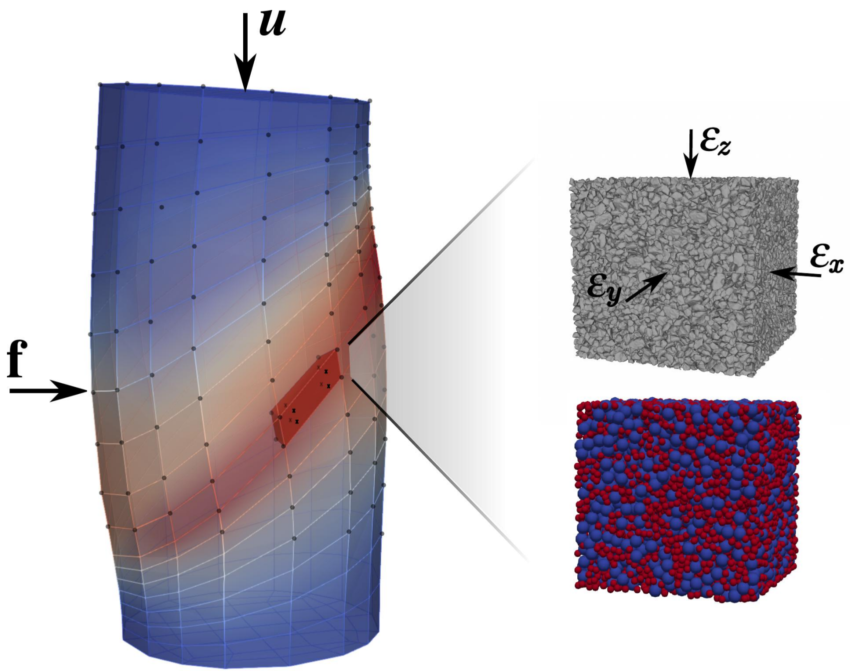


CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 7

From last time

General DEM algorithm

Update particle positions

Forces and moments on particles (contact check):

$$\boldsymbol{f}_i^c = f_i^n \boldsymbol{n}^c + f_i^t \boldsymbol{t}^c$$

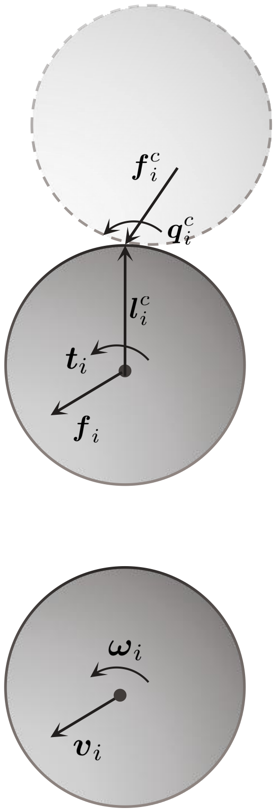
$$\boldsymbol{f}_i = \sum_c \boldsymbol{f}_i^c$$: Total force acting on particle i

$$\boldsymbol{t}_i = \sum_c (\boldsymbol{l}_i^c \times \boldsymbol{f}_i^c + \boldsymbol{q}_i^c)$$: Total torque acting on particle i

Equations of motion:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{f}_i$$: Linear momentum balance

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \boldsymbol{t}_i$$: Angular momentum balance



Quiz

The critical time step for a DEM simulation:

a. increases with contact stiffness

b. increases with particle density

c. is a function of the number of contacts

d. is not a function of damping

Note: One or more answers might be correct.

Quiz

The critical time step for a DEM simulation:

a. increases with contact stiffness

b. increases with particle density

c. is a function of the number of contacts

d. is not a function of damping

Note: One or more answers might be correct.

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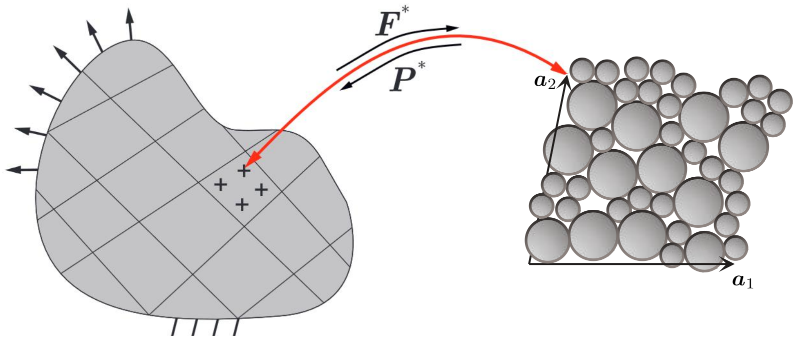
Multiscale modeling in granular systems

Does scale separation hold (approximately)?

