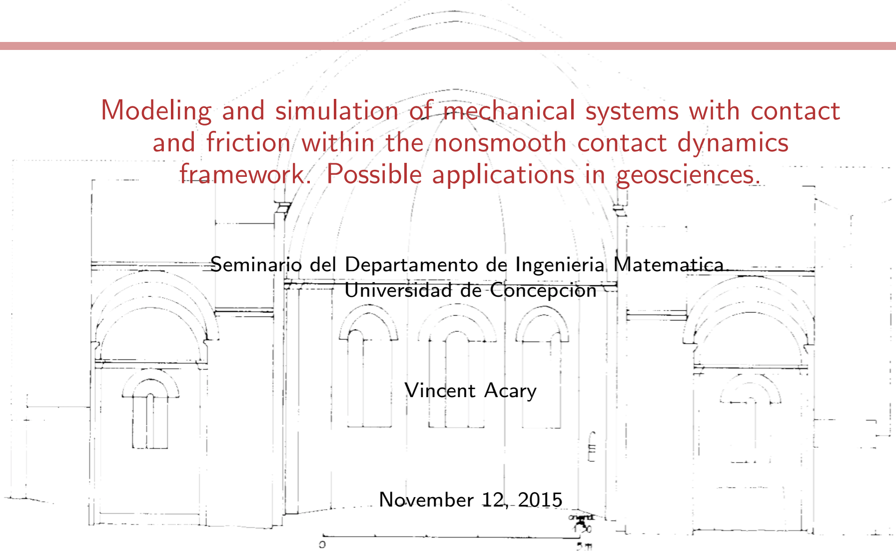
Modeling and simulation of mechanical systems with contact and friction within the nonsmooth contact dynamics framework. Possible applications in geosciences.



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Motivations

- Simulation of the mechanical behavior (statics and dynamics) of large collection of bodies in interaction through:
  - contact and impact,
  - Coulomb dry friction,
  - cohesive interfaces with damage and plasticity.
- Nonsmooth mechanics modeling framework:
  - dedicated time–integration schemes,
  - numerical optimization solvers for SOCCP.
- Applications in geosciences.
  - granular flows, rock avalanches,
  - fracture processes,
  - rock stability,
  - friction instabilities (seismic waves).


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Nonsmooth modeling of mechanical systems

Smooth multibody dynamics

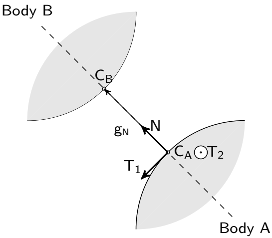
Equations of motion

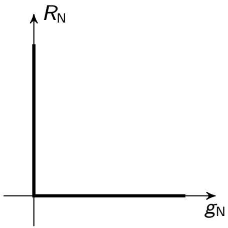
$$\begin{cases} M(q)\dfrac{dv}{dt} + F(t,q,v) = 0, \\ v = \dot{q} \\ q(t_0) = q_0 \in \boldsymbol{R}^n, \quad v(t_0) = v_0 \in \boldsymbol{R}^n, \end{cases} \tag{1}$$

where

- $F(t,q,v) = N(q,v) + F_{int}(t,q,v) - F_{ext}(t)$

Unilateral contact and impact





- Unilateral contact (Signorini condition)

$$0 \leqslant g_{\mathrm{N}}(q) \perp R_{\mathrm{N}} \geqslant 0 \qquad (2)$$

Complementarity condition

- Local relative velocity at contact

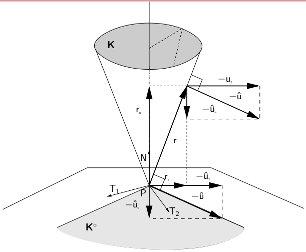
$$U = \begin{bmatrix} U_{\mathrm{N}} \\ U_{\mathrm{T}} \end{bmatrix} = G^T(q)v \qquad (3)$$

- Impact Law (Newton Impact law)

$$U_{\mathrm{N}}^{+} = -e\, U_{\mathrm{N}}^{-} \qquad (4)$$

e is the coefficient of restitution.

Coulomb's friction



Coulomb's friction

Coulomb's friction says the following:
If $g_{\mathrm{N}}(q) = 0$ then:

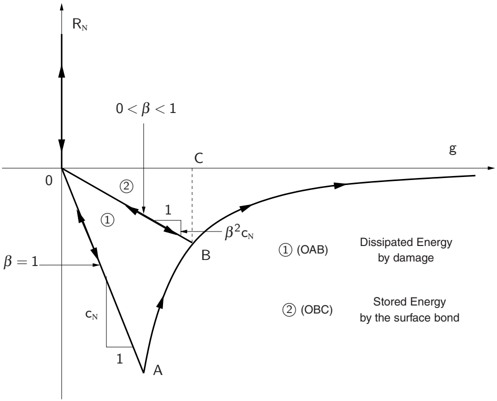
$$\left\{\begin{array}{lll} \text{If } U_{\mathrm{T}} = 0 & \text{then } R \in \ \mathbf{K} \\ \text{If } U_{\mathrm{T}} \neq 0 & \text{then } ||R_{\mathrm{T}}(t)|| = \mu |R_{\mathrm{N}}| \text{ and there exists a scalar } a \geqslant 0 \\ & \text{such that } R_{\mathrm{T}} = -a U_{\mathrm{T}} \end{array}\right. \tag{5}$$

where $K = \{R, ||R_{\mathrm{T}}|| \leqslant \mu |R_{\mathrm{N}}| \ \}$ is the Coulomb friction cone

Maximum dissipation principle in the tangent plane [Moreau, 1974].

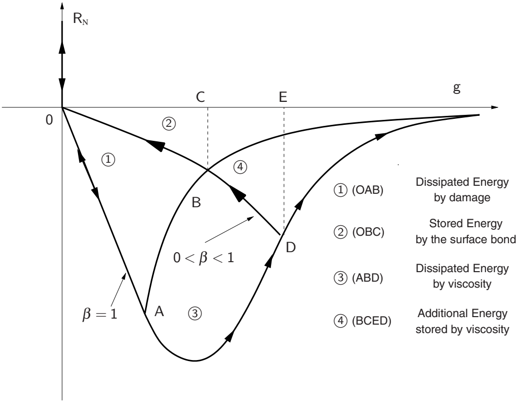
$$\max_{R_{\mathrm{T}} \in D(\mu R_{\mathrm{N}})} -U_{\mathrm{T}}^T R_{\mathrm{T}} \tag{6}$$

Nonsmooth cohesive zone model



(a) Rate independent law

Nonsmooth cohesive zone model



(b) Rate dependent law (viscosity)

Why a nonsmooth modeling rather a smooth one ?

