Numerical Modeling of granular materials with multi physics coupling. Application to the analysis of granular flow

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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.
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.
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.
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).

 Various situations

“binary interaction”     “ ?? ”     “composite - continuous”

All the situations can’t be addressed easily by DEMs.
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.
Considering *divided media* it exists various space scales:

- **Microscopic**
- **Mesoscopic**
- **Macroscopic**
Considering **divided media** it exists various space scales:

- microscopic
- mesoscopic
- macroscopic

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

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

**Drawbacks**: building a model with the relevant phenomenological parameters and identifying the parameters.
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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
     - Equations of motion
     - Interaction treatment
     - Local-Global mapping
     - Interaction law
   - Non Smooth Dynamic
     - Equations of motion
     - Interaction law
     - Shock law
   - Conclusion

3 Numerical Strategies

4 Technical Aspects

5 NSCD Extensions

6 Multi-Physics

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

\[ M(q, t) \ddot{q} = F(q, \dot{q}, t) + P(t) + r, \]  

(1)

where

- \( q \in \mathbb{R}^n \) represents the vector of generalized degrees of freedom,
- \( \dot{q} \in \mathbb{R}^n \) the generalized velocities,
- \( r \in \mathbb{R}^n \) the contact forces,
- \( P(t) \) the external forces,
- \( F(q, \dot{q}, t) \) the internal force (deformable bodies) and the nonlinear inertia terms (centrifugal and gyroscopic),
- \( M(q, t) : \mathbb{R}^n \mapsto M^{n \times n} \) the inertia matrix.

Initial and boundary conditions must be added to fully describe the evolution of the system.
Considering a rigid component, a more suitable dynamical equation may be used introducing the \( \mathbf{v} \) and \( \omega \), the translation and rotation velocities of the center of mass.

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

\[
\begin{align*}
\mathbf{M} \ddot{\mathbf{v}} &= \mathbf{P}(t) + \mathbf{r} \\
\mathbf{I} \dot{\omega} &= -\omega \wedge (\mathbf{I} \omega) + \mathbf{M}_p(t) + \mathbf{M}_r
\end{align*}
\]

where

- \( \mathbf{P}(t) \) and \( \mathbf{r} \) represent respectively the resultant of external and contact forces,
- \( \mathbf{M}_p(t) \) and \( \mathbf{M}_r \) represent respectively the momentum due to external and contact forces,
- \( \mathbf{M} \) and \( \mathbf{I} \) represents respectively the mass and the inertia matrices.

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

The choice of angle parameters is very important, especially in 3D (inertia frame mapping, Euler angles, quaternion, etc.)
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.
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

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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.
Implicitly DEMs rely on the following hypotheses:

1. The deformation concerns only the contact point neighborhood.
2. Components of the system may be considered as rigid.
3. The contact area is small behind the size of the component; the locus of interaction may be supposed as punctual.
4. Interactions are binary (no effect of connected interaction by particle on their behavior); interaction law depends only on related component.

At least, for every potential contact $\alpha$, it will be determined:

- Contact point coordinates ($t_\alpha, n_\alpha, s_\alpha$);
- The gap ($g_\alpha$), i.e., the algebraic distance between two bodies;
- The contact relative velocity between the two bodies ($U_\alpha$).

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Contact description is a key point of DEMs.
Two sets of unknowns:

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

Related by kinematic relations:

\[
g = D(q)\\
U = \mathbb{H}^*(q)\dot{q} = \nabla_q D(q)\dot{q}
\]
Lets consider two rigid bodies.

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

\[ \mathbf{v}(M) = \mathbf{v}(G) + \omega \times \mathbf{l} \]

where \( \mathbf{l} \) represents the vector between the inertia center \( (G) \) and the contact point \( (M) \),

Then it is possible to write the relative velocity between the two points \( (M_i) \) \((i \text{ bodies})\) and \( (M_j) \) \((j \text{ bodies})\):

\[ \mathbf{U}_{X,Y,Z} = \mathbf{v}(M_i) - \mathbf{v}(M_j) = \mathbf{v}(G_i) - \mathbf{v}(G_j) + \omega_i \times \mathbf{l}_i - \omega_j \times \mathbf{l}_j \]

which can be written in a "matricial" way:

\[
\begin{bmatrix}
\mathbf{v}(G_i) \\
\omega_i \\
\mathbf{v}(G_j) \\
\omega_j 
\end{bmatrix} = H_{i,j}^*(\mathbf{q}) \dot{\mathbf{q}}
\]

And expressed in a local frame as:

\[
\begin{bmatrix}
\mathbf{t}^T \\
\mathbf{n}^T \\
\mathbf{s}^T
\end{bmatrix} H_{i,j}^*(\mathbf{q}) \dot{\mathbf{q}} = \mathbb{H}_{i,j}^*(\mathbf{q}) \dot{\mathbf{q}}
\]
More generally, using kinematic relations, one can write for a given contact $\alpha$:

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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:

$$r_\alpha = H_\alpha(q) R_\alpha,$$

where $H_{\alpha}^*(q)$ is the transpose of $H_\alpha(q)$. 

Remark: even if $H_{\alpha}^*(q)$ and $H_\alpha(q)$ have good theoretical properties (surjectivity and injectivity), it is not necessary the case for $H_{\alpha}^*$ and $H_\alpha$. Loose of these properties is due to the introduction of kinematic relations between contacts.
More generally, using kinematic relations, one can write for a given contact $\alpha$:

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In the following, operators mapping all the local and global unknowns are introduced:

$$\mathbb{H}(q) : R = \{R_{\alpha}\} \rightarrow r = \sum_{\alpha=1}^{n_c} \mathbb{H}_{\alpha}(q)R_{\alpha}$$

$$\mathbb{H}^*(q) : \dot{q} \rightarrow U = \{U_{\alpha}\} = \{\mathbb{H}^*_{\alpha}(q)\dot{q}\}$$

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

1 - interaction behavior represents only what happens at the boundary scale: impenetrability, plastic deformation of asperities, capillarity effects, friction, wear, etc.

2 - interaction behavior represents 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.
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Recover elastic and plastic behavior of the media. No indeterminacy.

