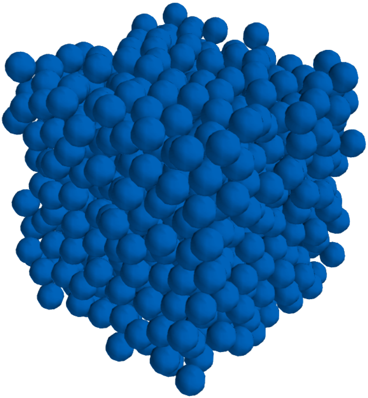
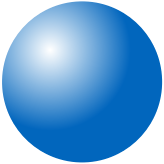
Mesoscale Discrete Element Model for Concrete and Its Combination with FEM

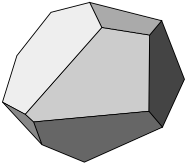
Jan Stránský
Department of Mechanics
Faculty of Civil Engineering
Czech Technical University in Prague
26th April 2018

- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws

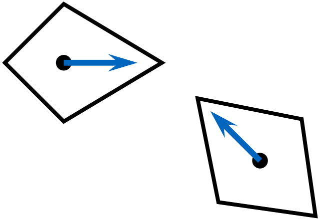


- **set of rigid particles**
- **various particle shapes**
- motion, contact detection
- Newton's laws of motion
- contact laws

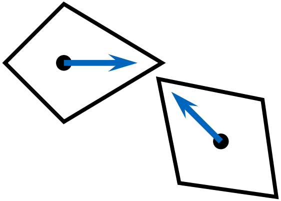




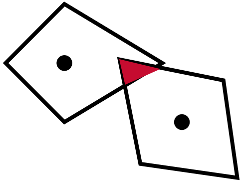
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



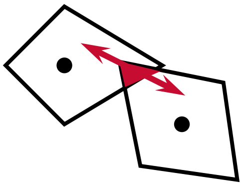
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



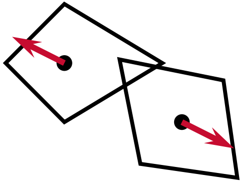
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



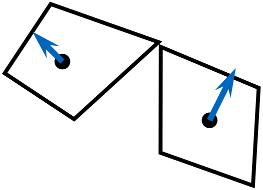
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



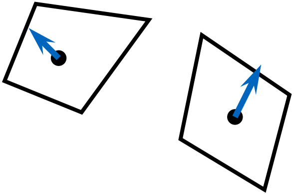
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



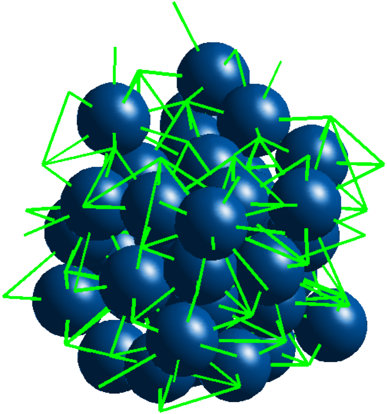
- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws



- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton's laws of motion
- contact laws

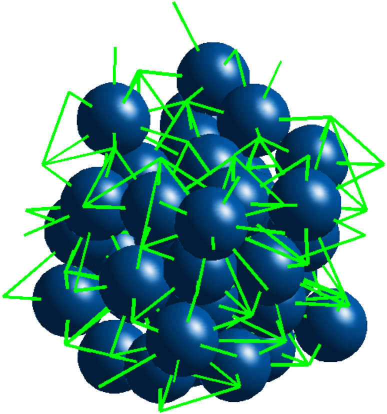


- set of rigid particles
- various particle shapes
- motion, contact detection
- Newton’s laws of motion
- contact laws

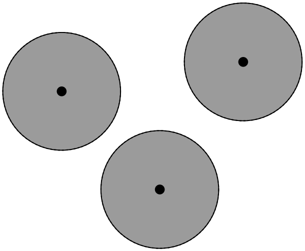


- **by Šmilauer & Jirásek**
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration

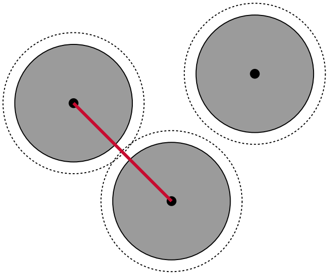
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



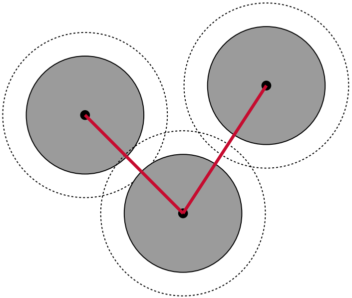
- **by Šmilauer & Jirásek**
- **uniform spheres**
- **artificial discretization**
- **random close packing**
- **cohesive links**
- **interaction ratio**
- **normal and shear stress**
- **damage and plasticity**
- **uniaxial tests illustration**



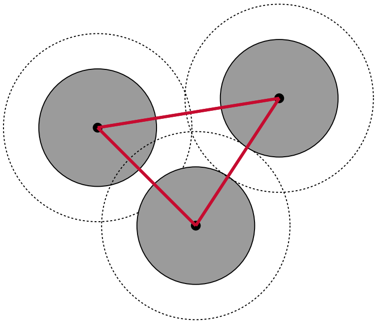
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



