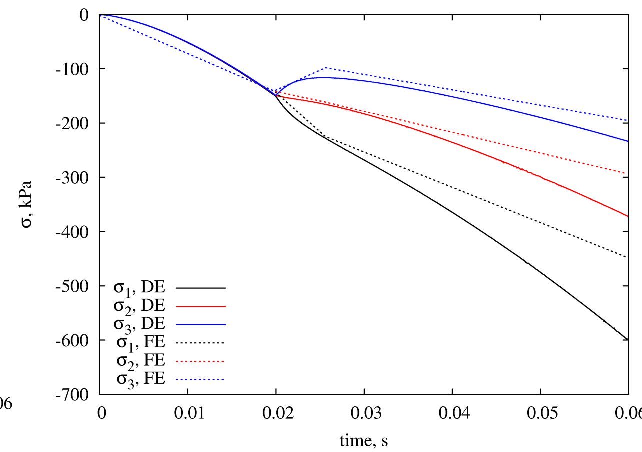
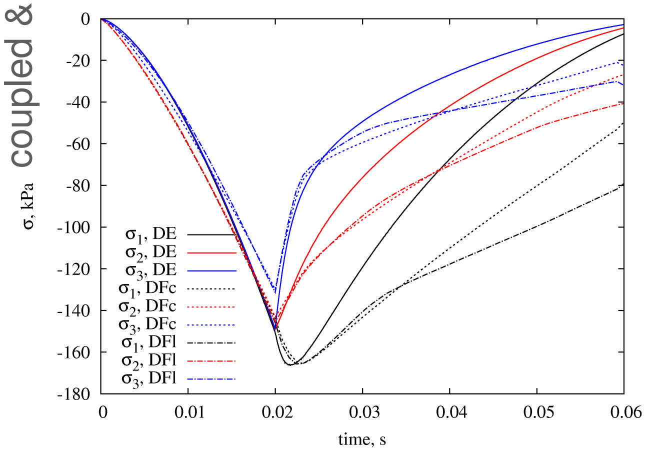
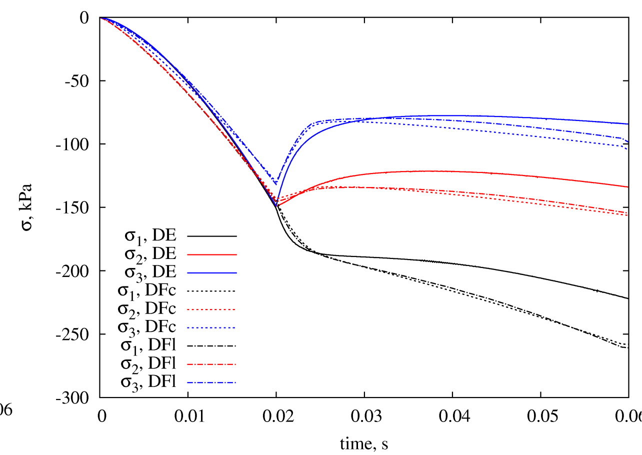


