



Discrete Element Methods for the simulation of divided media.

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DEM::Preamble

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DEM::Preamble

Many solid materials and structures are made of **components** in **interaction**:

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- Dry granular material (divided media)



- ▶ **component**: grain, cluster of grain, piece of grain, coarse grain, etc.
- ▶ **interaction**: unilateral contact, elasticity or/and cohesion, friction, etc.

DEM::Preamble

Many solid materials and structures are made of **components** in **interaction** :

- Masonry structures (divided structure)

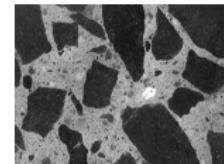
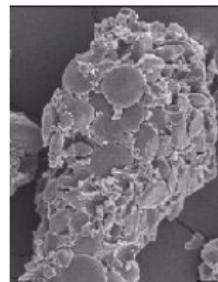


- ▶ **component**: brick, stone, mortar, mortar grain.
- ▶ **interaction**: unilateral contact, friction, cohesion, etc.

DEM::Preamble

Many solid materials and structures are made of **components** in **interaction** :

- solid grains in a solid matrix (composites, etc) and/or in a fluid matrix (colloids, concrete, etc)



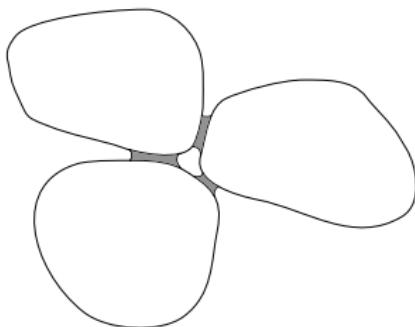
idem as before but a solid or fluid matrix should be concerned.

DEM::Preamble

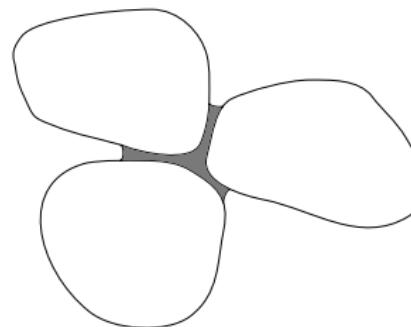
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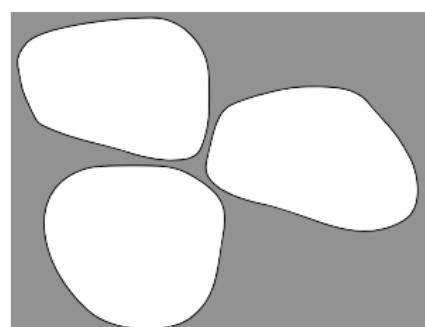
various situations



“binary interaction”
pendular regime



“multiple interaction”
funicular regime



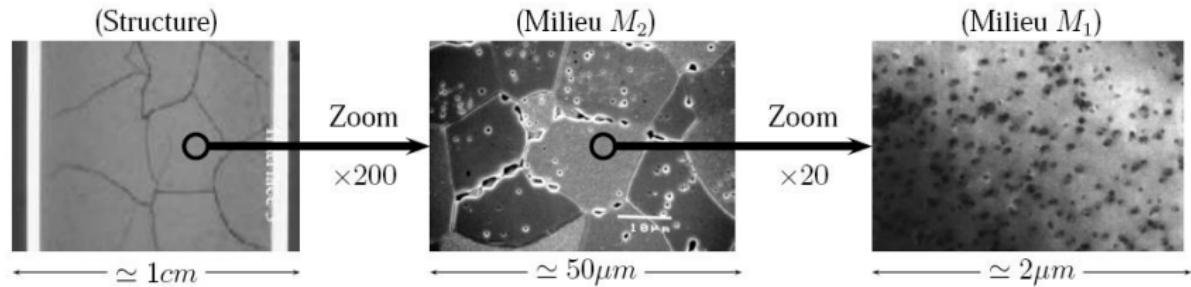
“composite - continuous”
saturated

All the situations can't be addressed easily by DEMs.

DEM::Preamble

Many solid materials and structures are essentially discontinuous or divided:

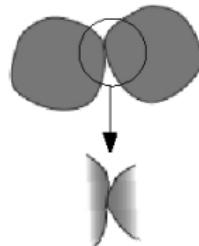
- changing the scale a continuous media may become discontinuous



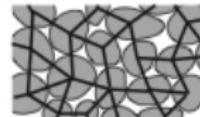
- ▶ **component**: metal grain, crystal in a poly-crystal, molecules, atoms;
- ▶ **interaction**: grain bond, defects, Wan der Waals effects, Lenhard-Jones potentials, atomic bonds, etc.

DEM::Preamble

Considering **divided media** it exists various space scales :



microscopic



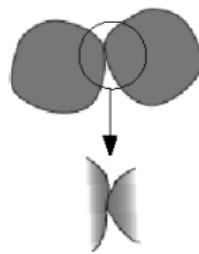
mesoscopic



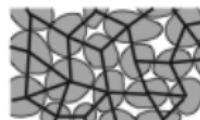
macroscopic

DEM::Preamble

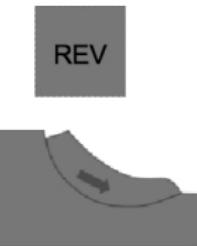
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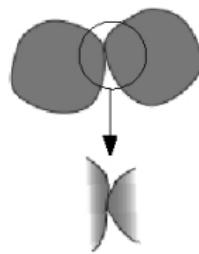
macroscopic

Behavior depends on :

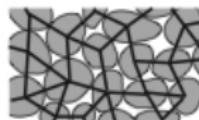
- composition: shape (angularity, elongation, etc), dispersity
- state: dense-loose, confining pressure, dry-wet-composite
- load: static-dynamic

DEM::Preamble

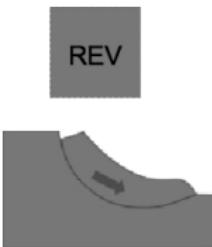
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microscopic



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macroscopic

Behavior depends on :

- composition: shape (angularity, elongation, etc), dispersity
- state: dense-loose, confining pressure, dry-wet-composite
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Depending on the solicitation it may behave like: a solid, a liquid or a gas



DEM::Preamble

It exists numerous methods to model these kind of media and structures.

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At the **macroscopic scale** the divided media is considered as continuous.

It is possible to use various discretization :

- classical methods (Finite Difference, Finite Element Method, Finite Volume Method, etc)
- dedicated methods (Thin Layer Model, Spreading-based model, etc)

it **needs an ad-hoc rheological model** to represent the complex behavior of the media (elasticity, plasticity, visco-plasticity with threshold, fracture, etc).

Advantages: cheap

Drawbacks: building a model with the relevant phenomenological parameters and identifying the parameters. Stiff transitions can't be represented.

DEM::Preamble

It exists numerous methods to model these kind of media and structures.

At the **microscopic or mesoscopic scale**, methods rely on a modeling of :

- the behavior of each component
- the behavior of the interactions of each component with its neighborhood

A lot of methods aim to model divided media (and/or structures) at the component and interaction scale: Cellular Automata, SPH, Lattice Element methods, Discontinuous Deformation Analysis (DDA), etc and **Discrete Element Methods (DEM)**.

Advantages: simpler model, less parameters, easier to identify

Drawback: computational cost.

DEM::Preamble

One can also consider DEMs to model fictitious divided media as in:

- coarse grain approach,
- domain decomposition approach.

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DEM can be mixed with continuous methods to model, for example, the transition between a continuous and a divided media :

- fragmentation of a media,
- wear,
- powder compaction to obtain ceramics.

DEM::Modeling

1 Preamble

2 Modeling

- Smooth Dynamic
- Non Smooth Dynamic
- Conclusion

3 Numerical Strategies

4 NSCD Extensions

5 Multi-Physics

6 Technical Aspects

7 Bibliography



DEM::Modeling::Smooth Dynamic::Equations of motion

Assuming a smooth evolution of the system allows to describe the motion of each mechanical component by a semi-discretized in space system:

$$\mathbb{M}(q, t)\dot{V} = F_{ext}(t) + F_{int}(q, V; t) + R \quad (1)$$

where

- $q \in \mathbb{R}^n$ represents the vector of generalized degrees of freedom,
- $V \in \mathbb{R}^n$ the generalized velocities,
- $R \in \mathbb{R}^n$ the resultant of contact forces,
- $F_{ext}(t)$ the external loads,
- $F_{int}(q, V; t)$ the internal force (deformable bodies) and the nonlinear inertia terms (centrifugal and gyroscopic),
- $\mathbb{M}(q, t) : \mathbb{R}^n \mapsto \mathcal{M}^{n \times n}$ the mass (inertia) matrix.

Initial and boundary conditions must be added to fully describe the evolution of the system.

▶ details

DEM::Modeling::Smooth Dynamic::Equations of motion

Considering a rigid component, a more suitable dynamics equation may be used introducing v the translation and ω the rotational velocities of the center of mass.

The Eq.(1) is replaced by the well-known Newton-Euler system of equations:

$$\begin{cases} \mathbb{M}_R \dot{v} &= \mathbf{F}_{ext}(t) + \mathbf{R} \\ \mathbb{J}_R(\mathbf{q}) \dot{\omega} &= \mathbf{M}_{ext}(t) + \mathbf{M} \end{cases}$$

where

- $\mathbf{F}_{ext}(t)$ and \mathbf{R} represent respectively the resultant of external and contact forces,
- $\mathbf{M}_{ext}(t)$ and \mathbf{M} represent respectively the momentum due to external and contact forces,
- \mathbb{M}_R and $\mathbb{J}_R(\mathbf{q})$ represents respectively the mass and the inertia matrices.

DEM::Modeling::Smooth Dynamic::Equations of motion

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The Eq.(1) is replaced by the well-known Newton-Euler system of equations with respect to a coordinate frame whose origin coincides with the body's center of mass (C):

$$\begin{cases} \mathbb{M}_R \ddot{v} &= \mathbf{F}_{ext}(t) + \mathbf{R} \\ \mathbb{J}_R \ddot{\omega} &= -\omega \wedge (\mathbb{J}_R \omega) + \mathbf{M}_{ext}(t) + \mathbf{M} \end{cases}$$

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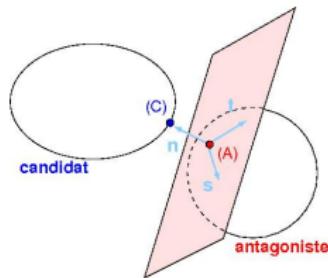
Note that for 2D components or 3D components with geometric isotropy, the vector $\omega \wedge (\mathbb{J}\omega)$ is equal to zero.

In the following: $V = \{v, \omega\}$, $\mathbb{M} = diag(\mathbb{M}_R, \mathbb{J}_R)$ and $q = \{x_c, \mathcal{R}_c\}$ are the generalized coordinates. Note $\dot{\mathcal{R}}_c = \omega_R \mathcal{R}_c^T$. The choice of orientation parameters is very important especially in 3D (inertia frame mapping, Euler angles, quaternion, etc.)

DEM::Modeling::Smooth dynamics::Interaction description

At any time of the evolution of the system one needs to define the interaction locus and an associated local frame in order to describe the interaction behavior.

→ implicit a priori.

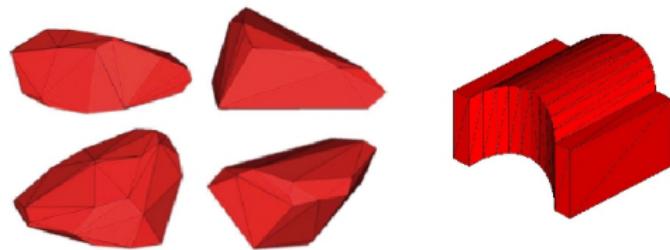


it is assumed that one is able to define for each point (C) of the candidate boundary its (unique) nearest point (A) on the antagonist boundary. It allows to define for each couple of points a local frame (t, n, s): with n the normal vector of the antagonist boundary and (s, t) two vectors of its tangential plane.

Only in simplest cases (rigid body with strictly convex boundary) the interaction locus may be considered as punctual.

DEM::Modeling::Smooth dynamics::Interaction description

Less trivial in usual cases :



- not strictly convex, i.e. cubes, bricks, etc.
- only locally convex, i.e. general polyhedron, triangulated surface
- not convex at all.
→ It may be decomposed in not strictly convex shapes.

DEM::Modeling::Smooth dynamics::Interaction description

In these cases many choices

- punctual contact with extended law (transmission of torque)
 - how to define the normal ? The interaction law depends on the objects shape ! etc.
- multi-punctual contacts with classical interaction laws
 - how many contact points ? normal choice ? It may introduce local indetermination of contact forces, etc.
- continuous surfaced description as in mortar methods
 - needs to perform integration on non-conforming triangulation, etc.
- etc.

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→ components of the system may be considered as rigid;
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- ③ interactions are binary (no effect of connected interaction by particle on their behavior);
→ interaction law depends only on related component;

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At least, for every potential contact α , one needs:

- Contact point coordinates;
- The local frame $(t^\alpha, n^\alpha, s^\alpha)$;
- The gap (g^α) , i.e. the algebraic distance between two bodies;
- The contact relative velocity between the two bodies (\mathcal{V}^α) .

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Contact description is a key point of DEMs.

DEM::Modeling::Smooth dynamic::Local-Global mapping

Two sets of unknowns:

- **global unknowns** (or kinematic space unknowns) related to the bodies: center of inertia or mesh node displacement and velocity (\mathbf{q}, \mathbf{V}), resulting force and momentum (\mathbf{R}), etc.
- **local unknowns** (or contact space unknowns) related to interactions: gap (\mathbf{g}), relative velocities (\mathcal{V}), forces (\mathcal{R}), etc.

Related by kinematic relations :

$$\mathbf{g} = D(\mathbf{q})$$

$$\mathcal{V} = \mathbb{H}^*(\mathbf{q})\mathbf{V} = \nabla_q D(\mathbf{q})\mathbf{V}$$

DEM::Modeling::Smooth dynamic::Local-Global mapping

Lets consider two **rigid bodies**.