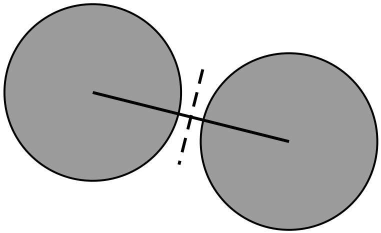
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



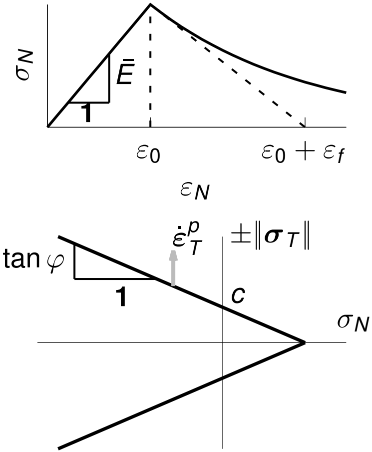
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



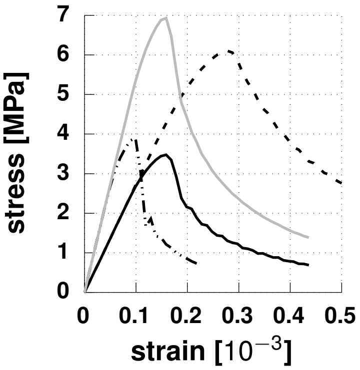
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



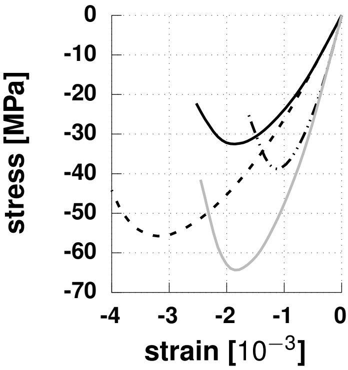
- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



- by Šmilauer & Jirásek
- uniform spheres
- artificial discretization
- random close packing
- cohesive links
- interaction ratio
- normal and shear stress
- damage and plasticity
- uniaxial tests illustration



MACROSCOPIC ELASTIC PROPERTIES OF DEM MODELS

micro parameters: $\bar{E}$, $\bar{G}$

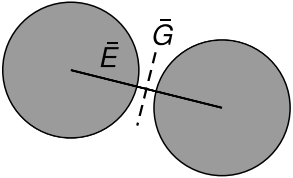
macro parameters: E, ν

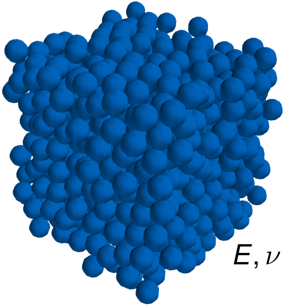
Numerical solution

- dynamic DEM, static FEM
- periodic BCs

Analytical solution

- affine displacement
- stiffness tensor
- uniform distribution of link directions





micro parameters: $\bar{E}$, $\bar{G}$

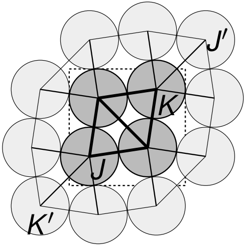
macro parameters: E, ν

Numerical solution

- **dynamic DEM, static FEM**
- **periodic BCs**

Analytical solution

- **affine displacement**
- **stiffness tensor**
- **uniform distribution of link directions**



micro parameters: $\bar{E}$, $\bar{G}$

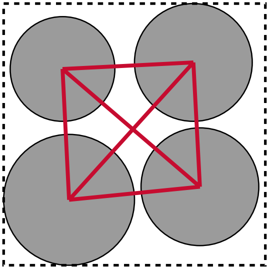
macro parameters: E, ν

Numerical solution

- **dynamic DEM, static FEM**
- **periodic BCs**

Analytical solution

- **affine displacement**
- stiffness tensor
- uniform distribution of link directions



micro parameters: $\bar{E}$, $\bar{G}$

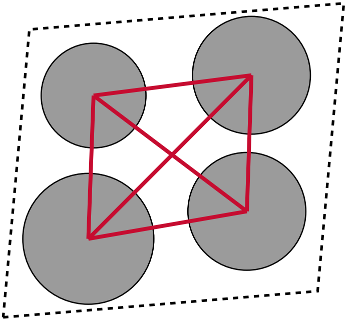
macro parameters: E, ν

Numerical solution

- **dynamic DEM, static FEM**
- **periodic BCs**

Analytical solution

- **affine displacement**
- stiffness tensor
- uniform distribution of link directions



micro parameters: $\bar{E}$, $\bar{G}$
macro parameters: E, ν

$$\mathbb{D}_e = \frac{1}{V}\sum_c L^c A^c \left(\bar{E}\mathbb{N}^c + \bar{G}\mathbb{T}^c\right)$$