From a “mathematical” point of view:

1 - Set value function, defined by an implicit law:
\[ h(R, U, g) = \text{true} \]

2 - Function, defined by an explicit law:
\[ R = f(U, g) \]
explicit laws

- Normal part: $\delta = \min(-g, 0)$
  - Hertz law: $R_n = k_n \delta^{3/2}$
  - Hook law with viscous damping: $R_n = \max(0, K_n \delta + \eta_n m_{\text{eff}} U_n \cdot d_{\text{eff}})$

- JKR cohesion law: $R_n = k_n \delta^{3/2} + \eta_n \sqrt{m_{\text{eff}} U_n} - \gamma_n \sqrt{\delta r_{\text{eff}}}$

where $K_n$ is the contact stiffness, $\eta_n$ viscosity coefficient and $\gamma_n$ contact cohesion.

$U_n$ represents the relative velocity between particles and $d (= d_n)$ is defined as center-center vector, $m_{\text{eff}}$ and $r_{\text{eff}}$ represent respectively the effective mass and radius associated to the contact.
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Normal part \((\delta =< -g >^+)\)

- Hertz law: \(R_n = k_n \delta^{3/2} = K_n(\delta)\delta\)
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explicit laws

Normal part ($\delta = < -g >^+$)

For Hertz law $K_n = \frac{E \sqrt{r_{\text{eff}} \delta}}{3(1-\nu^2)}$.

Behavior parameter are "structure" dependant (i.e. geometry).

For a given pressure $P$, the stiffness level may be characterized by:

$$\kappa = \left(\frac{E}{P}\right)^{2/3} \text{ (Hertz)} \quad \text{or} \quad \kappa = \frac{K_n}{P r_{\text{eff}}^{d-2}} \text{ (Hook)}$$

So the elastic deflection $\delta \propto \frac{r_{\text{eff}}}{\kappa}$

Remarks:

- rigid grains if $\kappa \to \infty$. "Good" value are 10000.
- Quasi-static problem: $\delta \ll < -g >^+$ ($< g >^+$ interstice between grains)
- Flow problem: $\tau \ll < g >^+ r_{\text{eff}}^{-\gamma}$ ($\tau$ duration of contact)
explicit laws

Normal part \((\delta = < -g >^+)\)

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

\[
\mathit{m}_\text{eff} \frac{d^2 \delta}{dt^2} + \eta_n \frac{d\delta}{dt} + K_n \delta = 0
\]

- critical damping \(\eta_n^c = 2\sqrt{\mathit{m}_\text{eff} K_n}\). \(\alpha_n = \frac{\eta_n}{\eta_n^c}\)

- pulsation \(\omega = \sqrt{\frac{K_n}{\mathit{m}_\text{eff}} (1 - \alpha_n^2)}\) and contact duration \(\tau = \pi / \omega\)

- restitution coefficient \(e_n = \exp[-\frac{\pi \alpha_n}{\sqrt{1 - \alpha_n^2}}]\)

Remarks:
- \(\eta_n \leq \eta_n^c\)
- For Hertz law, same results with a varying \(K_n\)
explicit laws

Tangential part

- viscous law with Coulomb threshold:
  \[ R_{t}^{Tr} = -\eta_t m_{eff} U_t \]
  if \( ||R_{t}^{Tr}|| \geq \mu |r_n| \) then \( R_t = \mu |r_n| \frac{R_{t}^{Tr}}{||R_{t}^{Tr}||} \) else \( R_t = R_{t}^{Tr} \)

- incremental elastic law with Coulomb threshold:
  a previous \( R_t \) is known, \( \Delta R_t = K_t h U_t \) and \( R_{t}^{Tr} = R_t + \Delta R_t \)
  if \( ||R_{t}^{Tr}|| \geq \mu |r_n| \) then \( R_t = \mu |r_n| \frac{R_{t}^{Tr}}{||R_{t}^{Tr}||} \) else \( R_t = R_{t}^{Tr} \)

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  else \( \mathbf{R}_t = \mathbf{R}_t^{Tr} \)
  with \( K_t = \frac{2(1-\nu)}{2-\nu} K_n \).

Remarks:

- compute \( \eta_t^c \) as before by taking \( m_{\text{eff}} = \frac{m_1 m_2}{m_1 + m_2} + m_1 m_2 \left( \frac{R_1^2}{l_1} + \frac{R_2^2}{l_2} \right) \) and replacing \( K_n \) by \( K_t \)
- \( \eta_t \leq \eta_t^c \)
- difficult to give a physical meaning to \( \eta_n \) and \( \eta_t \)
Explicit laws allow to substitute the displacement (or the velocity) to the force in the dynamical equation. If considering a simplified problem described by the Newton equation:

$$M \ddot{v} = F(q, \dot{q}, t) + P(t) + r$$

using

$$U = H \star (q, v), \quad g = D(q), \quad r = H(q)R$$

and

$$R = f(U, g)$$

one can write:

$$M \ddot{v} = P(t) + H(q)f(H \star (q, v), D(q))$$

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

The kinematic unknowns of each component are dependent due to the interactions.
explicit laws

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If considering a simplified problem described by the Newton equation:

$$ M \ddot{v} = F(q, \dot{q}, t) + P(t) + r $$

using $U = H^*(q)v$, $g = D(q)$, $r = H(q)R$ and $R = f(U, g)$ one can write:

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implicit laws
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Frictional contact: Signorini-Coulomb

\[ R_N \geq 0 \quad g \geq 0 \quad R_N \cdot g = 0 \]

\[ \| R_T \| \leq \mu R_N, \begin{cases} &\| R_T \| < \mu R_N \Rightarrow U_T = 0 \\ &\| R_T \| = \mu R_N \Rightarrow \exists \alpha \geq 0, U_T = -\alpha R_T \end{cases} \]

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

Assuming \( g(t_0) \geq 0 \) then \( \forall t > t_0 \) if \( g(t) \leq 0 \) then \( U_N \geq 0 \), \( R_N \geq 0 \), \( U_N R_N = 0 \) else \( R_N = 0 \).
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if \( g(t) \leq 0 \) then \( U_N \geq 0, \ R_N \geq 0, \ U_N R_N = 0 \)
else \( R_N = 0 \)
It's 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.
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An explicit law may be written as an implicit law.
Let's consider the basic example of a single ball bouncing on a plan:
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Question: Is the usual formalism adapted to describe a dynamical system with unilateral contact?
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![Diagram of a ball bouncing on a plane]

