Discrete Element Modeling

Bruno Chareyre

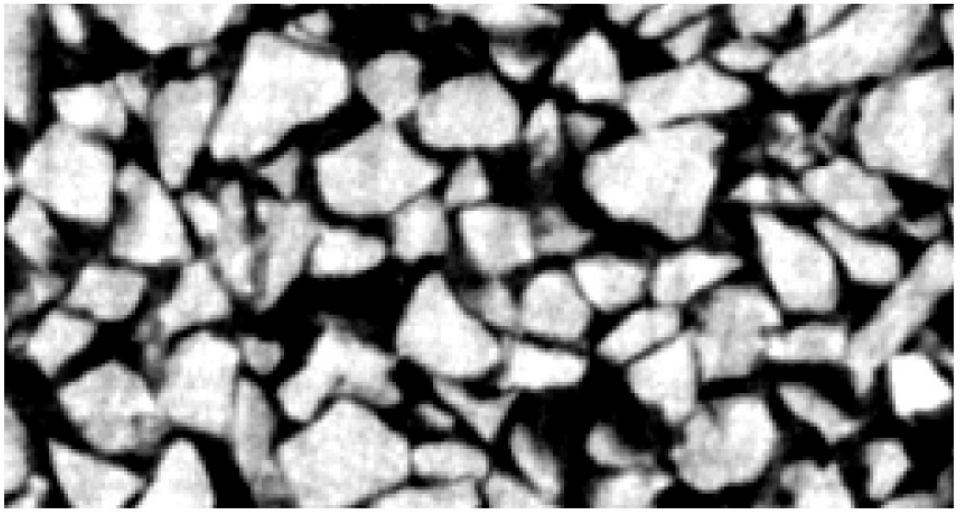
Yade Course, Amsterdam, 2022

Granular materials

Industrial and other anthropic materials

Source: wikipedia (2012)

Natural materials



Source: Ando et al. (2011)

Discrete **E**lement **M**ethod (DEM)

Selected examples:

Sandpile
Larger and cohesive
Rotating drum
Screw conveyor
Grid-type Structure
Soil+grid (1)(2)
Periodic boundaries
Fluid coupling

What is a “discrete” model?

* All numerical models in mechanics define a finite number of DOFs, they are all “discrete”.

* Here we call “*discrete*” a model for which the underlying conceptual model is *discontinuous*, as opposed to “*continuum”* mechanics.

* The discrete element method (DEM) is sometimes used even when the conceptual basis is continuous (see vision 2 in what follows)

What is a “discrete” model?

Conceptual model

Continuous

Finite element method (FEM)
Finite volume method (FVM)
Finite differences method (FDM)
Smooth particles hydrodynamics (SPH)
Lattice Boltzmann method (LBM)

Discrete

Molecular dynamics (MD)
Discrete element method (DEM)
Variants of Cundall's DEM (contact dynamics, event driven,...)

What is a “discrete” model?

Conceptual model

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Finite volume method (FVM)
Finite differences method (FDM)
Smooth particles hydrodynamics (SPH)
Lattice Boltzmann method (LBM)
Discrete element method (??)

Discrete

Molecular dynamics (MD)
Discrete element method (DEM)
Variants of Cundall's DEM (contact dynamics, event driven,...)

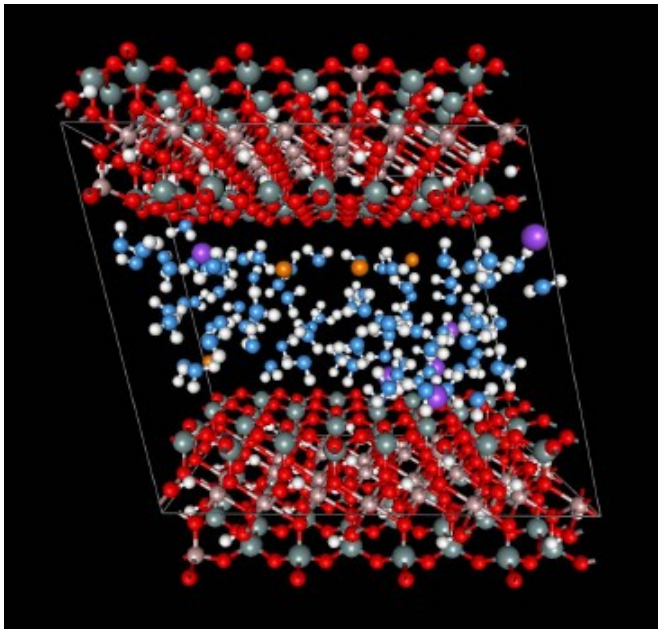
What is a “discrete” model?

Yet more semantic...

Molecular Dynamics (Alder, 1959)

“Molecular dynamics (MD) is a computer simulation of physical movements of atoms and molecules. [...] In the most common version, the trajectories of molecules and atoms are determined by numerically solving the Newton's equations of motion for a system of interacting particles, where forces between the particles and potential energy are defined by **molecular mechanics force fields**.” (wikipedia)

***Softwares**: OpenMM, Amber, LAMMPS,...*



Source: Park & Sposito, 2003.

Discrete Element Method (Cundall, 1979 – ISI 2469)

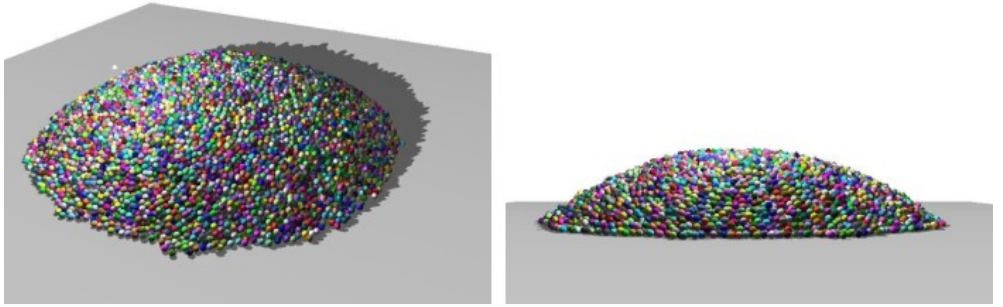
“A discrete element method (DEM), also called a distinct element method is any of family of numerical methods for computing the motion and effect of a large number of small particles. Though DEM is **very closely related to molecular dynamics**, the method is generally distinguished by its **inclusion of rotational degrees-of-freedom as well as stateful contact and often complicated geometries** (including polyhedra).” (wikipedia)

***Softwares**: PFC2D/3D, SDEC, YADE-DEM, EsyS-Particle,...*

Contact (a.k.a NSCD, Moreau, 1988)

“Contact dynamics deals with the motion of multibody systems subjected to **unilateral** contacts and friction.” (wikipedia)

***Softwares**: LMGC90,...*



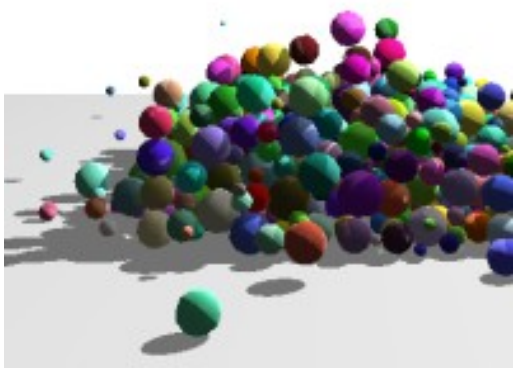
Source: Yade-DEM

MD ≠ DEM !

Explicit DEM

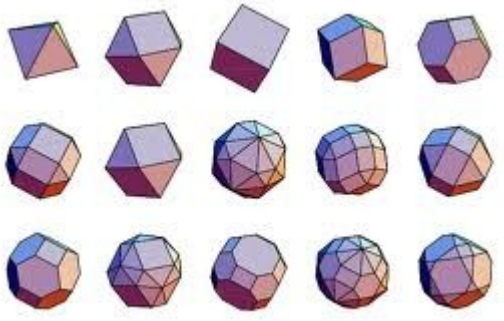
Idealized particle shapes

Spheres



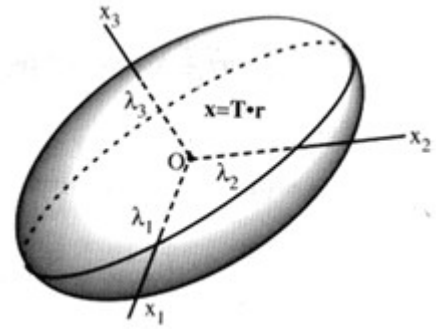
source: Yade-DEM

Polyhedra



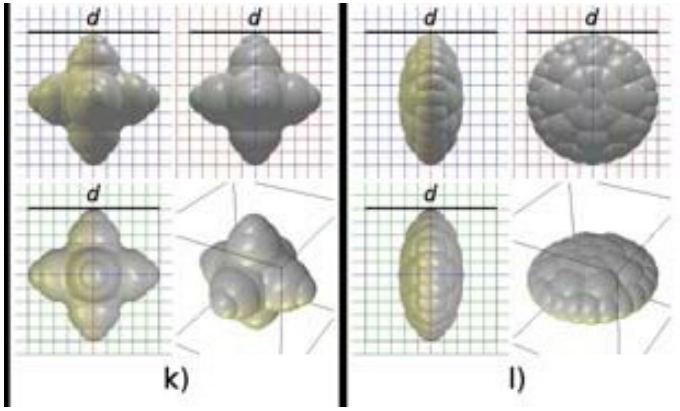
source: http://watermanpolyhedron.com/watermanpolyhedra1.html

Ellipsoids



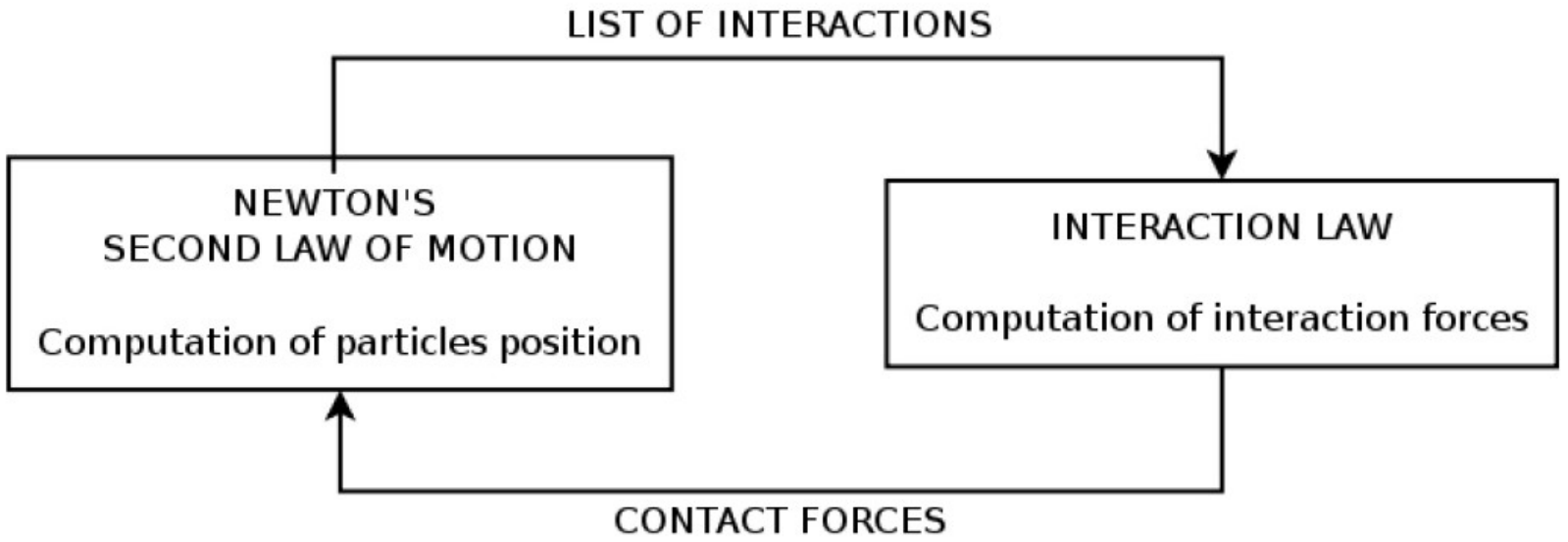
source: http://www.ruppweb.org/xray/comp/suptext.htm

Clusters



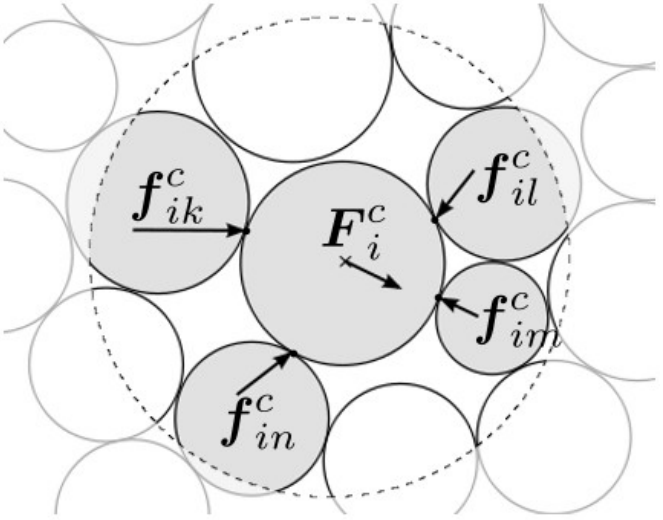
source: **KOZICKI AND TEJCHMAN, 2011 (Yade-DEM)**

Explicit FD scheme



(Source: E. Catalano, PhD, 2012)

Governing Equations



Newtons Law

Translation

$$\ddot{\mathbf{u}}^{\circ} = \mathbf{F}/m$$

Rotation

$$\mathbf{T}_i = \mathbf{I}_{ii}\dot{\boldsymbol{\omega}}_i + (\mathbf{I}_{kk} - \mathbf{I}_{jj})\boldsymbol{\omega}_j\boldsymbol{\omega}_k \qquad \text{or}$$

$$\dot{\boldsymbol{\omega}}_i^{\circ} = \mathbf{T}_i/\mathbf{I} \qquad \text{(isotropic case)}$$

Contact Laws

In the general case: $\mathrm{d}\{f_{ij},m_{ij}\}/\mathrm{d}t = L_{ij}(u_i, u_j, \dot{u}_i, \dot{u}_j)$

Content

Explicit FD scheme

Schéma classique (point commun entre la DEM et la dynamique moléculaire):
Seconde loi de Newton;

$$\Sigma F = m\ddot{x} \tag{1}$$

Schéma DF explicite:

$$\Sigma F(t) = m\ddot{x}(t) = \frac{x(t+dt) - 2x(t) + x(t-dt)}{dt^2} + O(dt^2) \tag{2}$$

Intégration:

$$x(t+dt) = 2x(t) - x(t-dt) + \frac{\Sigma F(t)}{m} dt^2 \tag{3}$$

(principe similaire pour les rotations...)