The mapping between inertia center and contact point velocities will be write as follow:

$$v(M) = v(C) + \omega \times \ell$$

where ℓ represents the vector between the inertia center (C) and the contact point (M). Then it is possible to write the relative velocity between the two points (M^i) (body i) and (M^j) (body j) :

$$\mathcal{V}_{X,Y,Z} = v(M^i) - v(M^j) = v(C^i) - v(C^j) + \omega^i \times \ell^i - \omega^j \times \ell^j$$

which can be written in a “matricial” way (here in 2D) :

$$\mathcal{V}_{X,Y}^\alpha = \begin{bmatrix} 1 & 0 & -\ell_Y^i & -1 & 0 & \ell_Y^j \\ 0 & 1 & \ell_X^i & 0 & -1 & -\ell_X^j \end{bmatrix} \begin{bmatrix} v_X(C^i) \\ v_Y(C^i) \\ \omega^i \\ v_X(C^j) \\ v_Y(C^j) \\ \omega^j \end{bmatrix} = H^{\alpha,*}(q) V^{ij}$$

DEM::Modeling::Smooth dynamic::Local-Global mapping

And expressed in a local frame as:

$$\mathcal{V}_{t,n,s}^\alpha = \begin{bmatrix} \mathcal{V}_{X,Y,Z}^\alpha \cdot t \\ \mathcal{V}_{X,Y,Z}^\alpha \cdot n \\ \mathcal{V}_{X,Y,Z}^\alpha \cdot s \end{bmatrix} = \begin{bmatrix} t^T \\ n^T \\ s^T \end{bmatrix} H^{\alpha,*}(q) V^{ij} = \mathbb{H}^{\alpha,*}(q) V^{ij}$$

which can be written in a “matricial” way (here in 2D) :

$$\mathcal{V}_{t,n}^\alpha = \begin{bmatrix} t_x & t_y & -t_x \ell_Y^i + t_y \ell_X^i & -t_x & -t_y & t_x \ell_Y^j - t_y \ell_X^j \\ n_x & n_y & -n_x \ell_Y^i + n_y \ell_X^i & -n_x & -n_y & n_x \ell_Y^j - n_y \ell_X^j \end{bmatrix} \begin{bmatrix} v_X(C^i) \\ v_Y(C^i) \\ \omega^i \\ v_X(C^j) \\ v_Y(C^j) \\ \omega^j \end{bmatrix}$$

One can note that with disks, since n and ℓ are colinear, $t \times \ell = \pm r$ and $n \times \ell = 0$ which simplify the previous expression:

$$\mathcal{V}_{t,n}^\alpha = \begin{bmatrix} t_x & t_y & r^i & -t_x & -t_y & r^j \\ n_x & n_y & 0 & -n_x & -n_y & 0 \end{bmatrix} V^{ij}$$

DEM::Modeling::Smooth dynamic::Local-Global mapping

More generally, using kinematic relations, one can write for a given contact α :

$$\mathcal{V}^\alpha = \mathbb{H}^{\alpha,\star}(q)V^{ij}$$

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Using duality consideration (equality of power expressed in terms of global or local unknowns), the local contact force may be mapped on the global unknowns :

$$\mathbf{R}^{ij} = \mathbb{H}^\alpha(\mathbf{q})\mathcal{R}^\alpha,$$

where $\mathbb{H}^{\alpha,*}(\mathbf{q})$ is the transpose of $\mathbb{H}^\alpha(\mathbf{q})$.

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In the following we note $\mathcal{R}, \mathbf{R}, \mathcal{V}, \mathbf{V}$ the vectors gathering all the reactions, resultants, local velocities and global velocities.

We can construct mapping between these vectors, assembling the local unknown we introduced before:

$$\begin{aligned}\mathbb{H}(\mathbf{q}) &= \cup_{\alpha=1}^{n_c} \mathbb{H}^\alpha(\mathbf{q}) \\ \mathbb{H}^*(\mathbf{q}) &= \cup_{\alpha=1}^{n_c} \mathbb{H}^{\alpha,*}(\mathbf{q})\end{aligned}$$

Remark : even if $\mathbb{H}^{\alpha,*}(\mathbf{q})$ and $\mathbb{H}^\alpha(\mathbf{q})$ have good theoretical properties (surjectivity and injectivity), it is not necessary the case for \mathbb{H}^* and \mathbb{H} . Loose of these properties is due to the introduction of kinematic relation between contacts.

DEM::Modeling::Smooth dynamic::Interaction law

In DEMs, a large part of the physics of the problem is described through interaction laws.

Two ways of thinking :

1 - interaction behavior is a coarse representation of what happens at the boundary scale: impenetrability, plastic deformation of asperities, capillarity effects, friction, wear, etc.

2 - interaction behavior is a fine representation of what happens both at the bulk and boundary scale: idem as 1 + bulk behavior, etc.

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The two ways have different space scales which imply different time scales.

When considering rigid bulk behavior, one is able to describe :

1 - rigid body motion.
→ “Large time scale”.
Recover plastic behavior of the media.

2 - motion due to wave propagation.
→ Fine time scale.
Recover elastic and plastic behavior of the media. No indeterminacy.

DEM::Modeling::Smooth dynamic::Interaction law

From a “mathematical” point of view :

1 - set valued function, defined by
an **implicit law** : $h(\mathcal{R}, \mathcal{V}, g) = 0$.

2 - function, defined by an **explicit
law** : $\mathcal{R} = f(\mathcal{V}, g)$

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws – Normal part

- Hertz law : $\mathcal{R}_n = k_n \delta^{\frac{3}{2}} = K_n(\delta) \delta$
- Hook law with viscous damping : $\mathcal{R}_n = \max(0, k_n \delta + \eta_n \mathcal{V}_n)$
- JKR cohesion law : $\mathcal{R}_n = k_n \delta^{\frac{3}{2}} + \eta_n \mathcal{V}_n - \gamma_n \sqrt{\delta}$.

where $\delta = \langle -g \rangle^+$, k_n is a contact stiffness, η_n viscosity coefficient and γ_n contact cohesion.

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws – Normal part

How to choose parameters ? parameter are “shape” dependant.

- For Hertz law $K_n(\delta) = \frac{E\sqrt{2r_{eff}\delta}}{3(1-\nu^2)}$.
- One can define parameter through the elastic deflection $\delta \propto \frac{r_{eff}}{\kappa}$:
 - ▶ rigid grains if $\kappa \rightarrow \infty$. “Good” value are 10000.
 - ▶ Quasi-static problem: $\delta \ll \langle g \rangle^+$ ($\langle g \rangle^+$ interstice between grains)
- One can define parameters through dynamics as in flow problem: $t_c \ll \frac{\langle g \rangle^+}{r_{eff}\dot{\gamma}}$ (t_c duration of contact).

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws – Normal part

Considering the oscillator made by two particles in contact (Hook law) :

$$m_{\text{eff}} \frac{d^2\delta}{dt^2} + \eta_n \frac{d\delta}{dt} + K_n \delta = 0$$

- critical damping $\eta_n^c = 2\sqrt{m_{\text{eff}} K_n}$. $\alpha_n = \frac{\eta_n}{\eta_n^c}$
- pulsation $\omega = \sqrt{\frac{K_n}{m_{\text{eff}}}(1 - \alpha_n^2)}$ and contact duration $\tau = \pi/\omega$
- restitution coefficient $e_n = \exp\left[-\frac{\pi\alpha_n}{\sqrt{1 - \alpha_n^2}}\right]$

Remarks :

- $\eta_n \leq \eta_n^c$
- For Hertz law, same results with a varying K_n

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws – Tangential part

- viscous law with Coulomb threshold:

$$\mathcal{R}_t^{Tr} = -\eta_t \mathcal{V}_t$$

if $\|\mathcal{R}_t^{Tr}\| \geq \mu |\mathcal{R}_n|$ then $\mathcal{R}_t = \mu |\mathcal{R}_n| \frac{\mathcal{R}_t^{Tr}}{\|\mathcal{R}_t^{Tr}\|}$ else $\mathcal{R}_t = \mathcal{R}_t^{Tr}$

- incremental elastic law with Coulomb threshold:

a previous \mathcal{R}_t is known, $\Delta \mathcal{R}_t = K_t h \mathcal{V}_t$ and $\mathcal{R}_t^{Tr} = \mathcal{R}_t + \Delta \mathcal{R}_t$

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with $K_t = \frac{2(1-\nu)}{2-\nu} K_n$.

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- incremental elastic law with Coulomb threshold:

a previous \mathcal{R}_t is known, $\Delta \mathcal{R}_t = K_t h \mathcal{V}_t$ and $\mathcal{R}_t^{Tr} = \mathcal{R}_t + \Delta \mathcal{R}_t$

if $\|\mathcal{R}_t^{Tr}\| \geq \mu |\mathcal{R}_n|$ then $\mathcal{R}_t = \mu |\mathcal{R}_n| \frac{\mathcal{R}_t^{Tr}}{\|\mathcal{R}_t^{Tr}\|}$ else $\mathcal{R}_t = \mathcal{R}_t^{Tr}$

with $K_t = \frac{2(1-\nu)}{2-\nu} K_n$.

Remarks :

- compute η_t^c as before by taking $m_{eff} = \frac{m_1 m_2}{m_1 + m_2} + m_1 m_2 \left(\frac{R_1^2}{I_1} + \frac{R_2^2}{I_2} \right)$ and replacing K_n by K_t
- $\eta_t \leq \eta_t^c$
- difficult to give a physical meaning to η_n and η_t

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws

DEM::Modeling::Smooth dynamics::Interaction law

explicit laws

Explicit laws allow to substitute the displacement (or the velocity) to the force in the dynamics equation.

If considering a simplified problem described by the Newton equation :

$$\dot{M}\ddot{V} = F_{int}(q, V, t) + F_{ext}(t) + R$$

using $\mathcal{V} = \mathbb{H}^*(q)V$, $g = D(q)$, $R = \mathbb{H}(q)\mathcal{R}$ and $\mathcal{R} = f(\mathcal{V}, g)$ one can write :

$$\dot{M}\ddot{V} = F_{ext}(t) + \mathbb{H}(q)f(\mathbb{H}^*(q)V, D(q))$$

which is a “classical” non linear problem only written in term of kinematic unknowns.

The kinematic unknowns of all components are related due to the interactions.

DEM::Modeling::Smooth dynamic::Interaction law

implicit laws

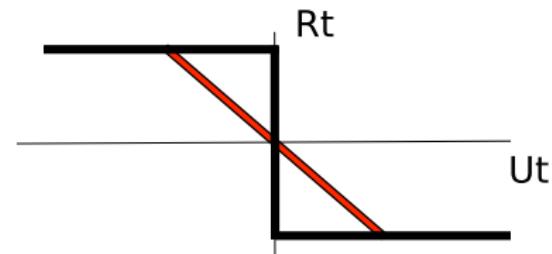
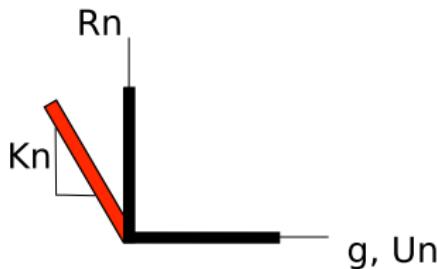
DEM::Modeling::Smooth dynamic::Interaction law

implicit laws

Frictional contact: Signorini-Coulomb

$$\mathcal{R}_n \geq 0 \quad g \geq 0 \quad \mathcal{R}_n \cdot g = 0$$

$$\|\mathcal{R}_t\| \leq \mu \mathcal{R}_n, \begin{cases} \|\mathcal{R}_t\| < \mu \mathcal{R}_n \Rightarrow \mathcal{V}_t = 0 \\ \|\mathcal{R}_t\| = \mu \mathcal{R}_n \Rightarrow \exists \alpha \geq 0, \mathcal{V}_t = -\alpha \mathcal{R}_t \end{cases}$$



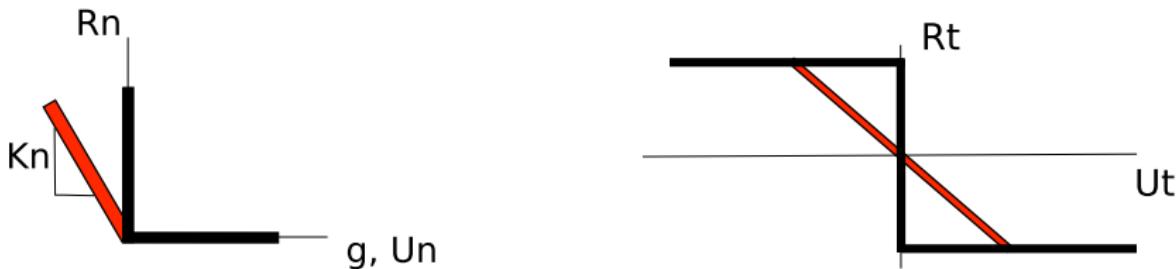
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Remark : for dynamical problems, it is more natural to formulate the unilateral contact in term of velocities

*Assuming $g(t_0) \geq 0$ then $\forall t > t_0$
 if $g(t) \leq 0$ then $\mathcal{V}_n \geq 0, \mathcal{R}_n \geq 0, \mathcal{V}_n \mathcal{R}_n = 0$
 else $\mathcal{R}_n \equiv 0$*

DEM::Modeling::Smooth dynamic::Interaction law

implicit laws

DEM::Modeling::Smooth dynamic::Interaction law

implicit laws

It is not possible to substitute reaction by kinematic unknowns, the problem remains implicit.

One can consider explicit law (smooth) as a regularization of implicit law (non smooth). In this case the parameters are not due to physical considerations but numerical ones.

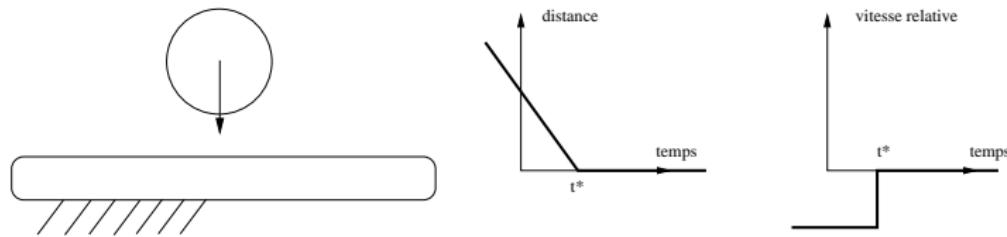
An explicit law may be written as an implicit law.