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

So let try to solve the (simplified) problem:

\[
M\ddot{q} = R \\
0 \leq q \perp R \geq 0 \\
\text{initial conditions : } q(0) = 0, \dot{q}(0) = -1
\]
Using an implicit Euler scheme, one obtains the following system:

\[
\begin{align*}
\ddot{q}_{i+1} &= \left(\dot{q}_{i+1} - \dot{q}_i\right)/h \\
q_{i+1} &= q_i + h\dot{q}_{i+1}
\end{align*}
\]

Thus the solution is:

\[
\begin{align*}
\dot{q}_{1+1} &= 0 \\
\dot{q}_1 &= 0 \\
R_1 &= M\dot{q}_0/h \\
\dot{q}_k &= 0 \\
R_k &= 0
\end{align*}
\]

So if \( h \to 0 \) 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.
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Thus the solution is:

\[
\begin{align*}
q^1 &= 0, \quad \dot{q}^1 = 0, \quad R^1 = M\dot{q}^0/h \\
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\end{align*}
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So if \( h \to 0 \) 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.
The differential system must be modified to describe collisions and other non smooth phenomena.

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

\[ M(q) + F(q, \dot{q}, s) + P(s) ds + p \]

where the impulse \( p \) will contain both the sum of the contribution of smooth load over the time interval \( (t+T-t) \), the percussion, denoted \( P \), at shock time (supposed instantaneous).

To describe \( \dot{q} \) one uses the local bounded variation framework over all sub-intervals of \( I^{T_p} = [0, T] \), i.e. \( \text{lbv}(I^{T_p}, R^n) \) and one introduces differential measures allowing the generalization of the equation of motion to non smooth phenomena (Moreau 1988).

Remark: Event driven approaches will consider smooth motion, but will re-initialize velocity (acceleration, etc.) at each non smooth event using shock law. Only reasonable to compute a granular gas or a loose flow of granular material.
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\[
M(\dot{q}^+ - \dot{q}^-) = \int_{t^-}^{t^+} (F(q, \dot{q}, s) + P(s)) ds + p
\]

where the impulse \( p \) will contain both the sum of

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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.
  Only reasonable to compute a granular gas or a loose flow of granular material.
More precisely the classical equation of motion is reformulated in terms of a differential measure equation:

\[
\mathbb{M} d\dot{q} = F(t, q, \dot{q}^+) dt + P(t, q, \dot{q}^+) dt + dp
\]

\[
q(t) = q(t_0) + \int_{t_0}^{t} \dot{q}^+ dt
\]

In the previous equation, \(d\dot{q}\) is the differential measure of \(\dot{q}\) (atomistic at the discontinuity and \(\ddot{q} dt\) on the continuous part), \(dt\) is the Lebesgue measure on \(\mathbb{R}\) while \(dp\) is the differential measure of contact forces.

The measure \(dp\) contains:

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

\[ U^+ = H^*(q)q^+ \]
\[ dp = H(q)dP \]
Local - global mapping:

\[ U^+ = \mathbb{H}^*(q) \dot{q}^+ \]
\[ dp = \mathbb{H}(q)dP \]

Frictional contact:

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

if \( g(t) \leq 0 \) then \( U_N^+ \geq 0, \ dP_N \geq 0, \ U_N^+dP_N = 0 \)
else \( dP_N = 0 \)

Coulomb friction (threshold law):

\[ \| dP_T \| \leq \mu dP_N, \]
\[ \left\{ \begin{array}{l}
\| dP_T \| < \mu dP_N \Rightarrow U_T^+ = 0 \\
\| dP_T \| = \mu dP_N \Rightarrow \exists \alpha \geq 0, \ U_T^+ = -\alpha dP_T
\end{array} \right. \]
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
In the case of binary shocks, three kind of restitution can be used:

- Newton restitution, which relates the velocity after ($U_+$) to the velocity before ($U_-$) impact:
  \[ U_+ = -e U_- \]

- Poisson restitution, which relates restitution impulsion ($R_r$) to the compression impulsion ($R_c$) according to the decomposition of the shocks in a compression and restitution phase:
  \[ R_r = e_p R_c \]

- Energy or Stronge restitution, which relates restitution energy to compression energy:
  \[ e_s = R_{tr} R_{tc} \]

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).
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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).
Various modeling choices are possible for DEM depending on:

- space scale: interaction $\rightarrow$ smooth, component $\rightarrow$ non-smooth
- time scale: waves $\rightarrow$ smooth, rigid body motion with impact $\rightarrow$ non-smooth
- the shape of the components $\rightarrow$ non-smooth easier but introduce indetermination.
- etc.
3 Numerical Strategies

- Introduction
- smooth-DEM
  - Generality
  - Time integrator
  - Technical aspects
- Non Smooth Contact Dynamics
  - Time stepping
  - Managing interactions :
  - Contact problem formulation
  - Solvers
  - Practical view

4 Technical Aspects

5 NSCD Extensions

6 Multi-Physics
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 solver if necessary (Lemke, Gauss-Seidel, bi-potential, etc.)
- technical aspects: contact detection, rotation integration, etc.
- etc.
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- technical aspects: contact detection, rotation integration, etc.
- etc.

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.
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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In a different way, Moreau (1988) developed the Contact Dynamics method for implicit non smooth interaction model. It uses an implicit time integrator. It needs a dedicated contact solver. Further works lead to the extension of the method to multi-contact simulations of collections of deformable bodies (Jean 1999) and the method becomes the so-called Non Smooth Contact Dynamics method (NSCD). This kind of methods refer to NSCD.
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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.
Using explicit interaction law leads to solve:

\[ M \dot{v} = F(q, \dot{q}, t) + P(t) + r \]

with \( r = H(q)R, \) \( R = f(U, g) \) and \( U = H^*(q)v, \) \( g = D(q). \)

\[ \rightarrow \text{This is a non-linear problem.} \]

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

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

\[ M(v_{n+1} - v_n) = hF(q_n, \dot{q}_n, t_n) + hP(t_n) + hr_n \]

Different explicit time integrator can be used to integrate the motion of particle:
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with $r = \mathcal{H}(q)R$, $R = f(U, g)$ and $U = \mathcal{H}^*(q)v$, $g = D(q)$.