Explicit FD scheme

This centered 2nd order explicit scheme is also known as:

*“leap-frog” for the positions are known at times $i\Delta t$ while velocities are known at times $i\Delta t+\Delta t/2$

* Störmer's method or Verlet algorithm, especially in the context of MD (Teukolsky, 2007)

It belongs to the family of *symplectic integrators* for Hamiltonian systems. It implies the following properties, that even higher-order schemes may not have (e.g. Runge-Kutta):

* Energy conservation over the time steps (with bounded oscillations)

* Time reversibility

Classical contact laws

Kinematic description

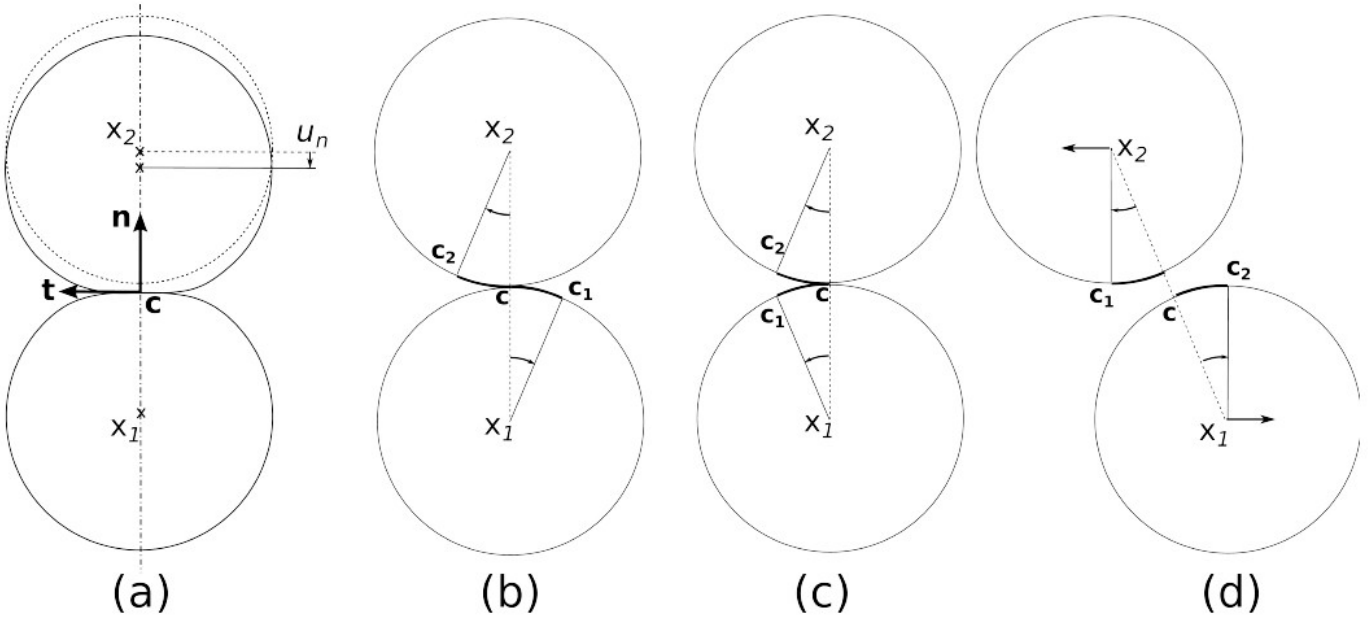


Figure: Mouvements relatifs 2D de deux particules en contact. (a) déplacement normal, (b) cisaillement pur, (c) roulement, (d) cisaillement simple.

Yade-DEM)

Classical contact laws

Force d'interaction définie la "loi de contact" $\mathcal{L}$

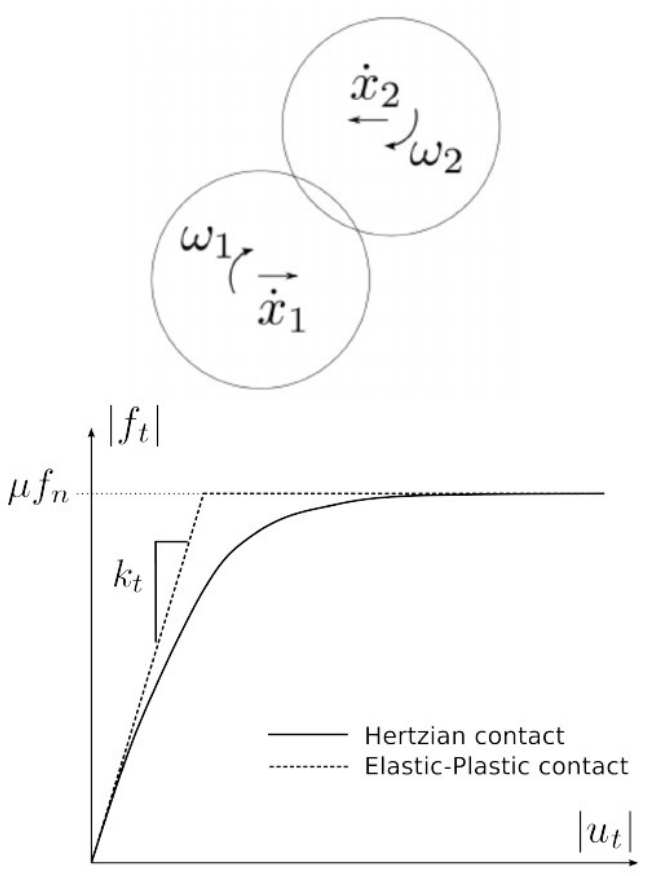
$$\mathbf{f} = \mathcal{L}(\mathbf{x_1}, \mathbf{x_2}, \dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2, \mathcal{H}) \qquad (4)$$

ou par la dérivée:

$$\dot{\mathbf{f}} = \mathcal{L}^*(\mathbf{x_1}, \mathbf{x_2}, \dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2, \mathcal{H}, \mathbf{f}) \qquad (5)$$

Cas particuliers:
élastique linéaire: $\mathbf{f} = \mathcal{L}(\mathbf{x_1}, \mathbf{x_2})$
visco-élastique: $\mathbf{f} = \mathcal{L}(\mathbf{x_1}, \mathbf{x_2}, \dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2)$
visco-élasto-plast.: $\dot{\mathbf{f}} = \mathcal{L}^*(\mathbf{x_1}, \mathbf{x_2}, \dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2, \mathbf{f})$
+ couple (roulement et/ou torsion)

$> 2R$



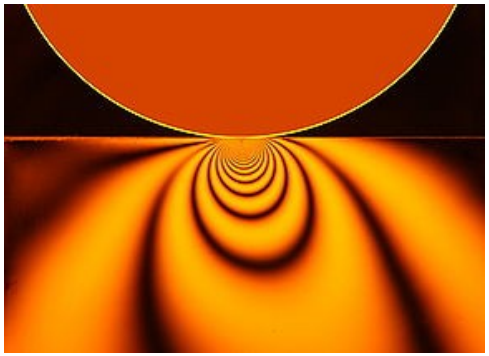
Hertzian model and the elastic-plastic idealization.

Classical contact laws

Normal force-displacement relation

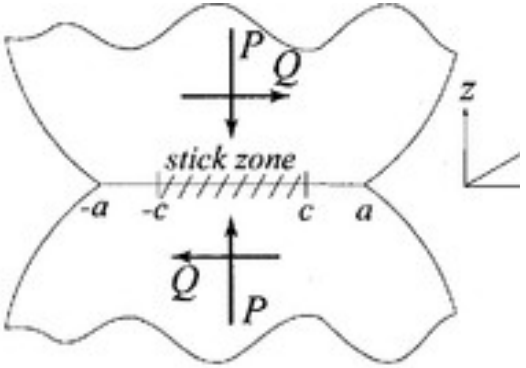
* Hertz contact (non-linear elasticity)

$$F = \frac{4}{3} E^* R^{1/2} d^{3/2}$$



Source: wikipedia

* Mindlin and Deresiewicz (inelastic)



(a) Contact in partial slip

Source: Young Ju Ahn, Response of coupled frictional contacts to cyclic loading, PhD dissertation, 2009.

Classical contact laws

Simplified linear elastic law in the normal direction

$$u_N = |\mathbf{C}_2^\circ - \mathbf{C}_1^\circ| - d_0$$

$$\mathbf{F}_N = K_N u_N \mathbf{n}$$

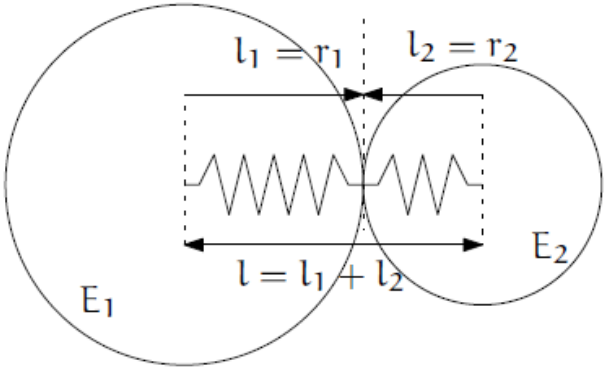
A convenient definition of K_N

$$K_i = E_i \tilde{l}_i$$

$$K_1^{-1} + K_2^{-1} = K_N^{-1}$$

$$K_N = \frac{K_1 K_2}{K_1 + K_2}$$

$$K_N = \frac{E_1 \tilde{l}_1 E_2 \tilde{l}_2}{E_1 \tilde{l}_1 + E_2 \tilde{l}_2}$$



Series of 2 springs representing normal stiffness of contact between 2 spheres.

(Source: Yade-DEM)

Classical contact laws

Simplified linear elastic law: tangential direction

Relative velocity at the contact point:

$$\boldsymbol{v}_{12} = \left(\boldsymbol{v}_2^{\ominus} + \boldsymbol{\omega}_2^{-} \times (-\mathrm{d}_2\mathbf{n}^{\circ})\right) - \left(\boldsymbol{v}_1^{\ominus} + \boldsymbol{\omega}_1^{\ominus} \times (\mathrm{d}_1\mathbf{n}^{\circ})\right)$$

It has the tangential component:

$$\boldsymbol{v}_{12}^{\perp} = \boldsymbol{v}_{12} - (\mathbf{n}^{\circ} \cdot \boldsymbol{v}_{12})\mathbf{n}^{\circ}$$

Time integration of the force-displacement relation:

$\Delta \boldsymbol{F}^{\mathrm{t}}_{\mathrm{T}} = \boldsymbol{K}_{\mathrm{T}} \Delta \boldsymbol{u}_{\mathrm{T}} = \boldsymbol{K}_{\mathrm{T}} (\boldsymbol{v}_{\mathrm{T}} + \boldsymbol{\omega}_{\mathrm{r}} \times \boldsymbol{u}_{\mathrm{T}}) \Delta t = (\boldsymbol{K}_{\mathrm{T}} \boldsymbol{v}_{\mathrm{T}} + \boldsymbol{\omega}_{\mathrm{r}} \times \boldsymbol{F}^{\mathrm{t}}_{\mathrm{T}}) \Delta t.$

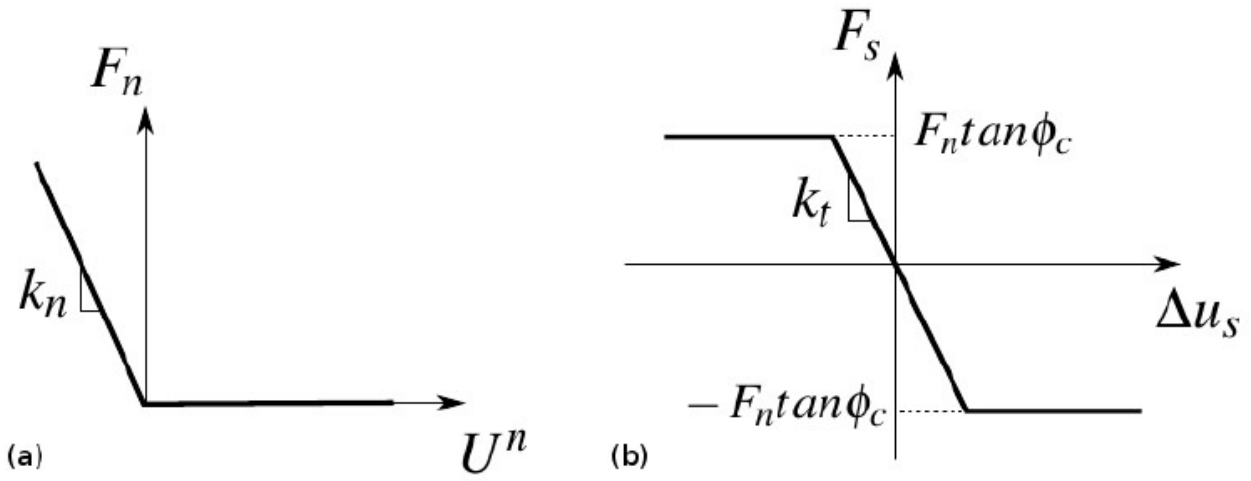
Attention must be paid to the global rotation of the contact represented by the spin $\boldsymbol{\omega}_{\mathrm{r}}$, which must also be reflected in $\mathbf{F}_{\mathbf{T}}$.

Like for K_N, K_T can be taken as the harmonic average of K_{T1} and K_{T2}

Classical contact laws

Coulomb's friction

$$\mathbf{F}_T = \begin{cases} \mathbf{F}_T^t \dfrac{|\mathbf{F}_N| \tan \varphi}{\mathbf{F}_T^t} & \text{if } |\mathbf{F}_T| > |\mathbf{F}_N| \tan \varphi \\ \mathbf{F}_T^t & \text{otherwise.} \end{cases}$$



(Source: Scholtès L., PhD, 2012)

Classical contact laws

Additional features:

* normal adhesion (tensile strength)
* shear adhesion (shear strength summed with friction)
* Viscosity
* irreversibility
* etc.

Higher degree laws (6D)

* rotational stiffness (bending and twisting)
* rotational strength (in the form of adhesion + “rolling” friction)

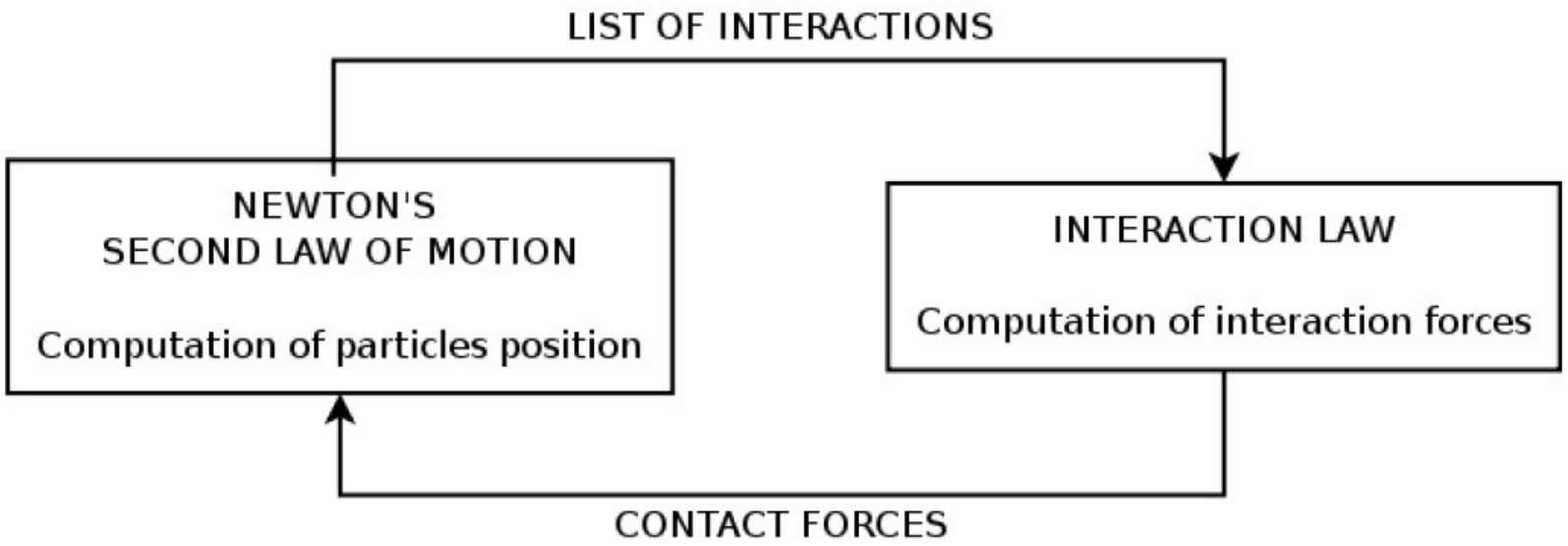
Classical contact laws

The force-displacement relations and motion equations are all defined in the current (deformed) configuration, as in the “updated Lagrangian” methods.

Hence there is no limitation in the deformation/displacement.