√

Hierarchical

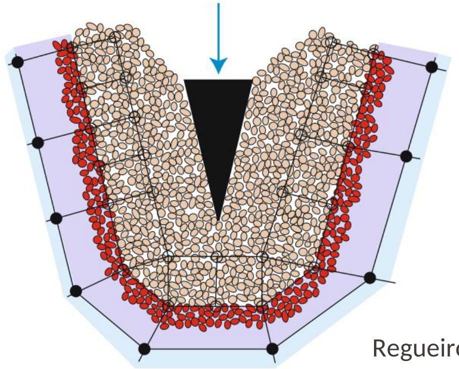


Macroscale FE problem

Microscale DEM problem (periodic RVE)

X

Concurrent

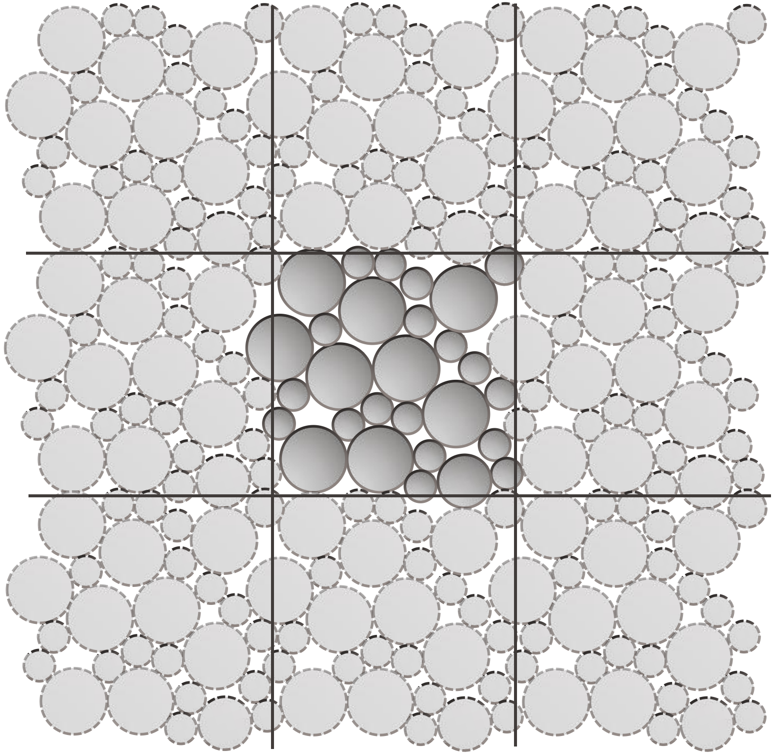


Regueiro et al., 2011

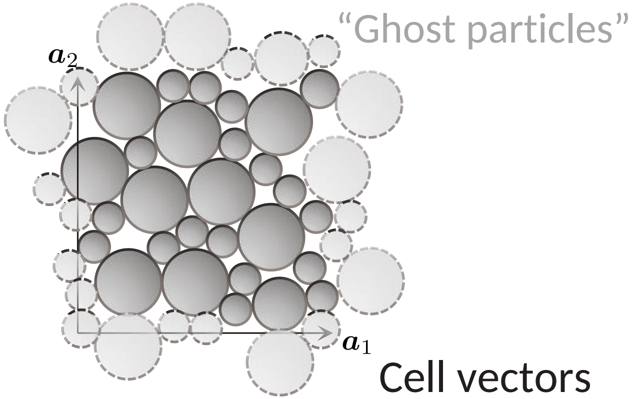
Passing of information from DEM domain to continuum domain and vice-versa

Computational homogenization

Similarly to the continuum problem, the most accurate way to compute the average (homogenized) behavior in a discrete problem is via **periodic boundary conditions:**