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

- Gear integrator for Molecular Dynamics
Using explicit interaction law leads to solve:

\[ \mathbf{M} \mathbf{v} = \mathbf{F}(\mathbf{q}, \mathbf{\dot{q}}, t) + \mathbf{P}(t) + \mathbf{r} \]

with \( \mathbf{r} = \mathbf{H}(\mathbf{q})\mathbf{R} \), \( \mathbf{R} = f(U, g) \) and \( \mathbf{U} = \mathbf{H}^*(\mathbf{q})\mathbf{v}, \ g = D(\mathbf{q}) \).

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

\[ \mathbf{M} (\mathbf{v}_{n+1} - \mathbf{v}_n) = h\mathbf{F}(\mathbf{q}_n, \mathbf{\dot{q}}_n, t_n) + h\mathbf{P}(t_n) + h\mathbf{r}_n \]

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

- Gear integrator for Molecular Dynamics
- Velocity verlet
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with \( r = H(q)R, R = f(U, g) \) and \( U = H^*(q)v, g = D(q) \).

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

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

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

\[
q_{p}(t + h) = q(t) + h\dot{q}(t) + \frac{h^2}{2!}\ddot{q}(t) + \frac{h^3}{3!}b(t) + \frac{h^4}{4!}c(t) + \ldots
\]

\[
\dot{q}_{p}(t + h) = \dot{q}(t) + h\ddot{q}(t) + \frac{h^2}{2!}b(t) + \frac{h^3}{3!}c(t) + \ldots
\]

\[
\ddot{q}_{p}(t + h) = \ddot{q}(t) + h\dddot{q}(t) + \frac{h^2}{2!}b(t) + \frac{h^3}{3!}c(t) + \ldots
\]

\[
b_{p}(t + h) = b(t) + h\dot{c}(t) + \frac{h^2}{2!}c(t) + \ldots
\]

\[
c_{p}(t + h) = c(t) + \ldots
\]

Perform detection in the predicted configuration, compute contact forces, compute the acceleration (\(\ddot{q}_{c}\)):

\[
\ddot{q}_{c}(t + h) = M^{-1}F + P + r(t + h).
\]

Correction:
Considering \(\mathcal{T}_q = \ddot{q}_c(t + h) - \ddot{q}_{p}(t + h)\) perform the correction:

\[
q_{c}(t + h) = q_{p}(t + h) + c_0\mathcal{T}_q
\]

\[
\dot{q}_{c}(t + h) = \dot{q}_{p}(t + h) + c_1\mathcal{T}_q
\]

\[
\ddot{q}_{c}(t + h) = \ddot{q}_{p}(t + h) + c_2\mathcal{T}_q
\]

\[
b_{c}(t + h) = b_{p}(t + h) + c_3\mathcal{T}_q
\]

\[
c_{c}(t + h) = c_{p}(t + h) + c_4\mathcal{T}_q.
\]

The correction step may be repeated.
Predictor-corrector Gear integrator

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

\[
\begin{align*}
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) + \ldots \\
\dot{q}^P(t + h) &= \dot{q}(t) + h\ddot{q}(t) + \frac{h^2}{2!}b(t) + \frac{h^3}{3!}c(t) + \ldots \\
\ddot{q}^P(t + h) &= \ddot{q}(t) + hb(t) + \frac{h^2}{2!}c(t) + \ldots \\
b^P(t + h) &= b(t) + hc(t) + \ldots \\
c^P(t + h) &= c(t) + \ldots
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Perform detection in the predicted configuration, compute contact forces, compute the acceleration ($\ddot{q}^c(t + h) = M^{-1}F + P + r(t + h)$).
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\end{align*}
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Perform detection in the predicted configuration, compute contact forces, compute the acceleration (\(\ddot{q}^c(t + h) = M^{-1}F + P + r(t + h))\).

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

\[
\begin{align*}
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} \\
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Perform detection in the predicted configuration, compute contact forces, compute the acceleration (\(\ddot{q}^c(t + h) = \mathbf{M}^{-1} \mathbf{F} + \mathbf{P} + \mathbf{r}(t + h)\)).

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

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\begin{align*}
q^c(t + h) &= q^P(t + h) + c_0 \Delta \dot{q} \\
\dot{q}^c(t + h) &= \dot{q}^P(t + h) + c_1 \Delta \dot{q} \\
\ddot{q}^c(t + h) &= \ddot{q}^P(t + h) + c_2 \Delta \dot{q} \\
b^c(t + h) &= b^P(t + h) + c_3 \Delta \dot{q} \\
c^c(t + h) &= c^P(t + h) + c_4 \Delta \dot{q}
\end{align*}
\]

The correction step may be repeated.
Velocity Verlet scheme

\[
\begin{align*}
q(t + h) &= q(t) + h \dot{q}(t) + \frac{1}{2} h \ddot{q}(t) \\
\dot{q}(t + h/2) &= \dot{q}(t) + \frac{1}{2} h \ddot{q}(t) \\
\ddot{q}(t + h) &= M^{-1} F(t + h) + P + r(t + h)
\end{align*}
\]

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

It's also a predictor-corrector approach.

**Prediction:**

\[
\begin{align*}
q(t + h) &= q(t) + h\dot{q}(t) + \frac{1}{2} h^2 \ddot{q}(t) \\
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**Correction:**

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\dot{q}(t+h) = \dot{q}(t+h/2) + \frac{1}{2}h\ddot{q}(t+h)
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Time-centered scheme

Knowing $q(t)$ and $\dot{q}(t-h/2)$ one performs contact detection, computes contact forces and updates acceleration $\ddot{q}(t)$. Then one updates $
abla \dot{q}(t+h/2) = \dot{q}(t-h/2) + h \ddot{q}(t)$.

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Some cares must be taken to obtain numerical results that keep a mechanical sense.
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- The time step $h$ depends explicitly on the mechanical parameters of the system ($h = \frac{1}{N} \sqrt{\frac{m_{\text{eff}}}{K_n}}$) and must be small enough to ensure numerical stability and describe with accuracy the contact.