DEM::Modeling::Smooth dynamic::Interaction

Lets consider the basic example of a single ball bouncing on a plan:

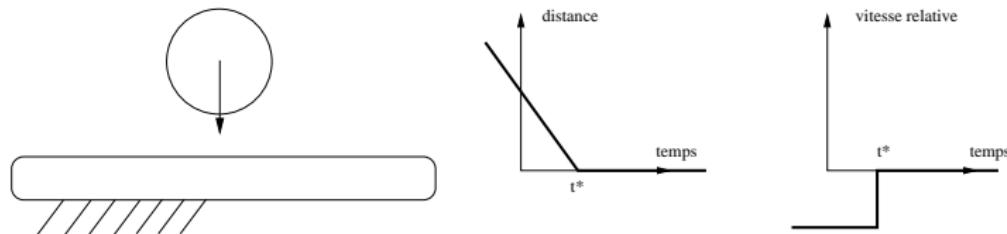
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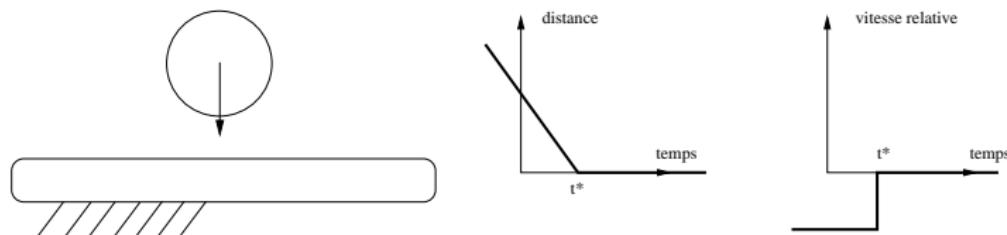
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Question: Is the usual formalism adapted to describe a dynamical system with unilateral contact?

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So let try to solve the (simplified) problem:

$$M\ddot{q} = R$$

$$0 \leq q \perp R \geq 0$$

$$\text{initial conditions : } q(0) = 0, \dot{q}(0) = -1$$

DEM::Modeling::Smooth dynamic::Interaction

Using an implicit Euler scheme, one obtains the following system:

$$\begin{cases} \ddot{q}_{i+1} = (\dot{q}_{i+1} - \dot{q}_i)/h \\ q_{i+1} = q_i + h\dot{q}_{i+1} \end{cases}$$

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So if $h \rightarrow 0$ then $R^1 = \infty$!

Two solutions are possible:

- Using smooth interaction law as before but needs **reasonably small** time steps
- Adapting the formalism to face the problem

Introducing a deformable body will not solve the problem.

DEM::Modeling::Non smooth dynamic::Equations of motion

The differential system must be modified to describe collisions and other non smooth phenomena.

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The “spirit” of the approach is to consider a weaken form of the dynamical system, e.g. balance of momentum :

$$\mathbb{M}(V^+ - V^-) = \int_{t^-}^{t^+} (F_{int}(q, V, s) + F_{ext}(s)) ds + I$$

where the impulse I will contain both the sum of

- the contribution of smooth load over the time interval ($\int_{t^-}^{t^+} R dt$),
- the percussion, denoted P , at *shock* time (supposed instantaneous).

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Remark :

- Event driven approaches will consider smooth motion, but will re-initialize velocity (acceleration, etc.) at each non-smooth event using shock law.

DEM::Modeling::Non smooth dynamic::Equations of motion

More precisely the classical dynamics equation is reformulated in terms of a differential measure equation:

$$\begin{aligned}\mathbb{M}dV &= F_{int}(t, q, V^+)dt + F_{ext}(t)dt + dl \\ q(t) &= q(t_0) + \int_{t_0}^t V^+ dt\end{aligned}$$

In the previous equation, dV is the differential measure of V ($dV = \dot{V}dt + d\hat{V}$), dt is the Lebesgue measure on \mathbb{R} while dl is the differential measure of contact forces ($dl = Rdt + dP$).

The measure dl contains:

- The contribution of smooth contact (diffuse contribution Rdt):
- The contribution of local impulsion densities exerted by shocks $P\delta$ (atomic contributions),

A differential measure df is integrated such that :

$$\int_{[t_a, t_b]} df = f(t_b) - f(t_a)$$



DEM::Modeling::Non smooth dynamic::Interaction law

- Local - global mapping:

$$\begin{aligned}\mathcal{V}^+ &= \mathbb{H}^*(q)\mathbf{V}^+ \\ d\mathbf{l} &= \mathbb{H}(q)d\mathcal{I}\end{aligned}$$

DEM::Modeling::Non smooth dynamic::Interaction law

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Assuming $g(t_0) \geq 0$ then $\forall t > t_0$

if $g(t) \leq 0$ then $\mathcal{V}_n^+ \geq 0$, $d\mathcal{I}_n \geq 0$, $\mathcal{V}_n^+ d\mathcal{I}_n = 0$
else $d\mathcal{I}_n = 0$

- Coulomb friction (threshold law):

$$\|d\mathcal{I}_t\| \leq \mu d\mathcal{I}_n, \begin{cases} \|d\mathcal{I}_t\| < \mu d\mathcal{I}_n \Rightarrow \mathcal{V}_t^+ = 0 \\ \|d\mathcal{I}_t\| = \mu d\mathcal{I}_n \Rightarrow \exists \alpha \geq 0, \mathcal{V}_t^+ = -\alpha d\mathcal{I}_t \end{cases}$$

DEM::Modeling::Non smooth dynamic::Shock law

When shocks occur in a rigid body collection, the equation of motion and the interaction law are not sufficient to describe properly all the physics of the problem.

It must take into account:

- Local phenomena as inelastic behavior of materials at the interface depending on both the contact geometry and the material behavior.
- Global phenomena as the wave propagation in the body bulk, body geometry dependency and boundary conditions.
- More complex effects: long distance effects due to simultaneous impact

DEM::Modeling::Non smooth dynamic::Shock law

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Impact law for the normal component is well understood, it is not the case of the tangential component. The choice of the restitution coefficient is a difficult task for complex structures.

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Impact law for the normal component is well understood, it is not the case of the tangential component. The choice of the restitution coefficient is a difficult task for complex structures.

In the case of dense granular material, the effect of impacts may be neglected and previous laws can be used.

Binary impact law are not sufficient to model phenomena such as Newton cradle (multiple impacts).

DEM::Modeling::Conclusion

Various modeling choices are possible for DEM depending on:

- space scale: interaction → smooth, component → non-smooth
- time scale: waves → smooth, rigid body motion with impact → non-smooth
- the shape of the components → non-smooth easier but introduce indetermination.
- etc.

DEM::Numerical Strategies

1 Preamble

2 Modeling

3 Numerical Strategies

- Introduction
- smooth-DEM
- Non Smooth Contact Dynamics

4 NSCD Extensions

5 Multi-Physics

6 Technical Aspects

7 Bibliography

8 Annexes

DEM::Numerical Strategies::Introduction

Depending on modeling choices numerical strategies are build to solve the evolution problem.

They depend on :

- time evolution strategy: **time stepping** or event driven
- time integrator over a time step: explicit or implicit
- implicit contact law needs a contact solver (Lemke, Gauss-Seidel, bi-potential, etc.)
- technical aspects: contact detection, rotation integration, etc.
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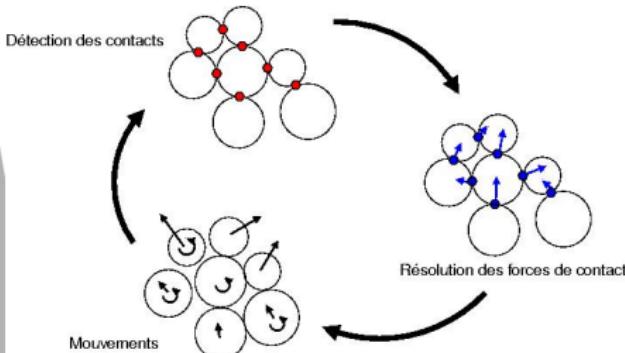
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Over a time step $[t, t + h[$, three important tasks can be underlined:



- The contact detection
- The computation of contact forces, called contact problem
- The motion of the different element of the media.

DEM::Numerical Strategies::Introduction

Pioneer DEMs (Cundall et al. 1979, Allen et al. 1987) consider explicit interaction model (smooth) and use explicit time integration scheme. This kind of methods refer to **smooth-DEM**.

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Carpenter et al. (1991) proposed a method to solve implicit interaction model using explicit time integrator.

Thus the *end-user* has various possibilities to perform numerical modeling.

DEM::Numerical Strategies::smooth-DEM::Generality

Using explicit interaction law leads to solve :

$$\dot{M}V = F_{int}(q, V, t) + F_{ext}(t) + R$$

with $R = \mathbb{H}(q)\mathcal{R}$, $\mathcal{R} = f(\mathcal{V}, g)$ and $\mathcal{V} = \mathbb{H}^*(q)V$, $g = D(q)$.

→ This is a non-linear problem.

Using an implicit time integrator, a non-linear solver (Newton-Raphson) will be necessary.

Assuming linear contact laws and fixed contact network it may be solved directly (see GEM of Kishino).

Using an explicit time integrator leads to an uncoupled set of equations :

$$M(V_{n+1} - V_n) = hF_{int}(q_n, V_n, t_n) + hF_{ext}(t_n) + hR_n$$

Different explicit time integrator can be used to integrate the motion of particle:

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- Gear integrator for Molecular Dynamics
- Velocity verlet
- Time-centered scheme for the Distinct Element Method (Cundall)



DEM::Numerical Strategies::smooth-DEM::Time integrator

Predictor-corrector Gear integrator

DEM::Numerical Strategies::smooth-DEM::Time integrator

Predictor-corrector Gear integrator

Prediction: Using classical Taylor expansion (b and c are first and second time derivative of acceleration) :

$$\left\{ \begin{array}{l} q^P(t+h) = q(t) + h\dot{q}(t) + \frac{h^2}{2!}\ddot{q}(t) + \frac{h^3}{3!}b(t) + \frac{h^4}{4!}c(t) + \dots \\ \dot{q}^P(t+h) = \dot{q}(t) + h\ddot{q}(t) + \frac{h^2}{2!}b(t) + \frac{h^3}{3!}c(t) + \dots \\ \ddot{q}^P(t+h) = \ddot{q}(t) + hb(t) + \frac{h^2}{2!}c(t) \dots \\ b^P(t+h) = b(t) + hc(t) + \dots \\ c^P(t+h) = c(t) + \dots \end{array} \right.$$

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Perform detection in the predicted configuration, compute contact forces, compute the acceleration ($\ddot{q}^c(t+h) = \mathbb{M}^{-1}(\mathbf{F}_{int} + \mathbf{F}_{ext} + \mathbf{R})$).

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Predictor-corrector Gear integrator

Prediction: Using classical Taylor expansion (b and c are first and second time derivative of acceleration) :

$$\left\{ \begin{array}{l} q^P(t+h) = q(t) + h\dot{q}(t) + \frac{h^2}{2!}\ddot{q}(t) + \frac{h^3}{3!}b(t) + \frac{h^4}{4!}c(t) + \dots \\ \dot{q}^P(t+h) = \dot{q}(t) + h\ddot{q}(t) + \frac{h^2}{2!}b(t) + \frac{h^3}{3!}c(t) + \dots \\ \ddot{q}^P(t+h) = \ddot{q}(t) + hb(t) + \frac{h^2}{2!}c(t) \dots \\ b^P(t+h) = b(t) + hc(t) + \dots \\ c^P(t+h) = c(t) + \dots \end{array} \right.$$

Perform detection in the predicted configuration, compute contact forces, compute the acceleration ($\ddot{q}^c(t+h) = \mathbb{M}^{-1}(F_{int} + F_{ext} + R)$).

Correction: considering $\Delta\ddot{q} = \ddot{q}^c(t+h) - \ddot{q}^P(t+h)$ perform the correction

$$\left\{ \begin{array}{l} q^c(t+h) = q^P(t+h) + c_0\Delta\ddot{q} \\ \dot{q}^c(t+h) = \dot{q}^P(t+h) + c_1\Delta\ddot{q} \\ \ddot{q}^c(t+h) = \ddot{q}^P(t+h) + c_2\Delta\ddot{q} \\ b^c(t+h) = b^P(t+h) + c_3\Delta\ddot{q} \\ c^c(t+h) = c^P(t+h) + c_4\Delta\ddot{q} \end{array} \right.$$

DEM::Numerical Strategies::smooth-DEM::Time integrator

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DEM::Numerical Strategies::smooth-DEM::Time integrator

Velocity Verlet scheme

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Velocity Verlet scheme

Its also predictor-corrector approach.

Prediction:

$$\begin{cases} q(t+h) &= q(t) + h\dot{q}(t) + \frac{1}{2}h^2\ddot{q}(t) \\ \dot{q}(t+h/2) &= \dot{q}(t) + \frac{1}{2}h\ddot{q}(t) \end{cases} .$$

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Perform detection in the predicted configuration, compute contact forces, compute the acceleration knowing $q(t+h)$ and $\dot{q}(t+h/2)$ ($\ddot{q}(t+h) = \mathbb{M}^{-1}(F_{int} + F_{ext} + R)$).

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Note that the classical Verlet scheme (*leap-frog*) is not usable for DEM.

DEM::Numerical Strategies::smooth-DEM::Time integrator

Time-centered scheme

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Knowing $q(t)$ and $\dot{q}(t - h/2)$ one perform contact detection, computes contact forces and update acceleration $\ddot{q}(t)$.

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Then one updates

$$\begin{cases} \dot{q}(t + h/2) &= \dot{q}(t - h/2) + h\ddot{q}(t) \\ q(t + h) &= q(t) + h\dot{q}(t + h/2) \end{cases}.$$

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It is not written as a predictor-corrector scheme.

But it's the same as velocity verlet.