Tribological reasons

- complexity of the behavior of the interface/interphase : elasticity, viscosity, damage, plasticity, wear, ...
- parameters are difficult to identify and to measure
- multi–scale problems: high stiffness coefficients, uncertainties on parameters.

smoothing techniques and regularized models

Regularization enables to use of standard PDE and/or ODE solvers, BUT

- the regularization parameters are in general not physical
- the results are highly sensible the regularization parameters
- the numerical tools are inefficient: stiff ODES, numerical instabilities.
- the intrinsic set–valuedness of the model is not well-represented (sticking state).
- The quasi–static process needs also unrealistic viscosity regularization.

Nonsmooth Lagrangian Dynamics

Fundamental assumptions.

- The velocity $v = \dot{q}$ is assumed to of Bounded Variations (B.V) and right–continuous
$$v^+ = \dot{q}^+ \tag{7}$$
- q is an absolutely continuous function such that
$$q(t) = q(t_0) + \int_{t_0}^{t} v^+(t)\,dt \tag{8}$$
- The acceleration ($\ddot{q}$ in the usual sense) is hence a differential measure dv associated with v such that
$$dv((a,b]) = \int_{(a,b]} dv = v^+(b) - v^+(a) \tag{9}$$

Nonsmooth Lagrangian Dynamics

Definition 1 (Nonsmooth Lagrangian Dynamics)

$$\begin{cases} M(q)dv + F(t,q,v^+)dt = di \\ \\ v^+ = \dot{q}^+ \end{cases} \tag{10}$$

where di is the reaction measure and dt is the Lebesgue measure.

Remarks

- The nonsmooth Dynamics contains the impact equations and the smooth evolution in a single equation.
- The formulation allows one to take into account very complex behaviors, especially, finite accumulation (Zeno-state).
- This formulation is sound from a mathematical Analysis point of view.

References

[Schatzman, 1973, 1978, Moreau, 1983, 1988]

Nonsmooth Lagrangian Dynamics

Measures Decomposition (for dummies)

$$\begin{cases} dv = & \gamma\, dt + & (v^+ - v^-)\, d\nu + & dv_s \\ di = & f\, dt + & p\, d\nu + & di_s \end{cases} \tag{11}$$

where

- $\gamma = \ddot{q}$ is the acceleration defined in the usual sense.
- f is the Lebesgue measurable force,
- $v^+ - v^-$ is the difference between the right continuous and the left continuous functions associated with the B.V. function $v = \dot{q}$,
- $d\nu$ is a purely atomic measure concentrated at the time t_i of discontinuities of v, i.e. where $(v^+ - v^-) \neq 0$,i.e. $d\nu = \sum_i \delta_{t_i}$
- p is the purely atomic impact percussions such that $pd\nu = \sum_i p_i \delta_{t_i}$
- dv_S and di_S are singular measures with the respect to $dt + d\eta$.

Impact equations and Smooth Lagrangian dynamics

Substituting the decomposition of measures into the nonsmooth Lagrangian Dynamics, one obtains

Impact equations

$$M(q)(v^+ - v^-)d\nu = pd\nu, \tag{12}$$

or

$$M(q(t_i))(v^+(t_i) - v^-(t_i)) = p_i, \tag{13}$$

Smooth Dynamics between impacts

$$M(q)\gamma dt + F(t,q,v)dt = fdt \tag{14}$$

or

$$M(q)\gamma^+ + F(t,q,v^+) \quad = \quad f^+ \quad [dt - a.e.] \tag{15}$$

The Moreau's sweeping process of second order

Moreau [1983, 1988]

A key stone of this formulation is the inclusion in terms of velocity.

$$\begin{cases} M(q)dv + F(t,q,v^+)dt = di = G(q)dI \\ v^+ = \dot{q}^+ \\ U^+ = G^T(q)v^+ \\ g_N(q) \leqslant 0 \implies 0 \leqslant U^+ + eU^- \perp dI \geqslant 0 \end{cases} \quad (16)$$

Comments

$$-dI \in N_{T_{\mathbb{R}_+}(g_N(q))}(U^+) \quad (17)$$

This formulation provides a common framework for the nonsmooth dynamics containing inelastic impacts without decomposition.

➜ Foundation of the time–stepping approaches.

Numerical methods for the simulation

Principle of nonsmooth event capturing methods (Time–stepping schemes)

1. A unique formulation of the dynamics is considered. For instance, a dynamics in terms of measures.

$$\begin{cases} -mdv = di \\ q = \dot{v}^+ \\ 0 \leqslant di \perp \dot{v}^+ \geqslant 0 \text{ if } q \leqslant 0 \end{cases} \quad (18)$$

2. The time-integration is based on a consistent approximation of the equations in terms of measures. For instance,

$$\int_{]t_k,t_{k+1}]} dv = \int_{]t_k,t_{k+1}]} dv = (v^+(t_{k+1}) - v^+(t_k)) \approx (v_{k+1} - v_k) \quad (19)$$

3. Consistent approximation of measure inclusion.

$$-di \in N_{T_C(t)}(v^+(t)) \quad (20) \quad \rightarrow \quad \begin{cases} p_{k+1} \approx \int_{]t_k,t_{k+1}]} di \\ \\ p_{k+1} \in N_{K(t)}(v_{k+1}) \end{cases} \quad (21)$$

Time Discretization of the nonsmooth dynamics

For sake of simplicity, the linear time invariant case is only considered.

$$\begin{cases} Mdv + (Kq + Cv^+)\,dt = F_{ext}\,dt + di. \\ v^+ = \dot{q}^+ \end{cases} \tag{22}$$

Integrating both sides of this equation over a time step $]t_k, t_{k+1}]$ of length h,

$$\begin{cases} \displaystyle\int_{]t_k,t_{k+1}]} Mdv + \int_{t_k}^{t_{k+1}} Cv^+ + Kq\,dt = \int_{t_k}^{t_{k+1}} F_{ext}\,dt + \int_{]t_k,t_{k+1}]} di\ , \\ \displaystyle q(t_{k+1}) = q(t_k) + \int_{t_k}^{t_{k+1}} v^+\,dt\ . \end{cases} \tag{23}$$

By definition of the differential measure dv,

$$\int_{]t_k,t_{k+1}]} M\,dv = M \int_{]t_k,t_{k+1}]} dv = M\,(v^+(t_{k+1}) - v^+(t_k))\ . \tag{24}$$

Note that the right velocities are involved in this formulation.