Numerical solution

- **dynamic DEM, static FEM**
- **periodic BCs**

Analytical solution

- **affine displacement**
- **stiffness tensor**
- **uniform distribution of link directions**

$$E = \frac{\sum L^c A^c}{3V} \cdot \frac{\bar{E}\left(2\bar{E}+3\bar{G}\right)}{4\bar{E}+\bar{G}}$$

$$\nu = \frac{\bar{E}-\bar{G}}{4\bar{E}+\bar{G}}$$

micro parameters: $\bar{E}$, $\bar{G}$

macro parameters: E, ν

Numerical solution

- **dynamic DEM, static FEM**
- **periodic BCs**

$$\mathbb{D}_e = \frac{1}{V}\sum_c L^c A^c \left(\bar{E}\mathbb{N}^c + \bar{G}\mathbb{T}^c\right)$$

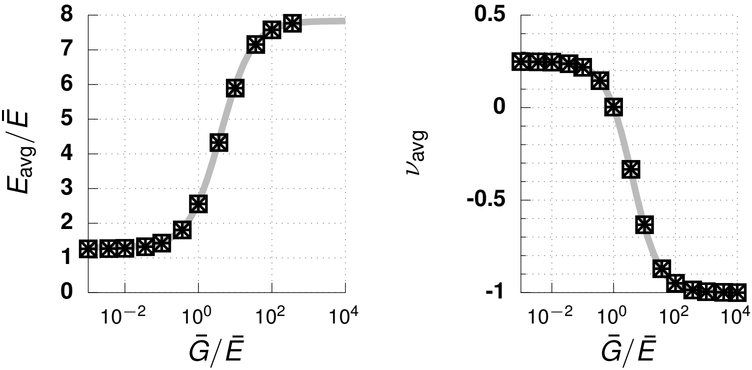
Analytical solution

- **affine displacement**
- **stiffness tensor**
- **uniform distribution of link directions**

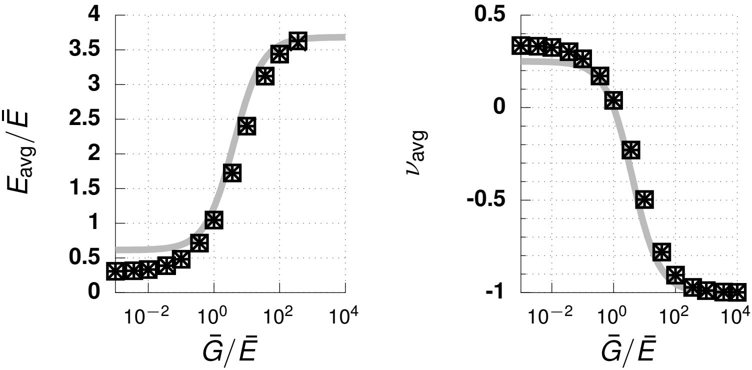
$$E = \frac{\sum L^c A^c}{3V} \cdot \frac{\bar{E}\left(2\bar{E} + 3\bar{G}\right)}{4\bar{E} + \bar{G}}$$

$$\nu = \frac{\bar{E} - \bar{G}}{4\bar{E} + \bar{G}}$$

interaction ratio = 1.50

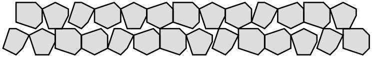


interaction ratio = 1.05



DEM

discrete domains

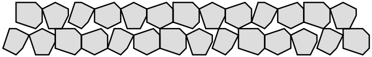


FEM

continuous domains

DEM

discrete domains

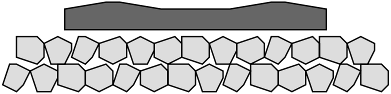


FEM

continuous domains

Combination

- monolithic application – redoing what already exists
- combination of existing codes



CTU
CZECH TECHNICAL UNIVERSITY IN PRAGUE

DEM – FEM COUPLING
MOTIVATION

YADE

- DEM analysis
- free
- open source
- C++ core
- Python user interface

OOFEM

OOFEM.ORG

- FEM analysis
- free
- open source
- C++ core
- Python user interface

YADE

- **DEM analysis**
- free
- open source
- C++ core
- Python user interface

OOFEM

OOFEM.ORG

- **FEM analysis**
- free
- open source
- C++ core
- Python user interface

YADE

- DEM analysis
- free
- open source
- C++ core
- Python user interface

OOFEM

- FEM analysis
- free
- open source
- C++ core
- Python user interface

YADE

- DEM analysis
- free
- open source
- C++ core
- Python user interface

OOFEM

- FEM analysis
- free
- open source
- C++ core
- Python user interface

YADE

- DEM analysis
- free
- open source
- C++ core
- Python user interface

OOFEM

- FEM analysis
- free
- open source
- C++ core
- Python user interface

YADE

- DEM analysis
- free
- open source
- C++ core
- Python user interface

OOFEM

- FEM analysis
- free
- open source
- C++ core
- Python user interface

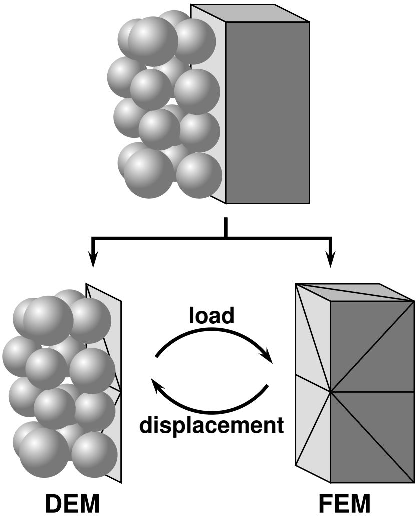
YADE

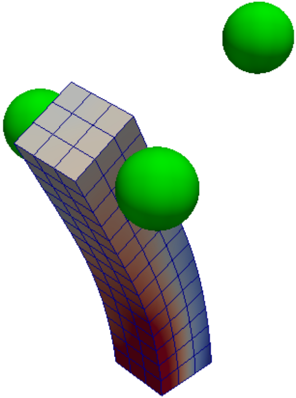
- DEM analysis
- free
- open source
- C++ core
- Python user