DEM::Numerical Strategies::smooth-DEM::Practical aspects

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- Dissipation must be added to stabilize the problem (i.e. over-shoots). For example non viscous dissipation can be added to study granular flow :

$$F_d = -\alpha \ r \ \text{sign}(V)$$

α is chosen depending on the studied problem: 0.7 for quasi-static problem, less for dynamic problem, and 0.1 for wave propagation

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Thus control parameter of the simulation are:

- the time step discretization (N),
- the local stiffness (normal K_n and tangential K_t),
- the viscous (η) or non viscous (α) dissipation.

Evaluation criteria related to the computation quality:

- Respect of interaction law,
- Control of numerical damping.

DEM::Numerical Strategies::NSCD::Time stepping

Time integration of the equation of motion leads to:

$$\begin{aligned}\mathbb{M}(V_{i+1} - V_i) &= \int_{t_i}^{t_{i+1}} (F_{int}(q, V, s) + F_{ext}(s)) ds + I_{i+1} \\ &= I_{free} + I_{i+1} \\ q_{i+1} &= q_i + \int_{t_i}^{t_{i+1}} V ds\end{aligned}$$

where

- $I_{i+1} = \int_{t_i}^{t_{i+1}} dI$ represents the value of the total impulsion over the time step **the unknown in the following**
- I_{free} the integral of applied forces over the time step;

DEM::Numerical Strategies::NSCD::Time stepping

A θ -method (Crank-Nicholson) is used to evaluate $\int_{t_i}^{t_{i+1}} (F_{int}(q, V, s) + F_{ext}(s)) ds$ and $\int_{t_i}^{t_{i+1}} V ds$:

$$\begin{aligned} I_{free} &= h(1 - \theta)(F_{int}(q_i, V_i, t_i) + F_{ext}(t_i)) + \\ &\quad h\theta(F_{int}(q_{i+1}, V_{i+1}, t_{i+1}) + F_{ext}(t_{i+1})) \\ q_{i+1} &= q_i + h((1 - \theta)V_i + \theta V_{i+1}) = q_m + h\theta V_{i+1} \end{aligned}$$

with $q_m = q_i + h(1 - \theta)V_i$.

- If $\theta \in [0.5, 1]$ the scheme is implicit and stable unconditionally.
- If $\theta = 0.5$ the scheme is conservative for smooth evolution problem,
- If $\theta = 0$ the scheme is explicit

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The order of the time integrator is weak (1 or 2).

The time discretization is imposed arbitrarily. Its mainly driven by the precision of the contact treatment.

If discontinuities occur they are treated simultaneously. No limitation on the number of interactions but the time order is lost.

DEM::Numerical Strategies::NSCD::Time stepping

If now we use this formulation for the previous elementary contact problem, one obtains:

$$M(V_{i+1} - V_i) = l_{i+1}$$

$$\text{If } q_i \leq 0, 0 \leq V_{i+1} \perp l_{i+1} \geq 0$$

$$\text{Initial conditions : } q(0) = 0, V(0) = -1$$

The implicit euler scheme gives:

$$\begin{cases} q_1 = 0, V_1 = 0, l_1 = M V_0 \\ q_k = 0, V_k = 0, l_k = 0 \end{cases}$$

The obtained solution is independent of the time step.

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The obtained solution is independent of the time step.

If $q(0) = \epsilon$ then $V_1 = 0$ and $l_1 = M V_0$ and $q_k = \epsilon$.

The error made on the gap decreases with the size of the time step.

DEM::Numerical Strategies::NSCD::Interaction management

The two mappings \mathbb{H}^* and \mathbb{H} depend of the solution.

They may be evaluated in a “mean” configuration : $\tilde{\mathbf{q}}_{k+1} = \mathbf{q}_k + h(\gamma_1 \mathbf{V}_k + \gamma_2 \mathbf{V}_{k+1})$

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If the time step is small enough (small sliding motions, etc) and the curvature of component shapes is small the mapping \mathbb{H}^* and \mathbb{H} can be considered as constant on a whole time interval.

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Remarks:

- Usually the contact problem is solved in a pseudo-explicit configuration :
 $\mathbf{q}_m = \mathbf{q}_i + h(1 - \theta)\mathbf{V}_i$.
- The pseudo configuration of the next time step will be determined by the final velocity \mathbf{V}_{i+1} : $\mathbf{q}_{m+1} = \mathbf{q}_m + h\mathbf{V}_{i+1}$. This is a *Leap-Frog* technique.

DEM::Numerical Strategies::NSCD::Contact problem formulation

The problem to solve is written in terms of :

- discretized equations of motion for each body expressed with global unknowns :

$$\mathbf{V}_{i+1} = \mathbf{V}_{free} + \mathbb{M}^{-1} \mathbf{l}_{i+1}$$

- interaction relations expressed with local unknowns (contact α):

$$Contact(g^\alpha, \mathcal{V}_n^\alpha, \mathcal{I}_n^\alpha) = 0 \quad Friction(\mathcal{V}_t^\alpha, \mathcal{I}_t^\alpha) = 0$$

- mappings (\mathbb{H} and \mathbb{H}^*) to pass from local to global unknowns

$$\mathbf{q}, \mathbf{V} \quad \leftarrow \text{Equations of motion} \rightarrow \quad \mathbf{l}$$

$$\mathbb{H}^* \downarrow \qquad \qquad \qquad \uparrow \mathbb{H}$$

$$\boldsymbol{\nu} \quad \leftarrow \text{Interaction laws} \rightarrow \quad \boldsymbol{\mathcal{I}}$$

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Using basic algebraic transformations the equations of motion may be expressed in terms of local unknowns

$$\boldsymbol{\nu} = \boldsymbol{\nu}_{free} + \mathcal{W} \boldsymbol{\mathcal{I}}$$

where $\mathcal{W} = \mathbb{H}^* \mathbb{M}^{-1} \mathbb{H}$ and $\boldsymbol{\nu}_{free} = \mathbb{H}^* (\mathbf{V}_i + \mathbb{M}^{-1} \mathbf{l}_{free}) = \mathbb{H}^* \mathbf{V}_{free}$.

DEM::Numerical Strategies::NSCD::Resolution Scheme

Iteration matrix computation (\mathbb{M})

Time loop

Free velocity computation(V_{free})

Temporary configuration computation(q_m)

Contact detection

Contact problem resolution

Velocity correction($V_{i+1} = V_{free} + \mathbb{M}^{-1}l_{i+1}$)

Update of the kinematics and the configuration

Halt criteria

DEM::Numerical Strategies::NSCD::Contact Solvers

The classical NSCD approach rely on a Non Linear Gauss Seidel (NLGS) algorithm.

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considering one by one the contacts (α) of the local systems to solve :

$$\mathcal{V}^\alpha = \mathcal{V}_{free}^\alpha + \mathcal{W}^{\alpha\alpha} \mathcal{I}^\alpha + \sum_{\beta \neq \alpha} \mathcal{W}^{\alpha\beta} \mathcal{I}^\beta$$
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- updated values of \mathcal{I} if $\beta < \alpha$
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we solve the α local problem of 2 unknowns with 2 equations.

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we repeat the process until convergence

DEM::Numerical Strategies::NSCD::Contact Solvers

Local solvers:

2D

- explicit uncoupled resolution if $\mathcal{W}^{\alpha\alpha}$ is diagonal
- coupled (n, t) graph intersection ($b = \mathbf{V}_{free}^\alpha + \sum_{\beta \neq \alpha} \mathcal{W}^{\alpha\beta} \mathbf{I}^\beta$)

If $b_N \geq 0$

then $\mathbf{I} = 0$

status : no contact

Else

compute

$\epsilon = -1, 1$

$Dft_\epsilon = \mathcal{W}_{TN} + \epsilon \mu \mathcal{W}_{TT}$

$Dfn_\epsilon = \mathcal{W}_{NN} + \epsilon \mu \mathcal{W}_{NT}$

If $\epsilon(Dft_\epsilon b_N - Dfn_\epsilon b_T) \geq 0$ then

$\mathcal{I}_n = -b_N/Dfn_\epsilon, \mathbf{I}_t = \epsilon \mu \mathcal{I}_n$

status : sliding(ϵ)

Else

$\mathbf{I} = \mathcal{W}^{-1} b$

status : sticking

- pseudo-potential approach (bi-potential)
- LCP solver
- etc.

DEM::Numerical Strategies::NSCD::Contact Solvers

Local solvers:

3D

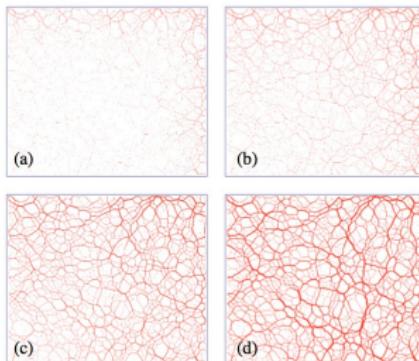
- explicit resolution if $\mathcal{W}^{\alpha\alpha}$ is diagonal
- Generalized Newton algorithm
- pseudo-potential approach
- LCP solver
- etc

NSCD : Framework

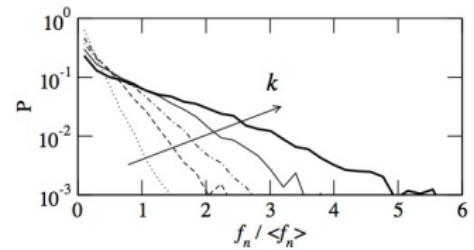
NLGS convergence :

- Once one has computed $\mathcal{I}^{k+1,\alpha}, \mathcal{V}^{k+1,\alpha} \forall \alpha$
- One performs a Jacobi loop (aka solving contacts as if uncoupled): $\mathcal{I}^{Jac,\alpha}, \mathcal{V}^{Jac,\alpha} \forall \alpha$
- One evaluates the distance between the two solutions.

Influence of convergence :



Evolution of contact forces in the course of iterations initialized by zero force at all contacts in a system subjected to equal top and right stresses.



DEM::Numerical Strategies::NSCD::Contact Solvers

Various implementation of NLGS are possible

DEM::Numerical Strategies::NSCD::Contact Solvers

Various implementation of NLGS are possible

Stored Delassus Loop strategy (SDL)

(0) Evaluating all the matrices $\mathcal{W}^{\alpha\beta} \forall \beta$

$k = k + 1$ (NLGS iteration)

$\alpha = \alpha + 1$ (Contact index)

(a) Evaluating the right-hand side

$$\mathbf{V}_{loc}^\alpha = \mathbf{V}_{free}^\alpha + \sum_{\beta < \alpha} \mathcal{W}^{\alpha\beta} \mathbf{I}^{\beta,k+1} + \sum_{\beta > \alpha} \mathcal{W}^{\alpha\beta} \mathbf{I}^{\beta,k}$$

(b) Solving the local problem

Convergence test for $k = 0 \dots k_{max}$

Rigid/deformable : performant in 2D and in 3D

DEM::Numerical Strategies::NSCD::Contact Solvers

Various implementation of NLGS are possible

Exchange Local Global Strategy (ELG)

(0) Evaluating the $\mathcal{W}^{\alpha\alpha}$ matrix

- $k = k + 1$ (NLGS iteration)
- $\alpha = \alpha + 1$ (Contact index)
 - (i) Identifying the contact bodies ($\alpha = jl$)
 - Computing an auxiliary value
 $\mathcal{V}_{aux}^\alpha = \mathbb{H}^{*,\alpha} (\mathbb{M}^{-1,j}|j,k - \mathbb{M}^{-1,k}|l,k)$
 - (a) Evaluating the right-hand side
 $\mathcal{V}_{loc}^\alpha = \mathcal{V}_{free}^\alpha + \mathcal{V}_{aux}^\alpha - \mathcal{W}^{\alpha\alpha} \mathcal{I}^{\alpha,k}$
 - (b) Solving the local problem
 - (i) Updating the resultant on bodies ($\alpha = jl$)
$$\begin{bmatrix} j \\ l' \end{bmatrix}^{k+1} = \begin{bmatrix} j \\ l' \end{bmatrix}^k + \mathbb{H}^\alpha (\mathcal{I}^{\alpha,k+1} - \mathcal{I}^{\alpha,k})$$
 - Convergence test for $k = 0 \dots k_{max}$

DEM::Numerical Strategies::NSCD::Contact Solvers

A parallel treatment of the NLGS is possible

DEM::Numerical Strategies::NSCD::Contact Solvers

A parallel treatment of the NLGS is possible

Store Delassus Loop strategy (SDL)

```
(0) Evaluating all the matrices  $\mathcal{W}^{\alpha\beta}$ 
    [  $k = k + 1$  (NLGS iteration)
      !$OMP PARALLEL PRIVATE (...) SHARED (...) ...
      !$OMP DO ...
        [  $\alpha = \alpha + 1$  (Contact index)
          (a) Evaluating the right-hand side
               $\mathcal{V}_{loc}^\alpha = \mathcal{V}_{free}^\alpha + \sum_{\beta < \alpha} \mathcal{W}^{\alpha\beta} \mathcal{I}^{\beta,k+1} + \sum_{\beta > \alpha} \mathcal{W}^{\alpha\beta} \mathcal{I}^{\beta,k}$ 
          (b) Solving the local problem
        !$OMP ENDDO
      !$OMP END PARALLEL
      Convergence test for  $k = 0 \dots k_{max}$ 
```

Needs equivalent parallel treatment of other CPU consuming parts of the code.

DEM::Numerical Strategies::NSCD::Contact Solvers

quasi NLGS may be derived, rewriting the system :

$$\mathcal{V}^\alpha = \mathcal{V}_{free}^\alpha + \mathcal{W}^{\alpha\alpha}(\mathcal{I}^\alpha - \mathcal{I}^{\alpha,est}) + \sum_\beta \mathcal{W}^{\alpha\beta} \mathcal{I}^\beta$$

$$Law(g^\alpha, \mathcal{V}_t^\alpha, \mathcal{I}_t^\alpha, \mathcal{I}_t^\alpha) = 0$$

where $\mathcal{I}^{\alpha,est}$ is the impulsion computed at the previous Gauss-Seidel iteration.

Noting that when the algorithm goes close to the solution, $\mathcal{I}^\alpha - \mathcal{I}^{\alpha,est} \rightarrow 0$ one may derive a quasi NLGS replacing the original $\mathcal{W}^{\alpha\alpha}$ by an arbitrary one.

