The nonsmooth contact dynamics method for the simulation of granular matter flows and fracture in mining applications

The nonsmooth contact dynamics method for the simulation of granular matter flows and fracture in mining applications Seminar CMM. Universidad de Chile Vincent Acary August 27, 2015 Ínnía informatics mathematics

Motivations

Nonsmooth modeling of mechanical systems

Numerical methods for the simulation

Applications in mining and geotechnical engineering

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 mining and geotechnical engineering.
 - granular flows,
 - fracture processes,
 - rock stability.

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Nonsmooth modeling of mechanical systems



Motivations - 5/49

Smooth multibody dynamics

Equations of motion

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

where

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

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Unilateral contact and impact



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Coulomb's friction Coulomb's friction Coulomb's friction says the following: If $g_N(q) = 0$ then: $\left\{ \begin{array}{ll} \text{If } U_{\mathsf{T}} = 0 & \text{then } R \in \mathbf{K} \\ \text{If } U_{\mathsf{T}} \neq 0 & \text{then } ||R_{\mathsf{T}}(t)|| = \mu |R_{\mathsf{N}}| \text{ and there exists a scalar } a \ge 0 \\ & \text{such that } R_{\mathsf{T}} = -a U_{\mathsf{T}} \end{array} \right.$ (5)where $K = \{R, ||R_T|| \leq \mu |R_N|\}$ is the Coulomb friction cone

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

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

Nonsmooth modeling of mechanical systems - 8/49

Coulomb's friction as a Second–Order Cone Complementarity Problem (SOCCP)

Let us introduce the modified velocity \widehat{U} defined by

$$\widehat{U} = [U_{\mathsf{N}} + \mu || U_{\mathsf{T}} ||, U_{\mathsf{T}}]^{\mathsf{T}}.$$
(7)

This notation provides us with a synthetic form of the Coulomb friction as

$$-\widehat{U} \in \mathbb{N}_{\mathbf{K}}(R),\tag{8}$$

or

$$\mathbf{K}^* \ni \widehat{U} \perp R \in \mathbf{K}.$$
 (9)

where $\mathbf{K}^* = \{ v \in \mathbb{R}^n \mid r^T v \ge 0, \forall r \in \mathbf{K} \}$ is the dual cone.

Nonsmooth cohesive zone model



Nonsmooth cohesive zone model



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Nonsmooth Lagrangian Dynamics

Fundamental assumptions.

• The velocity $v = \dot{q}$ is assumed to of Bounded Variations (B.V) and right–continuous

$$v^+ = \dot{q}^+ \tag{10}$$

q is an absolutely continuous function such that

$$q(t) = q(t_0) + \int_{t_0}^t v^+(t) dt$$
(11)

▶ The acceleration (\ddot{q} in the usual sense) is hence a differential measure dv associated with v such that

$$dv((a,b]) = \int_{(a,b]} dv = v^{+}(b) - v^{+}(a)$$
(12)

Nonsmooth Lagrangian Dynamics

Definition 1 (Nonsmooth Lagrangian Dynamics)

$$\begin{cases} M(q)dv + F(t, q, v^{+})dt = di \\ v^{+} = \dot{q}^{+} \end{cases}$$
(13)

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)

$$\begin{cases} dv = \gamma dt + (v^{+} - v^{-}) d\nu + dv_{s} \\ di = f dt + p d\nu + di_{s} \end{cases}$$
(14)

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 ν , i.e. where $(\nu^+ \nu^-) \neq 0$, 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 $dt + d\eta$.

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Impact equations and Smooth Lagrangian dynamics

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

Impact equations

$$M(q)(v^+ - v^-)d\nu = pd\nu, \qquad (15)$$

or

$$M(q(t_i))(v^+(t_i) - v^-(t_i)) = p_i,$$
(16)

Smooth Dynamics between impacts

$$M(q)\gamma dt + F(t, q, v)dt = fdt$$
(17)

or

$$M(q)\gamma^{+} + F(t, q, v^{+}) = f^{+} [dt - a.e.]$$
 (18)

Nonsmooth modeling of mechanical systems - 14/49

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The Moreau's sweeping process of second order Moreau [1983, 1988]

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

$$\begin{cases} M(q)dv + F(t, q, v^{+})dt = di = G(q)dl \\ v^{+} = \dot{q}^{+} \\ U^{+} = G^{T}(q)v^{+} \\ g_{\mathbb{N}}(q) \leq 0 \implies 0 \leq U^{+} + eU^{-} \perp dl \geq 0 \end{cases}$$
(19)

Comments

$$-dI \in N_{\mathcal{T}_{\mathbf{R}_{+}}(g_{\mathbb{N}}(q))}(U^{+})$$
(20)

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

→ Foundation of the time-stepping approaches.