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

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

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

Thus control parameter of the simulation are:

- the time step discretization ($\frac{1}{N}$),
- the local stiffness (normal $K_n$ and tangential $K_t$),
- the viscous ($\eta$) or non viscous ($\alpha$) dissipation.

Evaluation criteria related to the computation quality:

- Respect of interaction law,
- Control of numerical damping.
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- Respect of interaction law,
- Control of numerical damping.
Time integration of the equation of motion leads to:

\[ M(\dot{q}_{i+1} - \dot{q}_i) = \int_{t_i}^{t_{i+1}} (F(q, \dot{q}, s) + P(s))ds + p_{i+1} \]

\[ = p_{\text{free}} + p_{i+1} \]

\[ q_{i+1} = q_i + \int_{t_i}^{t_{i+1}} \dot{q}ds \]

where

- \( p_{i+1} = \int_{t_i}^{t_{i+1}} dp \) represents the value of the total impulsion over the time step the unknown in the following
- \( p_{\text{free}} \) the integral of applied forces over the time step;
A $\theta$-method (Crank-Nicholson) is used to evaluate $\int_{t_i}^{t_{i+1}} (F(q, \dot{q}, s) + P(s))ds$ and $\int_{t_i}^{t_{i+1}} \dot{q} ds$:

$$p_{\text{free}} = h(1 - \theta)(F(q_i, \dot{q}_i, t_i) + P(t_i)) +$$
$$h\theta(F(q_{i+1}, \dot{q}_{i+1}, t_{i+1}) + P(t_{i+1}))$$

$$q_{i+1} = q_i + h((1 - \theta)\dot{q}_i + \theta\dot{q}_{i+1}) = q_m + h\theta\dot{q}_{i+1}$$

with $q_m = q_i + h(1 - \theta)\dot{q}_i$.

- 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
A \( \theta \)-method (Crank-Nicholson) is used to evaluate \( \int_{t_i}^{t_{i+1}} (\mathbb{F}(q, \dot{q}, s) + \mathbb{P}(s)) ds \) and \( \int_{t_i}^{t_{i+1}} \dot{q} ds \):

\[
\begin{align*}
\rho_{\text{free}} &= h(1 - \theta)(\mathbb{F}(q_i, \dot{q}_i, t_i) + \mathbb{P}(t_i)) + \\
&

h\theta(\mathbb{F}(q_{i+1}, \dot{q}_{i+1}, t_{i+1}) + \mathbb{P}(t_{i+1})) \\
q_{i+1} &= q_i + h((1 - \theta)\dot{q}_i + \theta\dot{q}_{i+1}) = q_m + h\theta\dot{q}_{i+1}
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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.
If now we use this formulation for the previous elementary contact problem, one obtains:

\[ M(\dot{q}_{i+1} - \dot{q}_i) = p \]

If \( q_i \leq 0, 0 \leq \dot{q}_{i+1} \perp hR \geq 0 \)

Initial conditions: \( q(0) = 0, \dot{q}(0) = -1 \)

The implicit euler scheme gives:

\[
\begin{align*}
q^1 &= 0, \; \dot{q}^1 = 0, \; p^1 = M\dot{q}^0 \\
q^k &= 0, \; \dot{q}^k = 0, \; p^k = 0
\end{align*}
\]

The obtained solution is independent of the time step.
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q_k = 0, \dot{q}_k = 0, p_k = 0
\end{cases}$$

The obtained solution is independent of the time step.

If $q(0) = \epsilon$ then $\dot{q}_1 = 0$ and $p_1 = M\dot{q}_0$ and $q_k = \epsilon$.

The error made on the gap decreases with the size of the time step.
The two mappings $H^*$ and $H$ depend on the solution.

They may be evaluated in a “mean” configuration: $\ddot{q}_{k+1} = q_{k+1} + h(\gamma_1 \dot{q}_k + \gamma_2 \dot{q}_{k+1})$
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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 $H^*$ and $H$ can be considered as constant on a whole time interval.
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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 $H^*$ and $H$ can be considered as constant on a whole time interval.

Remarks:

- Usually the contact problem is solved in a pseudo-explicit configuration:
  \[ q_m = q_i + h(1 - \theta) \dot{q}_i. \]

- The pseudo configuration of the next time step will be determined by the final velocity $\dot{q}_{i+1}$:
  \[ q_{m+1} = q_m + h\dot{q}_{i+1}. \] This is a Leap-Frog technique.
The problem to solve is written in terms of:

- discretized equations of motion for each body expressed with global unknowns:
  \[ \mathbf{M} \ddot{\mathbf{q}}_{i+1} = \ddot{\mathbf{p}}_{\text{free}} + \mathbf{p}_{i+1} \]

- interaction laws expressed with local unknowns (contact \( \alpha \)):
  \[ \text{Contact}(g^\alpha, U^\alpha_n, P^\alpha_n) = \text{TRUE} \quad \text{Friction}(U^\alpha_t, P^\alpha_t) = \text{TRUE} \]

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

\[ \begin{align*} 
\mathbf{q}, \dot{\mathbf{q}} & \quad \leftarrow \text{Equations of motion} \rightarrow \mathbf{p} \\
\mathbb{H}^* \downarrow & \quad \uparrow \mathbb{H} \\
\mathbf{U} & \quad \leftarrow \text{Interaction laws} \rightarrow \mathbb{P} 
\end{align*} \]
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- mappings \((H\text{ and } H^*)\) to pass from local to global unknowns

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

\[ U = U_{\text{free}} + W P \]

where \( W = H^* M^{-1} H \) and \( U_{\text{free}} = H^* M^{-1} p_{\text{free}} \).
The classical NSCD approach rely on a Non Linear Gauss Seidel (NLGS) algorithm.

\[
U_\alpha = U_{\alpha,\text{free}} + W_{\alpha\alpha} P_\alpha + X_{\beta \neq \alpha} W_{\alpha\beta} P_\beta
\]

We freeze the contributions of other contact (\(\beta \neq \alpha\)) taking updated values if \(\beta < \alpha\) or old values if \(\beta > \alpha\).