DEM::Numerical Strategies::NSCD::Contact Solvers

quasi NLGS may be derived, rewriting the system :

$$\mathcal{V}^\alpha = \mathcal{V}_{\text{free}}^\alpha + \mathcal{W}^{\alpha\alpha}(\mathcal{I}^\alpha - \mathcal{I}^{\alpha,\text{esti}}) + \sum_\beta \mathcal{W}^{\alpha\beta} \mathcal{I}^\beta$$

$$\text{Law}(g^\alpha, \mathcal{V}_t^\alpha, \mathcal{I}_t^\alpha, \mathcal{I}_t^\alpha) = 0$$

where $\mathcal{I}^{\alpha,\text{esti}}$ is the impulsion computed at the previous Gauss-Seidel iteration.

Noting that when the algorithm goes close to the solution, $\mathcal{I}^\alpha - \mathcal{I}^{\alpha,\text{esti}} \rightarrow 0$ one may derive a *quasi NLGS* replacing the original $\mathcal{W}^{\alpha\alpha}$ by an arbitrary one.

Various alternatives are possible for the contact solver :

- Conjugate Projected Gradient Algorithm
- Lemke (for small collection of rigid bodies)
- Other possibilities, see Siconos NSSPack

DEM::Numerical Strategies::NSCD::Practical aspects

Numerical model parameters are:

- The θ value
- The time step
- The convergence norm of the Gauss-Seidel algorithm
- The direction of reading the contact set

Quality of the computation lays on:

- The respect of interaction laws
- The number of iteration performed
- The free evolution of bodies

DEM::NSCD Extensions

1 Preamble

2 Modeling

3 Numerical Strategies

4 NSCD Extensions

- Deformable bodies
- Interaction laws
- Explicit Integration

5 Multi-Physics

6 Technical Aspects

7 Bibliography

8 Annexes

DEM::NSCD extensions::Deformable bodies

When deformable bodies are used, the local dynamic system may be written in the same way

$$\mathcal{V} = \mathcal{V}_{\text{free}} + \mathcal{W} \mathcal{I}$$

with

- rigid: $\tilde{\mathbb{M}} = \mathbb{M}$
 $\mathcal{I}_{\text{free}} = h(1 - \theta)(\mathbf{F}_{\text{int}}(t_i) + \mathbf{F}_{\text{ext}}(t_i)) + h\theta(\mathbf{F}_{\text{int}}(t_{i+1}) + \mathbf{F}_{\text{ext}}(t_{i+1}))$
- linear: $\tilde{\mathbb{M}} = \mathbb{M} + h\theta\mathbb{C} + h^2\theta^2\mathbb{K}$
 $\mathcal{I}_{\text{free}} = [\mathbb{M} - h(1 - \theta)\mathbb{C} - h^2\theta(1 - \theta)\mathbb{K}] \mathbf{V}_i - h\mathbb{K}\mathbf{q}_i + h[\theta\mathbf{F}_{\text{ext}}(t_{i+1}) + (1 - \theta)\mathbf{F}_{\text{ext}}(t_i)]$
- non-linear: $\tilde{\mathbb{M}}^k = \mathbb{M} + h\theta\mathbb{C}^k + h^2\theta^2\mathbb{K}^k$
 $\mathcal{I}_{\text{free}} = \tilde{\mathbb{M}}^k \mathbf{V}_{i+1}^k + \mathbb{M}(\mathbf{V}_i - \mathbf{V}_{i+1}^k) + h[(1 - \theta)(\mathbf{F}_{\text{int}}(t_i) + \mathbf{F}_{\text{ext}}(t_i)) + \theta(\mathbf{F}_{\text{int}}^k(t_{i+1}) + \mathbf{F}_{\text{ext}}^k(t_{i+1}))]$

Remark :

- due to “energy conservation” one may replace $h[(1 - \theta)\mathbf{F}_{\text{int}}(t_i) + \theta\mathbf{F}_{\text{int}}^k(t_{i+1})]$ by a more suitable expression (Gonzalez, 2000)

DEM::NSCD extensions::Interaction laws

Different interaction laws may be used:

- Newton shock law using the variable $\tilde{\mathcal{V}}_n = \mathcal{V}_n + e\mathcal{V}_n^-$ and $\tilde{\mathcal{V}}_t = \mathcal{V}_t$

$$\tilde{\mathcal{V}}^\alpha = \mathcal{V}_{free}^\alpha + \max(e\mathcal{V}_i^\alpha, 0)^T + \mathcal{W}^{\alpha\alpha} \mathcal{I}^\alpha + \sum_{\beta \neq \alpha} \mathcal{W}^{\alpha\beta} \mathcal{I}_\beta$$

$$Law(\tilde{\mathcal{V}}^\alpha, \mathcal{I}^\alpha) = 0$$

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- Gap Signorini law using the variable $\tilde{\mathcal{V}}_n = g/h = g_0/h + \mathcal{V}_n$, $\tilde{\mathcal{V}}_t = \mathcal{V}_t$

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$$Law(\tilde{\mathcal{V}}^\alpha, \mathcal{I}^\alpha) = 0$$

- Elastic law using the variable $\tilde{\mathcal{V}}_n = g_0/h + \mathcal{V}_n + \mathcal{I}_n/h^2 k_n$

DEM::NSCD extensions::Interaction laws

Different interaction laws may be used:

- cohesive with damage law

$$(\mathcal{I}_n + \mathcal{I}_n^{coh}) \geq 0 \quad g \geq 0 \quad (\mathcal{I}_n + \mathcal{I}_n^{coh}) \cdot g = 0$$

$$\| (\mathcal{I}_t + \mathcal{I}_t^{coh}) \| \leq \mu \kappa(\beta) (\mathcal{I}_n + \mathcal{I}_n^{coh})$$

with : $\begin{cases} \| (\mathcal{I}_t + \mathcal{I}_t^{coh}) \| < \mu \kappa(\beta) (\mathcal{I}_n + \mathcal{I}_n^{coh}) \Rightarrow \mathbf{v}_t = 0 \\ \| (\mathcal{I}_t + \mathcal{I}_t^{coh}) \| = \mu \kappa(\beta) (\mathcal{I}_n + \mathcal{I}_n^{coh}) \Rightarrow \exists \alpha \geq 0, \mathbf{v}_t = -\alpha (\mathcal{I}_t + \mathcal{I}_t^{coh}) \end{cases}$

- ▶ intrinsic model:

$$\mathcal{I}^{coh} = K(\beta) \cdot \mathbf{v} \quad \text{and} \quad h(\dot{\beta}, \beta, \mathcal{V}_n, \mathbf{v}_t) = 0$$

$$K(\beta) = \beta \left(C_N n \otimes n + C_T \frac{\mathbf{v}_t \otimes \mathbf{v}_t}{\|\mathbf{v}_t\|^2} \right)$$

- ▶ extrinsic model:

$$\mathcal{I}^{coh} = \Upsilon(\beta) \quad \text{and} \quad h(\dot{\beta}, \beta, \mathcal{V}_n, \mathbf{v}_t) = 0$$

for example : $\mathcal{I}^{coh} = \beta \mathcal{I}_{max}^{coh}$

DEM::NSCD Extensions::Explicit Integration

In some cases it is necessary to decrease the time step (sharp body shape, impact with non linear bulk behavior, wave propagation, etc). It leads to reconsider the use of implicit time integrator. Carpenter et al. (1991) proposed a method to respect implicit law (impenetrability) when using an explicit time integrator.

DEM::NSCD Extensions::Explicit Integration

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The key point of the method is to apply the geometrical constraint in the actual (and unknown) configuration.

Considering the time increment $[t, t + h]$ it leads to

$$\begin{cases} \mathbb{M}\ddot{\mathbf{q}}_i = \mathbf{F}_{int}(\dot{\mathbf{q}}_i, \mathbf{q}_i) + \mathbf{F}_{ext}(t_i) + \mathbb{H}_{i+1}\mathbf{r}_i \\ \mathbb{H}_{i+1}^* \mathbf{q}_{i+1} \geq 0 \end{cases}, \quad (1)$$

where $\mathbf{F}_{int}(\dot{\mathbf{q}}_i, \mathbf{q}_i)$ represents the internal forces. As in the previous section, quantities indexed by i (resp. $i + 1$) refer to time t (resp. $t + h$).

DEM::NSCD Extensions::Explicit Integration

In this approach, a second order scheme is taken into account, using the first and second time derivatives of the configuration parameter that appears to be the primary unknown of the problem as contact forces. Thus acceleration and velocity are related to configuration parameter using, for example, a β method,

$$\begin{cases} \dot{q}_i = \frac{1}{1+2\beta} \{ \dot{q}_{i-1} + h(1-\beta)\ddot{q}_{i-1} + \frac{2\beta}{h}(q_{i+1} - q_i) \} \\ \ddot{q}_i = \frac{2}{h^2}(q_{i+1} - q_i - h\dot{q}_i) \end{cases}, \quad (2)$$

where β ($\in [0.5, 1]$) represents a numerical damping parameter.

DEM::NSCD Extensions::Explicit Integration

To take into account the displacement constraints in system (1), the displacement q_{i+1} is decomposed as

$$q_{i+1} = q_{i+1}^{free} + q_{i+1}^c$$

where q_{i+1}^{free} represents the prediction of the displacement without contact forces and q_{i+1}^c the correction due to the contact forces only.

DEM::NSCD Extensions::Explicit Integration

To take into account the displacement constraints in system (1), the displacement q_{i+1} is decomposed as

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where q_{i+1}^{free} represents the prediction of the displacement without contact forces and q_{i+1}^c the correction due to the contact forces only.

In the case of the central different method ($\beta = 0.5$), q_{i+1}^{free} is defined by

$$q_{i+1}^{free} = h^2 \mathbb{M}^{-1} \{ F_{ext}(t_i) - F_{int}(\dot{q}_i, q_i) \} + 2q_i - q_{i-1} \quad (3)$$

To solve the frictional contact problem and to determine the solution of the equation of motion, the couple of unknown (r_i, q_{i+1}^c) solution of the following system must be found

$$\begin{cases} h^2 \mathbb{H}_{i+1}^* \mathbb{M}^{-1} \mathbb{H}_{i+1} r_i = \mathbb{H}_{i+1}^* q_{i+1}^{free} \\ q_{i+1}^c = h^2 \mathbb{M}^{-1} \mathbb{H}_{i+1} r_i \end{cases}, \quad (4)$$

DEM::Multi-Physics

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5 Multi-Physics

- Generality
- Fluid
- Thermal
- Electricity

6 Technical Aspects

7 Bibliography

DEM::Multi-Physics::Generality

It appears more and more works related to the multi-physical extension of classical DEM, the classical feature refers to the mechanical one:

- fluid effect (...)
- thermal effect (Vargas et al., 2001) (Luding et al., 2005) ...
- electrical (Renouf et al., 2007)
- physico-chemical
- etc.

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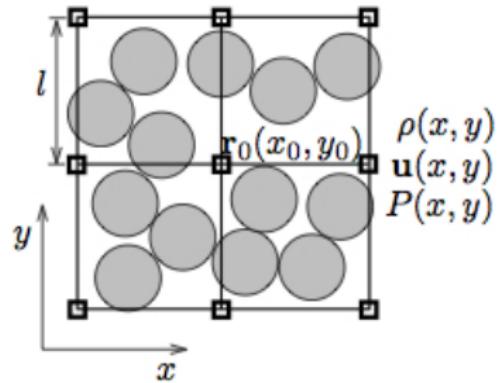
Coupling between mechanics and an added physical model could be performed using various approaches:

- **Serial treatment:** the results of the added physical model is used to compute the mechanical model without “retroaction”.
 - thermal dilatation effects in a granular assembly
- **Staggered treatment:** The new problem is computed using mechanical data in input and output are used to update some mechanical variables.
 - thermal conduction with thermal resistance at contact depending on pressure and thermal dilatation effects in a granular assembly
- **Monolithic treatment:** The problem is solved as a full multi-physical problem where the mechanics and the new physics are computed simultaneously.

DEM::Multi-Physics::Fluid

Modeling gaz grain mixture (see MacNamara et al., 2000).

- granular material with drag force due to fluid pressure (micro)
- fluid mechanics in an evolutive porous material (macro)
- Notations:
 - ▶ P : pressure.
 - ▶ η : fluid viscosity.
 - ▶ $\phi = 1 - \frac{V^G}{V}$: granular material porosity.
 - ▶ κ : permeability of the granular material.
 - ▶ \vec{u} : mean velocity of the grains.

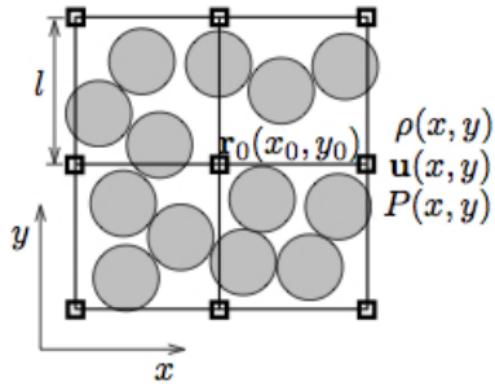


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 - ▶ κ : permeability of the granular material.
 - ▶ \bar{u} : mean velocity of the grains.
 - Hypotheses:
 - ▶ perfect gas.
 - ▶ neglect fluid inertia.
 - ▶ low Reynolds number (Darcy law).
 - ▶ spherical grains (radius r)
Carman-Kozeny :

$$\kappa(\phi) = (r^2/45) \phi^3 / (1 - \phi^2)$$



DEM::Multi-Physics::Fluid

Fluid pressure evolution

- Mass conservation of the fluid and grains :

$$\phi \left(\frac{\partial P}{\partial t} + \vec{u} \cdot \vec{\nabla} P \right) = \vec{\nabla} \cdot \left(P \frac{\kappa(\phi)}{\eta} \vec{\nabla} P \right) - P \vec{\nabla} \cdot \vec{u}$$

DEM::Multi-Physics::Fluid

Fluid pressure evolution

- Mass conservation of the fluid and grains :

$$\phi \left(\frac{\partial P}{\partial t} + \underbrace{\vec{u} \cdot \vec{\nabla} P}_{\text{convection term}} \right) = \vec{\nabla} \cdot \left(P \frac{\kappa(\phi)}{\eta} \vec{\nabla} P \right) - P \vec{\nabla} \cdot \vec{u}$$

- convection term: drag of the fluid due to the moving granular material.