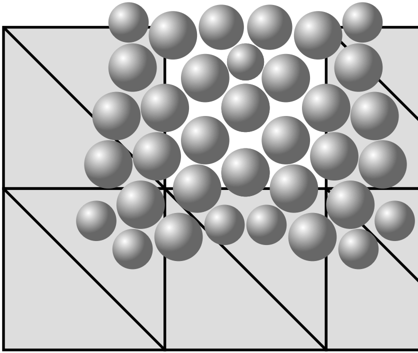
OOFEM

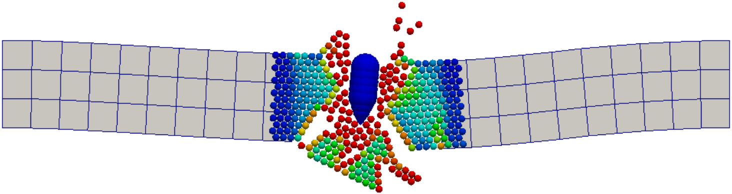
- lysis
- urce
- e
- user interface

DEM – FEM COUPLING
SURFACE COUPLING

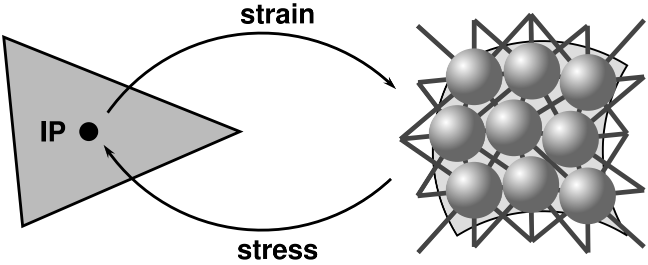


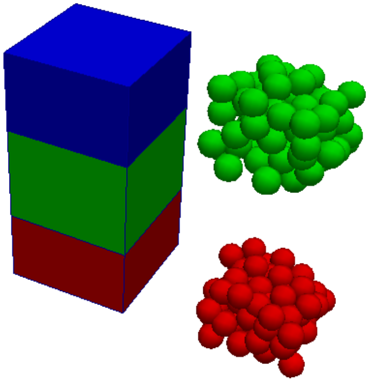


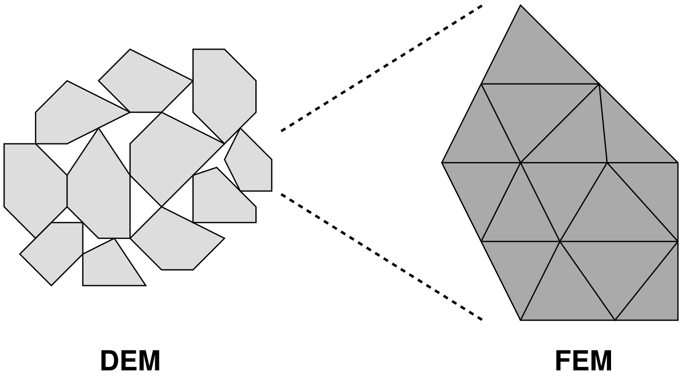


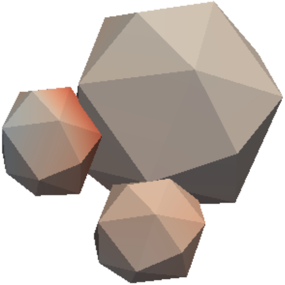


FE×DE (MULTISCALE) COUPLING

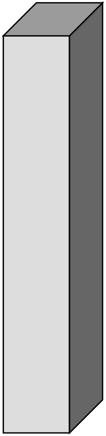




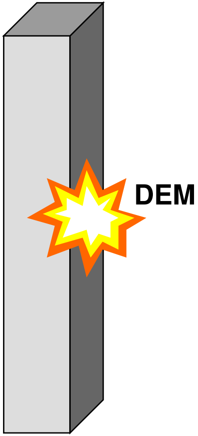

DEM
FEM



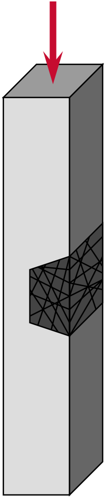
- **Processes separable in time**
- **FEM model for concrete by Grassl & Jirásek**
- **DEM ($\sigma_{DEM}, \Omega_{DEM}$) $\rightarrow$ $\rightarrow$ FEM ($\sigma, \omega, \kappa_D, \kappa_P$)**