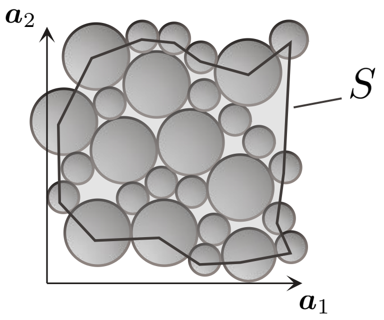
Periodic RVE

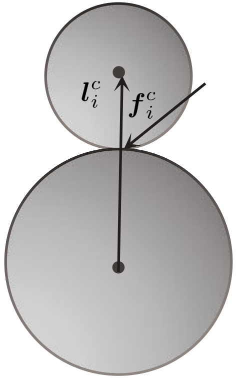


The determination of RVE size is subject to the conditions previously discussed.

Average stress - Quasistatic

Average stress (quasistatic)





$$\boldsymbol{\sigma} = \frac{1}{V} \sum_{c \in \mathcal{S}} \boldsymbol{x}_c \otimes \boldsymbol{f}_c$$

or:

$$\boldsymbol{\sigma} = \frac{1}{V} \sum_{c \in \mathcal{I}} \boldsymbol{l}_c \otimes \boldsymbol{f}_c$$

RVE volume

Set of contacts on the RVE boundary

Contact location

Contact force

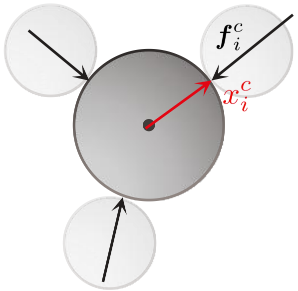
Set of contacts inside the RVE

Branch vector

Note:

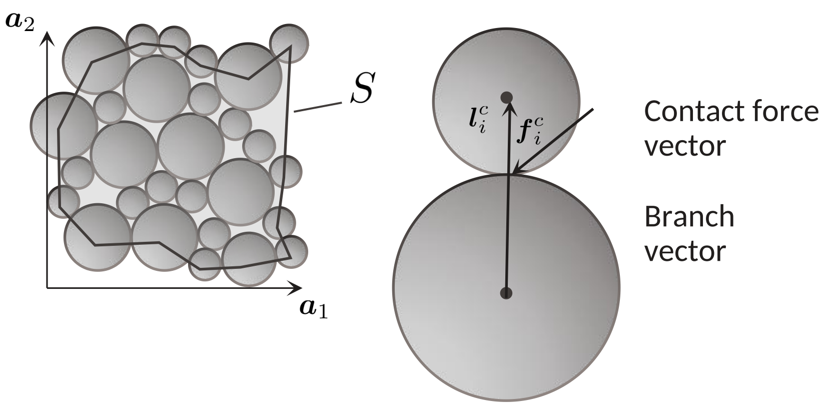
Not to be confused with the **average stress in a particle**:

$$\boldsymbol{\sigma}_p = \frac{1}{V_p} \sum_{c \in \mathcal{S}_p} \boldsymbol{x}_c \otimes \boldsymbol{f}_c$$



Average stress - Dynamic

Average stress (dynamic)



$$\boldsymbol{\sigma} = \frac{1}{V}\left(\sum_i m_i \tilde{\boldsymbol{v}}_i \otimes \tilde{\boldsymbol{v}}_i + \sum_c \boldsymbol{f}_c \otimes \boldsymbol{l}_c\right)$$

RVE volume — Kinetic contribution — Contact (quasistatic) contribution

where: $\tilde{\boldsymbol{v}}_i = \boldsymbol{v}_i - \langle \boldsymbol{v} \rangle$ is the velocity fluctuation

Note:

Care must be taken to ensure **consistent direction of forces** and **branch vectors.**

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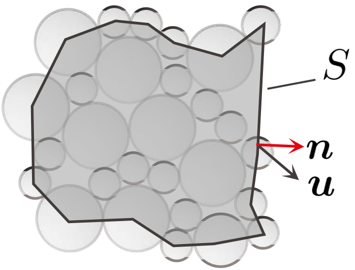
Average strain