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Numerical methods for the simulation

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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.

$$\begin{cases} -mdv = di \\ q = \dot{v}^+ \\ 0 \leqslant di \perp \dot{v}^+ \geqslant 0 \text{ if } q \leqslant 0 \end{cases}$$
(21)

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

$$\int_{]t_k,t_{k+1}]} dv = \int_{]t_k,t_{k+1}]} dv = (v^+(t_{k+1}) - v^+(t_k)) \approx (v_{k+1} - v_k)$$
(22)

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3. Consistent approximation of measure inclusion.

$$-di \in N_{\mathcal{T}_{\mathcal{C}}(t)}(v^{+}(t)) \quad (23) \quad \Rightarrow \qquad \begin{cases} p_{k+1} \approx \int_{]t_{k}, t_{k+1}]} di \\ p_{k+1} \in N_{\mathcal{K}(t)}(v_{k+1}) \end{cases}$$
(24)

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Time Discretization of the nonsmooth dynamics

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

$$\begin{cases} Mdv + (Kq + Cv^+) dt = F_{ext} dt + di.\\ v^+ = \dot{q}^+ \end{cases}$$
(25)

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

$$\begin{cases} \int_{]t_{k},t_{k+1}]} Mdv + \int_{t_{k}}^{t_{k+1}} Cv^{+} + Kq \, dt = \int_{t_{k}}^{t_{k+1}} F_{ext} \, dt + \int_{]t_{k},t_{k+1}]} di \,, \\ q(t_{k+1}) = q(t_{k}) + \int_{t_{k}}^{t_{k+1}} v^{+} \, dt \,. \end{cases}$$
(26)

By definition of the differential measure dv,

$$\int_{]t_k,t_{k+1}]} M \, dv = M \int_{]t_k,t_{k+1}]} dv = M \left(v^+(t_{k+1}) - v^+(t_k) \right). \tag{27}$$

Note that the right velocities are involved in this formulation.

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Time Discretization of the nonsmooth dynamics

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

$$\begin{cases} M\left(v(t_{k+1}) - v(t_k)\right) = \int_{t_k}^{t_{k+1}} -Cv^+ - Kq + F_{ext} dt + \int_{]t_k, t_{k+1}]} di, \\ q(t_{k+1}) = q(t_k) + \int_{t_k}^{t_{k+1}} v^+ dt. \end{cases}$$
(28)

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

$$p_{k+1} \approx \int_{]t_k, t_{k+1}]}^{t} dt$$

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

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

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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

 $\theta\text{-method}$ is used for the term supposed to be sufficiently smooth,

$$\int_{t_k}^{t_{k+1}} Cv + Kq \, dt \approx h \left[\theta (Cv_{k+1} + Kq_{k+1}) + (1-\theta) (Cv_k + Kq_k) \right]$$

$$\int_{t_k}^{t_{k+1}} F_{ext}(t) \, dt \approx h \left[\theta (F_{ext})_{k+1} + (1-\theta) (F_{ext})_k \right]$$

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 (27), one obtains:

$$\begin{bmatrix} M + h\theta C + h^{2}\theta^{2}K \end{bmatrix} (v_{k+1} - v_{k}) = -hCv_{k} - hKq_{k} - h^{2}\theta Kv_{k} + h[\theta(F_{ext})_{k+1}) + (1 - \theta)(F_{ext})_{k}] + p_{k+1},$$
(29)

which can be written :

$$v_{k+1} = v_{free} + \widehat{M}^{-1} p_{k+1}$$
(30)

where,

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

The vector

$$v_{free} = v_k + \widehat{M}^{-1} \left[-hCv_k - hKq_k - h^2\theta Kv_k + h\left[\theta(F_{ext})_{k+1}\right] + (1-\theta)(F_{ext})_k \right] \right]$$

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 ,

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

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

where

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

For the unilateral constraints, it is proposed

$$g_{k+1}^{lpha} = g_k^{lpha} + h \left[heta U_{k+1}^{lpha} + (1- heta) U_k^{lpha}
ight]$$