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- convection term: drag of the fluid due to the moving granular material.
- diffusion term: fluid diffusion in the porous granular material.

DEM::Multi-Physics::Fluid

Fluid pressure evolution

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- convection term: drag of the fluid due to the moving granular material.
- diffusion term: fluid diffusion in the porous granular material.
- Biot term: variation of the porous pressure due to evolution of the pore size.

DEM::Multi-Physics::Fluid

Hydrodynamic force

- Notations:

- ▶ V^G : grain volume.
- ▶ $\vec{\nabla} P$: pressure gradient at the center of the grain.

DEM::Multi-Physics::Fluid

Hydrodynamic force

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- Force on the grain due to the fluid pressure gradient :

$$\vec{F}_h = -\frac{V^G}{1-\phi} \vec{\nabla} P$$

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$$\vec{F}_h = -\frac{V^G}{1-\phi} \vec{\nabla} P$$

- the force increases proportionally to the fluid volume around the grain.

DEM::Multi-Physics::Fluid

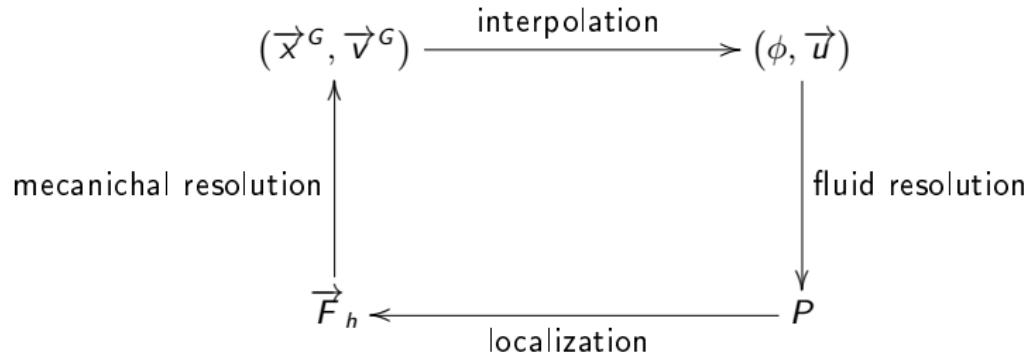
Numerical strategy

- coupling is solved with fixed point method on the grain velocity.

DEM::Multi-Physics::Fluid

Numerical strategy

- coupling is solved with fixed point method on the grain velocity.
- for one iteration :



DEM::Multi-Physics::Fluid

Numerical strategy

- interpolation: interpolation, aux nœuds du maillage utilisé pour le calcul de la pression, de la porosité locale : $\phi_{loc} = 1 - V^G/V_{ref}$, définie au centre des grains.

DEM::Multi-Physics::Fluid

Numerical strategy

- interpolation: interpolation, aux nœuds du maillage utilisé pour le calcul de la pression, de la porosité locale : $\phi_{loc} = 1 - V^G/V_{ref}$, définie au centre des grains.
- fluid resolution: compute pressure and pressure gradient on the mesh node :
 - ▶ “directional” operator splitting,
 - ▶ centered finite difference (space),
 - ▶ Crank-Nicholson (time),
 - ▶ Newton-Raphson (Non linearity)

DEM::Multi-Physics::Fluid

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- localization: compute hydrodynamic force by interpolating (at the grain center), $1/(1-\phi)\vec{\nabla}P$ known at the mesh load.

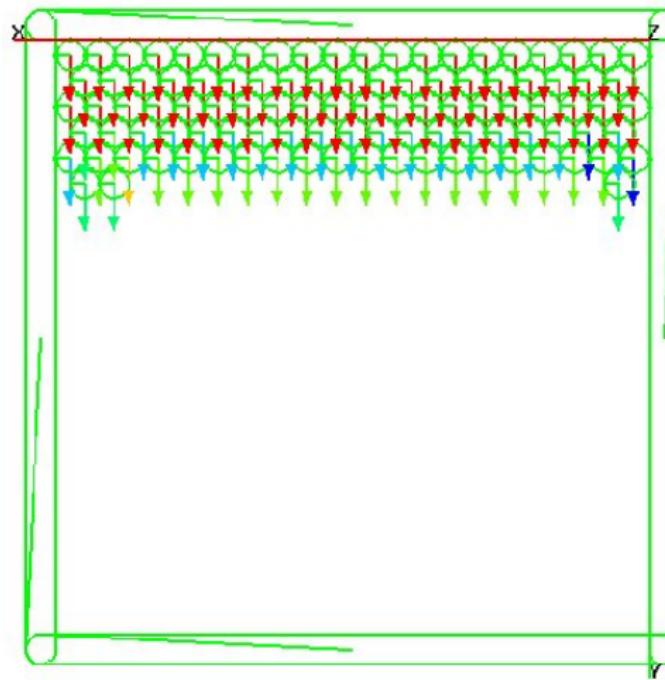
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- localization: compute hydrodynamic force by interpolating (at the grain center), $1/(1-\phi)\vec{\nabla}P$ known at the mesh load.
- mechanical resolution: compute velocity and position with a DEM code

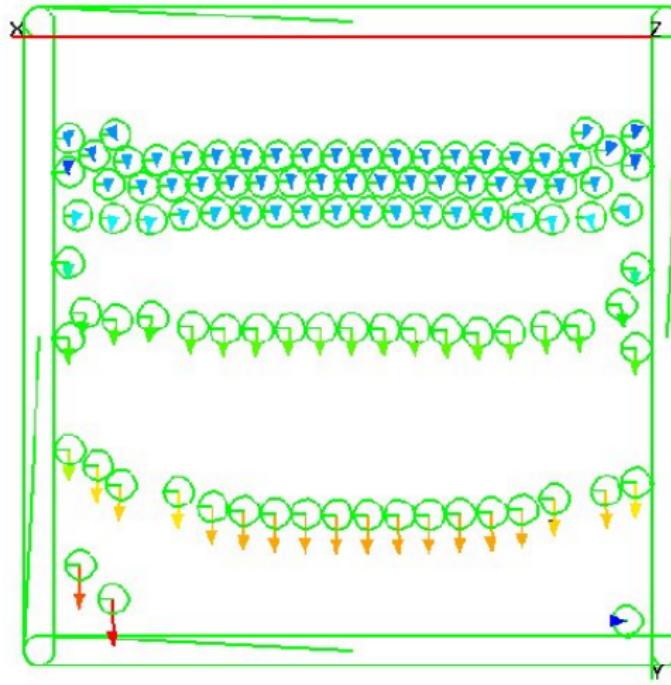
DEM::Multi-Physics::Fluid

Exemple: Sedimentation



DEM::Multi-Physics::Fluid

Exemple: Sedimentation



DEM::Multi-Physics::Thermal

Dilatation effect Resolution Scheme:

Iteration matrix computation (\mathbb{M})

Time loop

Compute temperature

Free velocity computation ($\dot{\mathbf{q}}_{free}$)

Temporary configuration computation(\mathbf{q}_m)

Contact detection (A)

Compute thermal velocity: $U_{th} = d_{th}/h$ (B)

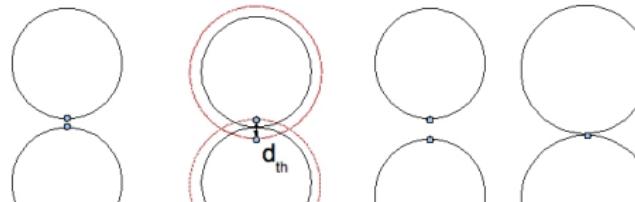
Contact problem resolution

Velocity correction ($\dot{\mathbf{q}}_{i+1}$)

Update of the kinematics and the configuration (C)

Update shapes (D)

Halt criteria



DEM::Multi-Physics::Electricity

As granular assemblies are considered, the formulation of the electrical problem relies on an analogy between an electrical and a contact network. Each particle of the granular assembly is considered as a node of the electrical network while each contact is considered as a branch of it. The formulation of the electrical problem relies on an analogy between an electrical and the contact network of a granular material.

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An linear electrical network is a set of linear dipoles, linked by conductor with weak resistivity. This network is composed of n_c branches (contacts) connected by n_b nodes (particles) and realizing n_m meshes. Thus, a node is a junction of several conductors, a branch a part of the network between two nodes and a mesh a closed run, composed of branch using a node only once.

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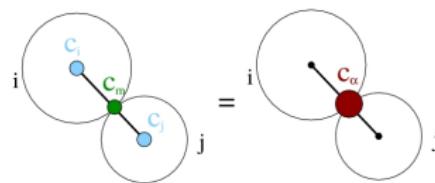
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To determine the global resistivity/conductivity of the sample, two aspect must be considered: the local conductivity of each branch and the relation between each branch of the network.

DEM::Multi-Physics::Electricity::Local formulation

To determine the conductivity of a contact between two particles, both the conductivity of particles and the mechanical conductivity (related to the contact force) must be determined. If the contact indexed by α involved particles i and j , their conductivity will be noted respectively C_i and C_j . The mechanical conductivity will be noted C_m .

Then, the contact conductivity can be expressed as a function of C_i , C_j and C_m :



$$C_\alpha = \frac{C_i C_j}{C_i + C_j + \frac{C_i C_j}{C_m}}. \quad (5)$$

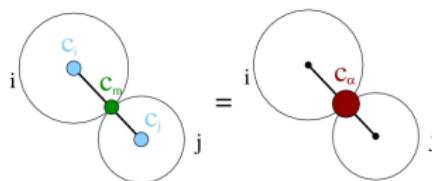
The equation (5) suppose that C_i and C_j as well as C_m are not equal to zero. If one of the conductivity is equal to zero (insulating particle or non contact) then $C_\alpha = 0$.

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Remark : it is possible to take into account more complex local phenomena (oxidation, breakdown,...). These ones will not be evoked here.

DEM::Multi-Physics::Electricity::Global formulation

The global formulation of the electrical problem refers to the first Kirchhoff law and to the Ohm law.

The first Kirchhoff law can be given under a matricial equation as:

$$\mathbb{N}\mathbf{I} = \mathbf{I}_0, \quad (6)$$

where $\mathbb{N} \in \mathbb{R}^{n_b \times n_c}$, $\mathbf{I} \in \mathbb{R}^{n_b}$ and $\mathbf{I}_0 \in \mathbb{R}^{n_b}$. The matrix \mathbb{N} denotes the incidence matrix between the nodes of the network. Its role is equivalent to the one of matrix \mathbb{H} defined in the mechanical section. The vector \mathbf{I}_0 is the intensity vector where each component \mathbf{I}_α is linked to one of the network branches.

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Thus writing the Ohm law for the set of contact, one obtains:

$$I = \mathbb{C}\mathbb{N}^T V. \quad (7)$$

Finally, using Equation (7) in Equation (6) one obtains:

$$\mathbb{N}\mathbb{C}\mathbb{N}^T V = -I_0. \quad (8)$$

where the electrical potential V , expressed in each node of the network, become the primary unknown of the problem. The matrix \mathbb{G} is equal to the product $\mathbb{N}\mathbb{C}\mathbb{N}^T$ and is, as the \mathcal{W} matrix, symmetric semi positive defined.

DEM::Multi-Physics::Electricity::Resolution

The resolution of the electrical problem is realized using the iterative Gauss-Seidel algorithm, used to solve the contact problem. On the same level as the mechanical problem, the electrical problem \mathbb{G} have a multiplicity of solution and thus is strongly dependant of initial condition and the direction of reading of the contact loop.

Gauss-Seidel algorithm

Step 0: Initialization with V^0 non negative.

Step 1: Iteration k

For all i in $\{1, \dots, n_b\}$

Compute $\tilde{V}_i = I_i^0 - \sum_{j < i} \mathbb{G}_{ij} V_j^k - \sum_{j > i} \mathbb{G}_{ij} V_j^{k-1}$

$$V_i^k = \frac{1}{\mathbb{G}_{ii}} \tilde{V}_i$$

Step 3: If error criterion is satisfied then V^k is solution

Else one iterates k and go to **Step 1**.

The error criteria used is a simple relative maximal variation criterion applied on the electrical potential.



DEM::MP::Electricity::Resolution

The construction of the electrical-mechanical problem is easy. For that, the different part of the electrical problem are introduced in the mechanical scheme after the contact resolution and before the correction of the position.

```
i = i + 1 (time loop)
q(i+1) prediction
Contact detection
q(i)free computation
  k = k + 1 (NSGS iteration)
    α = α + 1 (contact loop)
    bkα computation
    Contact problem resolution : (vk+1α, rk+1α) solution
    convergence test
  Electrical problem formulation
  Electrical problem resolution
q(i+1) correction
```

Then, the electrical problem construction is fully dependant of the mechanical problem.
In this scheme, the electrical problem have any influence on the mechanical problem.

DEM::Technical Aspects

1 Preamble

2 Modeling

3 Numerical Strategies

4 NSCD Extensions

5 Multi-Physics

6 Technical Aspects

- Contact detection
- Rotation

7 Bibliography

8 Annexes

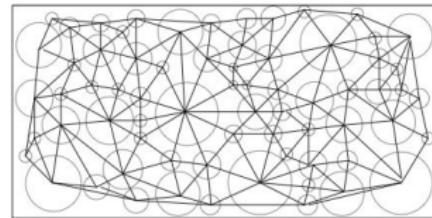
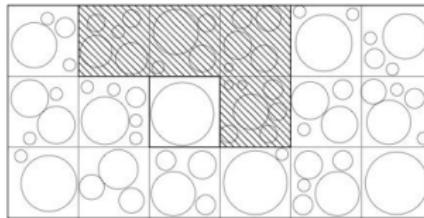
DEM::Technical Aspects::Contact detection

Contact detection becomes quickly a complex problem, using a large part of the CPU time.

This is directly related to the number and to the geometry of the different elements.

A first way to simplify and optimize the process is to perform:

- **a neighborhood construction** based on the sort of closed bodies (surrounding box method, tessellation,etc.)