Time Discretization of the nonsmooth dynamics

The equation of the nonsmooth motion can be written under an integral form as:

$$\begin{cases} M\,(v(t_{k+1}) - v(t_k)) = \displaystyle\int_{t_k}^{t_{k+1}} -Cv^+ - Kq + F_{ext}\,dt + \int_{]t_k,t_{k+1}]} di\;, \\[2ex] q(t_{k+1}) = q(t_k) + \displaystyle\int_{t_k}^{t_{k+1}} v^+\,dt\;. \end{cases} \tag{25}$$

The following notations will be used:

- $q_k \approx q(t_k)$ and $q_{k+1} \approx q(t_{k+1})$,
- $v_k \approx v^+(t_k)$ and $v_{k+1} \approx v^+(t_{k+1})$,

Impulse as primary unknown

The impulse $\displaystyle\int_{]t_k,t_{k+1}]} di$ of the reaction on the time interval $]t_k, t_{k+1}]$ emerges as a natural unknown. we denote

$$p_{k+1} \approx \int_{]t_k,t_{k+1}]} di$$

Time Discretization of the nonsmooth dynamics

Interpretation

The measure *di* may be decomposed as follows :

$$di = f\,dt + pd\nu$$

where

- $f\,dt$ is the abs. continuous part of the measure *di*, and
- $pd\nu$ the atomic part.

Two particular cases:

- Impact at $t_* \in]t_k, t_{k+1}]$: If $f = 0$ and $pd\nu = p\delta_{t_{k+1}}$ then

$$p_{k+1} = p$$

- Continuous force over $]t_k, t_{k+1}]$: If $di = fdt$ and $p = 0$ then

$$p_{k+1} = \int_{t_k}^{t_{k+1}} f(t)\,dt$$

Time Discretization of the nonsmooth dynamics

Remark

- A pointwise evaluation of a (Dirac) measure is a non sense. It practice using the value
$$f_{k+1} \approx f(t_{k+1})$$
yield severe numerical inconsistencies, since
$$\lim_{h \to 0} f_{k+1} = +\infty$$
- Since discontinuities of the derivative v are to be expected if some shocks are occurring, i.e. di has some Dirac atoms within the interval $]t_k, t_{k+1}]$, it is not relevant to use high order approximations integration schemes for di. It may be shown on some examples that, on the contrary, such high order schemes may generate artefact numerical oscillations.

Time Discretization of the nonsmooth dynamics

Discretization of smooth terms

θ-method is used for the term supposed to be sufficiently smooth,

$$\begin{aligned} \int_{t_k}^{t_{k+1}} Cv + Kq \, dt \quad &\approx \quad h\left[\theta(Cv_{k+1} + Kq_{k+1}) + (1-\theta)(Cv_k + Kq_k)\right] \\ \int_{t_k}^{t_{k+1}} F_{ext}(t) \, dt \quad &\approx \quad h\left[\theta(F_{ext})_{k+1} + (1-\theta)(F_{ext})_k\right] \end{aligned}$$

The displacement, assumed to be absolutely continuous is approximated by:

$$q_{k+1} = q_k + h\,\left[\theta v_{k+1} + (1-\theta)v_k\right]\ .$$

Time Discretization of the nonsmooth dynamics

Finally, introducing the expression of q_{k+1} in the first equation of (24), one obtains:

$$\left[M + h\theta C + h^2\theta^2 K\right](v_{k+1} - v_k) = -hCv_k - hKq_k - h^2\theta K v_k \\ +h\left[\theta(F_{ext})_{k+1}) + (1-\theta)(F_{ext})_k\right] + p_{k+1}\;, \tag{26}$$

which can be written :

$$v_{k+1} = v_{free} + \widehat{M}^{-1} p_{k+1} \tag{27}$$

where,

- the matrix $\widehat{M} = \left[M + h\theta C + h^2\theta^2 K\right]$ is usually called the iteration matrix and,
- The vector

$$\begin{aligned} v_{free} \quad = \quad & v_k + \widehat{M}^{-1}\Big[- hCv_k - hKq_k - h^2\theta K v_k \\ & +h\left[\theta(F_{ext})_{k+1}) + (1-\theta)(F_{ext})_k\right]\Big] \end{aligned}$$

is the so-called "free" velocity, i.e. the velocity of the system when reaction forces are null.

Time Discretization of the kinematics relations

According to the implicit mind, the discretization of kinematic laws is proposed as follows.
For a constraint α,

$$U^{\alpha}_{k+1} = H^{\alpha\,T}(q_k)\, v_{k+1} \,,$$

$$p^{\alpha}_{k+1} = H^{\alpha}(q_k)\, P^{\alpha}_{k+1} \,, \quad p_{k+1} = \sum_{\alpha} p^{\alpha}_{k+1} \,,$$

where

$$P^{\alpha}_{k+1} \approx \int_{]t_k, t_{k+1}]} d\lambda^{\alpha}.$$

For the unilateral constraints, it is proposed

$$g^{\alpha}_{k+1} = g^{\alpha}_{k} + h\left[\theta U^{\alpha}_{k+1} + (1-\theta) U^{\alpha}_{k}\right] \,.$$

Discretization of the unilateral constraints

Recall that the unilateral constraint is expressed in terms of velocity as

$$-di \in N_{T_C(q)}(v^+) \tag{28}$$

or in local coordinates as

$$-d\lambda^\alpha \in N_{T_{\mathbb{R}_+}(g(q))}(U^{\alpha,+}) \tag{29}$$

The time discretization is performed by

$$-P^\alpha_{k+1} \in N_{T_{\mathbb{R}^+}(g^\alpha(\tilde{q}_{k+1}))}(U^\alpha_{k+1}) \tag{30}$$

where $\tilde{q}_{k+1}$ is a forecast of the position for the activation of the constraints, for instance,

$$\tilde{q}_{k+1} = q_k + \frac{h}{2} v_k$$

In the complementarity formalism, we obtain

$$\text{if } g^\alpha(\tilde{q}_{k+1}) \leqslant 0, \text{ then } \quad 0 \leqslant U^\alpha_{k+1} \perp P^\alpha_{k+1} \geqslant 0$$