Image: A state of the simulation - 23/49

Discretization of the unilateral constraints

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

$$-di \in N_{\mathcal{T}_{\mathcal{C}}(q)}(v^{+}) \tag{31}$$

or in local coordinates as

$$-d\lambda^{\alpha} \in N_{\mathcal{T}_{\mathrm{IR}_{+}}(g(q))}(U^{\alpha,+})$$
(32)

The time discretization is performed by

$$-P_{k+1}^{\alpha} \in N_{\mathcal{T}_{\mathrm{IR}^+}(g^{\alpha}(\tilde{q}_{k+1}))}(U_{k+1}^{\alpha})$$
(33)

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

$$ilde{q}_{k+1} = q_k + rac{h}{2} v_k$$

In the complementarity formalism, we obtain

$$\text{if }g^{\alpha}(\tilde{q}_{k+1})\leqslant0, \text{ then } \quad 0\leqslant U_{k+1}^{\alpha}\perp P_{k+1}^{\alpha}\geqslant0$$

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Summary of the time discretized equations

One step linear problem
$$\begin{cases} v_{k+1} = v_{free} + \widehat{M}^{-1} p_{k+1} \\ q_{k+1} = q_k + h \left[\theta v_{k+1} + (1 - \theta) v_k \right] \end{cases}$$
Relations
$$\begin{cases} U_{k+1}^{\alpha} = H^{\alpha T}(q_k) v_{k+1} \\ p_{k+1}^{\alpha} = H^{\alpha}(q_k) P_{k+1}^{\alpha} \end{cases}$$
Nonsmooth Law
$$\begin{cases} \text{if } g^{\alpha}(\tilde{q}_{k+1}) \leq 0, \text{ then} \\ 0 \leq U_{k+1}^{\alpha} \perp P_{k+1}^{\alpha} \geq 0 \end{cases}$$

One step LCP

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

$$\text{if } g_p^{\alpha} \leqslant 0, \text{ then } 0 \leqslant U_{k+1}^{\alpha} \perp P_{k+1}^{\alpha} \geqslant 0 \\$$

Moreau's Time stepping scheme

$$M(q_{k+\theta})(v_{k+1}-v_k)-h\tilde{F}_{k+\theta}=H(q_{k+\theta})P_{k+1}, \tag{34a}$$

$$q_{k+1} = q_k + h v_{k+\theta}, \tag{34b}$$

$$U_{k+1} = H^{T}(q_{k+\theta}) v_{k+1}$$
(34c)

$$-P_{k+1} \in \partial \psi_{\mathcal{T}_{\mathrm{IR}^{m}_{+}}(\tilde{y}_{k+\gamma})}(U_{k+1} + eU_{k}), \tag{34d}$$

$$\tilde{y}_{k+\gamma} = y_k + h\gamma U_k, \quad \gamma \in [0, 1].$$
 (34e)

with $\theta \in [0, 1], \gamma \ge 0$ 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

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Schatzman–Paoli's Time stepping scheme

$$M(q_{k}+1)(q_{k+1}-2q_{k}+q_{k-1})-h^{2}F(t_{k+\theta},q_{k+\theta},v_{k+\theta})=p_{k+1},$$
 (35a)

$$v_{k+1} = \frac{q_{k+1} - q_{k-1}}{2h},\tag{35b}$$

$$\left(-p_{k+1}\in N_{K}\left(\frac{q_{k+1}+eq_{k-1}}{1+e}\right),$$
(35c)

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

$$0 \leq g\left(\frac{q_{k+1} + eq_{k-1}}{1+e}\right) \perp \nabla g\left(\frac{q_{k+1} + eq_{k-1}}{1+e}\right) P_{k+1} \geq 0$$
(36)

Properties

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

Numerical methods for the simulation - 27/49

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State-of-the-art

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

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Nonsmooth event capturing methods (Time-stepping methods)

- $\oplus \,$ robust, stable and proof of convergence
- \oplus low kinematic level for the constraints
- ⊕ able to deal with finite accumulation
- \ominus 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.