We solve the \(\alpha\) block of equations using:

- 2D: Explicit uncoupled resolution if \(W_{\alpha\alpha}\) is diagonal
- Coupled (\(n, t\)) graph intersection
- Pseudo-potential approach (bi-potential)
- LCP like local solver

3D: Explicit resolution if \(W_{\alpha\alpha}\) is diagonal
- Pseudo-potential approach
- Generalized Newton algorithm
- LCP like local solver

We repeat the process until convergence.
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Considering, one by one, the local systems to solve for each contact $\alpha$,

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$$

$$
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We repeat the process until convergence.
A parallel treatment of the NLGS is possible
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*quasi NLGS* may be derived, rewriting the system:

\[
U_\alpha = U_{\alpha,free} + W_{\alpha\alpha}(P_\alpha - P_{\alpha,esti}) + \sum_\beta W_{\alpha\beta}P_\beta
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\]

where \(P_{\alpha,esti}\) is the impulsion computed at the previous Gauss-Seidel iteration.

Noting that when the algorithm goes close to the solution, \(P_\alpha - P_{\alpha,esti} \to 0\) one may derive a *quasi NLGS* replacing the original \(W_{\alpha\alpha}\) by an arbitrary one.
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Various alternatives are possible for the contact solver:
- Conjugate Projected Gradient Algorithm
- Lemke (for small collection of rigid bodies)
- Other possibilities, see Siconos NSSPack
Resolution Scheme:

<table>
<thead>
<tr>
<th>Iteration matrix computation ($\mathbf{M}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time loop</td>
</tr>
<tr>
<td>Free velocity computation ($\dot{\mathbf{q}}_{\text{free}}$)</td>
</tr>
<tr>
<td>Temporary configuration computation ($\mathbf{q}_m$)</td>
</tr>
<tr>
<td>Contact detection</td>
</tr>
<tr>
<td><strong>Contact problem resolution</strong></td>
</tr>
<tr>
<td>Velocity correction ($\dot{\mathbf{q}}_{i+1}$)</td>
</tr>
<tr>
<td>Update of the kinematics and the configuration</td>
</tr>
<tr>
<td>Halt criteria</td>
</tr>
</tbody>
</table>
Numerical model parameters are:

- The $\theta$ 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. Technical Aspects
   - Contact detection
   - Rotation

5. NSCD Extensions

6. Multi-Physics

7. Bibliography

8. Annexes:
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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- **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.)
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 \((\mathcal{R})\).

Integrating Euler equation: \(\omega^f - \omega^i = hI^{-1}M\)

\[\Rightarrow \text{update the locate frame through the transformation matrix} \quad \mathcal{R}_f = \mathbb{P}\mathcal{R}_i\]

Various possibility:
- Euler angles
  \[\omega = \dot{\psi}e_1 + \dot{\phi}e_2 + \dot{\zeta}e_3\]
  \[\int_i^f \dot{\psi} ds \Rightarrow \Delta\Omega_1, \int_i^f \dot{\phi} ds \Rightarrow \Delta\Omega_2 \text{ and } \int_i^f \dot{\zeta} ds \Rightarrow \Delta\Omega_3\]
  \[\mathbb{P} = \Delta\Omega_3 \cdot \Delta\Omega_2 \cdot \Delta\Omega_1\]
  **drawback:** indeterminacy

- quaternion

- transformation matrix:
  - linearization: for each frame vector \(v_k = \omega \otimes e_k\) then \(e^f_k = e^i_k + hv_k\)
  - **drawback:** lose orthogonality and normality
  - incremental objective integrator (Hughes, 1980), (Geradin et al.,)
5 NSCD Extensions
   • Deformable bodies
   • Interaction laws
   • Explicit Integration

6 Multi-Physics

7 Bibliography

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

\[ \mathbf{U} = \mathbf{U}_{\text{free}} + \mathbf{W} \mathbf{P} \]

with

- **rigid**: \( \tilde{\mathbf{M}} = \mathbf{M} \)
  \[ p_{\text{free}} = h(1 - \theta)(\mathbf{F}_i + \mathbf{P}_i) + h\theta(\mathbf{F}_f + \mathbf{P}_f) \]

- **linear**: \( \tilde{\mathbf{M}} = \mathbf{M} + h\theta \mathbf{C} + h^2 \theta^2 \mathbf{K} \)
  \[ p_{\text{free}} = [\mathbf{M} - h(1 - \theta)\mathbf{C} - h^2 \theta(1 - \theta)\mathbf{K}] \mathbf{u}_i - h\mathbf{K}\mathbf{q}_i + h[\theta \mathbf{P}_f + (1 - \theta)\mathbf{P}_i] \]

- **non-linear**: \( \tilde{\mathbf{M}}^k = \mathbf{M} + h\theta \mathbf{C}^k + h^2 \theta^2 \mathbf{K}^k \)
  \[ p_{\text{free}} = \tilde{\mathbf{M}}^k \mathbf{u}_f^k + \mathbf{M}(\mathbf{u}_i - \mathbf{u}_f^k) + h[(1 - \theta)(\mathbf{F}_i + \mathbf{P}_i) + \theta(\mathbf{F}_f^k + \mathbf{P}_f^k)] \]

**Remark:**

- due to “energy conservation” one may replace \( h[(1 - \theta)\mathbf{F}_i + \theta \mathbf{F}_f^k] \) by more suitable expression (Gonzalez, 2000)
Different interaction laws may be used:

- Newton shock law using the variable $\tilde{u}_n = u_n + e u_n^-$ and $\tilde{u}_t = u_t$

\[
\tilde{u}^\alpha = u_\alpha,\text{free} + \max(eu^i_\alpha, 0)^T + W_{\alpha\alpha} hr^\alpha + \sum_{\beta \neq \alpha} W_{\alpha\beta} hr_\beta
\]

\[
\text{Law}(\tilde{u}_\alpha, r_\alpha) = \text{TRUE}
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  $$

  \[Law(\tilde{u}_\alpha, r_\alpha) = \text{TRUE}\]

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

  $$
  \tilde{u}_\alpha = u_{\alpha, \text{free}} + \max(g_0 / h, 0)^T + W_{\alpha\alpha} h r^\alpha + \sum_{\beta \neq \alpha} W_{\alpha\beta} h r_\beta
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\text{Law}(\tilde{u}^{\alpha}, r^{\alpha}) = \text{TRUE}
$$