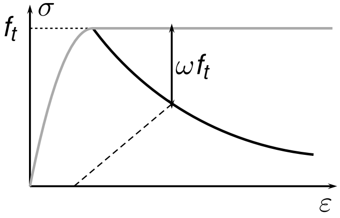
- **Processes separable in time**
- FEM model for concrete by Grassl & Jirásek
- DEM $(\sigma_{DEM}, \Omega_{DEM}) \rightarrow$ $\rightarrow$ FEM $(\sigma, \omega, \kappa_D, \kappa_P)$



- **Processes separable in time**
- FEM model for concrete by Grassl & Jirásek
- DEM ($\sigma_{DEM}, \Omega_{DEM}$) $\rightarrow$ $\rightarrow$ FEM ($\sigma, \omega, \kappa_D, \kappa_P$)



- **Processes separable in time**
- **FEM model for concrete by Grassl & Jirásek**
- **DEM ($\sigma_{DEM}, \Omega_{DEM}$) $\rightarrow$ $\rightarrow$ FEM ($\sigma, \omega, \kappa_D, \kappa_P$)**



$\omega = 0$
$\kappa_D = 0$
$\kappa_P < 1$

$\omega > 0$
$\kappa_D > 0$
$\kappa_P = \kappa_D + 1$

- **Processes separable in time**
- **FEM model for concrete by Grassl & Jirásek**
- **DEM ($\boldsymbol{\sigma}_{DEM}, \boldsymbol{\Omega}_{DEM}$) $\rightarrow$ $\rightarrow$ FEM ($\boldsymbol{\sigma}, \omega, \kappa_D, \kappa_P$)**

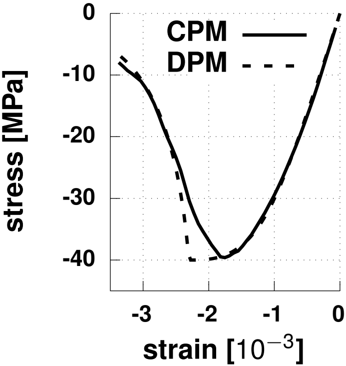
$$\boldsymbol{\Omega} = -\frac{1}{2}\mathbf{tr}(\boldsymbol{\Omega})\,\mathbf{1} + \frac{15}{2N}\sum_c \hat{\omega}^c \mathbf{n}^c \otimes \mathbf{n}^c =$$

$$= -\mathbf{1}\frac{3}{2N}\sum_c \hat{\omega}^c + \frac{15}{2N}\sum_c \hat{\omega}^c \mathbf{n}^c \otimes \mathbf{n}^c$$

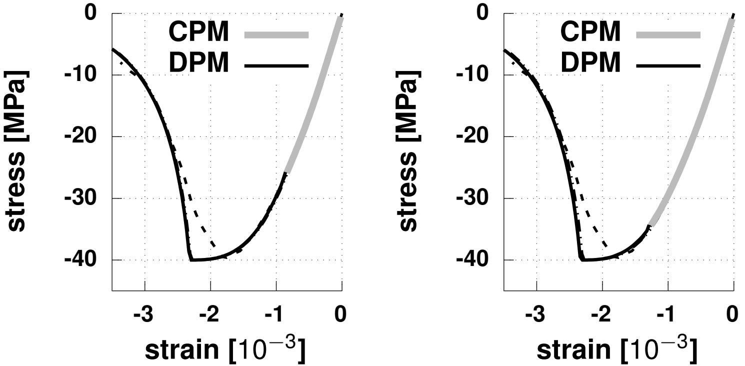
$$\omega_{FEM} = \omega(\boldsymbol{\Omega}) = \omega(\Omega_1, \Omega_2, \Omega_3)$$