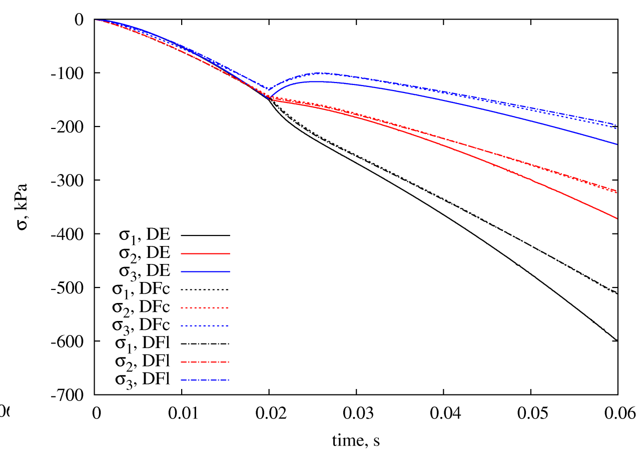
3



coupled & full DE







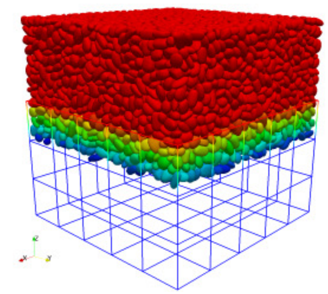
penalty factor & loading direction

- 3 penalty factors

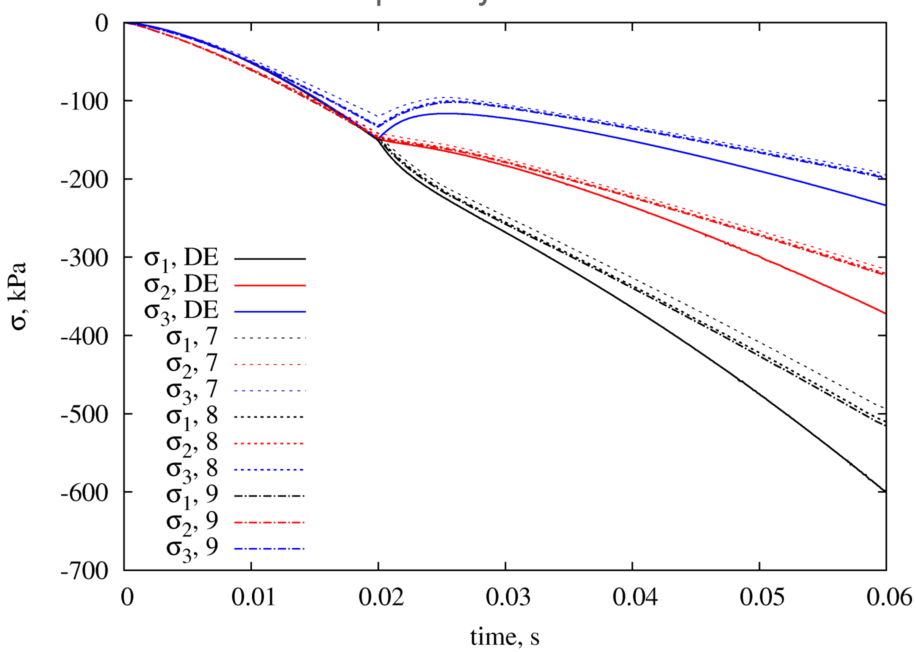
$$\epsilon = 10^7,\ 10^8,\ 10^9\ \mathrm{Pa/mm^2}$$

- => 10^8 is sufficient

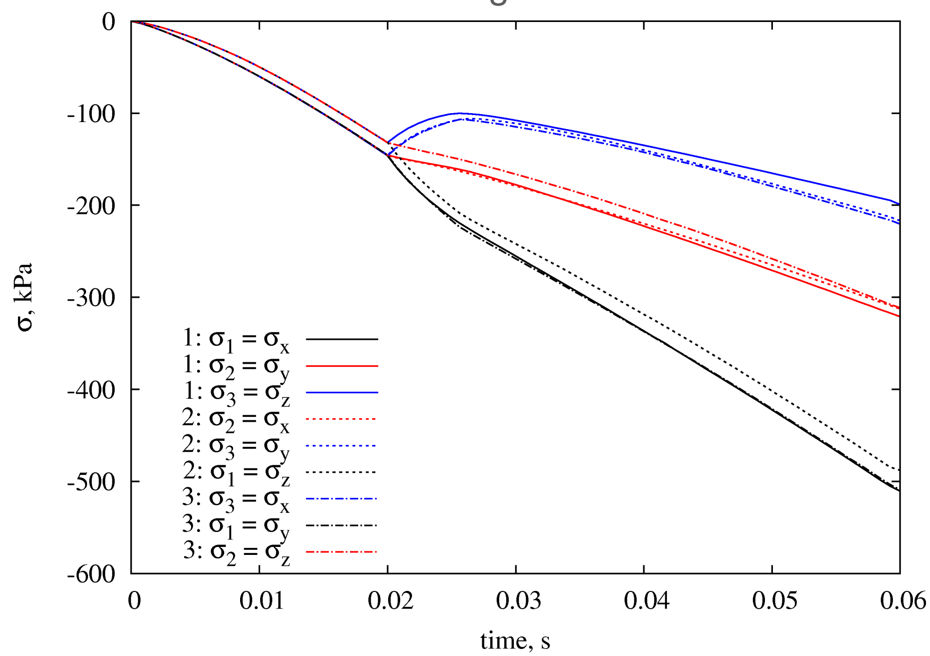
- switched loading directions
- small deviations in isotropic compression