Based on a boundary integral:



$$\boldsymbol{\varepsilon} = \frac{1}{V} \int_S \boldsymbol{u} \otimes \boldsymbol{n} \, dS$$

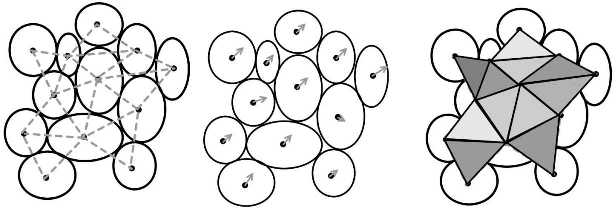
RVE boundary surface

Displacement

Boundary normal

Alternative definitions:

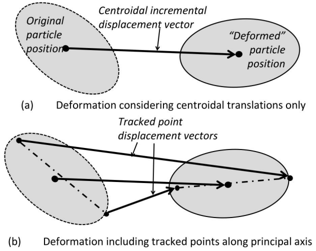
- Triangulation-based



- Best-fit

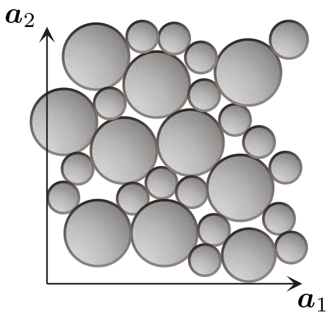
$$\arg_{\boldsymbol{\varepsilon}} \min ||\boldsymbol{u} - \boldsymbol{\varepsilon}\boldsymbol{x}||$$

- Methods that account for rotations



Packing fraction and fabric

Packing fraction



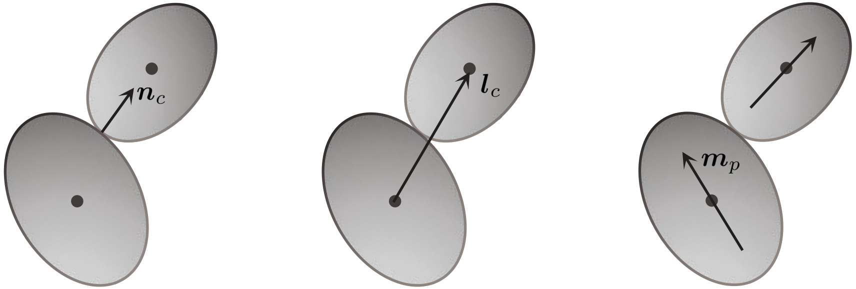
$$\phi = \frac{\sum_p V_p}{V}$$

Correlated with the coordination number

$$Z = \frac{2N_c}{N_p}$$

Fabric tensor

Can be defined on the basis of contact normals, branch vectors, major axis orientations

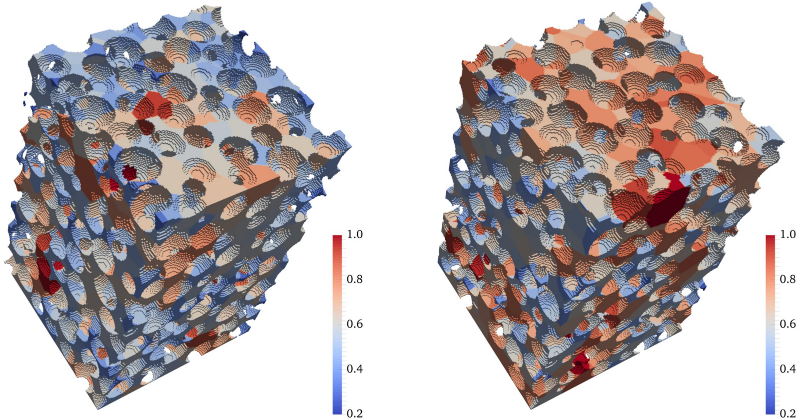


$$\boldsymbol{F} = \frac{1}{N_c}\sum_c \boldsymbol{n}_c \otimes \boldsymbol{n}_c \qquad \boldsymbol{F} = \frac{1}{N_c}\sum_c \boldsymbol{l}_c \otimes \boldsymbol{l}_c \qquad \boldsymbol{F} = \frac{1}{N_p}\sum_p \boldsymbol{m}_p \otimes \boldsymbol{m}_p$$