Summary of the time discretized equations

One step linear problem
$$\begin{cases} v_{k+1} = v_{free} + \widehat{M}^{-1} p_{k+1} \\ q_{k+1} = q_k + h\,[\theta v_{k+1} + (1-\theta) v_k] \end{cases}$$

Relations
$$\begin{cases} U^{\alpha}_{k+1} = H^{\alpha\,T}(q_k)\, v_{k+1} \\ p^{\alpha}_{k+1} = H^{\alpha}(q_k)\, P^{\alpha}_{k+1} \end{cases}$$

Nonsmooth Law
$$\begin{cases} \text{ if } g^{\alpha}(\tilde{q}_{k+1}) \leqslant 0, \text{ then} \\ 0 \leqslant U^{\alpha}_{k+1} \perp P^{\alpha}_{k+1} \geqslant 0 \end{cases}$$

One step LCP

$$U_{k+1} = H^T(q_k) v_{free} + H^T(q_k) \widehat{M}^{-1} H(q_k)\, P_{k+1}$$

$$\text{if } g^{\alpha}_{p} \leqslant 0, \text{ then } 0 \leqslant U^{\alpha}_{k+1} \perp P^{\alpha}_{k+1} \geqslant 0$$

Moreau's Time stepping scheme

$$
\begin{cases}
M(q_{k+\theta})(v_{k+1}-v_k) - h\tilde{F}_{k+\theta} = H(q_{k+\theta})P_{k+1}, & (31a)\\
q_{k+1} = q_k + hv_{k+\theta}, & (31b)\\
U_{k+1} = H^T(q_{k+\theta})\, v_{k+1} & (31c)\\
-P_{k+1} \in \partial\psi_{T_{\mathbb{R}^m_+}(\tilde{y}_{k+\gamma})}(U_{k+1} + eU_k), & (31d)\\
\tilde{y}_{k+\gamma} = y_k + h\gamma U_k, \quad \gamma \in [0,1]. & (31e)
\end{cases}
$$

with $\theta \in [0,1], \gamma \geqslant 0$ and $x_{k+\alpha} = (1-\alpha)x_{k+1} + \alpha x_k$ and $\tilde{y}_{k+\gamma}$ is a prediction of the constraints.

Properties

- Convergence results for one constraints
- Convergence results for multiple constraints problems with acute kinetic angles
- No theoretical proof of order

Schatzman–Paoli's Time stepping scheme

$$\begin{cases} M(q_k+1)(q_{k+1}-2q_k+q_{k-1}) - h^2F(t_{k+\theta}, q_{k+\theta}, v_{k+\theta}) = p_{k+1}, & (32a) \\ v_{k+1} = \dfrac{q_{k+1}-q_{k-1}}{2h}, & (32b) \\ -p_{k+1} \in N_K\left(\dfrac{q_{k+1}+eq_{k-1}}{1+e}\right), & (32c) \end{cases}$$

where N_K defined the normal cone to K.
For $K = \{q \in \mathbb{R}^n, y = g(q) \geqslant 0\}$

$$0 \leqslant g\left(\frac{q_{k+1}+eq_{k-1}}{1+e}\right) \perp \nabla g\left(\frac{q_{k+1}+eq_{k-1}}{1+e}\right) P_{k+1} \geqslant 0 \qquad (33)$$

Properties

- Convergence results for one constraints
- Convergence results for multiple constraints problems with acute kinetic angles
- No theoretical proof of order

State–of–the–art

Numerical time–integration methods for Nonsmooth Multibody systems (NSMBS):

Nonsmooth event capturing methods (Time–stepping methods)

- ⊕ robust, stable and proof of convergence
- ⊕ low kinematic level for the constraints
- ⊕ able to deal with finite accumulation
- ⊖ very low order of accuracy even in free flight motions

Two main implementations

- Moreau–Jean time–stepping scheme
- Schatzman–Paoli time–stepping scheme

Comparison

Shared mathematical properties

- Convergence results for one constraints
- Convergence results for multiple constraints problems with acute kinetic angles
- No theoretical proof of order

Mechanical properties

- Position vs. velocity constraints
- Respect of the impact law in one step (Moreau) vs. Two-steps(Schatzman)
- Linearized constraints rather than nonlinear.

Signorini's condition and Coulomb's friction

Modeling assumption

Let μ be the coefficient of friction. Let us define the Coulomb friction cone K which is chosen as the isotropic second order cone

$$K = \{r \in \mathbb{R}^3 \mid \|r_\mathrm{T}\| \leqslant \mu r_n\}. \tag{34}$$

The Coulomb friction states

- for the sticking case that

$$u_\mathrm{T} = 0, \quad r \in K \tag{35}$$

- and for the sliding case that

$$u_\mathrm{T} \neq 0, \quad r \in \partial K, \exists\, \alpha > 0, r_\mathrm{T} = -\alpha u_\mathrm{T}. \tag{36}$$

Disjunctive formulation of the frictional contact behavior

$$\begin{cases} r = 0 & \text{if } g_\mathrm{N} > 0 \quad \text{(no contact)} \\ r = 0, u_\mathrm{N} \geqslant 0 & \text{if } g_\mathrm{N} \leqslant 0 \quad \text{(take–off)} \\ r \in K, u = 0 & \text{if } g_\mathrm{N} \leqslant 0 \quad \text{(sticking)} \\ r \in \partial K, u_\mathrm{N} = 0, \exists\, \alpha > 0, u_\mathrm{T} = -\alpha r_\mathrm{T} & \text{if } g_\mathrm{N} \leqslant 0 \quad \text{(sliding)} \end{cases} \tag{37}$$

Signorini's condition and Coulomb's friction

Second Order Cone Complementarity (SOCCP) formulation De Saxcé [1992]