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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

$$\mathcal{K} = \{ r \in \mathbf{R}^3 \mid ||r_{\mathsf{T}}|| \leqslant \mu r_n \}.$$
(37)

The Coulomb friction states

for the sticking case that

$$u_{\rm T}=0, \quad r\in K \tag{38}$$

and for the sliding case that

$$u_{\mathrm{T}} \neq 0, \quad r \in \partial K, \exists \alpha > 0, r_{\mathrm{T}} = -\alpha u_{\mathrm{T}}.$$
 (39)

Disjunctive formulation of the frictional contact behavior

 $\left\{ \begin{array}{ll} r=0 & \text{if } g_{N} > 0 \quad (\text{no contact}) \\ r=0, u_{N} \ge 0 & \text{if } g_{N} \leqslant 0 \quad (\text{take-off}) \\ r\in K, u=0 & \text{if } g_{N} \leqslant 0 \quad (\text{sticking}) \\ r\in \partial K, u_{N} = 0, \exists \, \alpha > 0, u_{T} = -\alpha r_{T} & \text{if } g_{N} \leqslant 0 \quad (\text{sliding}) \end{array} \right.$ (40)

Numerical methods for the simulation - 30/49

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Signorini's condition and Coulomb's friction

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

• Modified relative velocity $\hat{u} \in \mathbf{R}^3$ defined by

1

$$\hat{u} = u + \mu \| u_{\mathsf{T}} \| \mathsf{N}.$$
 (41)

Second-Order Cone Complementarity Problem (SOCCP)

$$K^* \ni \hat{u} \perp r \in K$$
 (42)

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

$$K^{\star} = \{ u \in \mathbf{R}^3 \mid r^{\top} u \ge 0, \quad \text{for all } r \in K \}.$$
(43)

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The nonsmooth contact dynamics method for the simulation of granular matter flows and fracture in mining applications
UNumerical methods for the simulation



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

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3D frictional contact problem

Multiple contact notation

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

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

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

• the local reaction vector $r^{lpha} \in I\!\!R^3$

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

the local Coulomb cone

$$\mathcal{K}^{\alpha} = \{ \mathbf{r}^{\alpha}, \|\mathbf{r}^{\alpha}_{\mathsf{T}}\| \leqslant \mu^{\alpha} |\mathbf{r}^{\alpha}_{\mathsf{N}}| \} \subset \mathbf{R}^{3}$$

and the set ${\it K}$ is the cartesian product of Coulomb's friction cone at each contact, that

$$K = \prod_{\alpha = 1...n_c} K^{\alpha} \tag{44}$$

and K^* is dual.

Numerical methods for the simulation - 33/49

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 $w \in \mathbb{R}^m$,
- a vector of coefficients of friction $\mu \in \mathbf{R}^{n_c}$,

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

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

$$(45)$$
with $g(u) = [[\mu^{\alpha} || u_{T}^{\alpha} || \mathbf{N}^{\alpha}]^{\top}, \alpha = 1 \dots n_{c}]^{\top}.$

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Numerical methods for the simulation - 34/49

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 $\mu \in \mathbf{R}^{n_c}$ of coefficients of friction,

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

$$\begin{cases} u = Wr + q \\ \hat{u} = u + g(u) \\ K^* \ni \hat{u} \perp r \in K \end{cases}$$
(46)

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

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.

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The nonsmooth contact dynamics method for the simulation of granular matter flows and fracture in mining applications \Box Numerical methods for the simulation

From the mathematical programming point of view Nonmonotone and nonsmooth problem

$$K^* \ni Wr + q + g(Wr + q) \perp r \in K$$
(47)

- ▶ if we neglect g(·), (47) 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

$$-(Wr+q+g(Wr+q)) \stackrel{\Delta}{=} -F(r) \in N_{K}(r).$$
(48)

- Nonsmooth equations G(r) = 0
 - The natural map F^{nat} associated with the VI (48) $F^{\text{nat}}(z) = z P_X(z F(z))$.
 - 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

$$\mathsf{z}_{\mathsf{k}+1} \gets \mathsf{P}_{\mathsf{X}}(\mathsf{z}_{\mathsf{k}} - \rho_{\mathsf{k}} \, \mathsf{F}(\mathsf{z}_{\mathsf{k}}))$$

Extragradient method

$$\mathsf{z}_{\mathsf{k}+1} \gets \mathsf{P}_\mathsf{X}(\mathsf{z}_\mathsf{k} - \rho_\mathsf{k}\,\mathsf{F}(\mathsf{P}_\mathsf{X}(\mathsf{z}_\mathsf{k} - \rho_\mathsf{k}\,\mathsf{F}(\mathsf{z}_\mathsf{k}))))$$