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

$$
\tilde{u}^{\alpha} = u^{\alpha, free} + \max(g_0/h, 0)^T + W_{\alpha\alpha} hr^{\alpha} + \sum_{\beta \neq \alpha} W_{\alpha\beta} hr_{\beta}
$$

$$
\text{Law}(\tilde{u}^{\alpha}, r^{\alpha}) = \text{TRUE}
$$

- Elastic law using the variable $\tilde{u}_n = g_0/h + u_n + hr_n/h^2 k_n$
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.

\[
\ddot{M}q_i = F_i(\dot{q}_i, q_i) + P_i + H_{i+1}r_i H^*_{i+1}q_{i+1} \geq 0,
\]

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

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

\[
\begin{align*}
\mathcal{M}\ddot{q}_i &= F_i(\dot{q}_i, q_i) + P_i + H_{i+1}r_i \\
H_{i+1}^* q_{i+1} &\geq 0
\end{align*}
\]

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

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

where $\beta \in [0.5, 1]$ represents a numerical damping parameter.
To take into account the displacement constraints in system (1), the displacement \( q_{i+1} \) is decomposed as

\[
q_{i+1} = q_{i+1}^{\text{free}} + q_{i+1}^c
\]

where \( q_{i+1}^{\text{free}} \) represents the prediction of the displacement without contact forces and \( q_{i+1}^c \) the correction due to the contact forces only.
To take into account the displacement constraints in system (1), the displacement $q_{i+1}$ is decomposed as

$$q_{i+1} = q^\text{free}_{i+1} + q^c_{i+1}$$

where $q^\text{free}_{i+1}$ represents the prediction of the displacement without contact forces and $q^c_{i+1}$ the correction due to the contact forces only.

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

$$q^\text{free}_{i+1} = h^2 M^{-1} \{ P_i - F_i(\dot{q}_i, q_i) \} + 2q_i - q_{i-1} \quad (3)$$

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

$$\begin{align*}
h^2 H^*_i M^{-1} H_{i+1} r_i &= H^*_i q^\text{free}_{i+1} \\
q^c_{i+1} &= h^2 M^{-1} H_{i+1} r_i
\end{align*} \quad (4)$$
Preamble

Modeling

Numerical Strategies

Technical Aspects

NSCD Extensions

Multi-Physics
- Generality
- Fluid
- Thermal
- Electricity

Bibliography

Annexes:
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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- electrical (Renouf et al., 2007)
- physico-chemical
- etc.

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.
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.
- $\eta$: fluid viscosity.
- $\phi = 1 - \frac{V_G}{V}$: granular material porosity.
- $\kappa$: permeability of the granular material.
- $\overrightarrow{u}$: mean velocity of the grains.

Hypotheses:
- perfect gas.
- neglect fluid inertia.
- low Reynolds number (Darcy law).
- spherical grains (radius $r$)

Carman-Kozeny: $\kappa(\phi) = \frac{r^2}{45} \phi^3 \left(1 - \phi^2\right)$
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  Carman-Kozeny: \( \kappa (\phi) = \left( \frac{r^2}{45} \right) \phi^3 / (1 - \phi^2) \)
Fluid pressure evolution

- Mass conservation of the fluid and grains:

\[
\phi \left( \frac{\partial P}{\partial t} + \bar{u} \cdot \nabla P \right) = \nabla \cdot \left( \frac{\kappa(\phi)}{\eta} \nabla P \right) - P \nabla \cdot \bar{u}
\]
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- 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.
  - Biot term: variation of the porous pressure due to evolution of the pore size.
Hydrodynamic force

- Notations:
  - $V^G$: grain volume.
  - $\nabla P$: pressure gradient at the center of the grain.

The force on the grain due to the fluid pressure gradient increases proportionally to the fluid volume around the grain.
Hydrodynamic force

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  - \( V^G \): grain volume.
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- Force on the grain due to the fluid pressure gradient:

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\]
Hydrodynamic force

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

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

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- for one iteration:

\[
(\vec{x}^G, \vec{v}^G) \xrightarrow{\text{interpolation}} (\phi, \vec{u})
\]

- mecanichal resolution
- fluid resolution
- localization
- $F_h$ $\downarrow$ $P$
Numerical strategy

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

- interpolation: interpolation, aux nœuds du maillage utilisé pour le calcul de la pression, de la porosité locale : \( \phi_{\text{loc}} = 1 - \frac{V^G}{V_{\text{ref}}} \), 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)
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- interpolation: interpolation, aux nœuds du maillage utilisé pour le calcul de la pression, de la porosité locale : \( \phi_{loc} = 1 - \frac{V^G}{V_{ref}} \), définie au centre des grains.
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  \( \frac{1}{(1 - \phi)} \nabla P \) known at the mesh load.
- mechanical resolution: compute velocity and position with a DEM code
Exemple: Sedimentation
Exemple: Sedimentation
Dilatation effect Resolution Scheme:

- Iteration matrix computation ($M$)
- Time loop
  - Compute temperature
  - Free velocity computation ($\dot{q}_{\text{free}}$)
  - Temporary configuration computation ($q_m$)
  - Contact detection (A)
  - Compute thermal velocity: $U_{th} = d_{th}/h$ (B)
- Contact problem resolution
  - Velocity correction ($\dot{q}_{i+1}$)
  - Update of the kinematics and the configuration (C)
  - Update shapes (D)

Halt criteria
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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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.
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 $\alpha$ 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 $C_m$:

$$C_\alpha = \frac{C_i C_j}{C_i + C_j + \frac{C_i C_j}{C_m}}.$$  \hspace{1cm} (5)

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

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

\[ \mathbf{N} \mathbf{I} = \mathbf{I}_0, \]  

(6)

where \( \mathbf{N} \in \mathbb{R}^{n_b \times n_c} \), \( \mathbf{I} \in \mathbb{R}^{n_b} \) and \( \mathbf{I}_0 \in \mathbb{R}^{n_b} \). The matrix \( \mathbf{N} \) denotes the incidence matrix between the nodes of the network. Its role is equivalent to the one of matrix \( \mathbf{H} \) defined in the mechanical section. The vector \( \mathbf{I}_0 \) is the intensity vector where each component \( I_\alpha \) is linked to one of the network branches.
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Thus writing the Ohm law for the set of contact, one obtains:

$$\mathbf{I} = \mathbf{C}\mathbf{N}^T\mathbf{V}.$$  \hspace{1cm} (7)