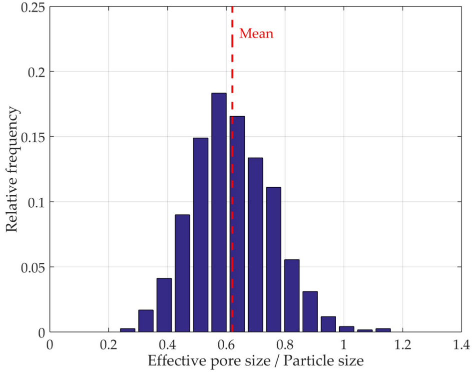
It is the 2nd-order descriptor of the probability distribution of the orientation of those vectors

Other metrics

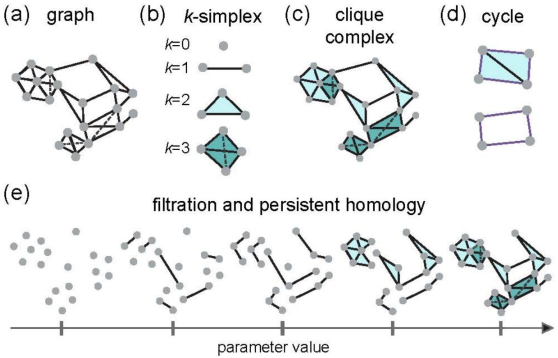
Void/pore space characterization



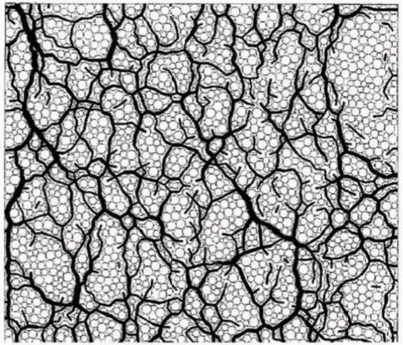
Roozbahani et al, 2017



Topological/Network metrics

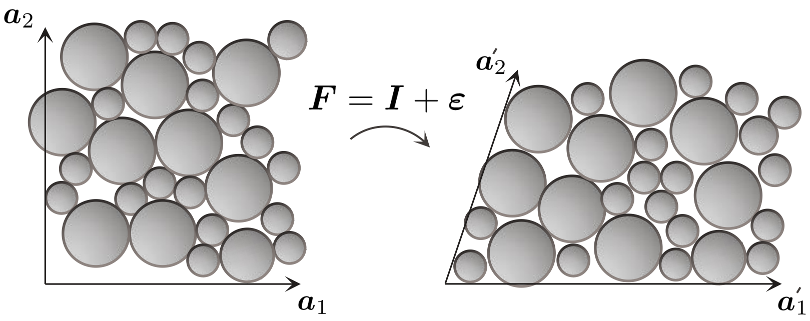


Papadopoulos et al, 2017



Strain and stress-control - Boundary motion

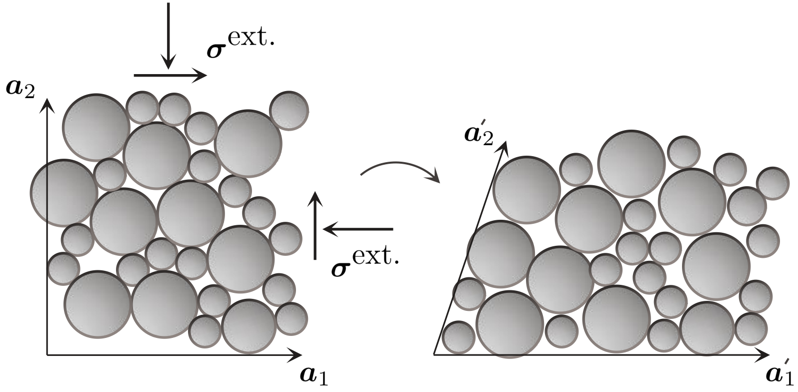
Strain-control



$$\boldsymbol{a}' = \boldsymbol{F}\boldsymbol{a} = (\boldsymbol{I} + \dot{\boldsymbol{\varepsilon}}\, dt)\, \boldsymbol{a}$$