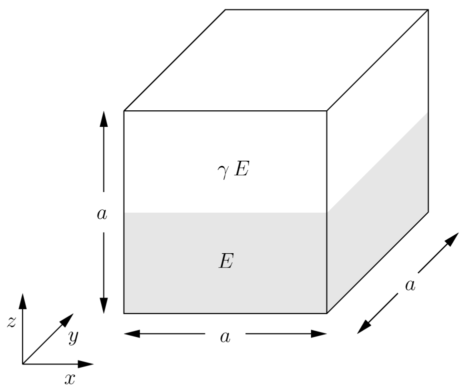
penalty factor



loading direction



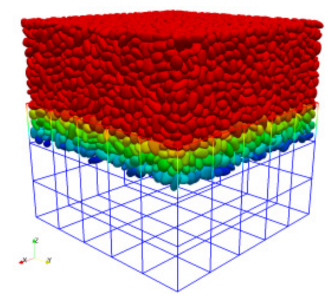
loading direction

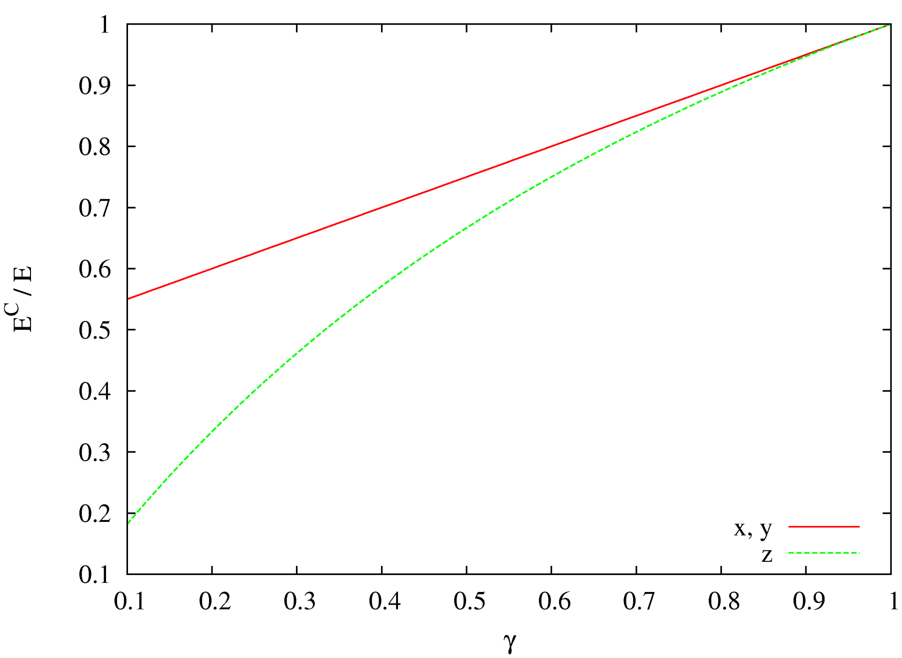


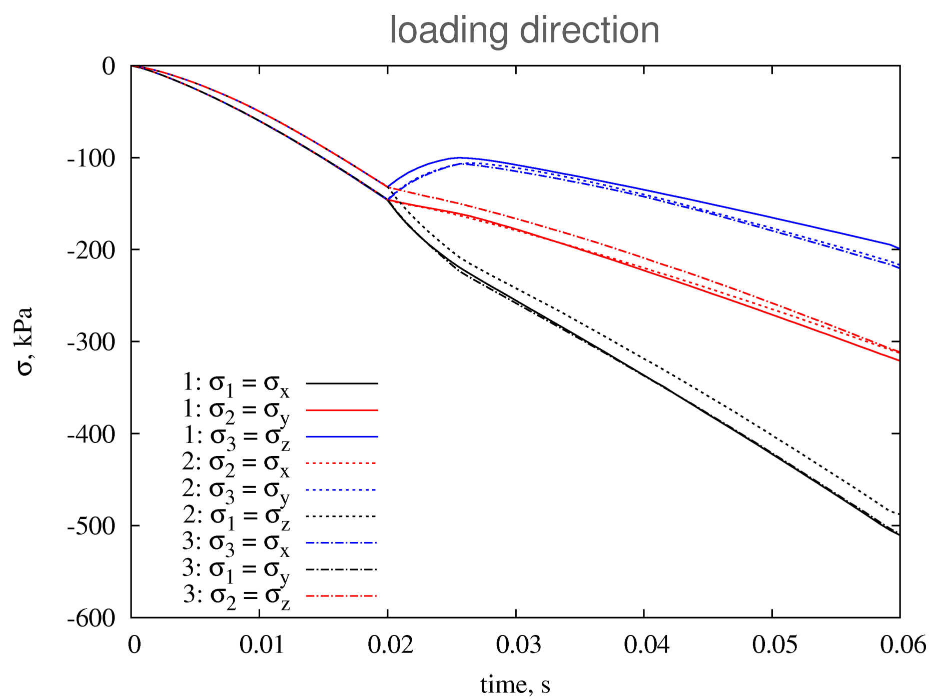
$$x, y \quad : \quad E^{\mathrm{C}} = \frac{1+\gamma}{2} E$$