See this **example** with Yade

Implementation issues



* Contact detection

* Stability condition / automatic timestep determination

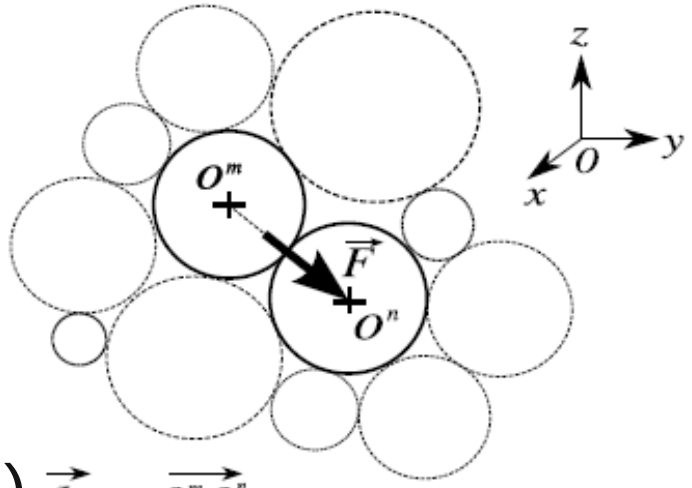
* Damping

Contact detection

The new contacts must be checked at each step.
The following naive algorithm scales with N^2 and needs a square root:

At each step:

```
For i in [1,N]:
    For j in [1,N]:
        (R_i + R_j) > sqrt(l_x²+l_y²+l_z²) ?
```

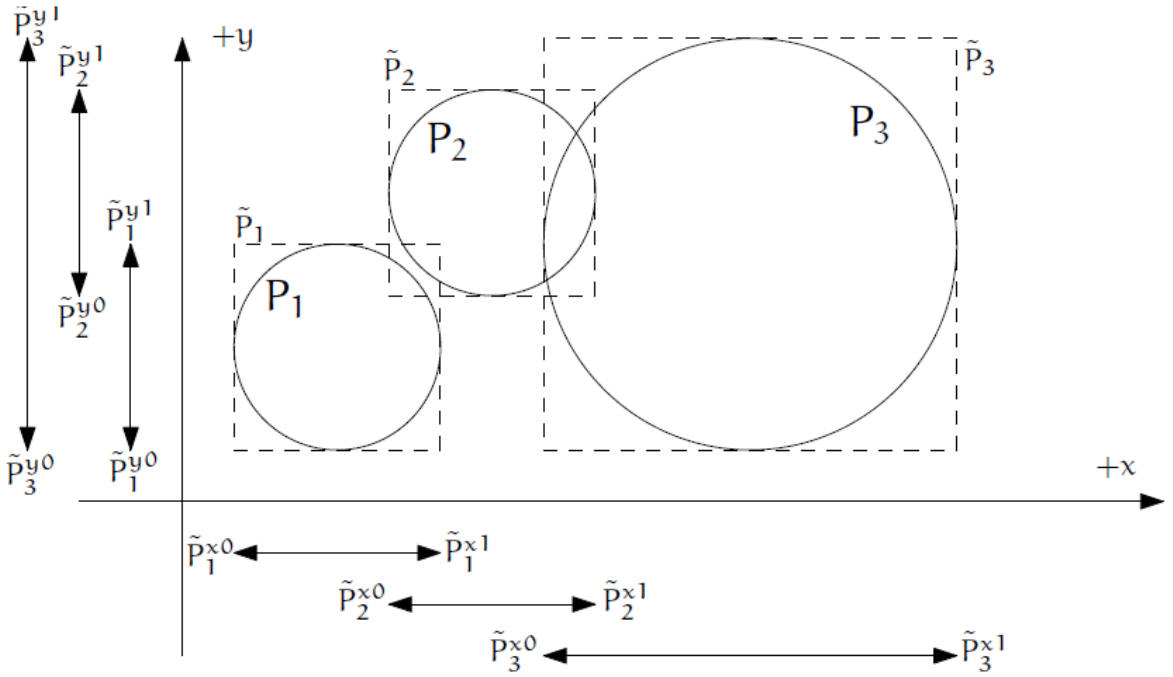


(and it is even worst for complex shapes...) $\vec{l} = \overrightarrow{o^m o^n}$

Contact detection

$(R_i + R_j) > \mathrm{sqrt}(l_x^2+l_y^2+l_z^2)$?

Bounding boxes let one exclude many potential interactions at a reduced cost



$$\left(\tilde{P}_i \cap \tilde{P}_j\right) \neq \emptyset \Leftrightarrow \bigwedge_{w\in\{x,y,z\}} \left[\left(\left(\tilde{P}_i^{w0}, \tilde{P}_i^{w1}\right) \cap \left(\tilde{P}_j^{w0}, \tilde{P}_j^{w1}\right)\right) \neq \emptyset\right]$$

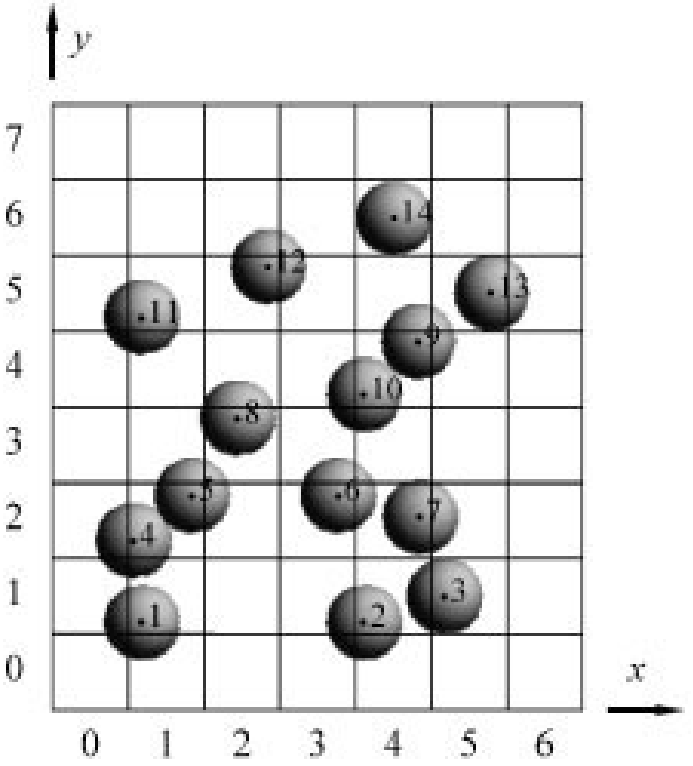
(Source: Yade-DEM)

Contact detection

For i in [1,N]:
    For j in [1,N]:
        fast check(i,j) ?
        $(R_i + R_j) > \mathrm{sqrt}(l_x^2+l_y^2+l_z^2)$?

Sorting in a regular grid results in a constant number of checks per particle, resulting in O(*N*) cost (Munjiza et al. 2006)

For i in [1,N]:
    For j in neighbour cells:
        fast check(i,j) ?
        $(R_i + R_j) > \mathrm{sqrt}(l_x^2+l_y^2+l_z^2)$?



(Munjiza et al. 2006)

Contact detection

At each step:

For i in [1,N]:

For j in [1,N]:

fast check(i,j) ?

$(R_i + R_j) > \mathrm{sqrt}(l_x^2+l_y^2+l_z^2)$?

If the bounding boxes are larger than the actual size of the bodies, then the extra length D^* let one define a number of iterations $n_{min}=D^*/(v_{max}\Delta t)$

in which no new contact can appear:

If $n > n_{max}$:

For i in [1,N]:

For j in neighbour cells:

fast check(i,j) ?

add virtual interaction (i,j)

A each step:

For (i,j) in virtual interactions:

fast check(i,j) ?

$(R_i + R_j) > \mathrm{sqrt}(l_x^2+l_y^2+l_z^2)$? (with the real values of R_i,R_j)

Explicit FD scheme

Stability condition

Before diving into the three-dimensional multibody problem, it may help to examine how the CFD scheme performs for a simple mass-spring system governed by

$$\ddot{x} = -\frac{k}{m}x. \tag{1.27}$$

This is practically what happens if we let one sphere subjected to gravity bounce on a plane without loosing the contact. The natural oscillations of this system have a period $T = 2\pi\sqrt{m/k}$

(Source)

Explicit FD scheme

Stability condition

Recall: Acceleration at time t is evaluated by

$$\ddot{\boldsymbol{x}}_n(t) = \frac{\boldsymbol{x}_n^{t-\Delta t} - 2\boldsymbol{x}_n^t + \boldsymbol{x}_n^{t+\Delta t}}{\Delta t^2} + \mathcal{O}(\Delta t^2) \tag{1.9}$$

$$\boldsymbol{x}_n^{t+\Delta t} = \boldsymbol{x}_n^t + \Delta t \left(\frac{\boldsymbol{x}_n^t - \boldsymbol{x}_n^{t-\Delta t}}{\Delta t} + \frac{\Delta t}{m_n} \boldsymbol{F}_n(\boldsymbol{X}^t) \right) + \mathcal{O}(\Delta t^4). \tag{1.10}$$

Apparently eq.1.10 implies that the positions of the last two steps (t and $t - \Delta t$) must be kept in computer's memory in order to calculate the next step, but concrete implementation are not doing this exactly. Instead the average velocity $\dot{\boldsymbol{x}}_n^{t-\Delta t/2} = \frac{\boldsymbol{x}_n^t - \boldsymbol{x}_n^{t-\Delta t}}{\Delta t}$ is stored directly. It uses the same amount of memory but it is much more useful in terms of post-processing. Is is commonly used for graphical representations

Using the average velocity, one iteration of the CFD sheme goes through the two-step update (equivalent to eq. 1.10)

$$\dot{\boldsymbol{x}}_n^{t+\Delta t/2} = \dot{\boldsymbol{x}}_n^{t-\Delta t/2} + \frac{\Delta t}{m_n} \boldsymbol{F}_n^t \tag{1.12}$$

$$\boldsymbol{x}_n^{t+\Delta t} = \boldsymbol{x}_n^{t-\Delta t} + \dot{\boldsymbol{x}}_n^{t+\Delta t/2} \Delta t \tag{1.13}$$

Explicit FD scheme

Stability condition

$$\dot{\boldsymbol{x}}_n^{t+\Delta t/2} = \dot{\boldsymbol{x}}_n^{t-\Delta t/2} + \frac{\Delta t}{m_n}\boldsymbol{F}_n^t \tag{1.12}$$

$$\boldsymbol{x}_n^{t+\Delta t} = \boldsymbol{x}_n^{t-\Delta t} + \dot{\boldsymbol{x}}_n^{t+\Delta t/2}\Delta t \tag{1.13}$$

In this situation we can write the state of the system after N iterations explicitly by introducing the vector $\boldsymbol{Y} = \{x^t, \dot{x}^{t-\frac{\Delta t}{2}}\Delta t\}^\top$. A matrix form of eqs. 1.13 and 1.12 using this vector is

$$\boldsymbol{Y}^k = \boldsymbol{M}\boldsymbol{Y}^{k-1} \tag{1.28}$$

where k denotes the number of iterations and

$$\boldsymbol{M} = \begin{bmatrix} 1-\beta & 1 \\ -\beta & 1 \end{bmatrix} \tag{1.29}$$

$$\beta = \frac{k\Delta t^2}{m} > 0$$

Consequently, the state after k iterations depends on the initial conditions and the k-th power of $\boldsymbol{M}$ as

$$\boldsymbol{Y}^k = \boldsymbol{M}^k\boldsymbol{Y}^0. \tag{1.30}$$

Explicit FD scheme

Stability condition

$$\boldsymbol{Y}^k = \boldsymbol{M}^k \boldsymbol{Y}^0$$

In principle, three possible situations can occur with such equation depending on the spectral radius $\rho(\boldsymbol{M})$ of the recursion matrix [4].

– If $\rho(\boldsymbol{M}) > 1$ then $\boldsymbol{M}^k$ is not bounded, the scheme diverges;

– If $\rho(\boldsymbol{M}) < 1$ then $\boldsymbol{M}^k$ converge to the null matrix as $k \to +\infty$, thus $\boldsymbol{Y}^k \to \boldsymbol{0}$ (unphysical since there is no damping);

– If $\rho(\boldsymbol{M}) = 1$ then $\boldsymbol{M}^k$ is finite (it may not have a limit), and the scheme is stable.

Explicit FD scheme

Stability condition

Here the eigenvalues of $\boldsymbol{M}$ are the roots of

$$\delta \equiv det(\boldsymbol{M} - \lambda \boldsymbol{I}) = \lambda^2 + (\beta - 2)\lambda + 1. \tag{1.31}$$

the discriminant of this polynomial is

$$\Delta = (\beta - 2)^2 - 4 \tag{1.32}$$

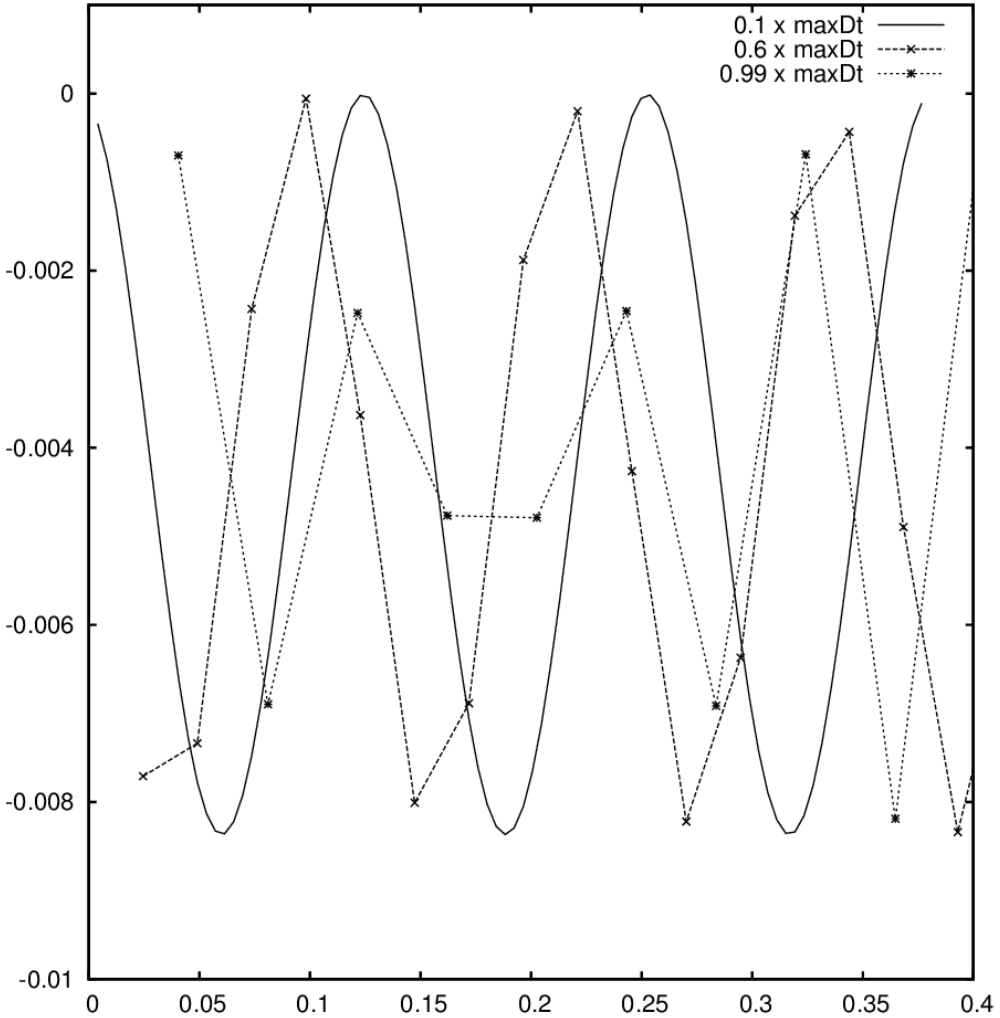
and its sign changes for $\beta = 4$, i.e. $\Delta t = 2\sqrt{m/k} = T/\pi$, hence:

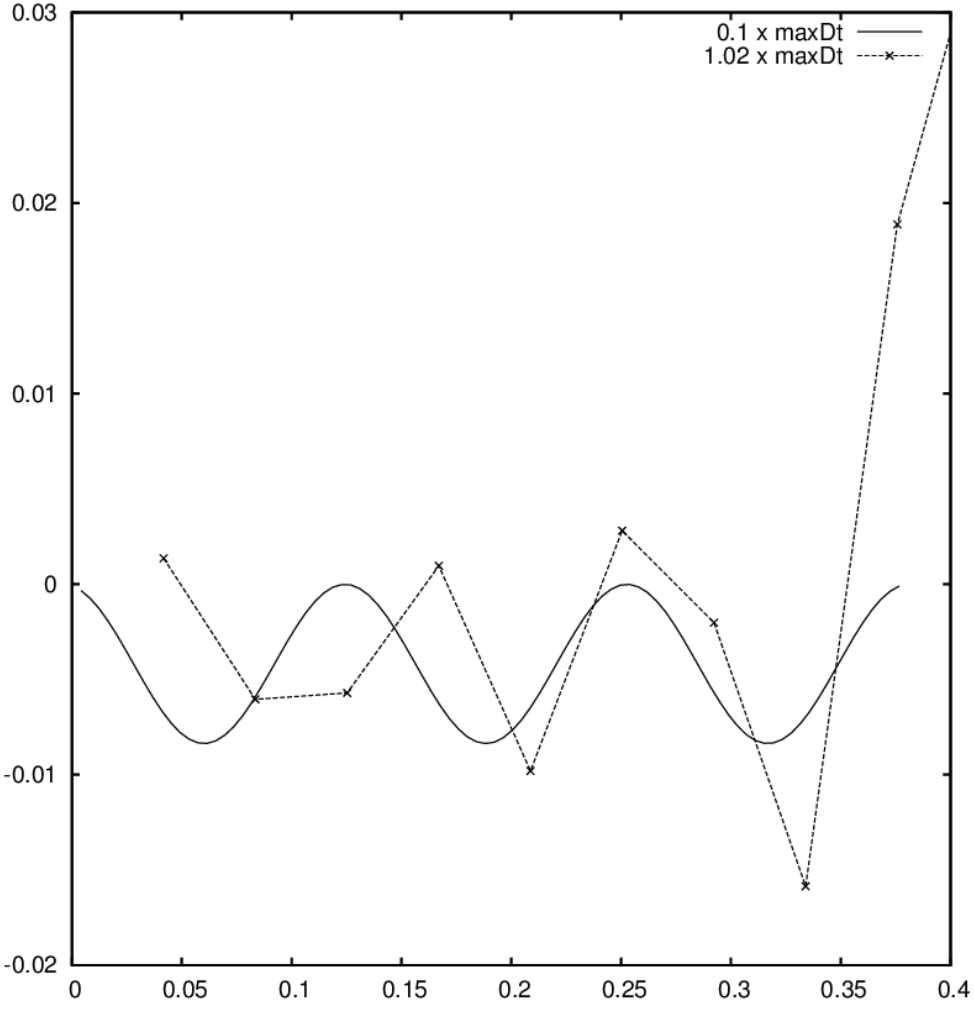
– If $\beta > 4$ (i.e. $\Delta t > 2\sqrt{m/k}$) the two eigenvalues are real numbers equal to $\lambda_1 = (2 - \beta + \sqrt{(\beta - 2)^2 - 4})/2$ and $\lambda_2 = (2 - \beta - \sqrt{(\beta - 2)^2 - 4})/2$, in which $|\lambda_2| > 1$, thus eq. 1.30 diverges.

– If $0 < \beta < 4$ (i.e. $\Delta t < 2\sqrt{m/k}$) the two eigenvalues are complex numbers equal to $\lambda_1 = (2 - \beta + i\sqrt{4 - (\beta - 2)^2})/2$ and $\lambda_2 = (2 - \beta - i\sqrt{4 - (\beta - 2)^2})/2$, and $\rho(\boldsymbol{M}) = |\lambda_1| = |\lambda_2| = 1$. It implies that the numerical solution - in terms of real number - is the superposition of two complex modes of oscillation of constant amplitude.

Explicit FD scheme

Stability condition





Explicit FD scheme

Stability condition

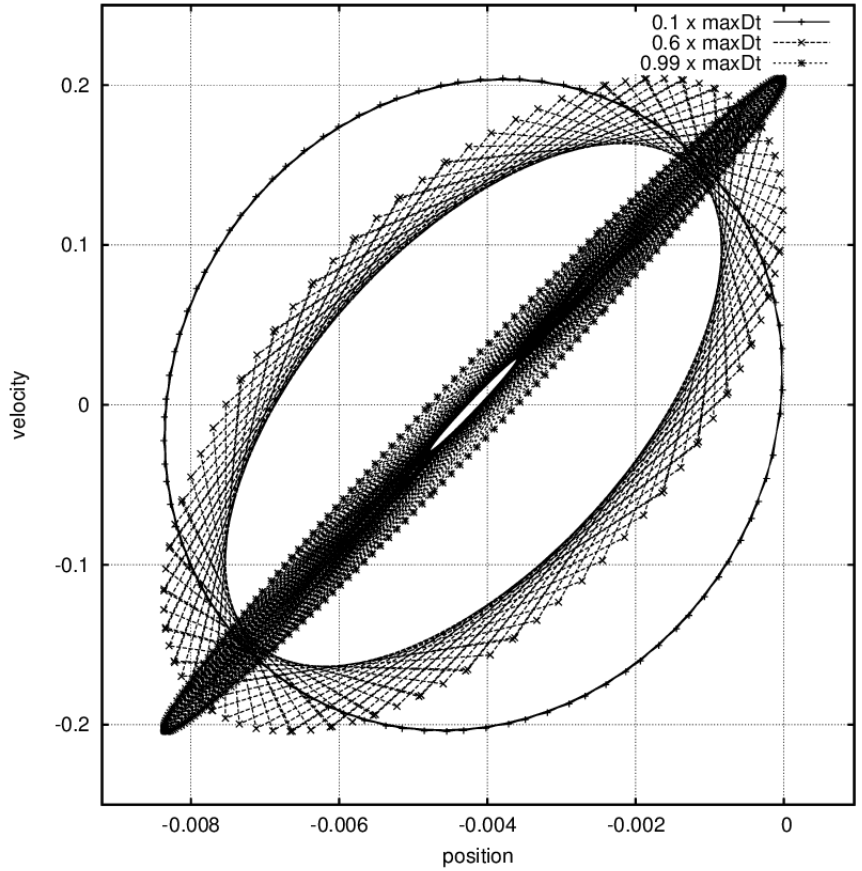
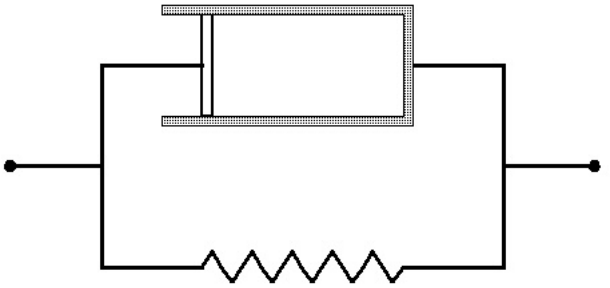


Figure 1.4 – The bouncing sphere in the position-velocity phase space, for different values of Δt.[fig:dispVel]

Damping



Physical origin of dissipation:

* plastic dissipation at contacts

* viscous effects at contacts (e.g. Kelvin's spring-dashpot model, lubrication,...)

Plastic dissipation is sometimes very small. Viscous dissipation can help stabilizing the particles, but it can be at the price of a smaller timestep.

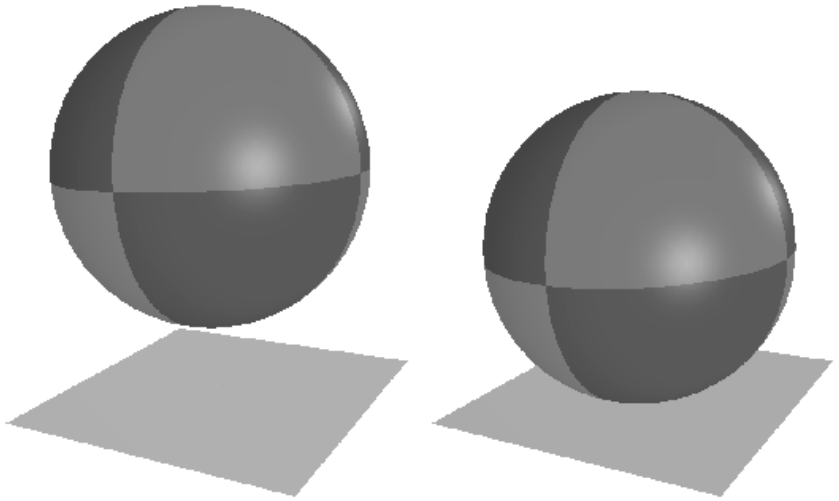
Numerical (non-physical) dissipation

* Cundall's non-viscous damping $\frac{(\Delta \mathrm{F})_{\mathrm{d}w}}{\mathrm{F}_w} = -\lambda_{\mathrm{d}} \operatorname{sgn}(\mathrm{F}_w \dot{\mathrm{u}}_w^{\ominus}), \quad w \in \{\mathrm{x}, \mathrm{y}, \mathrm{z}\}$

* viscous effects at contact (yes, again!)

Damping

$$\frac{(\Delta \mathbf{F})_{dw}}{\mathbf{F}_w} = -\lambda_d \, \mathrm{sgn}(\mathbf{F}_w \dot{\mathbf{u}}_w^{\ominus}), \quad w \in \{x, y, z\}$$



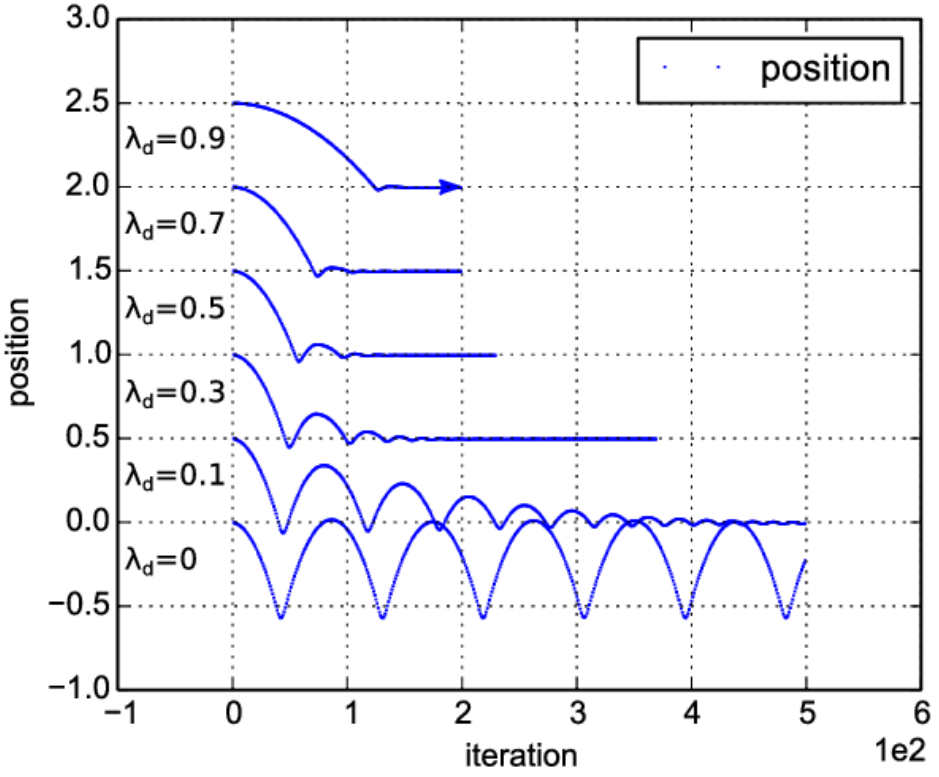


Figure 1.2 – A sphere bouncing on a plate with different values of non-viscous damping | `bouncing1`

Content

Element tests

How is DEM effectively used?

Vision 1: The conceptual model is particle-based

Model definition

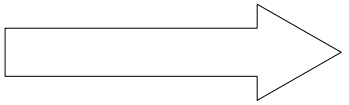
Particles
* shapes
* Particle Size Distribution
* Contact parameters

Packing
* porosity

Boundary conditions

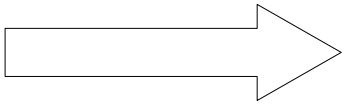
+ ***Static variables***
* *coordination*
* *initial distribution of forces*

Complex BVP



or

Element test



Result with complex boundary conditions
* rockfill,
* silos (e.g. A. Gladky, Yade-DEM),
* mixers (e.g. A. Gladky, Yade-DEM),
* …

Bulk behaviour in {σ,ε}
* elastic constants,
* friction coefficient,
* flow rule,
* ...

Element tests

How is DEM effectively used?

Vision 2: The conceptual model is continuous

Model definition

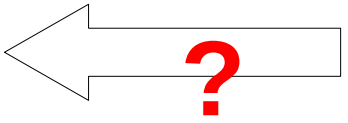
Particles
* shapes
* Particle Size Distribution
* Contact parameters

Packing
* porosity

Boundary conditions

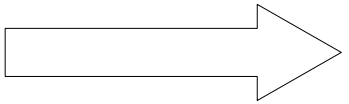
+ ***Static variables***
* *coordination*
* *initial distribution of forces*

Inverse problem



then

Complex BVP



Bulk behaviour in {σ,ε}
* elastic constants,
* friction coefficient,
* flow rule,
* ...

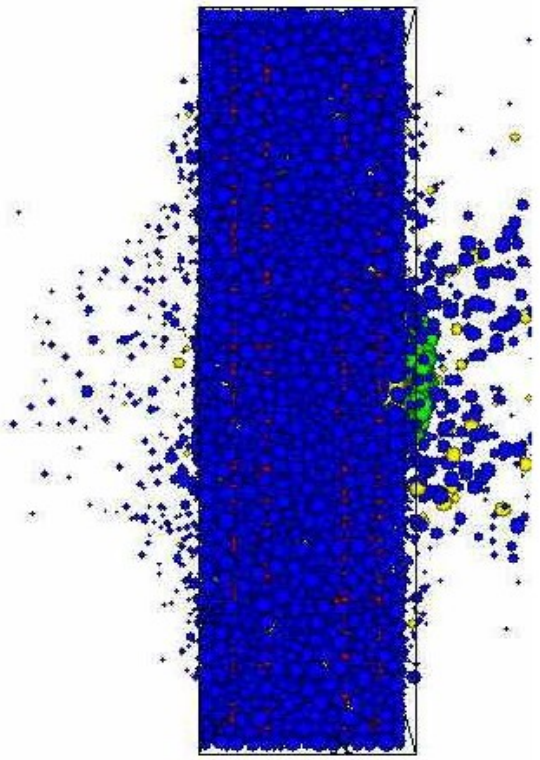
Result with complex boundary conditions
* structures (soil, rock, concrete),
* composite systems,
* fragmentation of blocks
* ...

Element tests

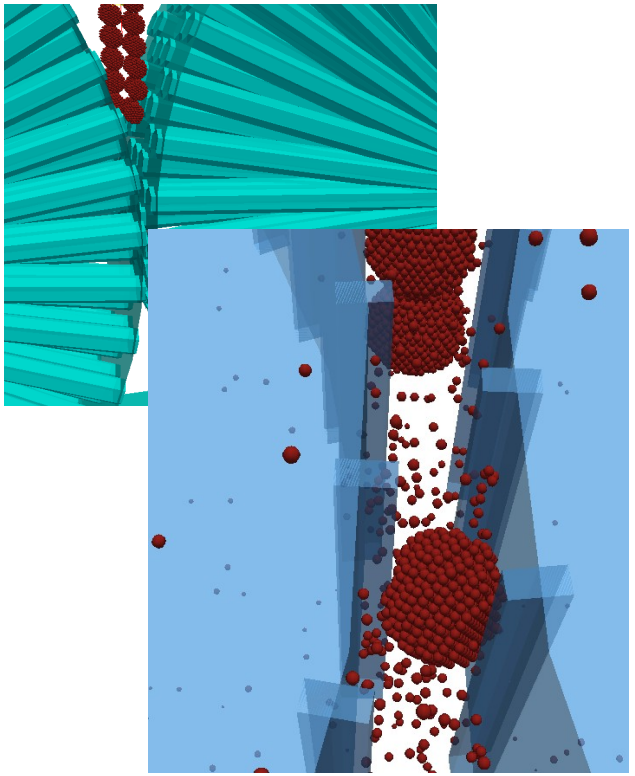
How is DEM effectively used?