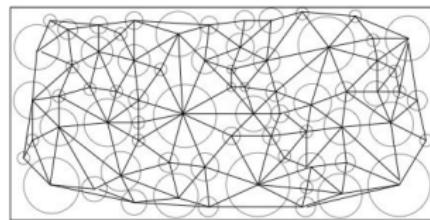
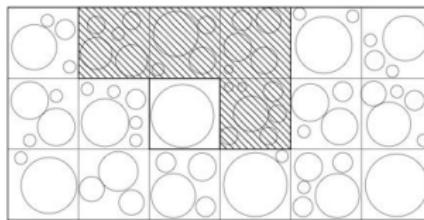
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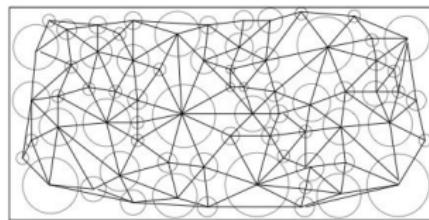
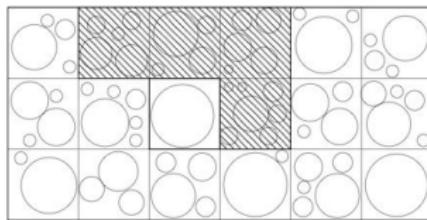
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- **a neighborhood construction** based on the sort of closed bodies (surrounding box method, tessellation,etc.)



- **a rough detection** based on the research of proximal objects (oct-tree, shadow-overlap, separator plan, etc.)
- **an accurate detection** based on the research of proximal points (intersection, projection, etc.)

DEM::Technical Aspects::Rotation

A relevant computation of “rotation” is necessary for

- interaction law: friction, cohesion, rolling friction, etc.
- numerical precision: respect objectivity

Usually geometry is represented in a moving frame (\mathcal{R}_f).

Integrating Euler equation : $\omega^f - \omega^i = h\mathbb{I}^{-1}\mathbf{M}$

→ update the locate frame through the transformation matrix $\mathcal{R}_f = \mathcal{P}\mathcal{R}_i$

Various possibility :

- Euler angles

$$\omega = \dot{\psi}e_1 + \dot{\phi}e_2 + \dot{\zeta}e_3$$

$$\int_i^f \dot{\psi} ds \rightarrow \Delta\Omega_1, \int_i^f \dot{\phi} ds \rightarrow \Delta\Omega_2 \text{ and } \int_i^f \dot{\zeta} ds \rightarrow \Delta\Omega_3$$

$$P = \Delta\Omega_3 \cdot \Delta\Omega_2 \cdot \Delta\Omega_1$$

drawback: indeterminacy

- quaternion

- transformation matrix :

- ▶ linearization : for each frame vector $v_k = \omega \otimes e_k$ then $e_k^f = e_k^i + hv_k$

drawback: lose orthogonality and normality

- ▶ incremental objective integrator (Hughes, 1980), (Geradin et al.,)

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Annexes::Deriving the Lagrangian system

Lets consider the smooth equations of motion of a collection of N continuum media.

The continuum medium is identified at time $t \in [0, T]$ by its volume in \mathbb{R}^d .

The integer $d = 1, 2, 3$ denotes the space dimension, of interior

$$\Omega(t) \subset \mathbb{R}^d, i \in \{1, \dots, N\}$$

and boundary $\partial\Omega(t)$.

If Ω is a deformable continuum medium, the equations of motion are introduced through the principle of virtual powers in a finite strain Lagrangian setting permitting a space-discretization based on a conventional finite element method.

If Ω is assumed to be a rigid body, the equation of motion will be described by a finite set of coordinates.

In both cases, possibly after a space-discretization, the equations of motion will be formulated and treated in a single finite-dimensional framework.

▶ back

Annexes::Deriving the Lagrangian system

A material particle is described by its position, X in a reference frame at $t = 0$ and by its current position $x = \varphi(X, t)$ at time t .

For a Lagrangian description, we also assume we know at least formally the function $X = \psi(x, t)$.

The displacement is defined by $u(x, t) = x - X = x - \psi(x, t)$ and the velocity and the acceleration are denoted by \dot{u} and \ddot{u} .

Most of the Lagrangian variables expressed in terms of X are denoted by capitals letters, for instance, $U(X, t)$ for the displacement, and denoted by lower case for the associated Eulerian variables, in this case $u(x, t)$.

This convention can be summarized by $u(x, t) = u(\varphi(X, t), t) = U(X, t)$.

▶ back

Annexes::Deriving the Lagrangian system

Starting from the equation of motion in Eulerian coordinates,

$$\operatorname{div} \sigma(x, t) + \rho(x, t)b(x, t) = \rho(x, t)\ddot{u}(x, t), \forall x \in \Omega(t),$$

where $\sigma(x, t)$ is the Cauchy stress tensor and $b(x, t)$ is the density of body forces, the principle of virtual power states that

$$\int_{\Omega(t)} (\ddot{u}(x, t) - b(x, t)) \hat{v}(x, t) dm(x, t) = \int_{\Omega(t)} \operatorname{div} \sigma(x, t) \hat{v}(x, t) d\omega(x, t), \quad (9)$$

for all virtual velocities denoted by $\hat{v}(x, t)$. The measure $d\omega(x, t)$ denotes the Lebesgue measure in \mathbb{R}^d at x and the measure $dm(x, t) = \rho(x, t) d\omega(x, t)$ is the mass measure. With the help of the Green formulas, the principle of virtual power is usually reformulated as

$$\begin{aligned} \int_{\Omega(t)} (\ddot{u}(x, t) - b(x, t)) \hat{v}(x, t) dm(x, t) &= - \int_{\Omega(t)} \sigma(x, t) : \nabla \hat{v}(x, t) d\omega(x, t) \\ &\quad + \int_{\partial\Omega_F(t)} t(x, t) \hat{v}(x, t) ds(x, t) + \int_{\Gamma_c^i(t)} r(x, t) \hat{v}(x, t) ds(x, t) \end{aligned} \quad (10)$$

where $A : B = A_{ij}B^{ij}$ is the double contracted tensor product, and $t(x, t) = \sigma(x, t).n(x, t)$ is the applied forces on the boundary of outward normal n and $r(x, t)$ the reaction forces due to the cohesive interface. The measure $ds(x, t)$ is the

Annexes::Deriving the Lagrangian system

The symmetry of the Cauchy stress tensor in absence of density of momentum allows one to introduce the symmetric deformation rate tensor,

$$D(x, t) = \frac{1}{2}(\nabla^T v(x, t) + \nabla v(x, t)) \quad (11)$$

leading to the standard expression of the virtual power of the internal forces of cohesion

$$\hat{\mathcal{P}}_{int} = - \int_{\Omega(t)} \sigma(x, t) : \nabla \hat{v}(x, t) d\omega(x, t) = - \int_{\Omega(t)} \sigma(x, t) : \hat{D}(x, t) d\omega(x, t) \quad (12)$$

In order to formulate the principle of virtual power in a total Lagrangian framework, the second Piola-Kirchhoff tensor,

$$S(X, t) = F^{-1} \det(F) \sigma^T F^{-T}$$

is introduced, where $F = \frac{\partial x}{\partial X} = \frac{\partial \varphi(X, t)}{\partial X}$ is the deformation gradient.

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Annexes::Deriving the Lagrangian system

The virtual power of the internal forces is then rewritten, as

$$\hat{\mathcal{P}}_{int} = - \int_{\Omega(t)} \sigma(x, t) : \nabla \hat{v}(x, t) d\omega(x, t) = - \int_{\Omega(0)} S(X, t) : \hat{L}(X, t) d\Omega(X, 0) \quad (13)$$

where $L = \dot{F}$.

Finally, the principle of virtual power in a total finite strain Lagrangian framework in terms of the convected Lagrangian variable X , is

$$\begin{aligned} \int_{\Omega(0)} (\ddot{U}(X, t) - B(X, t)) \hat{V}(X, t) dM(X, 0) &= - \int_{\Omega(0)} S(X, t) : \hat{L}(X, t) d\Omega(X, 0) \\ &\quad + \int_{\partial\Omega(0)} T(X, t) \hat{V}(X, t) dS(X, t) + \int_{\Gamma_c^i(0)} R(X, t) \hat{V}(X, t) dS(X, t) \end{aligned} \quad (14)$$

where the applied forces laws on the boundary satisfies

$T(X, t) = S(X, t) \cdot F^T(X, t) \cdot N(X, t)$ and $R(X, t) = S(X, t) \cdot F^T(X, t) \cdot N(X, t)$. It is noteworthy that the interactions between bodies that are taken into account in this model are only given by the forces through the interface with unilateral contact and friction.



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Annexes:: Deriving the Lagrangian system

For the constitutive material laws, a large panel of models can be taken into account in this framework and in the numerical applications. The formulation of the constitutive laws is based on the standard thermodynamics of irreversible processes or based on a variational formulation of incremental stress-strain relation deriving from a pseudo elastic potential.

If the bulk response of the material is linear elastic

$$S(X, t) = K(X, T) : E(X, t), \quad (15)$$

where E is the Green-Lagrange strain tensor,

$$E(X, t) = \frac{1}{2}(F^T(X, t)F(X, t) - I(X, t)), \quad (16)$$

the tensor I is the identity tensor and $K(X, T)$ is the fourth order tensor of elastic properties.

[▶ back](#)

Annexes::Deriving the Lagrangian system

The finite element discretization is conventional and is based on this principle of virtual power in this total Lagrangian framework. Choosing some isoparametric element leads to the following approximation

$$U(X, t) = \sum_h N^h(X, t) U_h(t), \quad \dot{u}(X, t) = \sum_h N^h(X, t) \dot{U}_h(t), \quad \ddot{u}(X, t) = \sum_h N^h(X, t) \ddot{U}_h(t) \quad (17)$$

where N^h are the shape functions and U_h the finite set of displacement at nodes.

Substituting this approximation into the principle of virtual power and simplifying with respect to the virtual field yields a space-discretized equation of motion of the form

$$M(U_h) \ddot{U}_h + F(t, U_h, \dot{U}_h) = R, \quad (18)$$

where $M(U_h)$ is the consistent or lumped mass matrix, the vector $F(t, U_h, \dot{U}_h)$ collects the internal and external discretized forces and R are the discretized forces due to the interaction.

▶ back

Annexes::Deriving the Lagrangian system

In rigid body mechanics, it is assumed that the power of the cohesion internal forces vanishes for a rigid motion given by the following set of virtual velocity field,

$$\mathcal{V} = \{\hat{v}(x, t) = \hat{v}_O(t) + \hat{\omega}(t) \times (x - x_O), \forall x \in \Omega(t)\}, \quad (19)$$

where O is a geometrical point fixed with respect to the body, x_O is the position of this point $v_O(t)$ is its velocity, and $\omega(t)$ the angular velocity of the body at O . This assumption yields

$$\int_{\Omega(t)} (\ddot{u}(x, t) - b(x, t)) \hat{v}(x, t) dm(x, t) = \int_{\partial\Omega(t)} t(x, t) \hat{v}(x, t) ds(x, t), \quad \forall \hat{v}(x, t) \in \mathcal{V} \quad (20)$$

The equation of motion can be derived choosing a particular virtual velocity as:

$$\left\{ \begin{array}{l} \frac{d}{dt} \int_{\Omega(t)} \dot{u}(x, t) dm(x, t) = \int_{\Omega(t)} b(x, t) dm(x, t) + \int_{\partial\Omega(t)} t(x, t) ds(x, t), \\ \frac{d}{dt} \int_{\Omega(t)} (x - x_O) \times \dot{u}(x, t) dm(x, t) = \int_{\Omega(t)} (x - x_O) \times g(x, t) dm(x, t) \\ \qquad \qquad \qquad + \int_{\partial\Omega(t)} (x - x_O) \times t(x, t) ds(x, t). \end{array} \right. \quad (21)$$

Annexes::Deriving the Lagrangian system

Various descriptions of the equations of motion of a rigid body can be deduced from the principle of virtual power choosing particular kinematics. Without going into further details, the Newton-Euler formulation can be chosen to write the kinematics with respect to the center of mass G_i of the body Ω in Eulerian coordinates:

$$\begin{cases} \dot{u}(x, t) = v_{G_i}(t) + \omega_i(t) \times (x - x_{G_i}), \\ \ddot{u}(x, t) = \dot{v}_{G_i}(t) + \dot{\omega}_i(t) \times (x - x_{G_i}) + \omega_i(t) \times (\omega_i(t) \times (x - x_{G_i})). \end{cases} \quad (22)$$

▶ back

Annexes::Deriving the Lagrangian system

Substituting (22) into the equations of motion (21) yields the well-known Newton-Euler equations,

$$\begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \frac{d}{dt} \begin{bmatrix} v_{G_i}(t) \\ \omega_i(t) \end{bmatrix} + \begin{bmatrix} 0 \\ \omega_i(t) \times I\omega_i(t) \end{bmatrix} = \begin{bmatrix} f_{ext}(t) \\ m_{ext}(t) \end{bmatrix}, \quad (23)$$

where

$$M = \int_{\Omega(t)} dm(x, t) = \int_{\Omega(0)} dM(X, 0),$$

$$I = \int_{\Omega(t)} (x - x_{G_i})^T (x - x_{G_i}) dm(x, t) = \int_{\Omega(0)} (X - X_{G_i})^T (X - X_{G_i}) dM(X, 0),$$

$$f_{ext}(t) = \int_{\Omega(t)} b(x, t) dm(x, t) + \int_{\partial\Omega(t)} t(x, t) ds(x, t),$$

$$m_{ext}(t) = \int_{\Omega(t)} (x - x_{G_i}) \times b(x, t) dm(x, t) + \int_{\partial\Omega(t)} (x - x_{G_i}) \times t(x, t) ds(x, t).$$

Annexes::Deriving the Lagrangian system

Usually, a second order form of the dynamics is obtained with the help of the following parametrization of the vector ω_i ,

$$\omega_i(t) = D_i(\Psi, t)\dot{\Psi}_i(t), \quad (25)$$

where $D(\Psi, t)$ is supposed to be a diffeomorphism. For a collection of N rigid bodies, a usual way is to introduce a set of generalized coordinates z such that

$$z = \left[[x_{G_i}, \Psi_i]_{i \in \{1 \dots N\}} \right]^T \quad (26)$$

assuming that the positions and the orientations of the bodies are uniquely determined by z . With this variable, after some algebraic manipulations, the equations of motion can be written as:

$$M(z)\ddot{z} + F(t, z, \dot{z}) = r \quad (27)$$

It is noteworthy that this formulation allows us to add some internal forces between bodies expressed in terms of the generalized coordinates z .