- Modified relative velocity $\hat{u} \in \boldsymbol{R}^3$ defined by

$$\hat{u} = u + \mu \|u_{\mathrm{T}}\| \mathrm{N}. \tag{38}$$

- Second-Order Cone Complementarity Problem (SOCCP)

$$K^\star \ni \hat{u} \perp r \in K \tag{39}$$

if $g_{\mathrm{N}} \leqslant 0$ and $r = 0$ otherwise. The set $K^\star$ is the dual convex cone to K defined by

$$K^\star = \{u \in \boldsymbol{R}^3 \mid r^\top u \geqslant 0, \quad \text{for all } r \in K\}. \tag{40}$$

Signorini's condition and Coulomb's friction

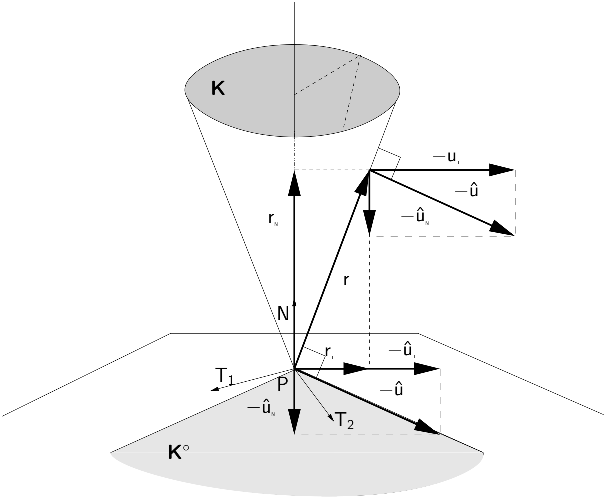


Figure: Coulomb's friction and the modified velocity $\hat{u}$. The sliding case.

3D frictional contact problem

Multiple contact notation

For each contact $\alpha \in \{1, \dots n_c\}$, we have

- the local velocity : $u^\alpha \in \boldsymbol{R}^3$, and

$$u = [[u^\alpha]^\top, \alpha = 1 \dots n_c]^\top$$

- the local reaction vector $r^\alpha \in \boldsymbol{R}^3$

$$r = [[r^\alpha]^\top, \alpha = 1 \dots n_c]^\top$$

- the local Coulomb cone

$$K^\alpha = \{r^\alpha, \|r^\alpha_{\mathrm{T}}\| \leqslant \mu^\alpha |r^\alpha_{\mathrm{N}}|\} \subset \boldsymbol{R}^3$$

and the set K is the cartesian product of Coulomb's friction cone at each contact, that

$$K = \prod_{\alpha=1\dots n_c} K^\alpha \tag{41}$$

and $K^\star$ is dual.

3D frictional contact problems

Problem 2 (General discrete frictional contact problem)

Given

- *a symmetric positive definite matrix* $M \in \mathbb{R}^{n\times n}$,
- *a vector* $f \in \mathbb{R}^n$,
- *a matrix* $H \in \mathbb{R}^{n\times m}$,
- *a vector* $w \in \boldsymbol{R}^m$,
- *a vector of coefficients of friction* $\mu \in \boldsymbol{R}^{n_c}$,

find three vectors $v \in \mathbb{R}^n$, $u \in \boldsymbol{R}^m$ *and* $r \in \boldsymbol{R}^m$, *denoted by* $\mathrm{FC/I}(M, H, f, w, \mu)$ *such that*

$$\begin{cases} Mv = Hr + f \\ u = H^\top v + w \\ \hat{u} = u + g(u) \\ K^\star \ni \hat{u} \perp r \in K \end{cases} \tag{42}$$

with $g(u) = [[\mu^\alpha \| u^\alpha_T \| \mathrm{N}^\alpha]^\top, \alpha = 1 \dots n_c]^\top$. □

3D frictional contact problems

Problem 3 (Reduced discrete frictional contact problem)

Given

- *a symmetric positive semi–definite matrix* $W \in \mathbb{R}^{m\times m}$,
- *a vector* $q \in \mathbb{R}^m$,
- *a vector* $\mu \in \boldsymbol{R}^{n_c}$ *of coefficients of friction,*

find two vectors $u \in \boldsymbol{R}^m$ *and* $r \in \boldsymbol{R}^m$, *denoted by* $\mathrm{FC/II}(W, q, \mu)$ *such that*

$$\begin{cases} u = Wr + q \\ \hat{u} = u + g(u) \\ K^\star \ni \hat{u} \perp r \in K \end{cases} \tag{43}$$

with $g(u) = [[\mu^\alpha \|u^\alpha_T\| \mathrm{N}^\alpha]^\top, \alpha = 1 \dots n_c]^\top$. □

Relation with the general problem

$W = H^\top M^{-1} H$ and $q = H^\top M^{-1} f + w$.

3D frictional contact problems

Wide range of applications

Origin of the linear relations .

$$Mv = Hr + f, \quad u = H^\top v + w$$

- Time–discretization of the discrete dynamical mechanical system
  - Event–capturing time–stepping schemes
  - Event–detecting time–stepping schemes (event-driven)
- Time–discretization and space discretization of the elasto dynamic problem of solids
- Space discretization of the quasi–static problem of solids.

with a possible linearization (Newton procedure.)

➜ These problems are really representative of a lot of applications.

From the mathematical programming point of view

Nonmonotone and nonsmooth problem

$$K^\star \ni Wr + q + g(Wr+q) \perp r \in K \tag{44}$$

- if we neglect $g(\cdot)$, (44) is a gentle monotone SOCLCP that is the KKT conditions of a convex SOCQP.
- otherwise, the problem is nonmonotone and nonsmooth since $g()$ is nonsmooth

➜ The problem is very hard to solve efficiently.

Possible reformulation

- Variational inequality or normal cone inclusion

$$-(Wr + q + g(Wr+q)) \triangleq -F(r) \in N_K(r). \tag{45}$$

- Nonsmooth equations $G(r) = 0$
  - The natural map F^{nat} associated with the VI (45) $F^{\text{nat}}(z) = z - P_X(z - F(z))$.
  - Variants of this map (Alart-Curnier formulation, ...)
  - one of the SOCCP-functions. (Fisher-Bursmeister function)
- and many other ...