Vision 2: The conceptual model is continuous

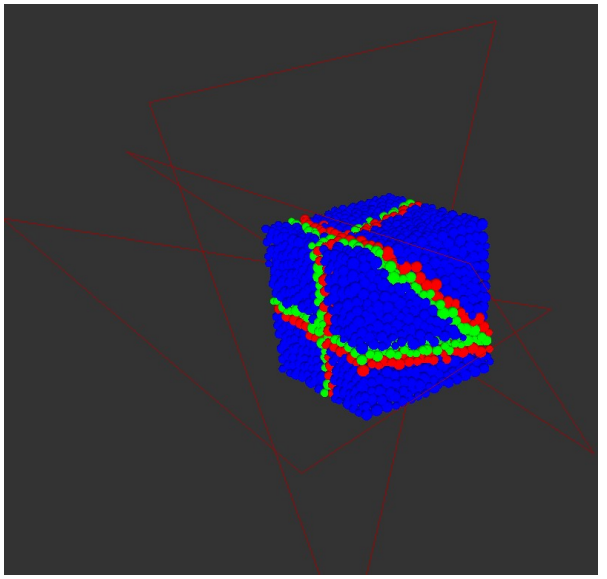
Missile impacts



Fragmentation



Fractured rock mass



Examples from Smilauer (2010a)

Element tests

How is DEM effectively used?

Vision 2: The conceptual model is continuous

Why DEM instead of classical continuous methods?

Advantages:

+ Fragmentation and/or creation of contacts
+ unlimited displacements
+ more or less realistic behaviour without defining explicitely all the parameters

Difficulties:

- scale effects
- inversion problem:

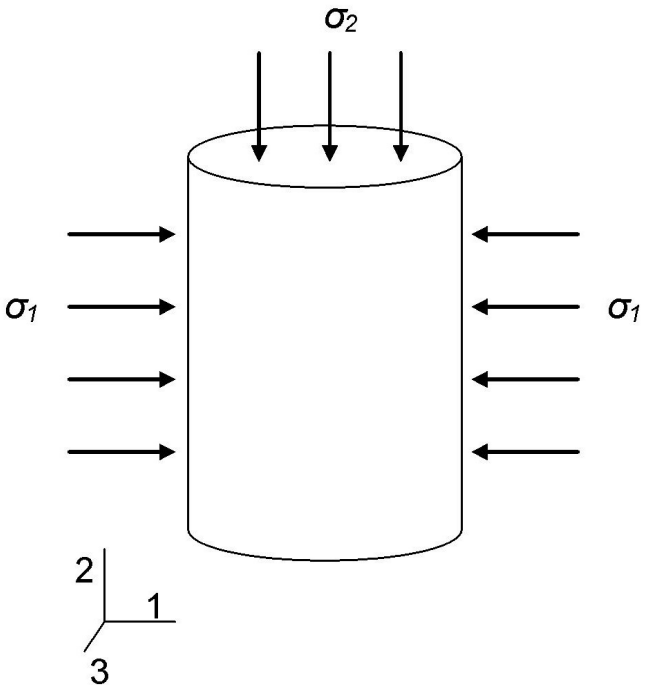
Q. *"I want to simulate a sand with f=30°, what contact friction should I use?"*

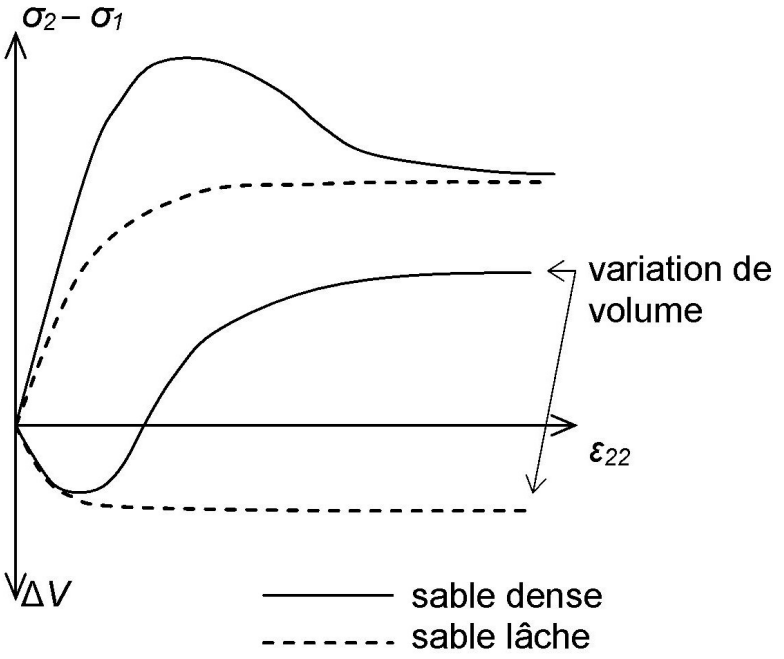
A. *"No clue. Let you start trial and error, through* ***element testing****."*

Examples from Smilauer (2010a)

Element tests

In both visions, the simulations of element tests appear as key point





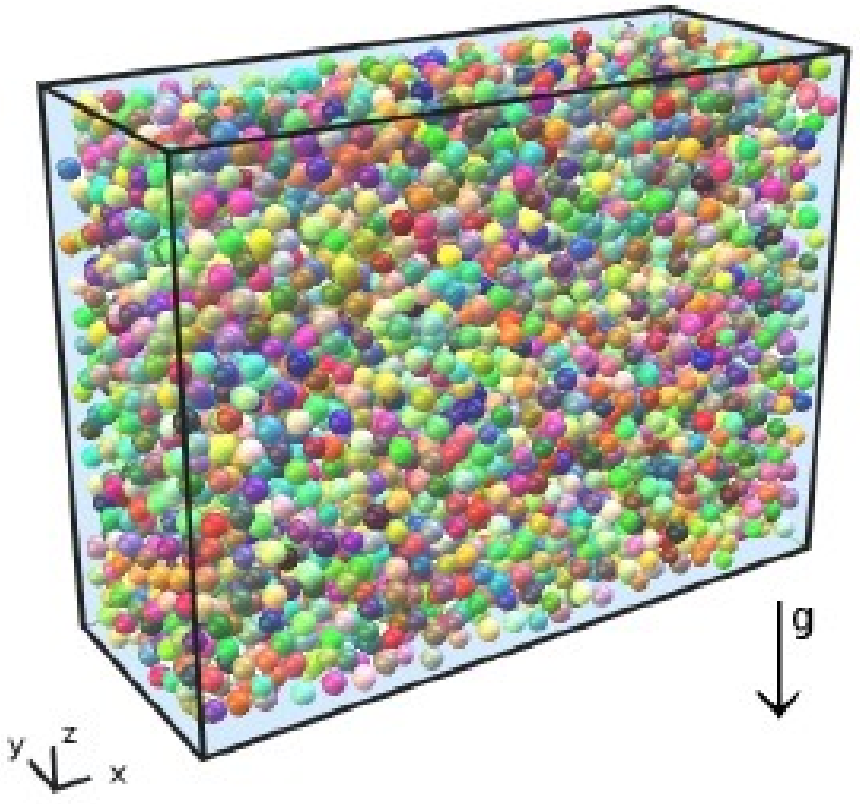
Element tests

1. Generate a (random) packing

2. Define and simulate a loading path

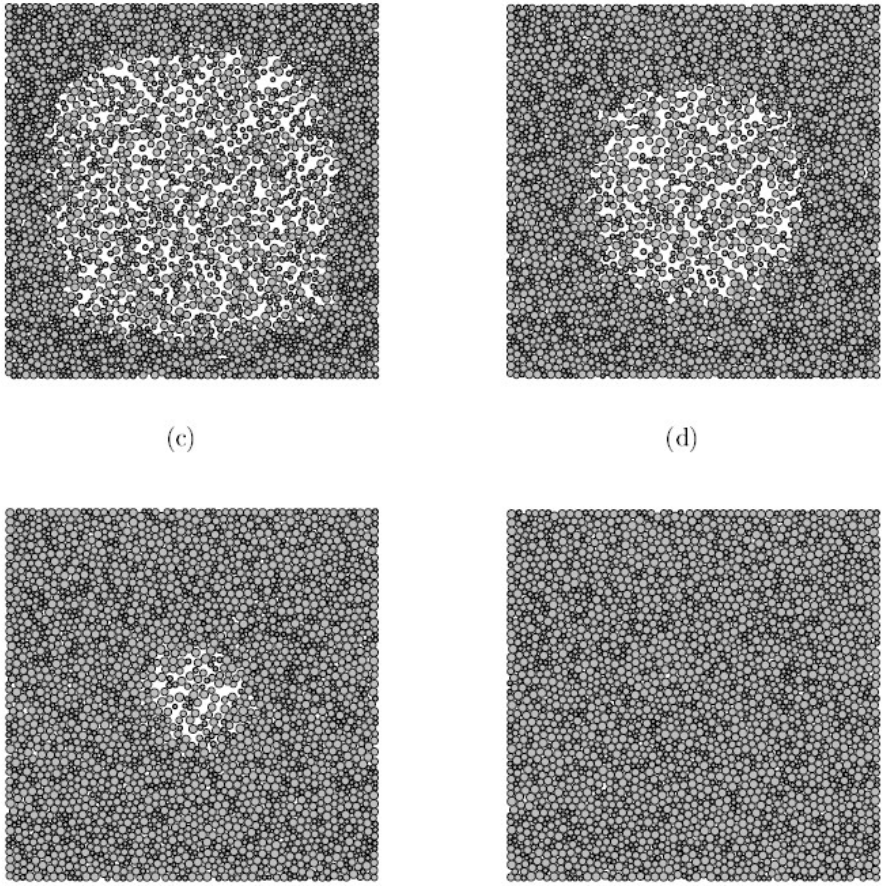
3. Analyze the results to get meaningful macro-scale quantities

Packing generation: deposition



Packing generation: compaction

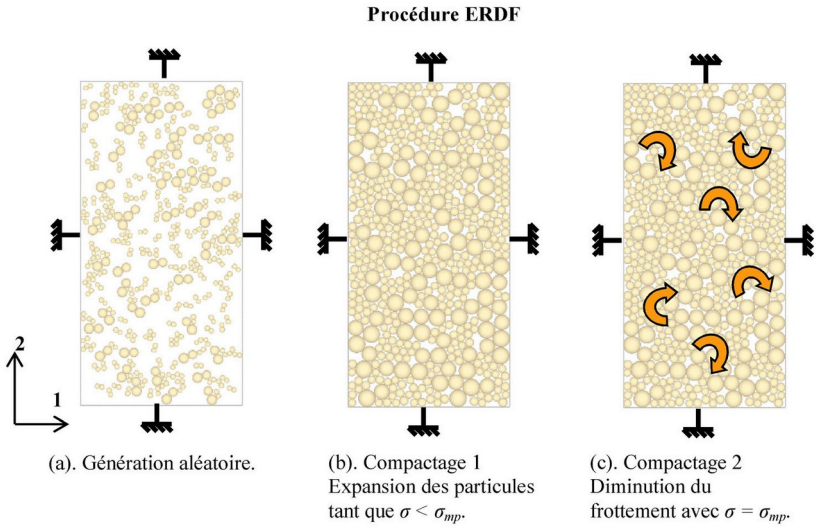
From the outside...

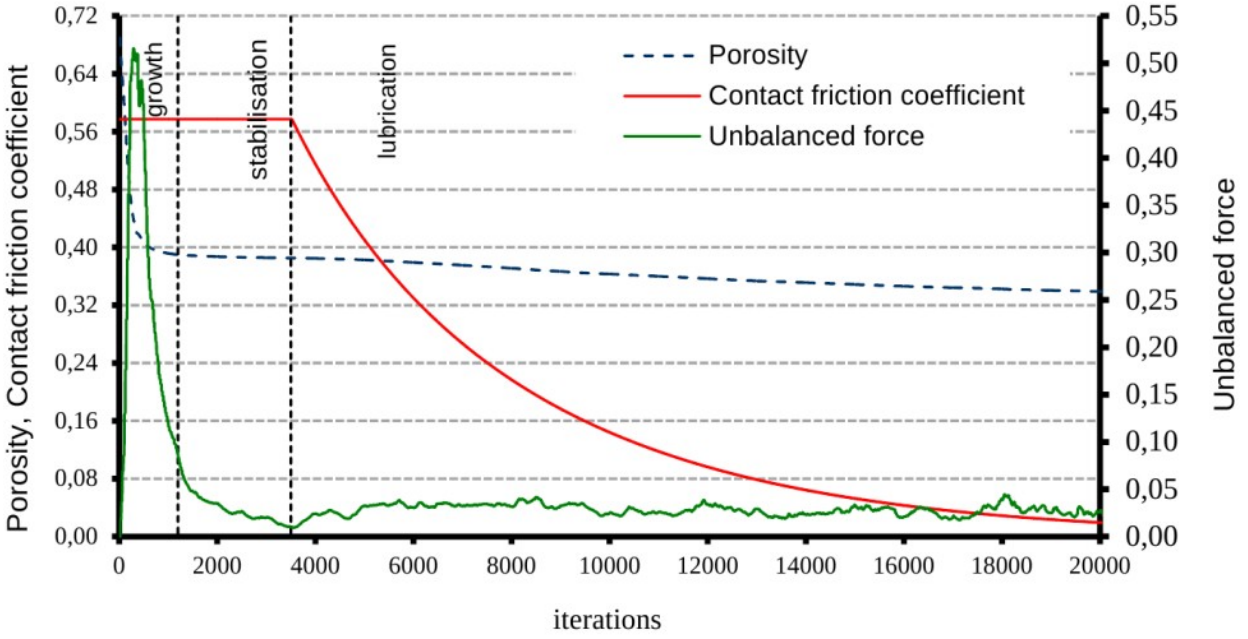


Source: Combe G., PhD Dissertation

Packing generation: compaction

… or from the inside (particles growth)

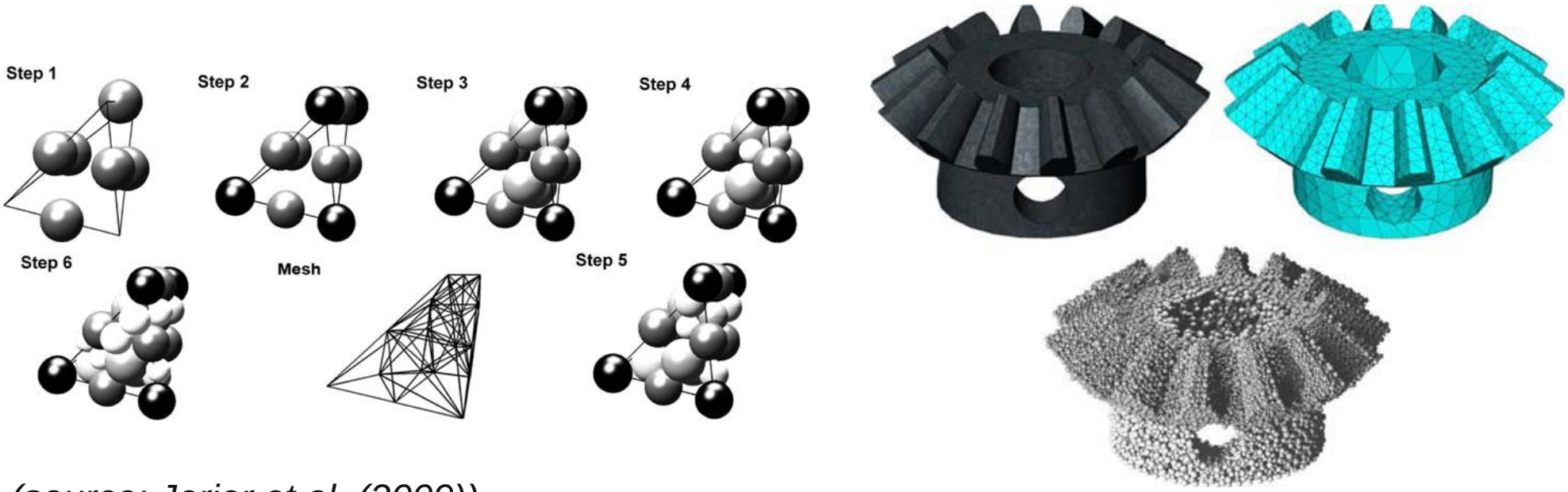




(Source: Tong et al., 2012)

Packing generation: geometric algorithms

* Example in Jerier et al. (2009) using tetrahedral mesh
* Many other algorithms, see for instance Bagi (2005)



(source: Jerier et al. (2009))

Packing generation: compaction

	Speed	Control PSD + porosity	Isotropic	Stable force network
Deposition	--	- / +	-	+
Geometric	+	-	+	-
Dynamic compaction	-	+	+	+

Loading path

Boundary conditions

Homogeneous conditions:

$$\mathbf{T} = \sigma\, \mathbf{n},$$

or

$$\mathbf{u} = \varepsilon\, \mathbf{x},$$

or combinations of the above.