$$\kappa_D = \kappa_D(\omega), \kappa_P = \kappa_P(\omega)$$

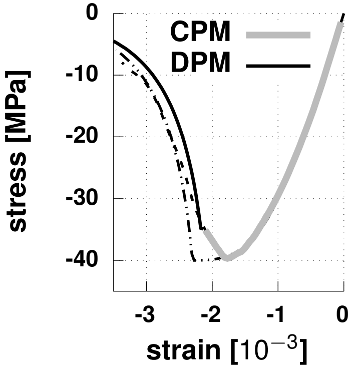
Results - uniaxial compression

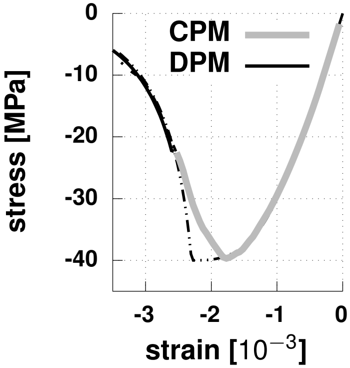


Results - uniaxial compression

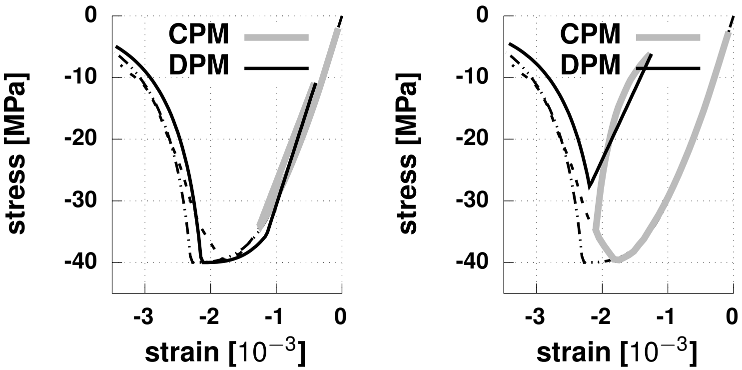


Results - uniaxial compression

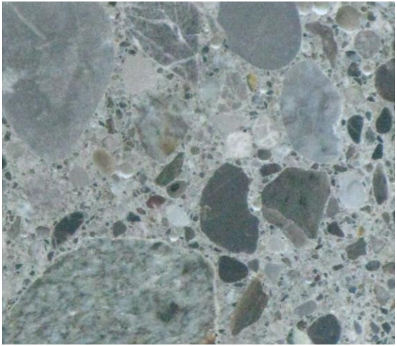




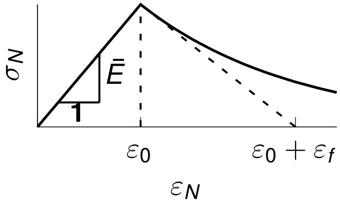
Results - uniaxial compression

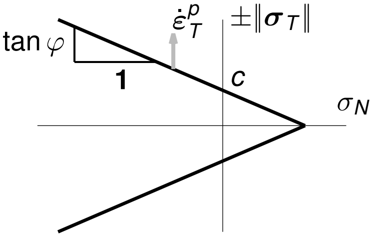


- three phase material
  - mortar matrix
  - aggregate inclusions
  - ITZ
- one material model
- 2 types of DEM particles
- 3 types of links
- ITZ link
  - weaker
  - less stiff
  - more brittle

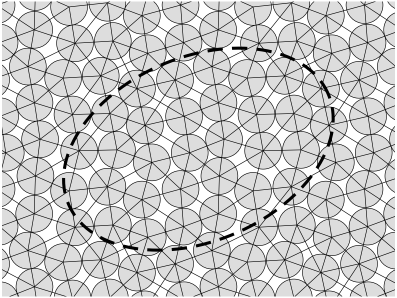


- **three phase material**
  - **mortar matrix**
  - **aggregate inclusions**
  - **ITZ**
- **one material model**
- **2 types of DEM particles**
- **3 types of links**
- **ITZ link**
  - **weaker**
  - **less stiff**
  - **more brittle**

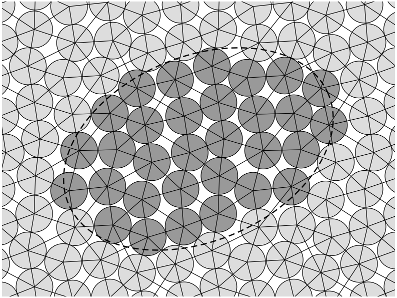




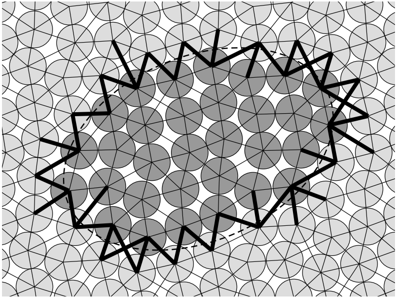
- three phase material
  - mortar matrix
  - aggregate inclusions
  - ITZ
- one material model
- 2 types of DEM particles
- 3 types of links
- ITZ link
  - weaker
  - less stiff
  - more brittle



- three phase material
  - mortar matrix
  - aggregate inclusions
  - ITZ
- one material model
- 2 types of DEM particles
- 3 types of links
- ITZ link
  - weaker
  - less stiff
  - more brittle



- three phase material
  - mortar matrix
  - aggregate inclusions
  - ITZ
- one material model
- 2 types of DEM particles
- 3 types of links
- ITZ link
  - weaker
  - less stiff
  - more brittle



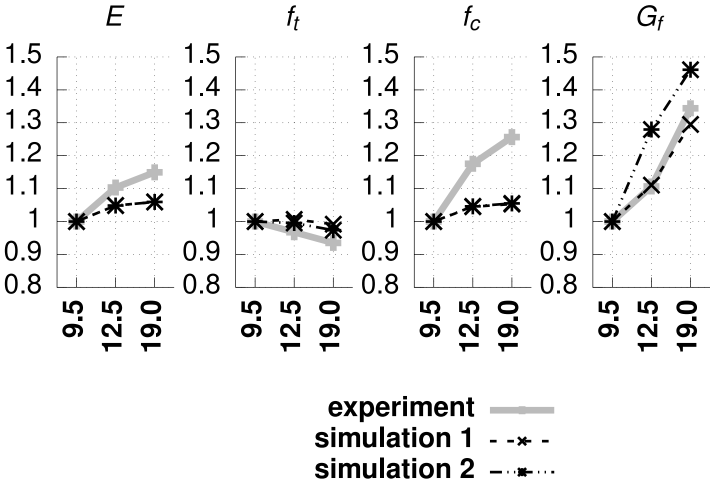
- **Experiment Beygi et al.**
- E, f_t, f_c, G_f
- **different grading curves**
- **same total amount of aggregates**
- **two types of concrete**