VI based methods

Standard methods

- Basic fixed point iterations with projection

$$z_{k+1} \leftarrow P_X(z_k - \rho_k F(z_k))$$

- Extragradient method

$$z_{k+1} \leftarrow P_X(z_k - \rho_k F(P_X(z_k - \rho_k F(z_k))))$$

- Hyperplane projection method

Self-adaptive procedure for ρ_k

For instance,

$$m_k \in \mathbb{N} \quad \text{such that} \quad \begin{array}{l} \rho_k = \rho 2^{m_k}, \\ \rho_k \|F(z_k) - F(\bar{z}_k)\| \leqslant \|z_k - \bar{z}_k\| \end{array} \tag{46}$$

Nonsmooth Equations based methods

Nonsmooth Newton on $G(z) = 0$

$$z_{k+1} = z_k - \Phi^{-1}(z_k)(G(z_k)), \qquad \Phi(z_k) \in \partial G(z_k)$$

- Alart–Curnier Formulation Alart and Curnier [1991]

$$\begin{cases} r_{\mathrm{N}} - P_{\mathbb{R}^{n_c}_+}(r_{\mathrm{N}} - \rho_{\mathrm{N}} u_{\mathrm{N}}) = 0, \\ r_{\mathrm{T}} - P_{D(\mu, r_{\mathrm{N},+})}(r_{\mathrm{T}} - \rho_{\mathrm{T}} u_{\mathrm{T}}) = 0, \end{cases} \tag{47}$$

- Direct normal map reformulation

$$r - P_K\left(r - \rho(u + g(u))\right) = 0$$

- Extension of Fischer-Burmeister function to SOCCP

$$\phi_{\mathrm{FB}}(x, y) = x + y - (x^2 + y^2)^{1/2}$$

with Jordan product and square root

Matrix block-splitting and projection based algorithms Moreau [1994], Jean and Touzot [1988]

Block splitting algorithm with $W^{\alpha\alpha} \in \mathbb{R}^3$

$$
\begin{cases}
u^\alpha_{i+1} - W^{\alpha\alpha} P^\alpha_{i+1} = q^\alpha + \sum_{\beta<\alpha} W^{\alpha\beta} r^\beta_{i+1} + \sum_{\beta>\alpha} W^{\alpha\beta} r^\beta_i \\
\widehat{u}^\alpha_{i+1} = \left[u^\alpha_{\mathrm{N},i+1} + \mu^\alpha \, ||u^\alpha_{\mathrm{T},i+1}||, u^\alpha_{\mathrm{T},i+1}\right]^T \\
\mathbf{K}^{\alpha,*} \ni \widehat{u}^\alpha_{i+1} \perp r^\alpha_{i+1} \in \mathbf{K}^\alpha
\end{cases}
\tag{48}
$$

for all $\alpha \in \{1 \dots m\}$.

One contact point problem

- closed form solutions
- Any solver listed before.

Proximal point technique Moreau [1962, 1965], Rockafellar [1976]

Principle

We want to solve

$$\min_x f(x) \tag{49}$$

We define the approximation problem for a given x_k

$$\min_x f(x) + \rho \|x - x_k\|^2 \tag{50}$$

with the optimal point $x^\star$.

$$x^\star \triangleq \text{prox}_{f,\rho}(x_k) \tag{51}$$

Proximal point algorithm

$$x_{k+1} = \text{prox}_{f,\rho_k}(x_k)$$

Special case for solving $G(x) = 0$

$$f(x) = \frac{1}{2} G^\top(x) G(x)$$

Optimization based methods

- Successive approximation with Tresca friction (Haslinger et al.)

$$\begin{cases} \theta = h(r_{\mathrm{N}}) \\ \min \ \frac{1}{2} r^\top W r + r^\top q \\ \quad \text{s.t.} \qquad r \in C(\mu, \theta) \end{cases} \tag{52}$$

  where $C(\mu,\theta)$ is the cylinder of radius $\mu\theta$.

- Fixed point on the norm of the tangential velocity [A., Cadoux, Lemaréchal, Malick(2011)] .

$$\begin{cases} s = \|u_{\mathrm{T}}\| \\ \min \ \frac{1}{2} r^\top W r + r^\top (q + \alpha s) \\ \quad \text{s.t.} \qquad r \in K \end{cases} \tag{53}$$

  Fixed point or Newton Method on $F(s) = s$

- Alternating optimization problems (Panagiotopoulos et al.)

Siconos/Numerics

Siconos

Open source software for modelling and simulation of nonsmooth systems

Siconos/Numerics

Collection of C routines to solve FC3D problem

- NonSmoothGaussSeidel : VI based projection/splitting algorithm
- TrescaFixedPoint : fixed point algorithm on Tresca fixed point
- LocalAlartCurnier : semi–smooth newton method of Alart–Curnier formulation
- ProximalFixedPoint : proximal point algorithm
- VIFixedPointProjection : VI based fixed-point projection
- VIExtragradient : VI based extra-gradient method
- . . .

http://siconos.gforge.inria.fr

use and contribute ...

Applications applications in mining and geotechnical engineering

Fields of expertise

Mechanical systems with contact, friction, impacts or cohesive interfaces

Modelling and numerical simulations of:

- Granular matter (flows, quasi-static equilibria, dense packing)
- Fracture dynamics.
- Jointed rock mechanics.
- Fluid/Granular flows (sedimentation).
- Multibody system dynamics.

Numerical methods are a kind of Discrete Element method (DEM), but

- Hard contact laws. (Nonsmooth Dynamics)
- Real Coulomb friction
- Enhanced cohesive zone model (CZM) with elasticity, damage

Existing software

LMGC90. CNRS Université de Montpellier II

- F90, Python, (1988–1999) 2000-2015
- Specialized in solid mechanics simulation with contact, friction and cohesion.
- Unilateral contact, friction cohesion laws.
- Pre and pro processing tools for granular matter and meshes. (DEM and FEM)

Siconos. INRIA France

- C++, Python, 2005-2015
- Specialized in simulation of abstract nonsmooth dynamical systems
- Unilateral contact, friction and multiple impacts
- Pre and pro processing tools for mechanisms and robotics

Future plans

- Python coupling in Saladyn project with Salomé and Code_Aster (EdF)
- Merge of the two codes.

Possible applications in geosciences and geotechnical engineering.