$$z \quad : \quad E^{\mathrm{C}} = \frac{2\,\gamma}{1+\gamma} E$$

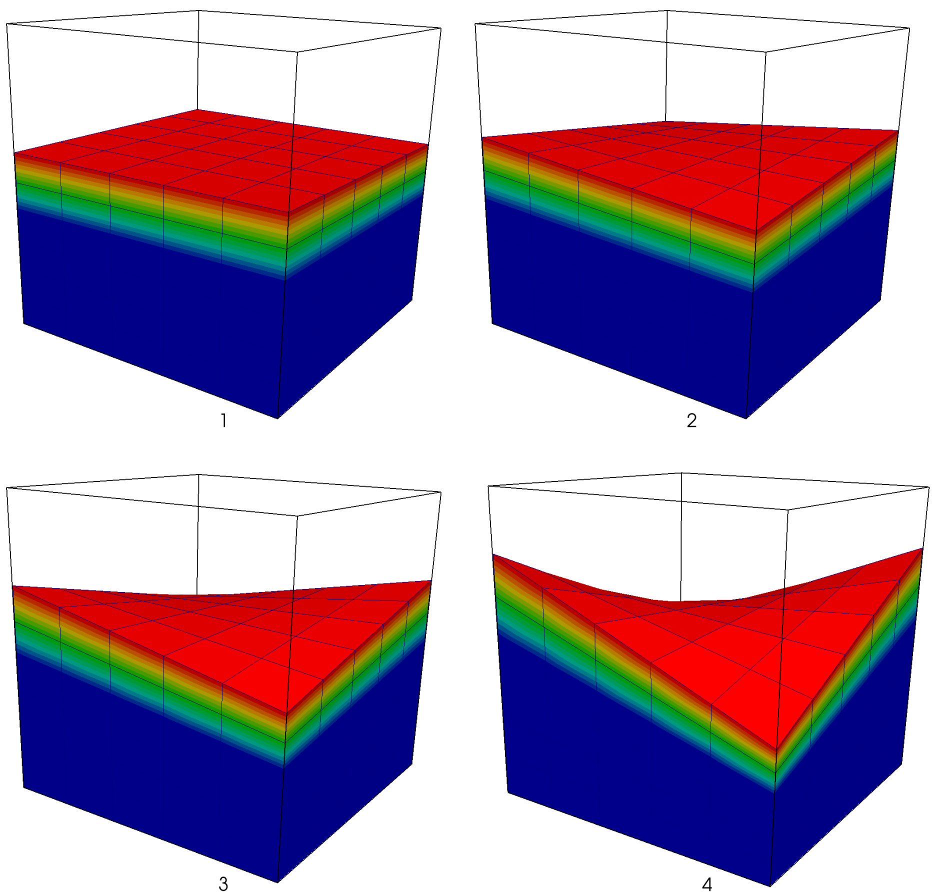
- switched loading directions
- small deviations in isotropic compression