▶ back

Annexes::Deriving the Lagrangian system

Clearly, the equations of motion can also be obtained straightforwardly thanks to the Lagrangian formalism postulating the existence of the Lagrangian of the system,

$$L(z, \dot{z}) = T(z, \dot{z}) - V(z),$$

composed of the kinetic energy,

$$T(z, \dot{z}) = \frac{1}{2} \dot{z}^T M(z) \dot{z}$$

and the potential energy of the system, $V(z)$. The Lagrange's equations can be written as

$$\frac{d}{dt} \left(\frac{\partial L(z, \dot{z})}{\partial \dot{z}_i} \right) - \frac{\partial L(z, \dot{z})}{\partial z_i} = Q_i(z, t), \quad i \in \{1 \dots n\}, \quad (28)$$

where the vector $Q(z, t) \in \mathbb{R}^n$ denotes the set of generalized forces.

 back

Annexes::Deriving the Lagrangian system

With some standard algebraic manipulations, the Lagrange equations (28) can be put in a more usual form:

$$M(z) \frac{d\dot{z}}{dt} + N(z, \dot{z}) = Q(z, t) - \nabla_z V(z) \quad (29)$$

where the vector $N(z, \dot{z}) = \left[\frac{1}{2} \sum_{k,l} \frac{\partial M_{ik}}{\partial z_l} + \frac{\partial M_{il}}{\partial z_k} - \frac{\partial M_{kl}}{\partial z_i}, i = 1 \dots n \right]^T$ collects the

nonlinear inertial terms i.e., the gyroscopic accelerations.

If we allow one to introduce non linear interactions between bodies of the system and external applied forces which do not derived from a potential, we will use the following more general form for the equation of motion:

$$M(z)\ddot{z} + F(t, z, \dot{z}) = 0 \quad (30)$$

where $F : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$ collects the internal non linear interactions between bodies which are not necessarily derived from a potential and the external applied loads.

▶ back

Annexes:: Deriving the linear system

En linéaire : petites déformations, comportement linéaire, etc.

$$\underline{\underline{F}}(q, u, t) = -Kq - Cu$$

où : $K \in \mathcal{M}^{n \times n}$ matrice de rigidité, $C \in \mathcal{M}^{n \times n}$ matrice de viscosité.

Le résidu libre s'écrit :

Annexes::Deriving the linear system

Aussi le problème global s'écrit :

$$\begin{aligned}\tilde{M}u_f &= h\tilde{r}_{free} + hr_f \\ q_f &= q_i + h((1-\theta)u_i + \theta u_f) = q_m + h\theta u_f\end{aligned}$$

avec

$$\begin{aligned}\tilde{M} &= M + h\theta C + h^2\theta^2 K \\ h\tilde{r}_{free} &= [M - h(1-\theta)C - h^2\theta(1-\theta)K] u_i - \\ &\quad hKq_i + h[\theta P(t_f) + (1-\theta)P(t_i)]\end{aligned}$$

Annexes::Deriving the linear system

Lecture; initialisations

Boucle en temps

Calcul du résidu libre (\tilde{r}_{free})

Calcul d'une position des corps (q_m)

Détection du contact

Résolution du problème avec contact

Actualisations: cinématique, positions

Test d'arrêt

Annexes::Deriving the linear system

Passage au cas non linéaire quand :

- grandes déformations,
- comportement non linéaire,
- H et H^* dépendent de la solution.

Nécessite une méthode de résolution de système non linéaire (Newton-Raphson) adaptée pour traiter la non différentiabilité des fonctionnelles.

Annexes::Deriving the linear system

Nous utilisons une méthode de Newton dédiée aux équations généralisées [?, ?, ?].
On entend par équations généralisées une écriture comme suit :

$$0 \in f(x) + \mathcal{N}_C(x) \quad (31)$$

où $f(x)$ est un opérateur non linéaire régulier et $\mathcal{N}_C(x)$ est le cône normal à un convexe fermé non vide C de \mathbb{R}^n :

$$\mathcal{N}_C(x) = \begin{cases} \{y \in \mathbb{R}^n / y^T (x^* - x) \leq 0 \quad \forall x^* \in C\} & \text{si } x \in C \\ \emptyset & \text{si } x \notin C \end{cases}$$

Quand C est \mathbb{R}^n , on a $\mathcal{N}_{\mathbb{R}^n}(x) = \{0\}$ et l'équation à résoudre se résume à $f(x) = 0$.

Annexes::Deriving the linear system

De plus (31) est équivalente à l'inéquation variationnelle :

$$x \in C, \quad \forall x^* \in C, \quad f(x)^T (x^* - x) \geq 0$$

A chaque incrément de temps pour une itération $j + 1$ de la méthode de Newton, le problème à résoudre va s'écrire :

$$\begin{cases} \text{Trouver } x^{j+1} \text{ tel que :} \\ 0 \in f(x^j) + \nabla_x f(x^j)(x^{j+1} - x^j) + \mathcal{N}_C(x^{j+1}) \end{cases}$$

Annexes::Deriving the linear system

Le problème de contact frottant en vitesse, peut s'écrire sous une forme identique à (31) :

Trouver $u \in T_\varphi \Psi, R_N \in \mathbb{R}^+, R_T \in C(\mu R_N)$ telle que :

$$0 \in \begin{bmatrix} \mathcal{L}(u, R_N, R_T) \\ U_N \\ U_T \end{bmatrix} + \mathcal{N}_C \begin{bmatrix} u \\ R_N \\ R_T \end{bmatrix}$$

avec

$$\begin{aligned} \mathcal{L}(u, R_N, R_T) &= M(u - u_i) - \\ &\quad h((1 - \theta)(\underline{F}(q_i, u_i, t_i) + P(t_i)) + \\ &\quad \theta(\underline{F}(q, u, t_f) + P(t_f))) \\ &\quad - (\underline{H}_N(u)R_N + H_T(u)R_T) \end{aligned}$$

Avec $C = \mathbb{R}^{ndf} \times \mathbb{R}^+ \times C(\mu R_N)$.

Annexes::Deriving the linear system

A un incrément donné, à l'itération $(j + 1)$ de la méthode de Newton-Raphson, le problème à résoudre est :

soient (u^0, R_N^0, R_T^0) donnés; trouver

$u^{j+1} \in T_\varphi \Psi$, $R_N^{j+1} \in \mathbb{R}^+$ et $R_T^{j+1} \in C(\mu R_N^{j+1})$ tels que :

$$0 \in \begin{bmatrix} \mathcal{L}^j \\ U_N^j \\ U_T^j \end{bmatrix} + \begin{bmatrix} \nabla_{u, R_N, R_T} \mathcal{L}^j \\ \nabla_{u, R_N, R_T} U_N^j \\ \nabla_{u, R_N, R_T} U_T^j \end{bmatrix} \begin{bmatrix} du^{j+1} \\ R_N^{j+1} - R_N^j \\ R_T^{j+1} - R_T^j \end{bmatrix} \quad (32)$$

$$+ \mathcal{N}_C \begin{bmatrix} u^{j+1} \\ R_N^{j+1} \\ R_T^{j+1} \end{bmatrix}$$

...

Annexes::Deriving the linear system

...

avec:

$$\begin{aligned}
 \nabla_{u, R_N, R_T} \mathcal{L}^j &= [\nabla_u \mathcal{L}^j \quad -H_N(u^j) \quad -H_T(u^j)] \\
 \nabla_{u, R_N, R_T} U_N^j &= \begin{bmatrix} \nabla_u U_N^j & 0 & 0 \end{bmatrix} = \begin{bmatrix} \Delta H_N^*(u^j) & 0 & 0 \end{bmatrix} \\
 \nabla_{u, R_N, R_T} U_T^j &= \begin{bmatrix} \nabla_u U_T^j & 0 & 0 \end{bmatrix} = \begin{bmatrix} \Delta H_T^*(u^j) & 0 & 0 \end{bmatrix} \\
 \nabla_u \mathcal{L}^j &= M + h\theta C(u^j) + h^2 \theta^2 K(u^j) \\
 &\quad - \nabla_u H_N^j R_N^j - \nabla_u H_T^j R_T^j = \hat{M} \\
 \mathcal{L}^j &= \mathcal{L}(u^j, R_N^j, R_T^j) \\
 du^{j+1} &= u^{j+1} - u^j
 \end{aligned} \tag{33}$$

Annexes::Deriving the linear system

On peut extraire trois contributions :

- équation de la dynamique :

$$\begin{aligned}\hat{M} u_f^{j+1} &= h \hat{r}_{free}^{j+1} + h r_f^{j+1} \\ q_f^{j+1} &= q_i + h((1 - \theta)u_i + \theta u_f^{j+1}) = q_m + h\theta u_f^{j+1}\end{aligned}$$

où :

$$\begin{aligned}h \hat{r}_{free} &= \hat{M} u_f^j + M(u_i - u_f^j) + \\ &\quad h[(1 - \theta)(\underline{F}(q_i, u_i, t_i) + P(t_i)) + \\ &\quad \theta(\underline{\underline{F}}(q^j, u^j, t_f) + P(t_f))]\end{aligned}$$

Annexes::Deriving the linear system

- contact :

sous forme d'inégalité variationnelle :

$$\begin{cases} R_N^{j+1} \in \mathbb{R}^+ \quad \forall S_N \in \mathbb{R}^+ \\ \left[U_N^j + \Delta H_N^*(u^j) \ du^{j+1} \right] \left[S_N - R_N^{j+1} \right] \geq 0 \end{cases}$$

ou sous forme de relation de complémentarité :

$$R_N^{j+1} \geq 0 \quad \left[U_N^j + \Delta H_N^*(u^j) \ du^{j+1} \right] \geq 0$$

$$R_N^{j+1} \cdot \left[U_N^j + \Delta H_N^*(u^j) \ du^{j+1} \right] = 0$$

Annexes::Deriving the linear system

- frottement :

sous forme d'inégalité variationnelle :

$$\begin{cases} R_T^{j+1} \in C(\mu R_N^{j+1}) \quad \forall S_T \in C(\mu R_N^{j+1}) \\ \left[U_T^j + \Delta H_T^*(u^j) \ du^{j+1} \right] \left(S_T - R_T^{j+1} \right) \geq 0 \end{cases}$$

ou sous forme de loi à seuil :

$$\|(R_T^{j+1})\| \leq \mu R_N^{j+1} \text{ avec:}$$

$$\|(R_T^{j+1})\| < \mu R_N^{j+1} \Rightarrow \left[U_T^j + \Delta H_T^*(u^j) \ du^{j+1} \right] = 0$$

$$\|(R_T^{j+1})\| = \mu R_N^{j+1} \Rightarrow \exists \lambda \geq 0 \\ \left[U_T^j + \Delta H_T^*(u^j) \ du^{j+1} \right] = -\lambda R_T^{j+1}$$

Annexes::Deriving the linear system

Si on admet que H^* varie peu sur le pas de temps alors :

$$U^j + \Delta H^*(u^j) du^{j+1} = H^*(u^j) U^{j+1}$$

Annexes::Deriving the linear system

Boucle en temps

Calcul d'une position des corps (q_m)

Détection du contact

Boucle de Newton Raphson ($j + 1$)

Calcul de la matrice des itérations (\hat{M})

Calcul du résidu libre (\hat{r}_{free}^{j+1})

Résolution du problème avec contact

Correction du déplacement (q_f^{j+1})

Test de convergence de Newton-Raphson

Actualisations : cinématique, positions

Test d'arrêt

Annexes::Various writings of frictional contact

Contact :

- Condition de complémentarité en déplacement (loi de Signorini):

$$g \geq 0, \quad R_N \geq 0, \quad gR_N = 0$$

- Inégalité variationnelle :

$$\forall S_N \in \mathbb{R}^+ \quad g(S_N - R_N) \geq 0$$

- Inclusion sous différentielle :

$$-g \in \partial \Psi_{\mathbb{R}^+}(R_N) \text{ où } \Psi_{\mathbb{R}^+}(g) = \begin{cases} 0 & \text{si } R_N \geq 0 \\ +\infty & \text{sinon} \end{cases}$$

Annexes::Various writings of frictional contact

Frottement de Coulomb : $C(\mu R_N) = \{S_T; \|S_T\| \leq \mu R_N\}$

- loi à seuil :

$$\|R_T\| \leq \mu R_N \text{ si } U_T \neq 0 \text{ alors } \|R_T\| = -\mu R_N U_T / \|U_T\|$$

- Inégalité variationnelle :

$$\forall S_T \in C(\mu R_N) \quad U_T.(S_T - R_T) \geq 0$$

- Inclusion sous différentielle :

$$-U_T \in \partial \Psi_{C(\mu R_N)}(R_T)$$

$$\text{où } \Psi_{C(\mu R_N)}(R_T) = \begin{cases} 0 \text{ si } R_T \in C(\mu R_N) \\ +\infty \text{ sinon} \end{cases}$$

Annexes::Various writings of frictional contact

En dynamique il est plus naturel de formuler les relations de contact unilatéral en vitesse :
A un temps initial t_0 on a $g(t_0) \geq 0$

$$\forall t > t_0, \text{ si } g(t) \leq 0$$

alors

$$U_N \geq 0, R_N \geq 0, U_N R_N = 0$$

On peut préférer d'autres formulations :

- inégalité variationnelle :

$$\forall S_N \geq 0 \quad U_N(S_N - R_N) \geq 0$$

- inclusion sous différentielle :

$$-U_N \in \partial \Psi_{R^+}(R_N) \text{ où } \Psi_{R^+}(R_N) = \begin{cases} 0 \text{ si } R_N \geq 0 \\ +\infty \text{ sinon} \end{cases}$$

Se démontre en utilisant $\dot{g} = U_N$.

Attention non trivial !