Hyperplane projection method

Self-adaptive procedure for ρ_k For instance.

$$m_k \in \mathbf{N}$$
 such that $\begin{array}{l} \rho_k = \rho 2^{m_k}, \\ \rho_k \|F(z_k) - F(\bar{z}_k)\| \leqslant \|z_k - \bar{z}_k\| \end{array}$ (49)

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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]

$$\begin{cases} r_{\rm N} - P_{\boldsymbol{R}^{n_c}_+}(r_{\rm N} - \rho_{\rm N} u_{\rm N}) = 0, \\ r_{\rm T} - P_{D(\mu, r_{\rm N, +})}(r_{\rm T} - \rho_{\rm T} u_{\rm T}) = 0, \end{cases}$$
(50)

Direct normal map reformulation

$$r-P_{K}\left(r-\rho(u+g(u))\right)=0$$

Extension of Fischer-Burmeister function to SOCCP

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

with Jordan product and square root

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

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

$$\begin{cases} u_{i+1}^{\alpha} - W^{\alpha\alpha} P_{i+1}^{\alpha} = q^{\alpha} + \sum_{\beta < \alpha} W^{\alpha\beta} r_{i+1}^{\beta} + \sum_{\beta > \alpha} W^{\alpha\beta} r_{i}^{\beta} \\ \\ \widehat{u}_{i+1}^{\alpha} = \left[u_{\mathsf{N},i+1}^{\alpha} + \mu^{\alpha} || u_{\mathsf{T},i+1}^{\alpha} ||, u_{\mathsf{T},i+1}^{\alpha} \right]^{\mathsf{T}} \\ \\ \mathsf{K}^{\alpha,*} \ni \widehat{u}_{i+1}^{\alpha} \perp r_{i+1}^{\alpha} \in \mathsf{K}^{\alpha} \end{cases}$$
(51)

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

One contact point problem

- closed form solutions
- Any solver listed before.

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

We want to solve

$$\min_{x} f(x) \tag{52}$$

We define the approximation problem for a given x_k

$$\min_{x} f(x) + \rho \|x - x_k\|^2$$
(53)

with the optimal point x^* .

$$x^{\star} \stackrel{\Delta}{=} \operatorname{prox}_{f,\rho}(x_k) \tag{54}$$

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Numerical methods for the simulation - 41/49

Proximal point algorithm

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

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.)

$$\begin{cases} \theta = h(r_{N}) \\ \min \frac{1}{2}r^{\top}Wr + r^{\top}q \\ \text{s.t.} \quad r \in C(\mu, \theta) \end{cases}$$
(55)

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)].

$$\begin{cases} s = \|u_{\mathsf{T}}\|\\ \min \frac{1}{2}r^{\top}Wr + r^{\top}(q + \alpha s)\\ \text{s.t.} \quad r \in K \end{cases}$$
(56)

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

Possible applications in mining industry and geotechnical applications.

Mines engineering process of ore

- Ore (granular) transport and transfer chutes (conveyor)
- ▶ Stirred mills, SAG mills, crushers and High Pressure Grinding Rolls
- Efficient separation, screening performance,
- Surface wear.
- Fluid flows with grains (sedimentation and transports)

Geotechnical engineering

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

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Possible applications in mining industry.

Stability of Rock masses





Image: A math a math

Possible applications in mining industry.

Stability of Rock masses



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Applications in mining and geotechnical engineering - 47/49

Possible applications in mining industry. Stability of Rock masses



Possible applications in mining industry. Stability of Rock masses



Possible applications in mining industry. Stability of Rock masses



Possible applications in mining industry.

Stability of Rock masses



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Possible applications in mining industry.

Stability of Rock masses



47/49

Possible applications in mining industry.

Stability of Rock masses



Starting studies for mines in Chile Flows and filling process of a hopper



Starting studies for mines in Chile

Studies of fracture processes in block caving techniques



Ilustración 2.2-1 Diseño de Macro Bloques y Niveles de Explotación

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Starting studies for mines in Chile

Studies of fracture processes in block caving techniques



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Starting studies for mines in Chile

Studies of fracture processes in block caving techniques



Academic study in progress for the "Chuquicamata" mine (Codelco)

Thank you for your attention.

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