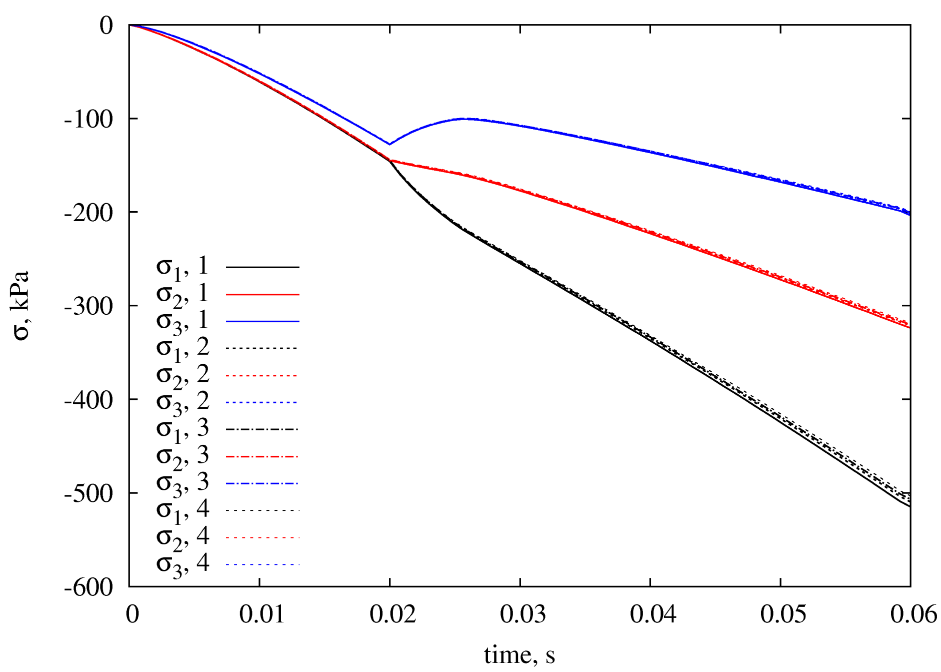






coupling geometry

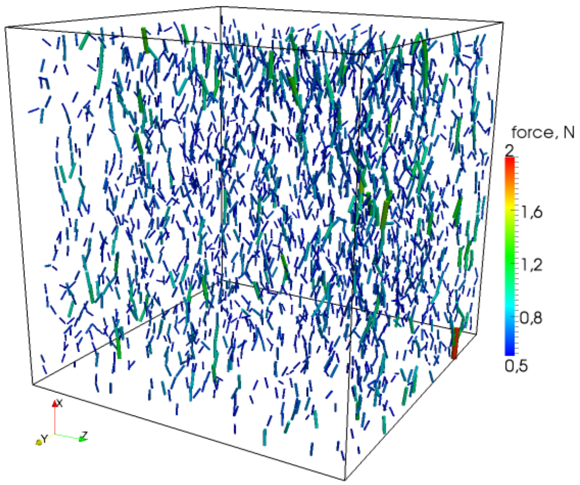




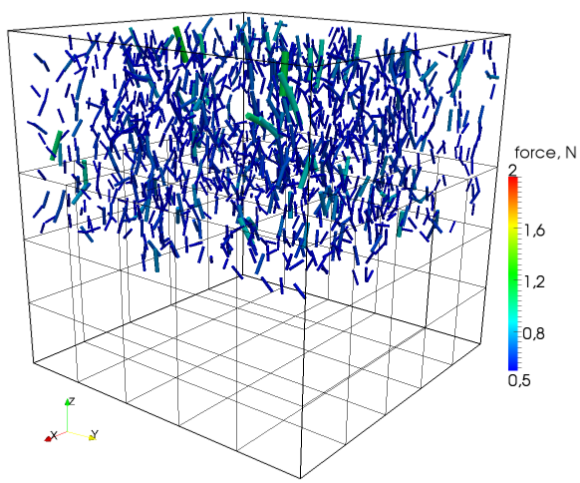
microstructure

contact force chains

full DE

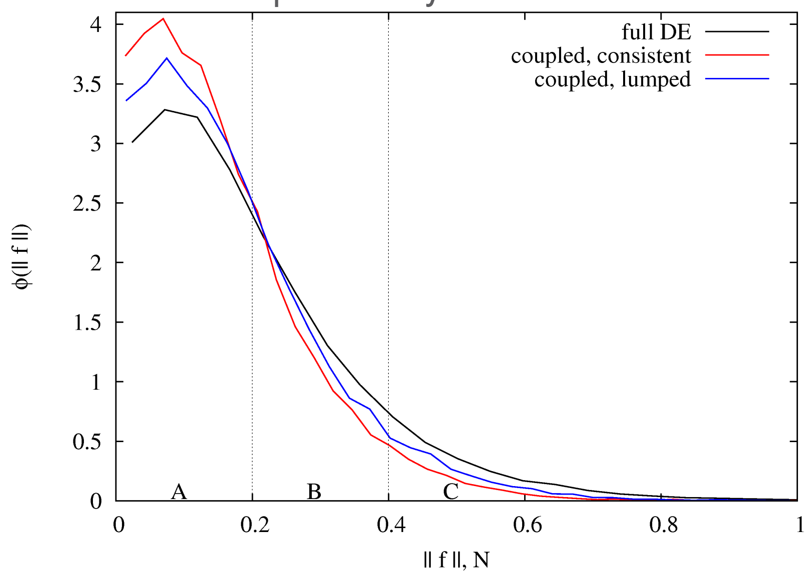


coupled