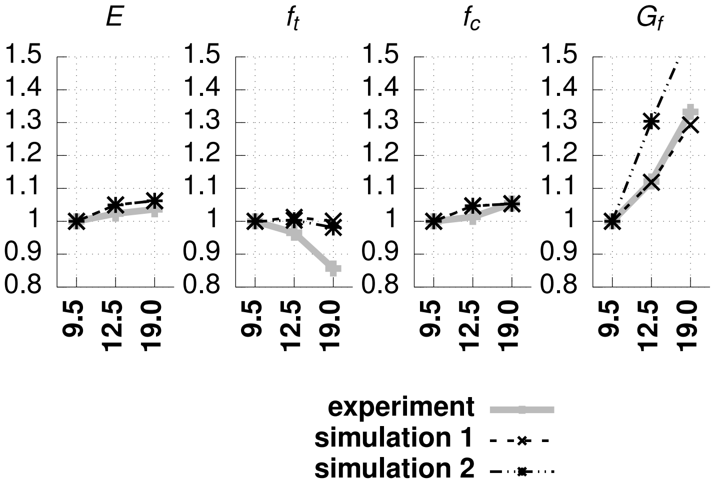
- **Experiment Beygi et al.**
- E, f_t, f_c, G_f
- **different grading curves**
- **same total amount of aggregates**
- two types of concrete

max. aggreg	9.5	12.5	19.0
powder	205	205	205
sand	917	917	917
4.75 - 9.5	750	300	300
9.5 - 12.5	-	450	300
12.5 - 19.0	-	-	150

- **Experiment Beygi et al.**
- E, f_t, f_c, G_f
- **different grading curves**
- **same total amount of aggregates**
- **two types of concrete**

	c	w
low s.	**325.8**	**187.0**
high s.	**422.4**	**160.7**


E
f_t
f_c
G_f
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
9.5
12.5
19.0
experiment
simulation 1
simulation 2


E
f_t
f_c
G_f
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
9.5
12.5
19.0
experiment
simulation 1
simulation 2

Conclusions

- macroscopic elastic properties of particle models
- discrete (couple) stress tensor
- DEM – FEM coupling, new open source package
- sequential DEM – FEM coupling
- mesoscale discrete element model for concrete

Future work

- new formula for discrete couple stress tensor verification
- more detailed parameter study of MCPM
- more examples of sequential DEM – FEM coupling
- more examples of concurrent DEM – FEM coupling

CTU

CZECH TECHNICAL
UNIVERSITY
IN PRAGUE

Question

What other formulas for the evaluation of the couple stress tensor in a discrete system are used? What are their differences, advantages and disadvantages compared to the newly derived formula?

Answer

Bardet & Vardoulakis and Chang & Kuhn:

$$\mu_{ji} + \varepsilon_{jkl}\Sigma_{jlk} = \dots$$

$$\Sigma_{kji} + \Sigma_{jki} = \dots$$

New formula

$$V\overline{\mu} = V\mathbf{x}^0 \otimes (\mathbf{1} \times \overline{\sigma}) + \sum_e \mathbf{x} \otimes \mathbf{c}^e$$

Question

Volume or surface coupling of discrete and continuum methods usually leads to undesirable reflection and dispersion of waves on their interface. Does any of the methods eliminate this problem?

Answer

No.

Question

The mesoscale model presented in part 3 is composed of spherical particles. Their size has no physical interpretation and it seems that it may be chosen almost arbitrarily. Is the response of the model independent on the size of these particles?

Answer

- **The model is NOT independent on particle size.**
- **For each particle size, the model should be calibrated independently.**

DISCUSSION
JAN ELIÁŠ, QUESTION 4

Question

It is stated that it is possible to split the summation assuming uniform distribution of the product of contact areas and lengths in the equation 3.35. However, I have the impression that the distribution may be considered arbitrary. For the presented summation split, it is necessary to assume independence of the normal direction n and the product of contact areas and lengths *AL*.

Answer

$$\mathbb{D}_e = \frac{1}{V}\sum_c L^c A^c \left(\bar{E}\mathbb{N}^c + \bar{G}\mathbb{T}^c\right)$$

$$E = \frac{\sum L^c A^c}{3V} \cdot \frac{\bar{E}\left(2\bar{E} + 3\bar{G}\right)}{4\bar{E} + \bar{G}}$$

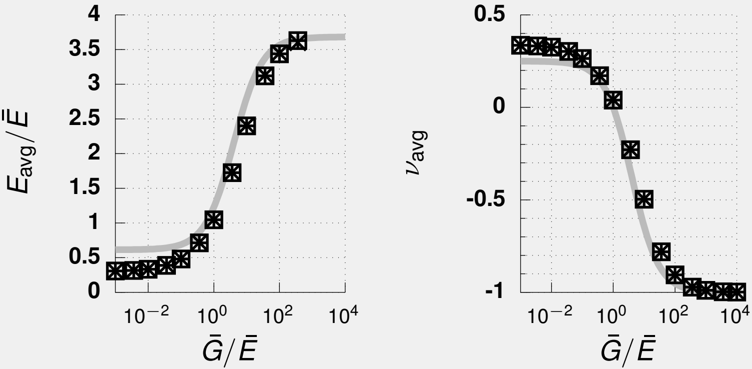
$$\nu = \frac{\bar{E} - \bar{G}}{4\bar{E} + \bar{G}}$$

- **I considered it as a part of the assumption of uniform distribution of link directions**
- **match of the results**
- **Least effect for low values of interaction ratio**

Question

Figures 3.8-3.11 show the difference of derived analytical formula and the real macroscopic response for low and high values of interaction ratio. Is there a simple explanation of the observed dependency on interaction ratio? Why is the estimation of elastic parameters so much different for low values of interaction ratio?