Deformation of unit cell vectors

Stress-control



$$\dot{\boldsymbol{\varepsilon}}^{\text{serv.}} = \dot{\boldsymbol{\varepsilon}}^{\text{serv.}} + \alpha(\boldsymbol{\sigma}^{\text{ext.}} - \boldsymbol{\sigma}^{\text{int.}})$$

$$\boldsymbol{a}' = (\boldsymbol{I} + \dot{\boldsymbol{\varepsilon}}^{\text{serv.}}\, dt)\, \boldsymbol{a}$$

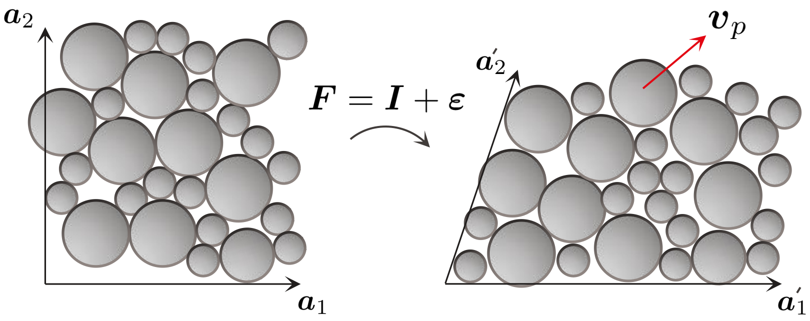
Externally imposed stress: $\boldsymbol{\sigma}^{\text{ext.}}$

Measured internal stress: $\boldsymbol{\sigma}^{\text{int.}}$

(Servo-control)