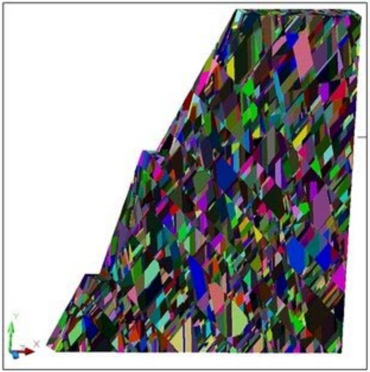
Geosciences

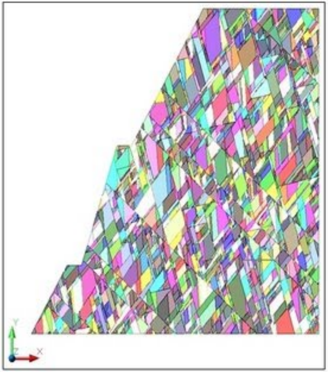
- Rheology, shear instabilities, avalanche in granular media (rocks)
- Fault propagation and Forced-fold
- Propagation of seismic waves
- study of erosion process (mixture Fluid/Granular)

Geotechnical engineering

- Rocky and snow avalanches
- Stability of jointed rock mass
- Earthquake engineering (friction and instability)

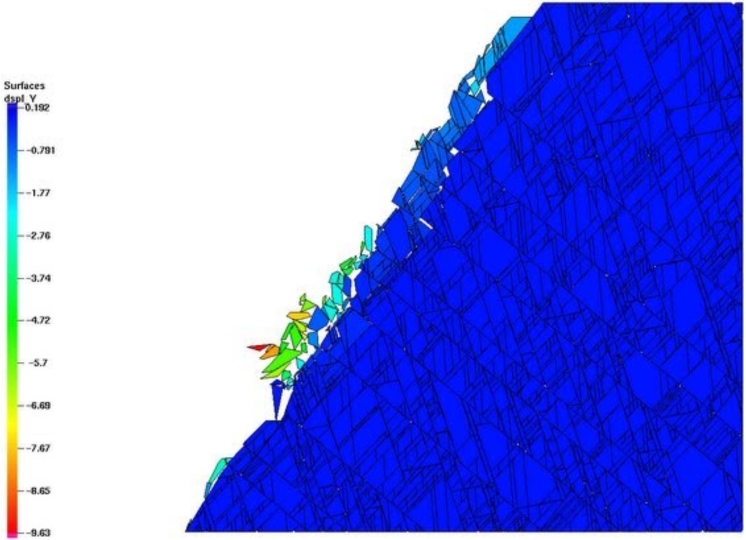
Rock mass Stability



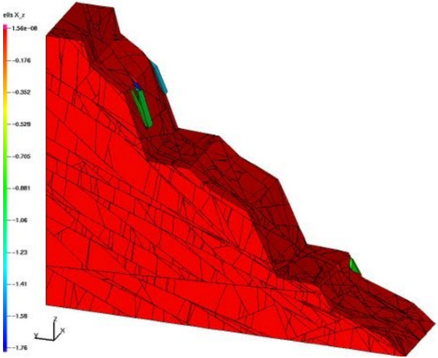


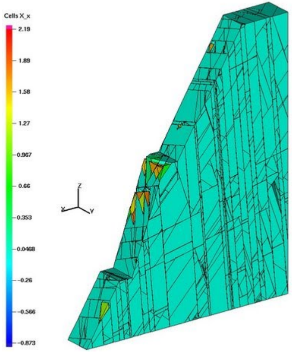
PhD
thesis of A. Rafiee
The Non-Smooth Contact Dynamics method applied to the mechanical simulation of a jointed rock mass Ali Rafiee, Marc Vinches, Frdric Dubois (2011)