Loading path

Boundary conditions

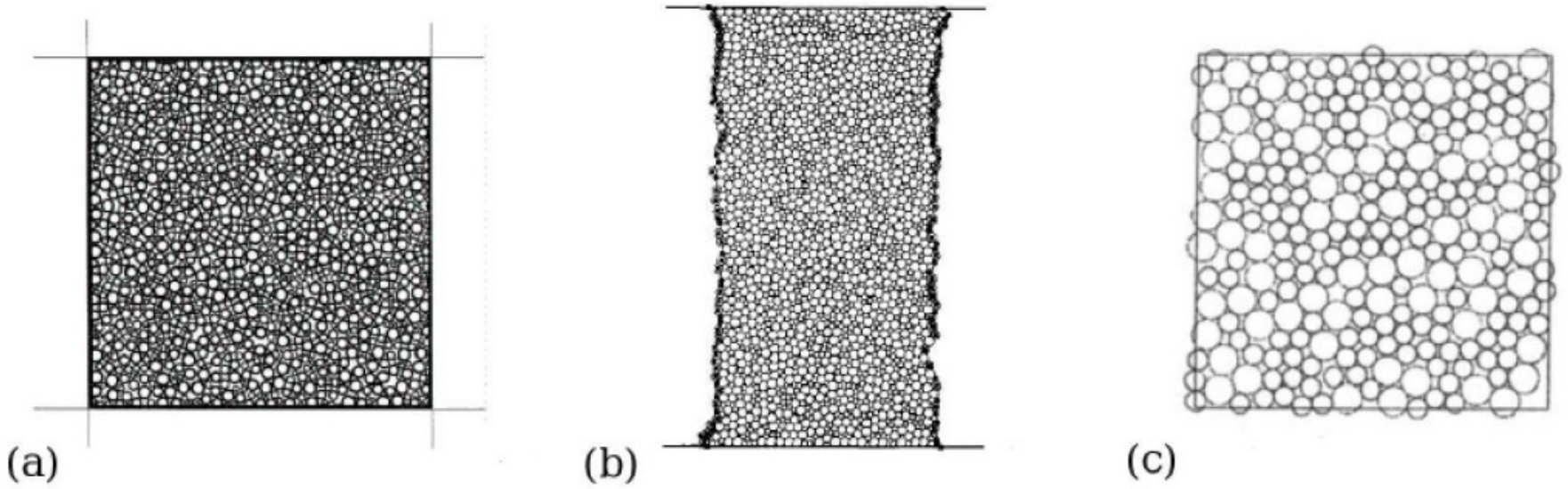


Figure 2.5: Types of boundary conditions: (a) rigid walls (b) flexible (c) periodic. [23]

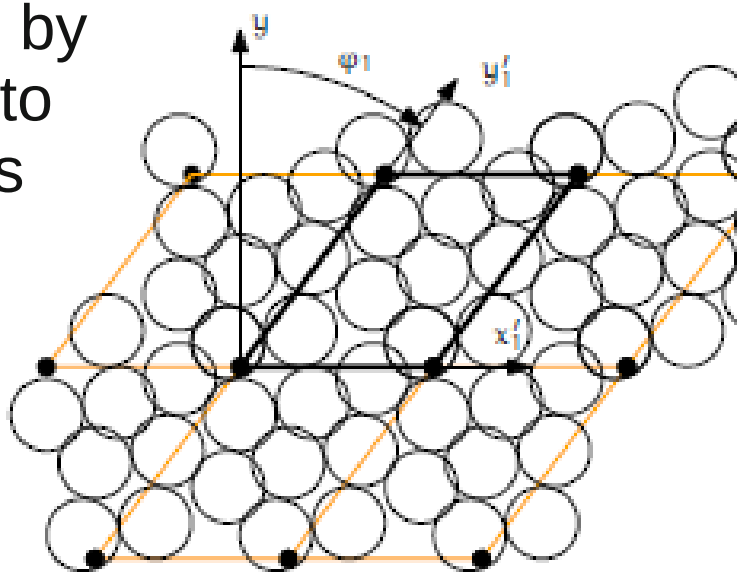
Loading path

Rigid walls:

* imposing displacement is straightforward
* imposing stress can be done with a dynamic method or by servo-control (more efficient)

Periodic boundary conditions (no boundaries!):

* stress and strains are controlled by deforming the period
* inhomogeneous effects are avoided by applying the same velocity gradient to the period and the particles positions



Loading path

Classical paths

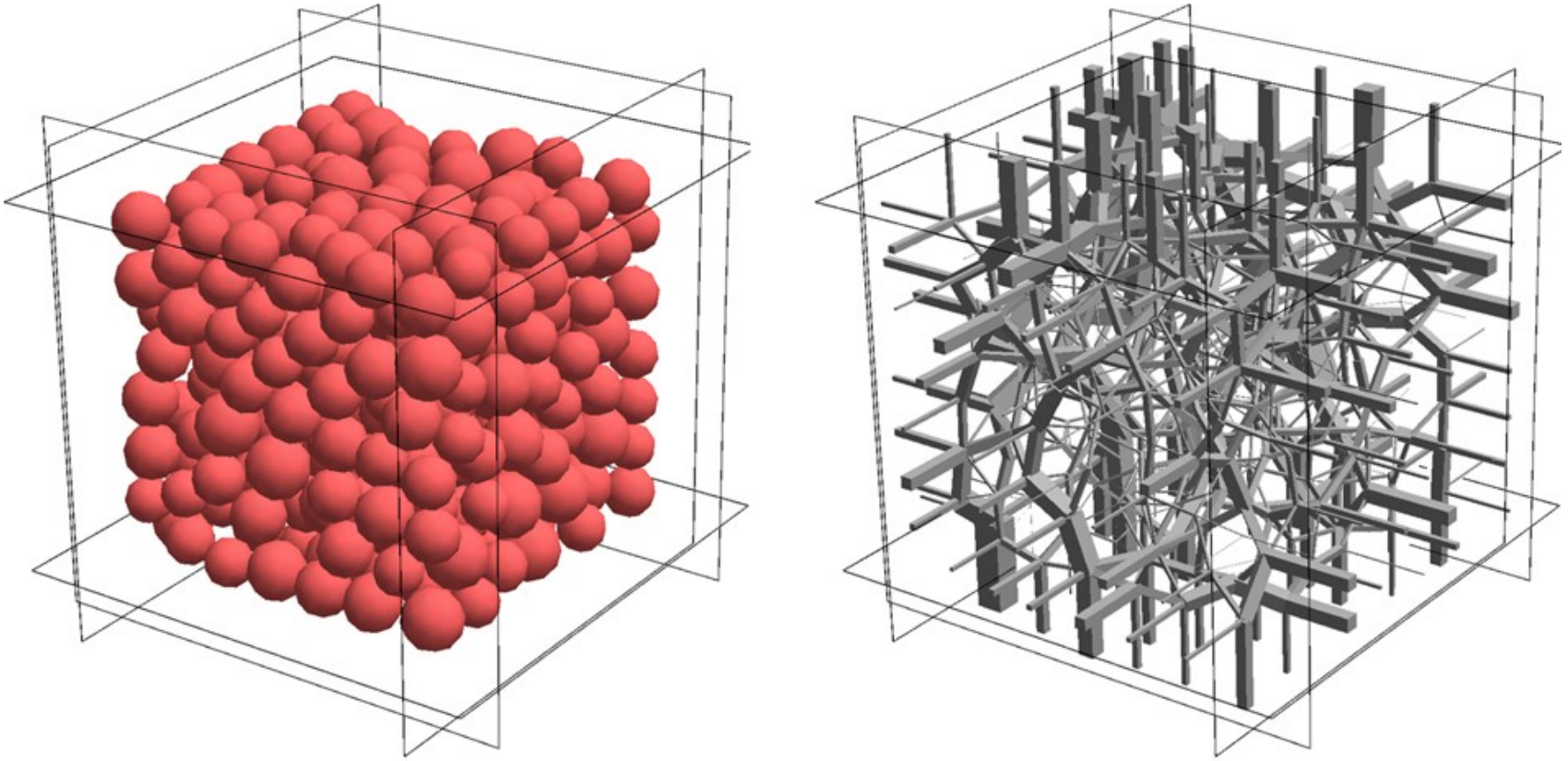
Triaxial compression
* The most classical test on soils

Simple shear
* Inspired by Couette flow. Mostly used with periodic boundary conditions (3-periodic or 2-periodic for very large shear)
* Introduces more complexity (hence harder analysis) due to non-coaxiality

Live examples with Yade

Post-processing

A. $\{\sigma,\varepsilon\}$ can be deduced simply by forces and displacements at the boundaries when rigid walls are used.

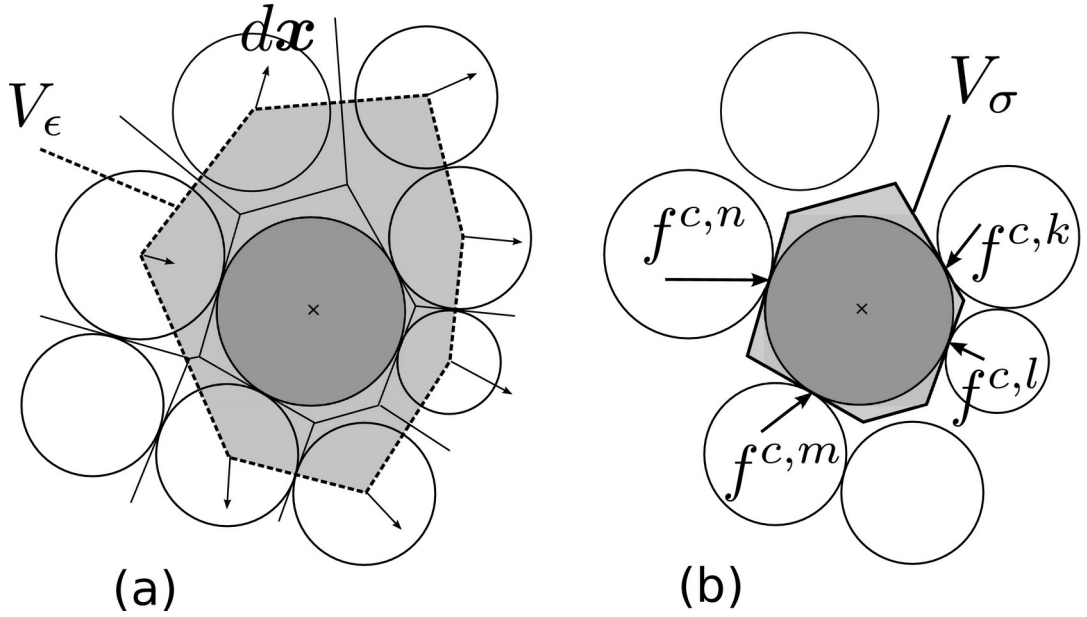


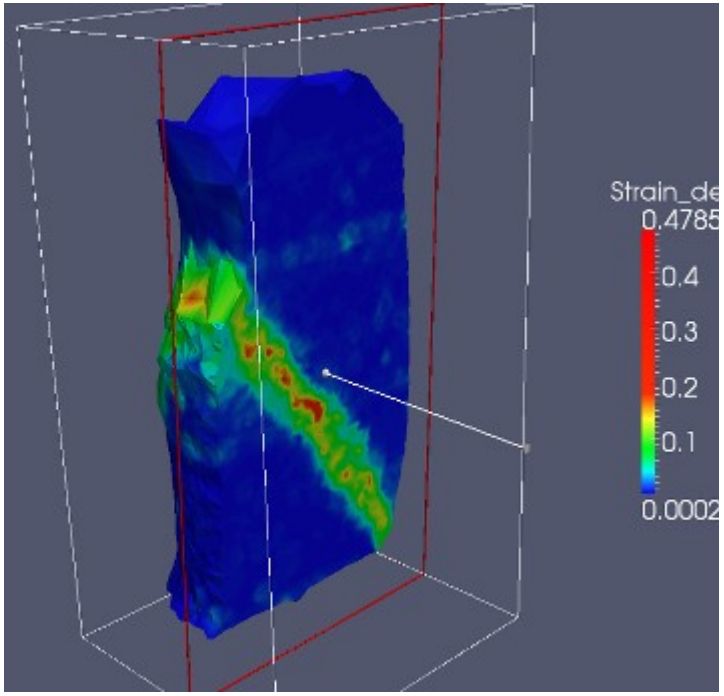
Post-processing

B. {σ,ε} can be defined from internal kinematic and static variables. Averaging the microscale definitions gives the same tensors as that defined at the boundaries (A). They also serve for analyzing heterogeneous disp./stress fields (e.g. shear banding)

$$< \nabla \mathbf{dX} >= \frac{1}{V_\varepsilon} \int_{V_\varepsilon} \nabla \mathbf{dX} dv = \frac{1}{V_\varepsilon} \int_{\partial V_\varepsilon} \mathbf{dX} \otimes \mathbf{n} ds$$

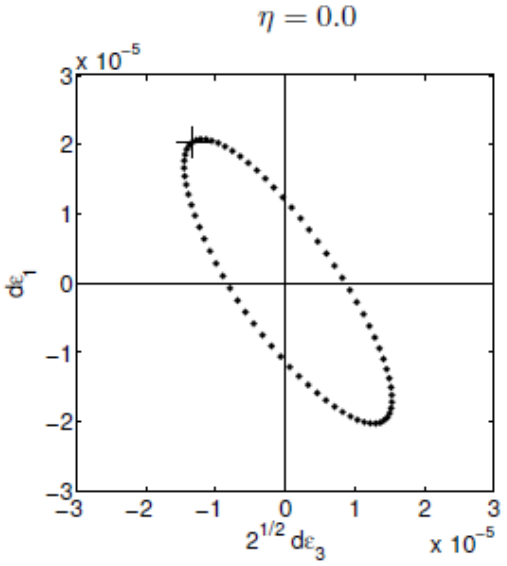
$$\overline{\sigma} = \frac{1}{V_\sigma} \sum_k \mathbf{x}^k \otimes \mathbf{f}^{c,k}$$