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

$$\mathbf{N}\mathbf{C}\mathbf{N}^T\mathbf{V} = -\mathbf{I}_0.$$  \hspace{1cm} (8)

where the electrical potential $\mathbf{V}$, expressed in each node of the network, become the primary unknown of the problem. The matrix $\mathbf{G}$ is equal to the product $\mathbf{N}\mathbf{C}\mathbf{N}^T$ and is, as the $\mathbf{W}$ matrix, symmetric semi positive defined.
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 \( G \) 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 \( \{1, \ldots, n_b\} \)

Compute \[
\tilde{V}_i = I_i^0 - \sum_{j<i} G_{ij} V_j^k - \sum_{j>i} G_{ij} V_j^{k-1}
\]

\[
V_i^k = \frac{1}{G_{ii}} \tilde{V}_i
\]

**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.
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.

\[
\begin{aligned}
i &= i + 1 \text{ (time loop)} \\
\mathbf{q}(i + 1) &\text{ prediction} \\
\text{Contact detection} \\
\dot{\mathbf{q}}(i)_{\text{free computation}} \\
&\quad k = k + 1 \text{ (NSGS iteration)} \\
&\quad \alpha = \alpha + 1 \text{ (contact loop)} \\
&\quad \mathbf{b}_\alpha^k \text{ computation} \\
&\quad \text{Contact problem resolution }:(v^{k+1}_\alpha, r^{k+1}_\alpha) \text{ solution} \\
&\quad \text{convergence test} \\
\text{Electrical problem formulation} \\
\text{Electrical problem resolution} \\
\dot{\mathbf{q}}(i + 1) &\text{ correction}
\end{aligned}
\]

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.
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Heat Conduction in GranularMaterials
Let's 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

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

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

If $\Omega$ 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 $\Omega$ 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.
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 $u(x, t) = u(\varphi(X, t), t) = U(X, t)$.
Annexes::Deriving the Lagrangian system

Starting from the equation of motion in Eulerian coordinates,

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

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

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

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

$$\int_{\Omega(t)} (\ddot{u}(x, t) - b(x, t))\hat{v}(x, t) \, dm(x, t) = -\int_{\Omega(t)} \sigma(x, t) : \nabla\hat{v}(x, t) \, d\omega(x, t)$$

$$+ \int_{\partial\Omega_F(t)} t(x, t)\hat{v}(x, t) \, ds(x, t) + \int_{\Gamma_c^i(t)} r(x, t)\hat{v}(x, t) \, ds(x, t),$$

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 Lebesgue measure at $x \in \partial\Omega$. 

F. Dubois & M. Renouf (CNRS)
The symmetry of the Cauchy stress tensor in absence of density of momentum allows one to introduce the symmetric deformation rate tensor,

\[ D(x, t) = \frac{1}{2} (\nabla^T \nu(x, t) + \nabla \nu(x, t)) \]  

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

\[ \hat{P}_{int} = - \int_{\Omega(t)} \sigma(x, t) : \nabla \hat{\nu}(x, t) \ d\omega(x, t) = - \int_{\Omega(t)} \sigma(x, t) : \hat{D}(x, t) \ d\omega(x, t) \]  

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.
Annexes:: Deriving the Lagrangian system

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

\[ \hat{P}_{\text{int}} = - \int_{\Omega(t)} \sigma(x, t) : \nabla \dot{\nu}(x, t) \, d\omega(x, t) = - \int_{\Omega(0)} S(X, t) : \hat{L}(X, t) \, d\Omega(X, 0) \]  

(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

\[ \int_{\Omega(0)} (\ddot{U}(X, t) - B(X, t)) \hat{V}(X, t) \, dM(X, 0) = - \int_{\Omega(0)} S(X, t) : \hat{L}(X, t) \, d\Omega(X, 0) \]

\[ + \int_{\partial\Omega(0)} T(X, t) \hat{V}(X, t) \, dS(X, t) + \int_{\Gamma_i^c(0)} R(X, t) \hat{V}(X, t) \, dS(X, t) \]  

(14)

where the applied forces laws on the boundary satisfies \( T(X, t) = S(X, t).F^T(X, t).N(X, t) \) and \( R(X, t) = S(X, t).F^T(X, t).N(X, t) \). 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.
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

\[ S(X, t) = K(X, T) : E(X, t), \]  \hspace{1cm} (15)

where \( E \) is the Green-Lagrange strain tensor,

\[ E(X, t) = \frac{1}{2} (F^T(X, t)F(X, t) - I(X, t)), \]  \hspace{1cm} (16)

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

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

(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

\[ M(U_h) \ddot{U}_h + F(t, U_h, \dot{U}_h) = R, \]

(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.
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,

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

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

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

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

$$\begin{align*}
\frac{d}{dt} \int_{\Omega(t)} \dot{u}(x, t) \, dm(x, t) &= \int_{\Omega(t)} b(x, t) \, dm(x, t) + \int_{\partial\Omega(t)} t(x, t) \, ds(x, t), \\
\frac{d}{dt} \int_{\Omega(t)} (x - x_O) \times \dot{u}(x, t) \, dm(x, t) &= \int_{\Omega(t)} (x - x_O) \times g(x, t) \, dm(x, t) \\
&\quad + \int_{\partial\Omega(t)} (x - x_O) \times t(x, t) \, ds(x, t). \quad (21)
\end{align*}$$
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 $\Omega$ in Eulerian coordinates:

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

(22)
Annexes:: Deriving the Lagrangian system

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

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

(23)

where

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

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

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

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

(24)
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Usually, a second order form of the dynamics is obtained with the help of the following parametrization of the vector $\omega_i$,

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

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 a generalized coordinates $z$ such that

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

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 $z$. 

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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

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

(28)

where the vector \( Q(z, t), \in \mathbb{R}^n \) denotes the set of generalized forces.
Annexes: Deriving the Lagrangian system

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

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

(29)

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

\[
M(z) \ddot{z} + F(t, z, \dot{z}) = 0
\]  

(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.