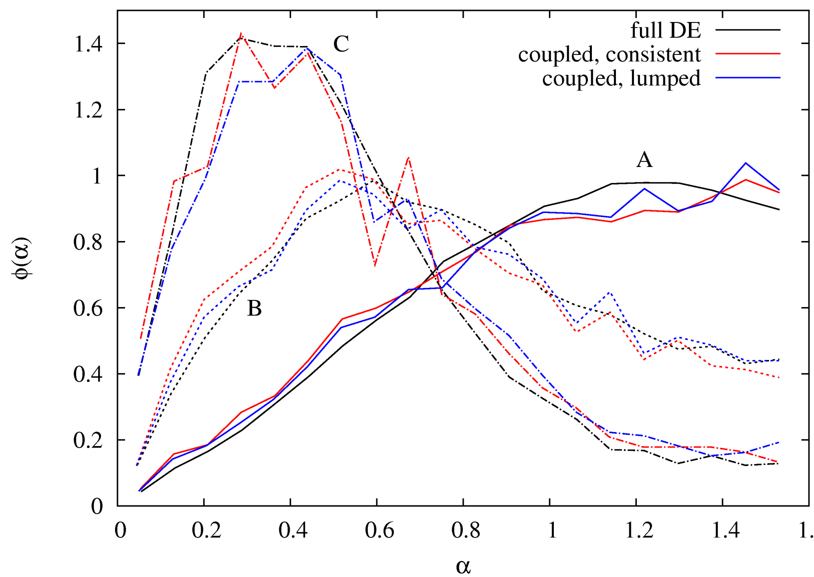


probability distributions

magnitude

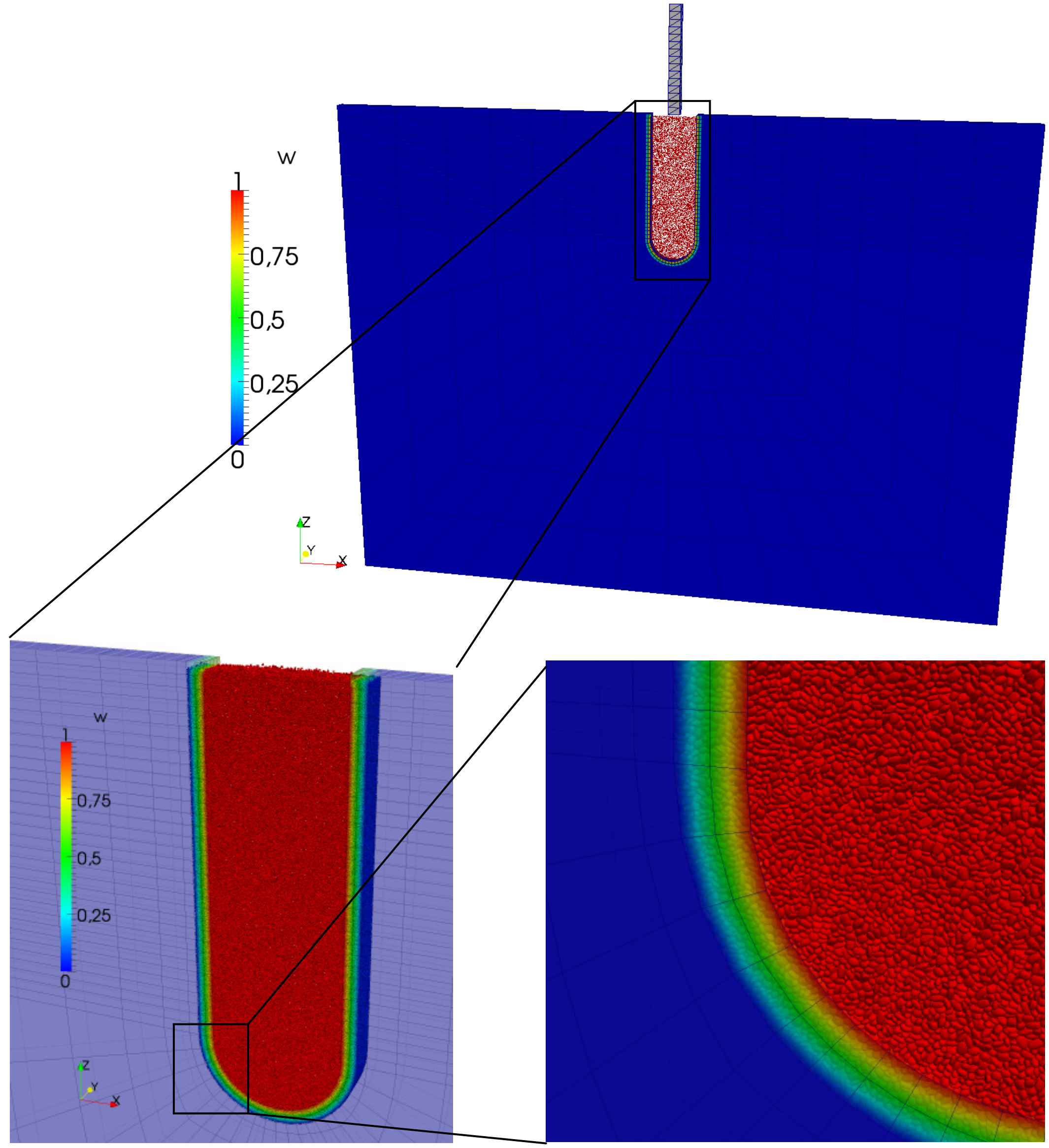


direction

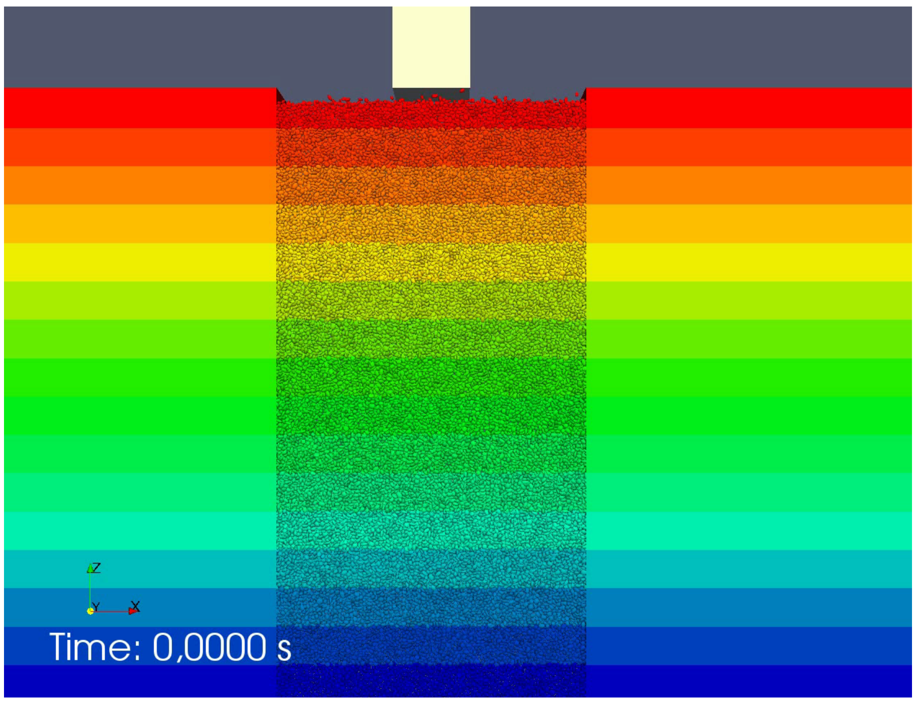


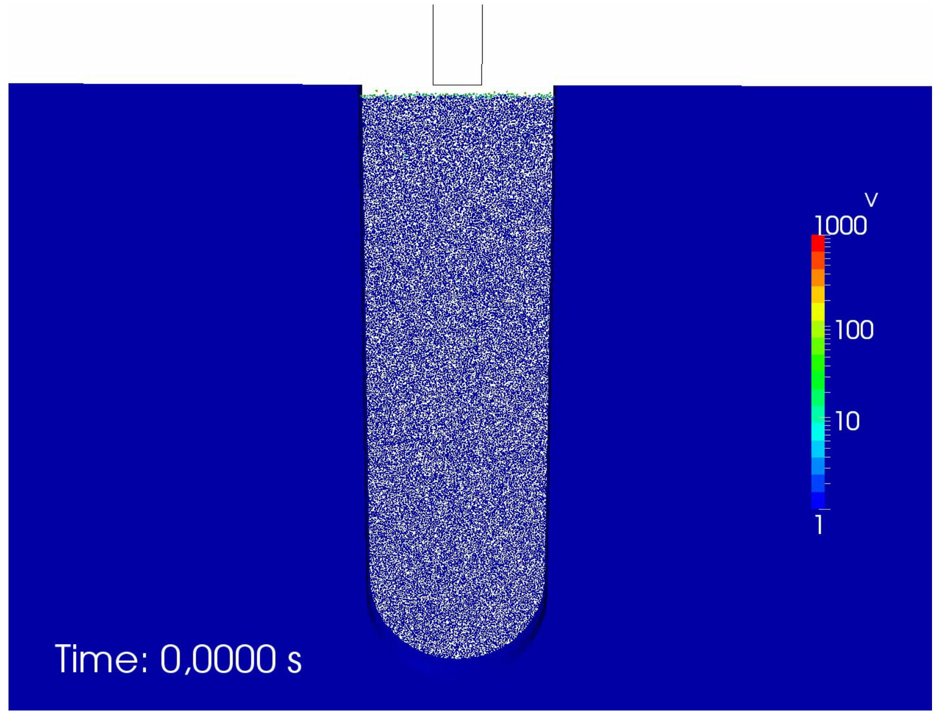
pile installation

- box: 1000 x 750 x 16.1mm
- pile cross section: 16.1 x 16.1 mm
- pile velocity: 1m/s
- friction pile-particles: 0.1
- full DE model: ~ 25×10^6 particles
- large deformations only in pile vicinity
- coupled simulation
  - 540,000 particles
  - 5040 trilinear bricks
  - 7560 nodes
  - 3.2×10^6 DOFs
  - lumped projection