Strain and stress-control - Particle motion

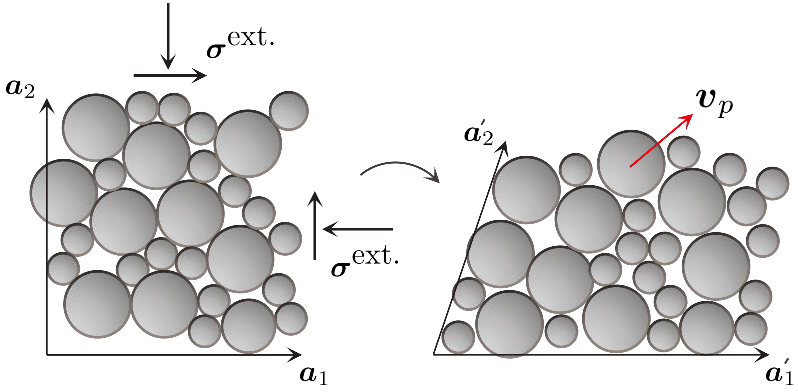
Strain-control



$$\boldsymbol{v}_p = \dot{\boldsymbol{\varepsilon}} \cdot \boldsymbol{x}_p$$

Velocity imparted to the particles due to global strain field

Stress-control

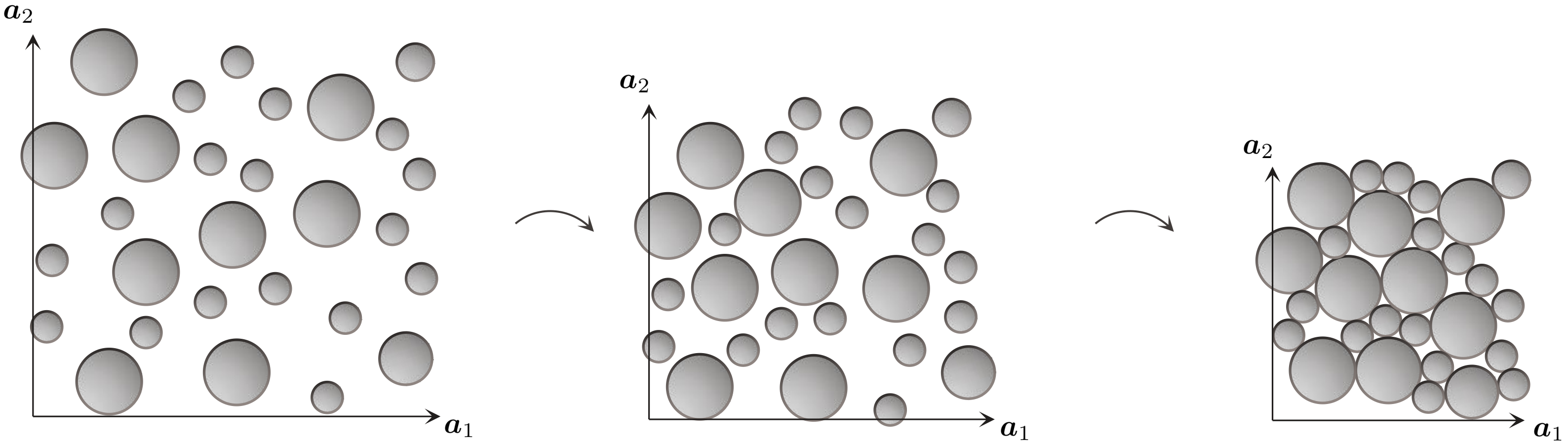


$$\boldsymbol{v}_p = \dot{\boldsymbol{\varepsilon}}^{\text{serv}} \cdot \boldsymbol{x}_p$$

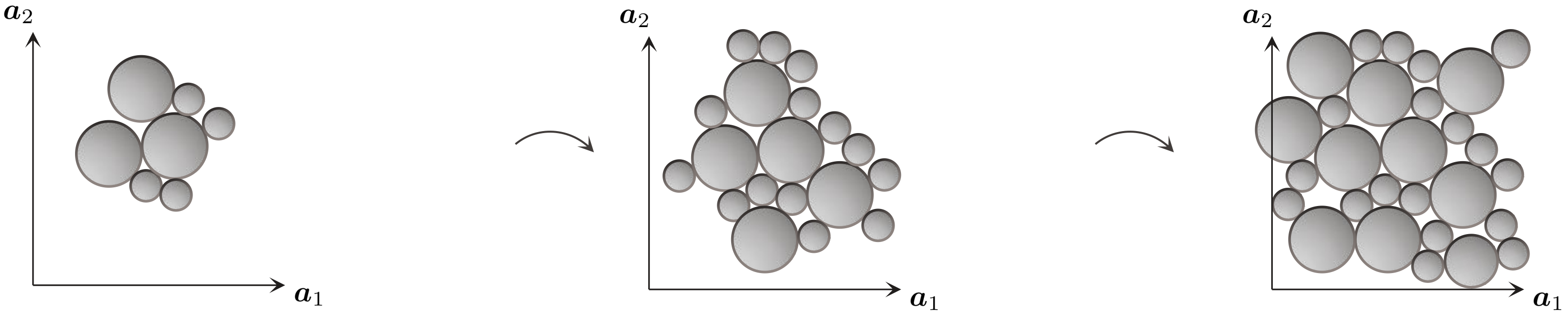
Velocity imparted to the particles due to global strain field

Sample preparation and simulation

Compression from gas state and relaxation



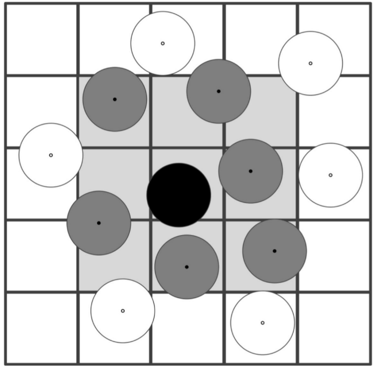
Random space-filling algorithms (hard for periodic boundary conditions)



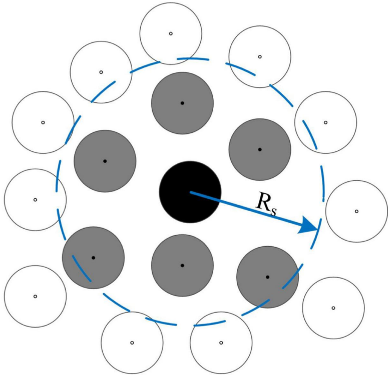
Computational aspects

Contact detection typically takes 70-80% of the computational effort.