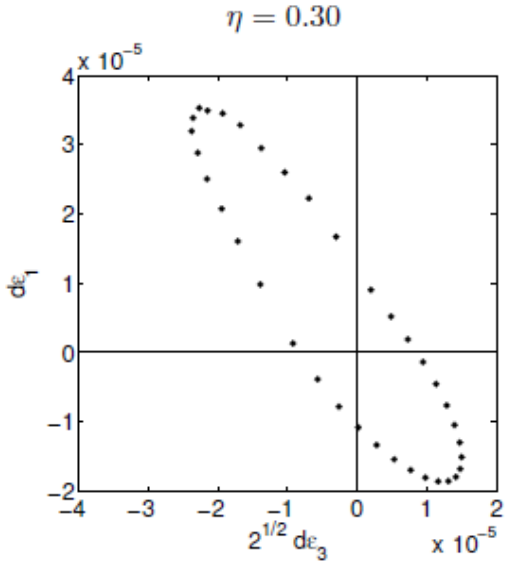


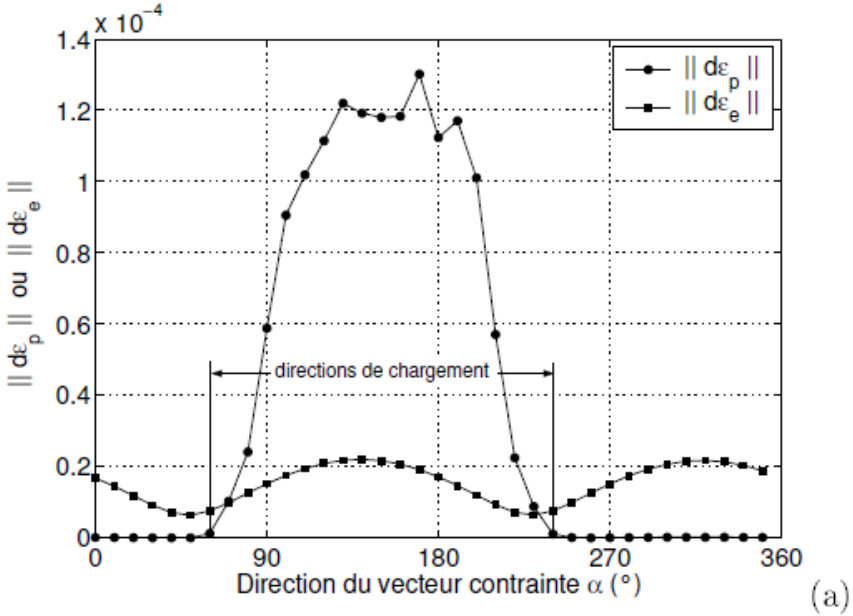


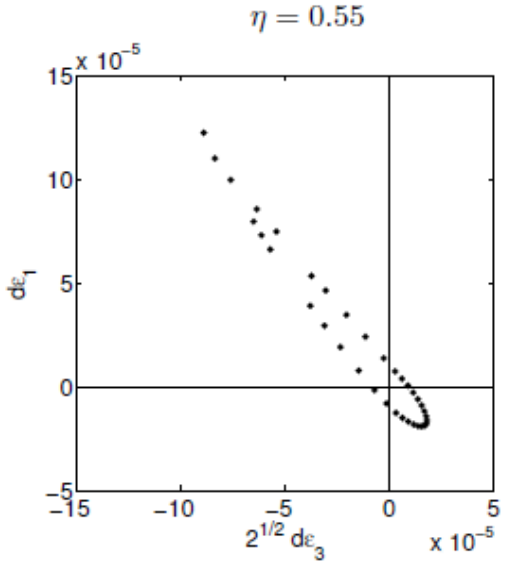
Source: Yade DEM, from E. Ando experiments

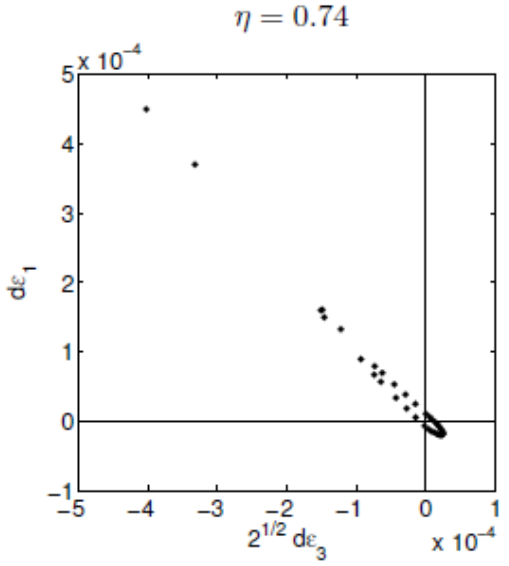
Advanced stress-strain probing

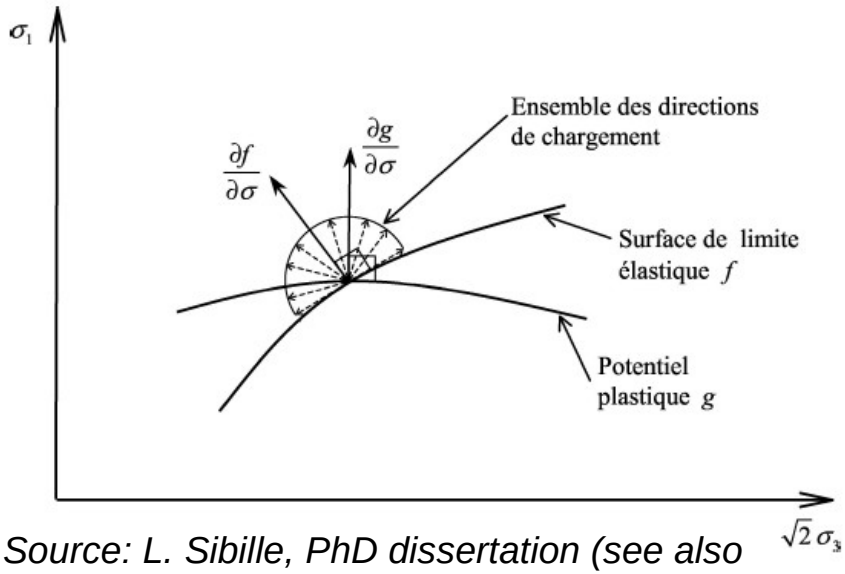










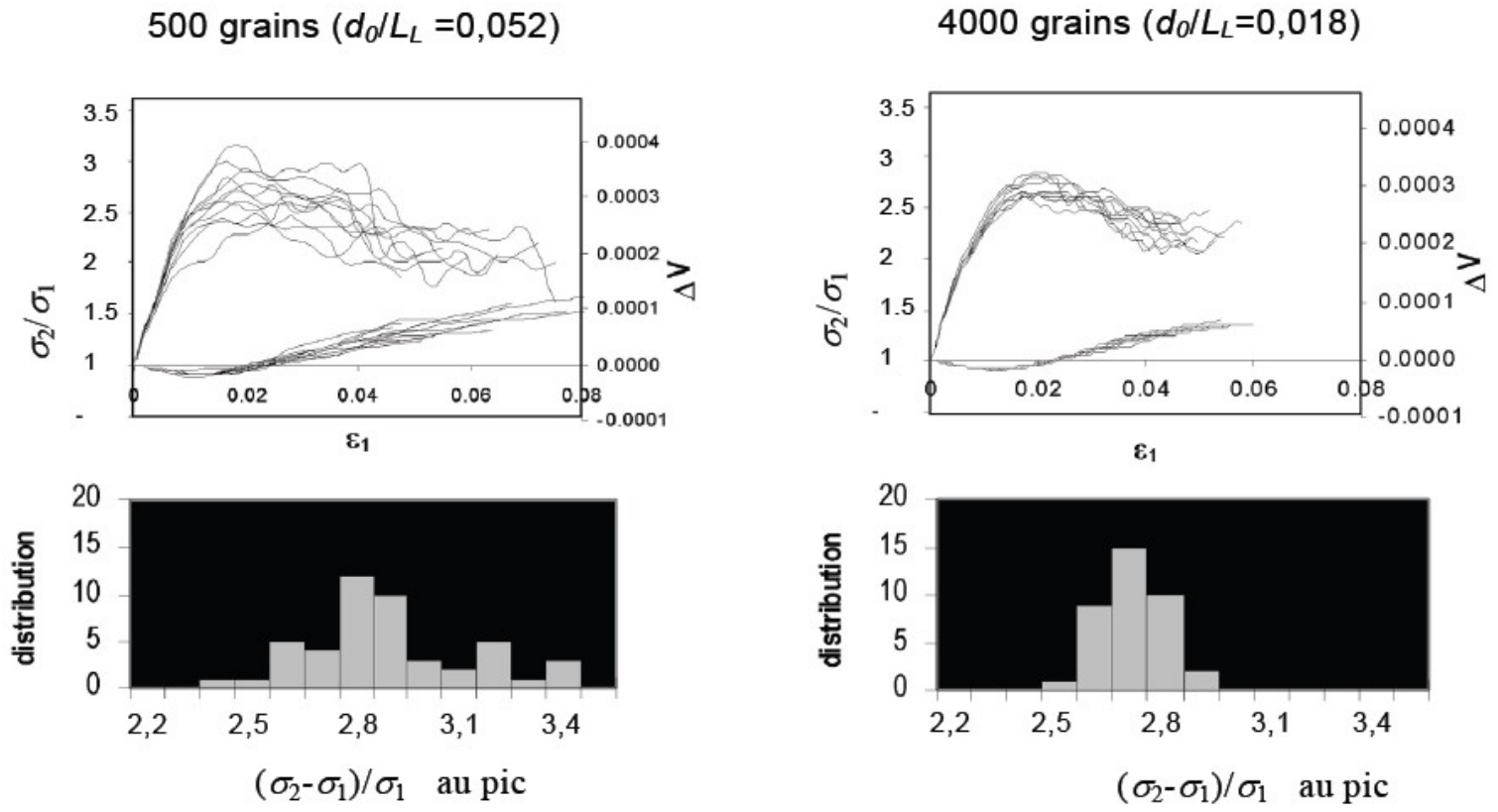


Source: L. Sibille, PhD dissertation (see also other papers from same author, e.g. Nicot et al. 2007)

Caveats

Variability, "*Representative Element Volume*", and the extreme sensitivity to initial conditions (butterfly effect)

* classical values: N>1k (2D) or N>10k (3D)
* variability is inherent (e.g. single thread vs. multithread)

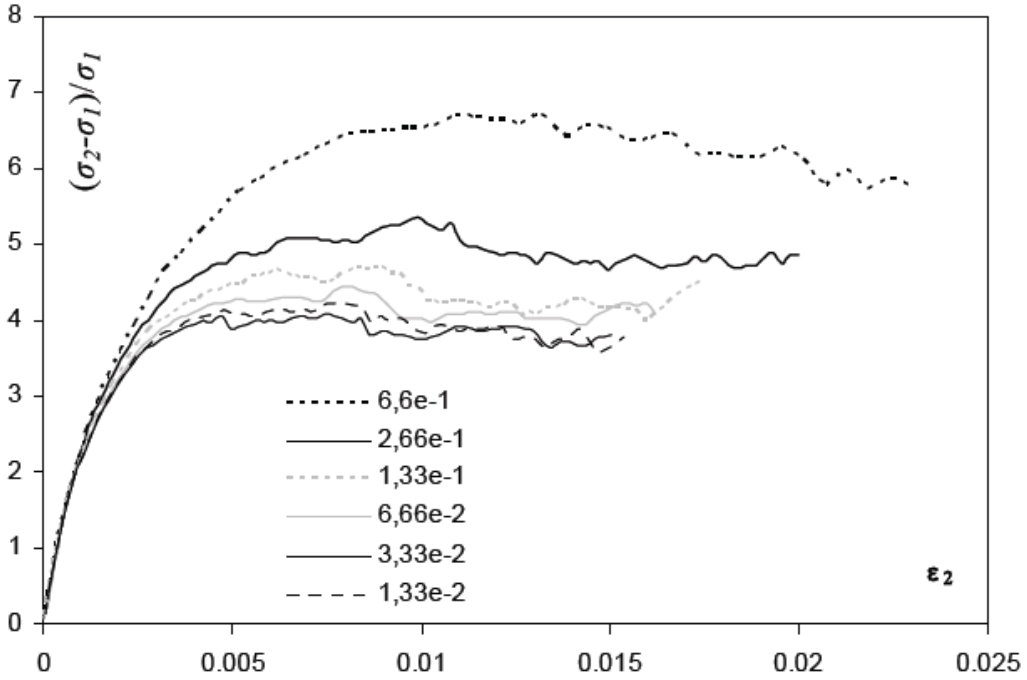


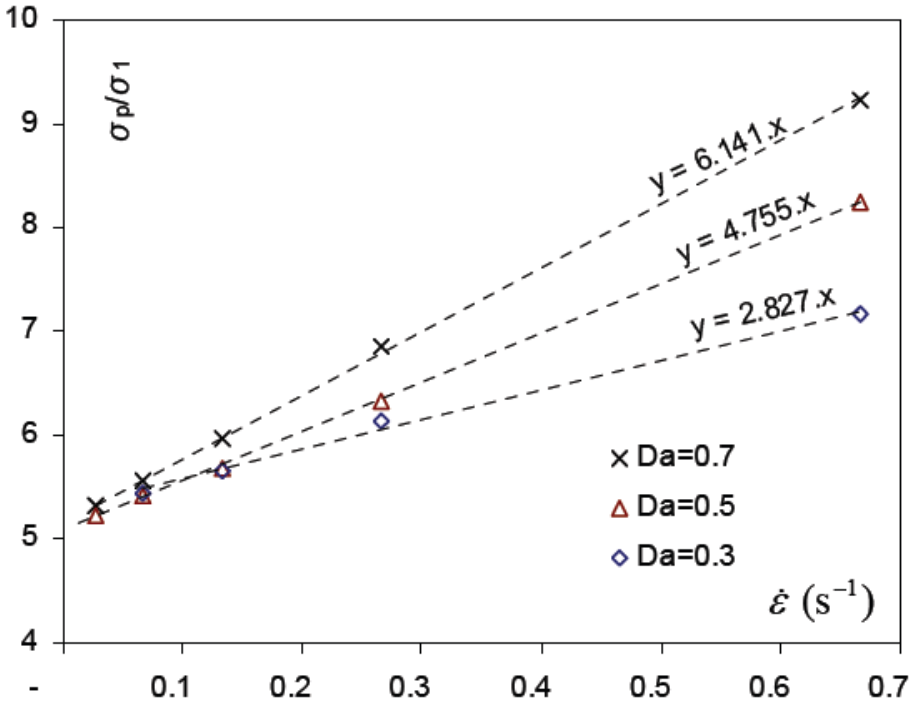
Source: Chareyre B., PhD Dissertation

Caveats

Quasistaticity

Strict quasistaticity is never found in granular soils (experimentaly nor numericaly). Of real interest is the impact of strain rate on the results. In most cases, authors refer to “quasistaticity” in this later sense.