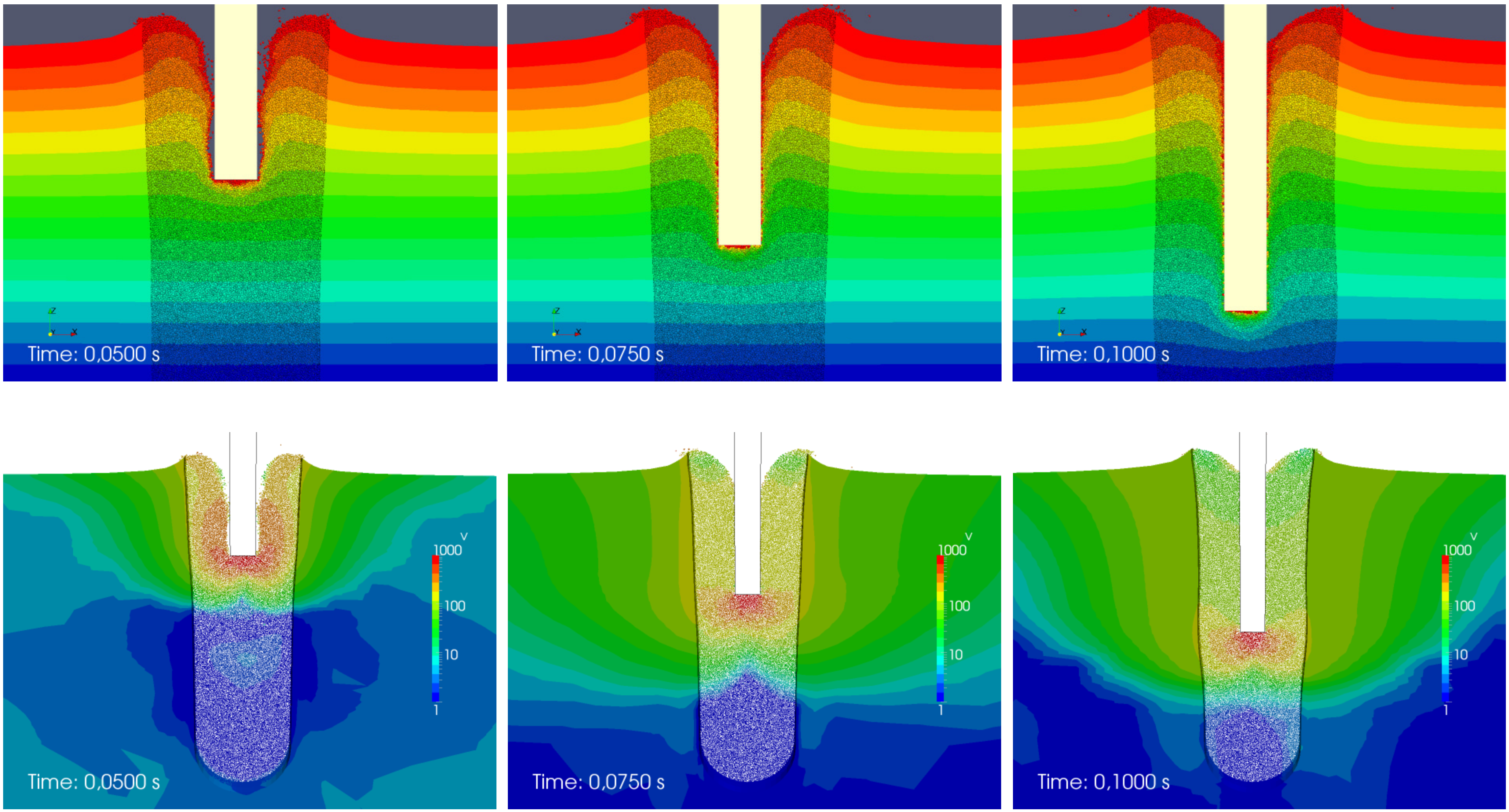
results



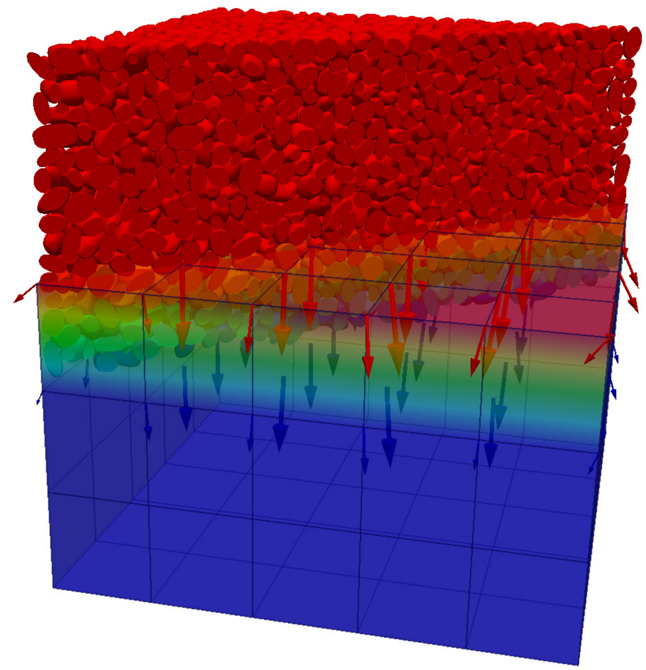


- particle cone forms at flat pile tip
- material is “spread” by cone and moves outside and upwards
- smooth transition between DE & FE domain

results


Time: 0,0500 s
Time: 0,0750 s
Time: 0,1000 s
v
1000
100
10
1
Time: 0,0500 s
Time: 0,0750 s
Time: 0,1000 s

summary & outlook



- DE-FE coupling scheme:
  - overlapping domain
  - weighted virtual work
  - coarse-fine split of DE displacements
- triaxial test:
  - similar results for consistent & lumped projection
  - works for distorted coupling geometry
  - preserves characteristic microstructure
- coupling scheme enables simulations not possible with mono-method model
- outlook:
  - enhance particle model to better represent shear strength of real granular materials
  - implement constitutive equation giving a better fit of the homogenized DE behavior
  - develop criteria and methods to adaptively control DE domain