Standard methods: **Linked cell, Verlet**



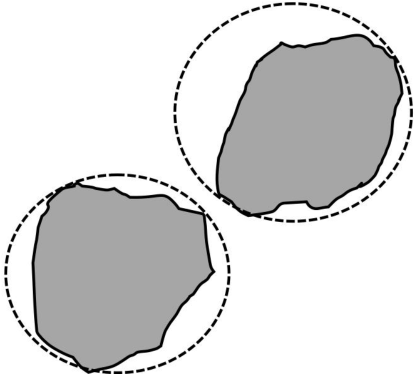
(a) Linked cell method



(b) Verlet table algorithm

Chen et al, Powder Technology (2024)

Bounding sphere



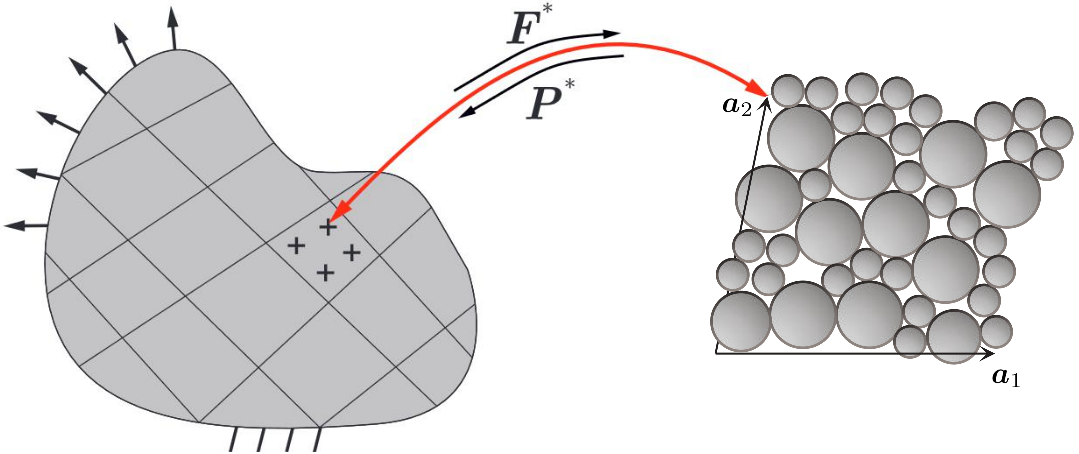
Useful for arbitrarily shaped particles

Parallelization:

OpenMP (shared memory), MPI (distributed memory), CUDA (GPU)

FEMxDEM

Similar to FE^2 but the microscale problem is replaced by DEM.



Macroscale FE problem

Microscale DEM problem

Futher reading

- Original paper by Cundall and Strack (1979):

" A discrete numerical model for granular assemblies"

- Book by B. Andreotti, Y. Forterre, O. Pouliquen (2013):

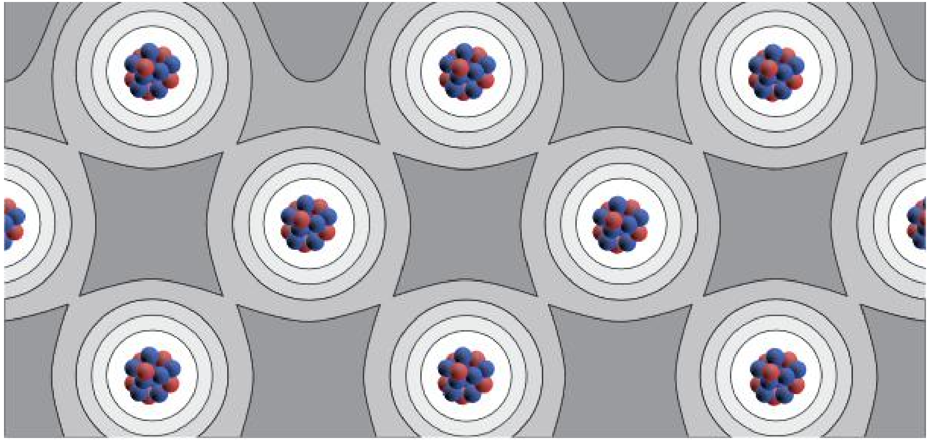
"Granular Media Between Fluid and Solid"

- Remaining chapters of our textbook by C. O'Sullivan (2011):

"Particulate Discrete Element Modeling"

Outlook

Atomistics and statistical mechanics



Discussion

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Multiscale Modeling, D. M. Kochmann

Chapters 12.5, 13, 15, 16