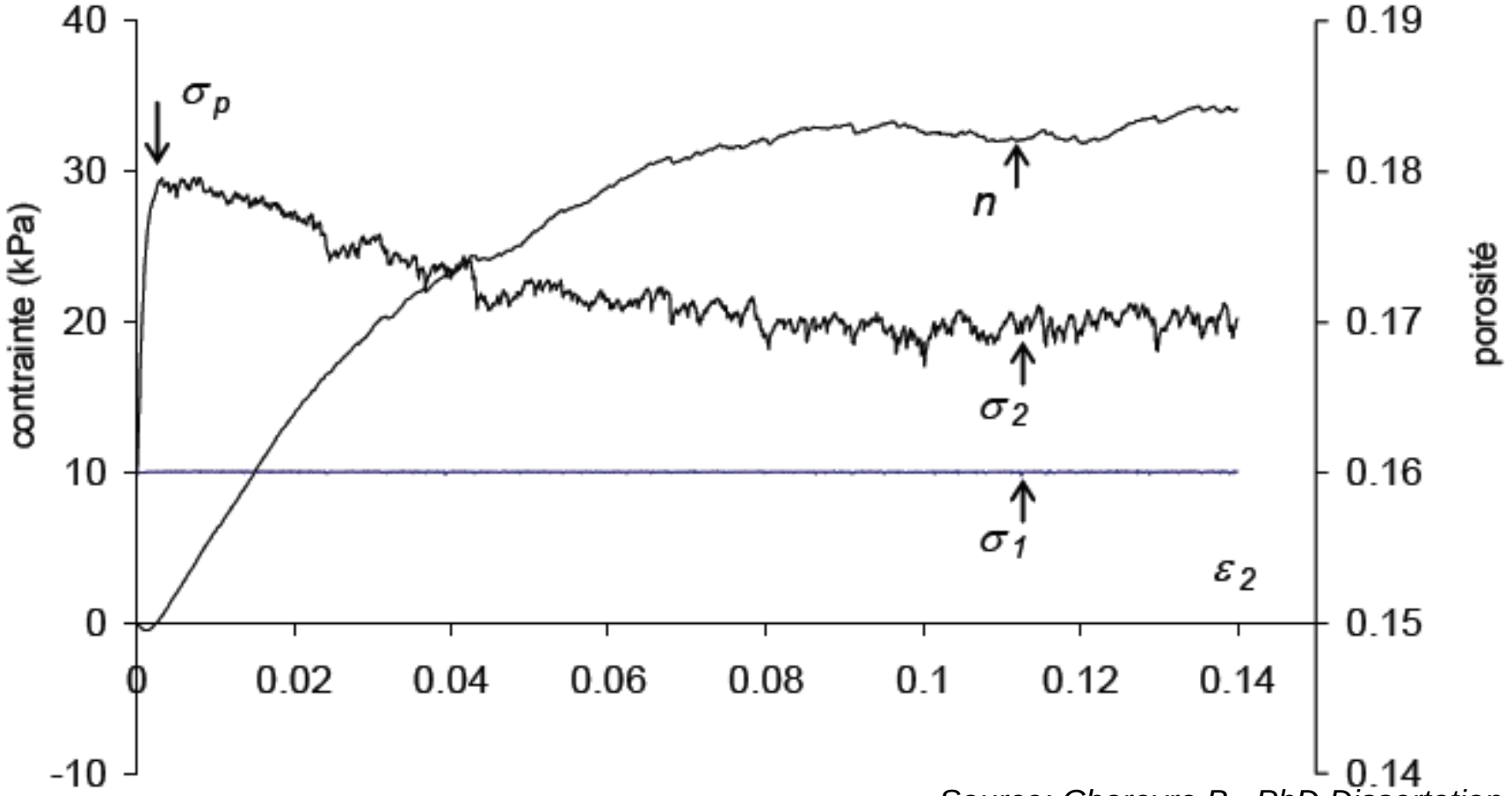


Source: Chareyre B., PhD Dissertation

Content

Classical results (elastic-frictional model)

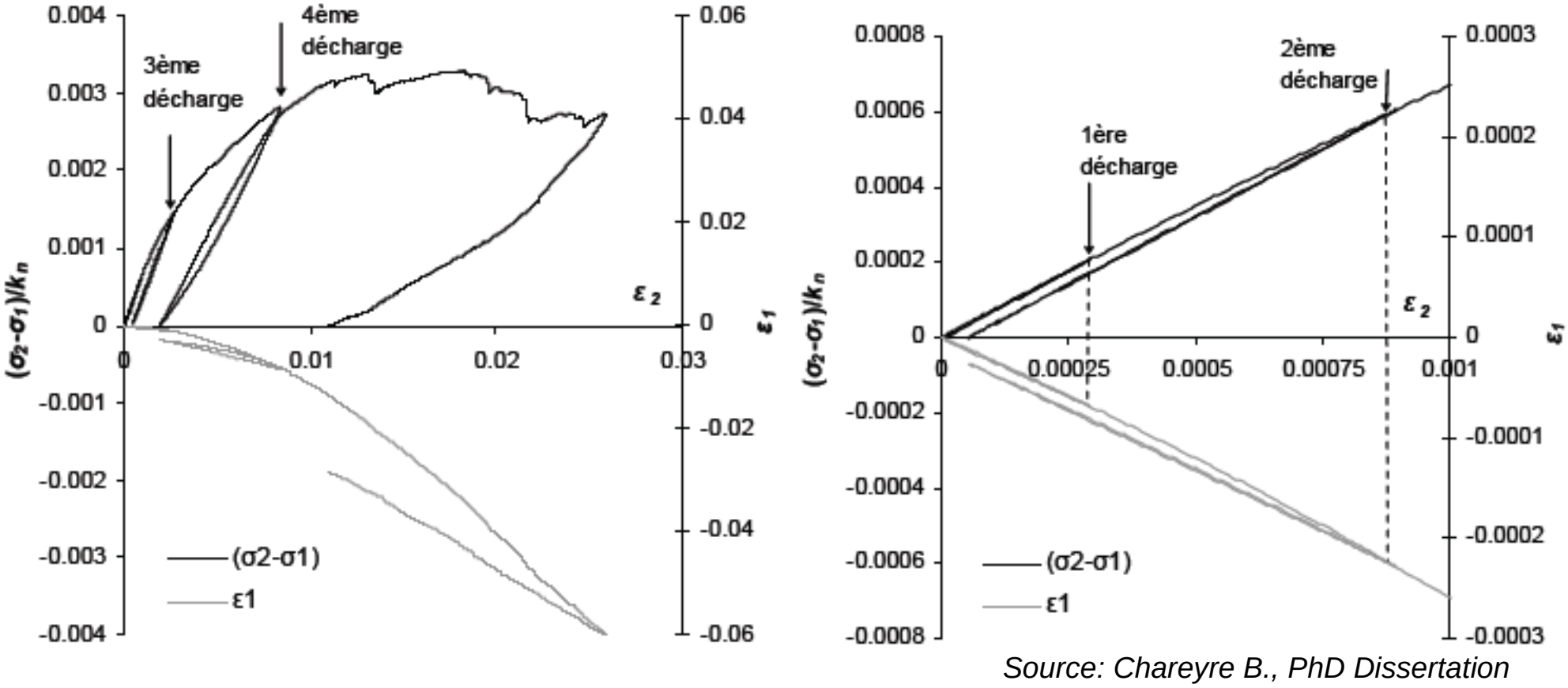
Qualitatively similar to experimental behavior of sands, but the shear strength of spheres is generally lower (typically, ϕ=18° at the critical state)



Source: Chareyre B., PhD Dissertation

Classical results (elastic-frictional model)

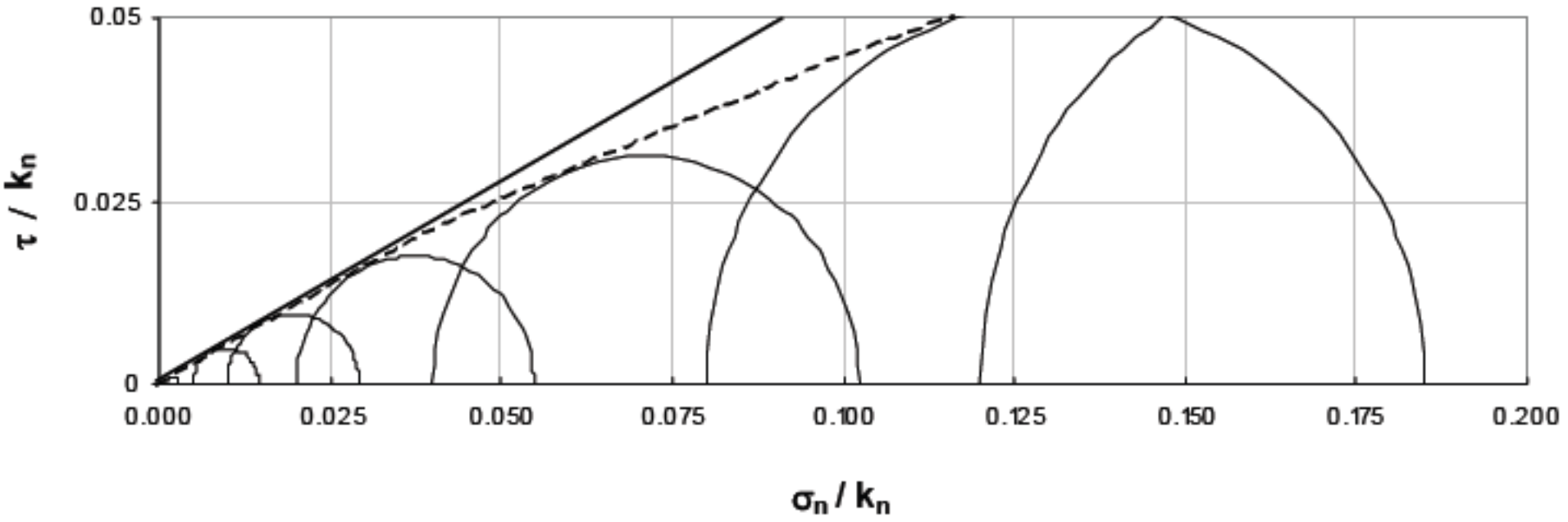
A quasi-elastic domain can be identified with linear elastic contact laws



Source: Chareyre B., PhD Dissertation

Classical results (elastic-frictional model)

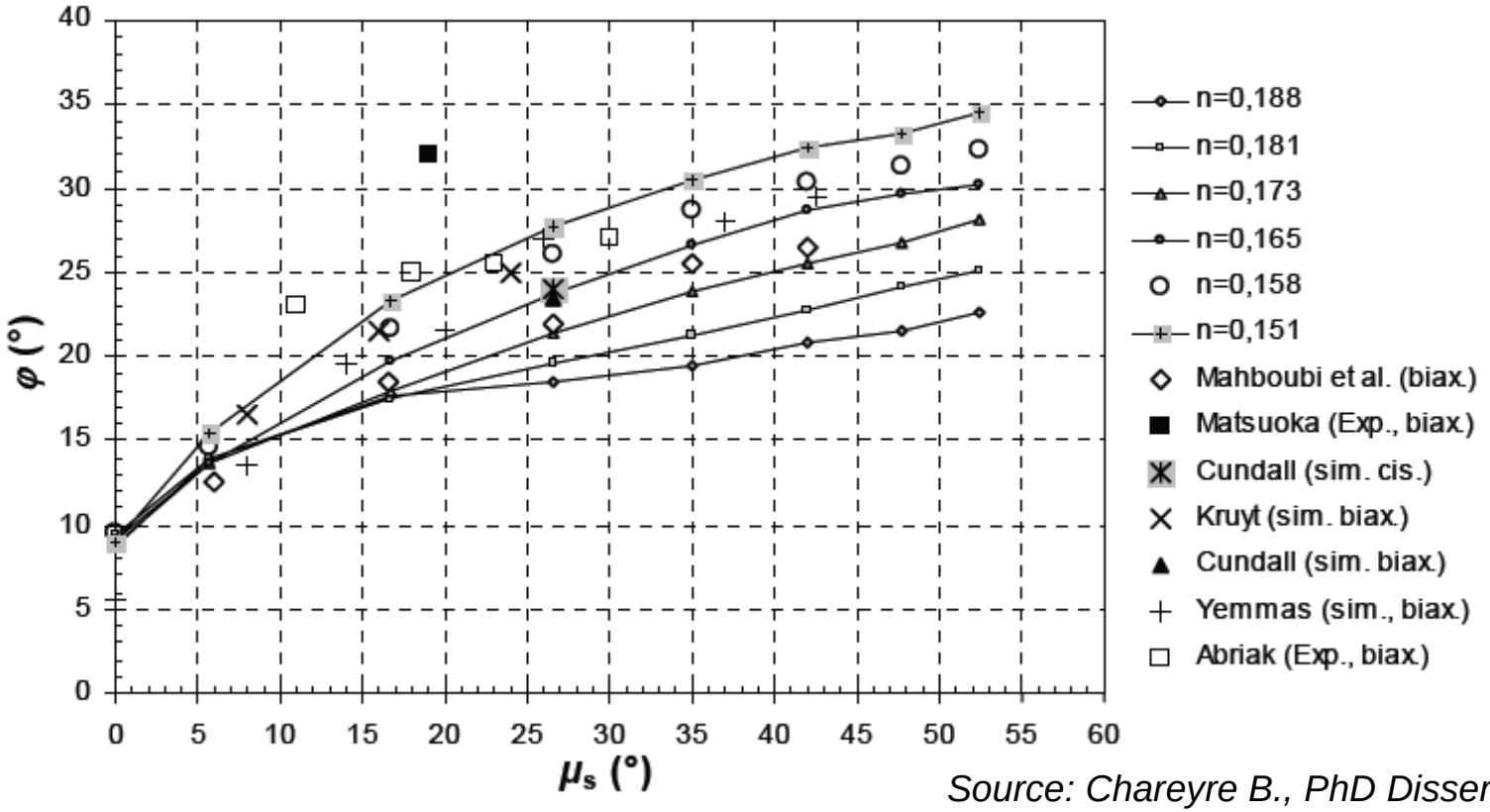
Coulomb friction rules the bulk behavior for elastic-plastic contacts as long as $\sigma/E < 100$



Source: Chareyre B., PhD Dissertation

Classical results (elastic-frictional model)

* The relation between peak friction and contact friction is highly non-linear.
* More contact friction induces more dilantancy
* Residual friction is almost constant (and very low)
* Realistic bulk friction is obtained at the price of <u>complex shapes or moments at contact</u>

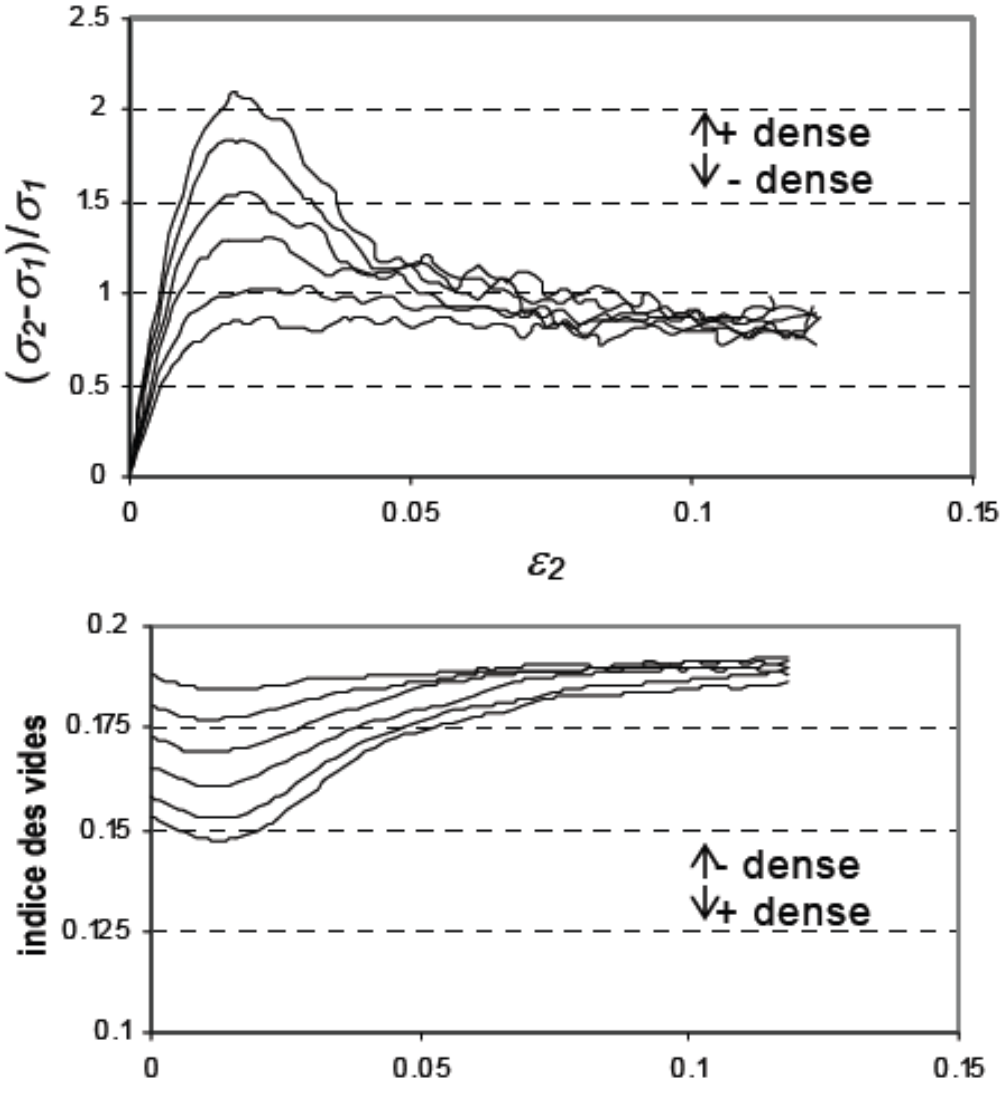


Source: Chareyre B., PhD Dissertation

Classical results (elastic-frictional model)

A critical state is observed, with a unique asymptotic behavior at large strain

Approximately $\varepsilon > 10\%$ in 2D, $\varepsilon > 20\%$ in 3D



Source: Chareyre B., PhD Dissertation