Answer



- systematic error in my evaluation
- not fulfilled assumptions of the gray estimation

DISCUSSION
JAN ELIÁŠ, QUESTION 5

Question

Is is possible to get such accurate estimation also for non-spherical particles (like ellipsoids) for the whole range of shear and normal stiffness?

Answer

I believe yes, but have not tested it nor did any research.

Question

Please, explain in more detail your statement from page 9:
A "small" change of positions of particles can cause a sudden ("big") change of the stiffness of the system. For this reason, implicit integration schemes are in general not suitable for numerical solution and an explicit time integration scheme is usually applied to solve equations of motion

Answer

- **not very good expressions, *not suitable* is too strong**
- ***sudden change of stiffness* = zero or nonzero stiffness**
- **What I meant: explicit time integration is "less complex"**

Question

You assume an affine displacement of individual particles. This kinematic assumption is not fulfilled for heterogeneous materials because of perturbations of displacement field due to spatially variable stiffness. What is the influence of this assumption of the accuracy of obtained properties, with respect to the results presented in section 3.4.2?

Answer

- method is designed for homogeneous materials
- for heterogeneous material, each phase could be evaluated independently and another homogenization method could be used to determine overall elastic parameters.

Question

Please, explain in more detail your statement on page 43:
The resulting (couple) stress tensor does not depend on the choice of the point of moment equilibrium.
The resulting (couple) stress tensor does not depend on the choice of particles' reference points.

Answer

These are necessary conditions for macro (couple) stress tensor according to Chang & Kuhn.

DISCUSSION

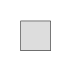
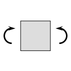
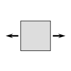
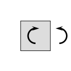
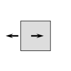
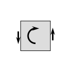
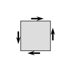
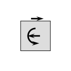
JAN ZEMAN, QUESTION 4

Question

Please, explain what you have tried to show with table 4.1 on page 46.

Answer

Simple illustration of (couple) stress tensor

	σ	μ		σ	μ
	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$		$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & 2 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$
	$\begin{bmatrix} 2 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$		$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$
	$\begin{bmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$		$\begin{bmatrix} \cdot & 2 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$
	$\begin{bmatrix} \cdot & 2 & \cdot \\ 2 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$		$\begin{bmatrix} \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$	$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$

DISCUSSION

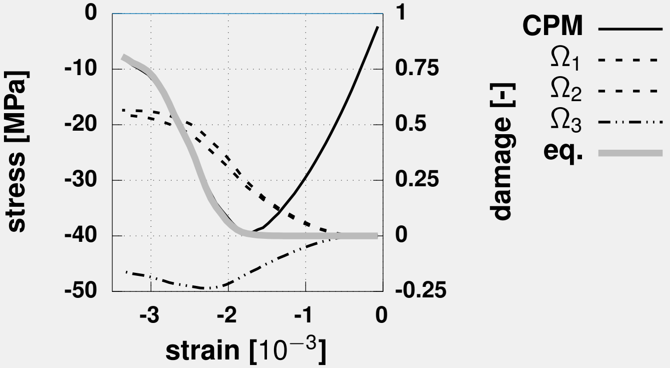
JAN ZEMAN, QUESTION 5

Question

Please, explain based on which considerations you got the calibration formulas in equations (6.17)-(6.19)

Answer

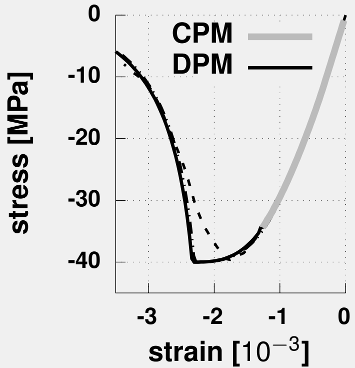
$$\omega = 2.09\,(0.85\Omega_1 + 0.15\Omega_3)^{4.7}$$



Answer

$$\textbf{if} \quad \omega \leq m \quad \textbf{then} \quad \kappa_D = 0, \kappa_P = \kappa_P(\omega), \omega = 0$$

$$m = 5 \cdot 10^{-4}, \quad \kappa_P = 0.3 + 900\omega$$



Question

Results in figure 8.6 should be explained better. For example, it is not clear what is the meaning of the vertical axis and how the results reflects the influence of the transition zone (as was declared in the objectives of the doctoral thesis).

Answer

- ***Since the absolute values of macroscopic quantities can be relatively easily estimated, only values relative to the results for the smallest aggregate size are plotted.***
- **More detailed parameter study could be done to assess influence of ITZ.**