Rock mass Stability

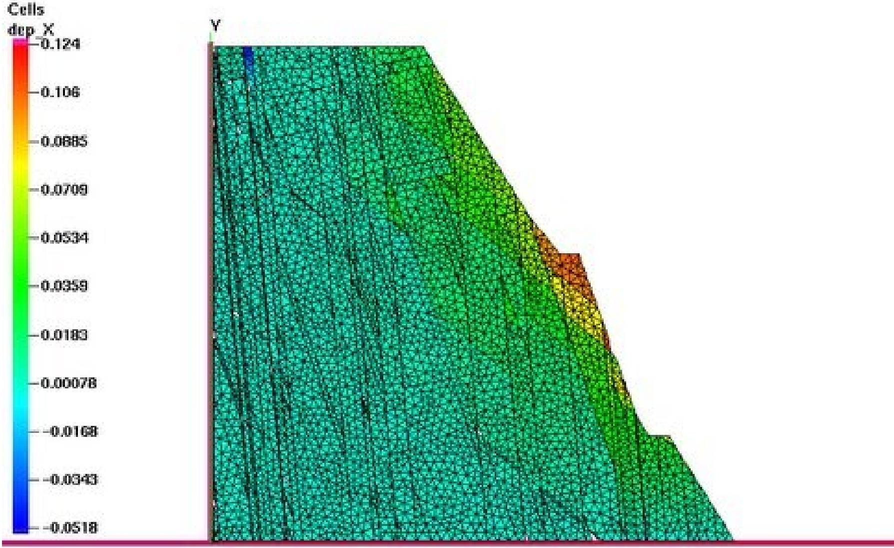


Rock mass Stability

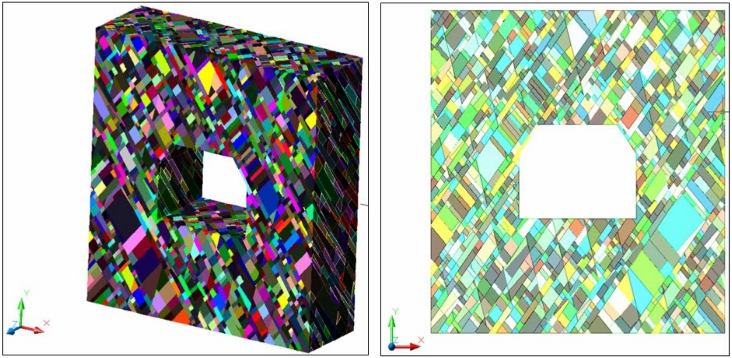




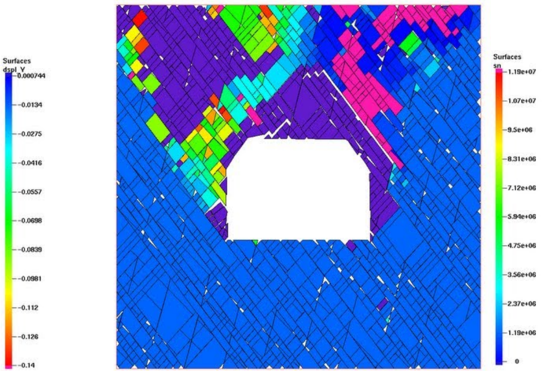
Rock mass Stability



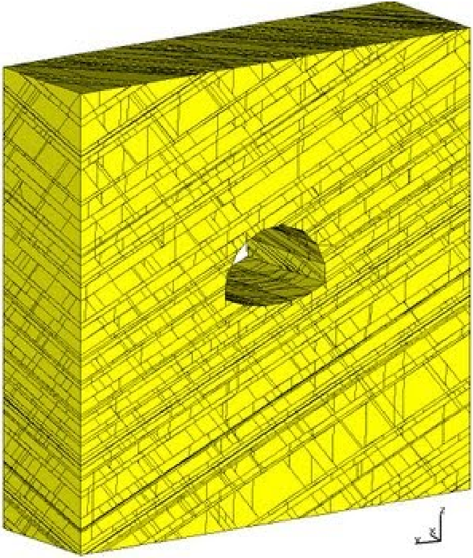
Rock mass Stability for tunnel



Rock mass Stability for tunnel



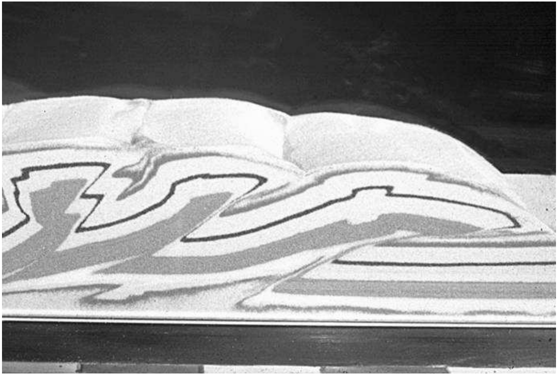
Rock mass Stability for tunnel



Fault propagation and Forced-fold

Numerical Investigations of Fault Propagation and Forced-Fold using a Non Smooth Discrete Element Method
Mathieu Renouf, Frederic Dubois and Pierre Alart (2006)

Experimental sandbox simulation.



Fault propagation and Forced-fold

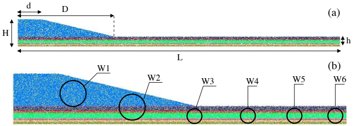


Figure 4. *(a) Initial state of the sample used for forced-fold evolution. (b) Definition of the different cells used for the structure analysis during the whole process.*

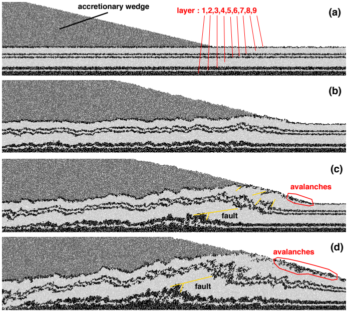


Figure 5. *Different snapshots of the forced-fold evolution : (a) the initial configuration, (b) $t = 200\ s$, (c) $t = 350\ s$ and (d) the final state at $t = 500\ s$*

Fault propagation and Forced-fold

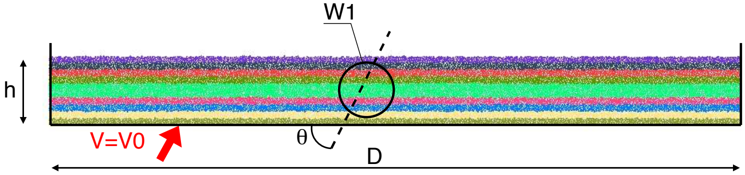


Figure 10. *Initial state of the sample used for fault-propagation.*

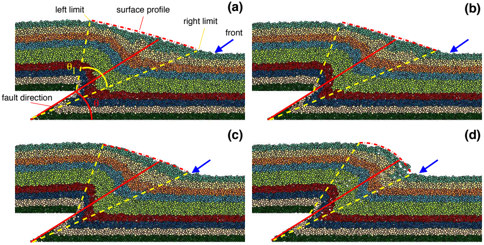


Figure 11. *Profiles for different values of* γ *: (a) 0 N, (b)* 10^3 *N, (c)* 10^4 *N and (d)* 10^5 *N.*

Rheology, shear instabilities, avalanche in granular media (rocks)

- Collaboration between LMGC (F.Radjai, E. Azéma) and Alfredo Taboada. Géosciences Montpellier and Nicolas Estrada, Departamento de Ingenieria Civil y Ambiental, Universidad de los Andes, Bogota, Colombia
- Collboration between LMGC (F. Radjai) and institut Physique du Globe and UMPC(J.P. Vilotte, L. Staron)

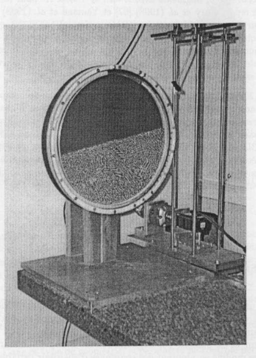


FIG. 2.2 – Photo du dispositif expérimental.

Rheology, shear instabilities, avalanche in granular media (rocks)

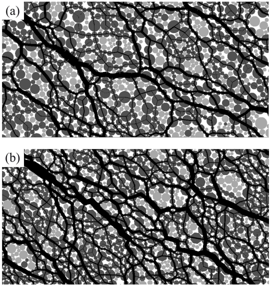


FIGURE 4. Snapshots of the force network in (a) a system composed of disks with rolling friction ($\mu_r = 0.05$) and (b) a system composed of octagonal particles. The line thickness is proportional to the normal force. The floating particles are represented in light grey.

Rheology, shear instabilities, avalanche in granular media (rocks)

Some movies

Many other applications

- Shear wave and friction instabilities between two dissimilar material (FEM + friction). Tectonic plate simulation. Work of L. Baillet
- Cohesive zone modeling with damage for geomaterials.
- ...

Thank you for your attention.

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