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Cone complementarity problems for solving large scale multi rigid body dynamics

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Model requirements and notation

Nonsmooth rigid multibody dynamics (NRMD) methods attempt to predict the position and velocity evolution of a group of rigid particles subject to certain constraints and forces.

- non-interpenetration.
- collision.
- joint constraints
- adhesion
- Dry friction – Coulomb model.
- global forces: electrostatic, gravitational.

■ These we cover in our approach.

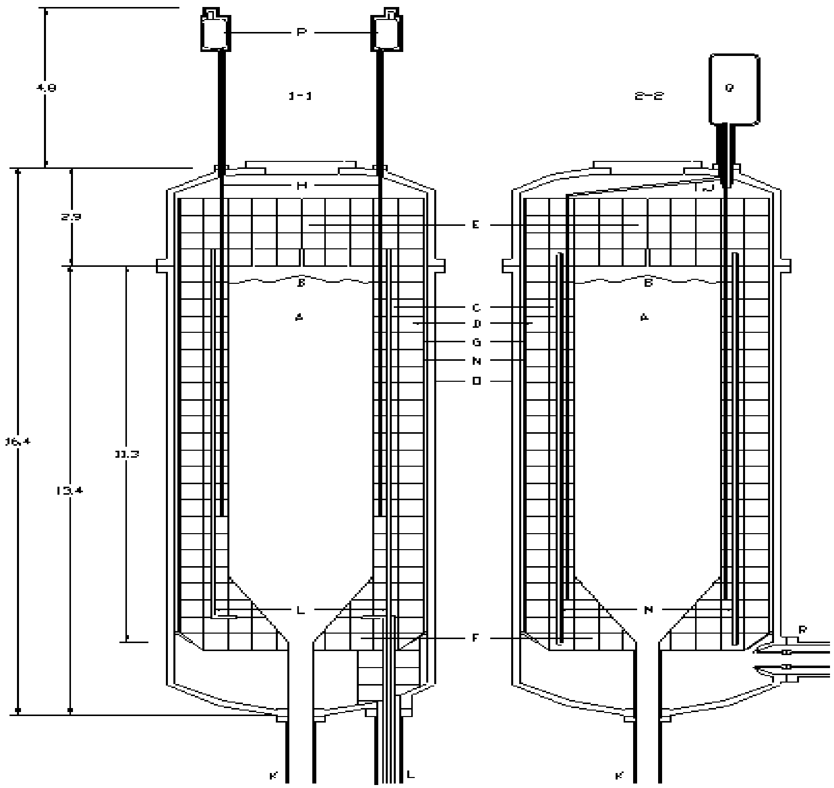
Areas that use NRMD

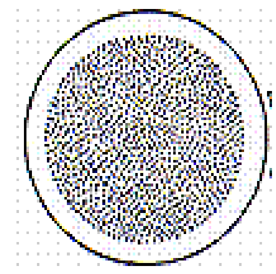
- granular and rock dynamics.
- masonry stability analysis.
- simulation of concrete obstacle response to explosion.
- tumbling mill design (mineral processing industry).
- interactive virtual reality.
- robot simulation and design.

The pebble bed nuclear reactor (PBR)

- In PBR, the fuel pebbles are moving as a slow granular flow. PBR is the leading NGNP candidate for an INL prototype (Pop mech, Oct, 2006)

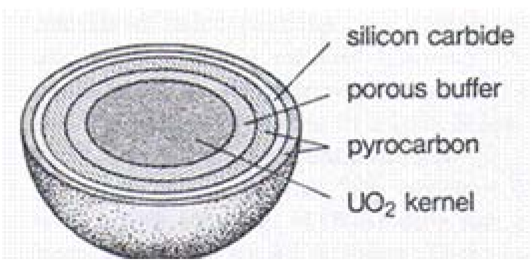
Sketch of a pebble bed reactor with 360,000 fuel pebbles





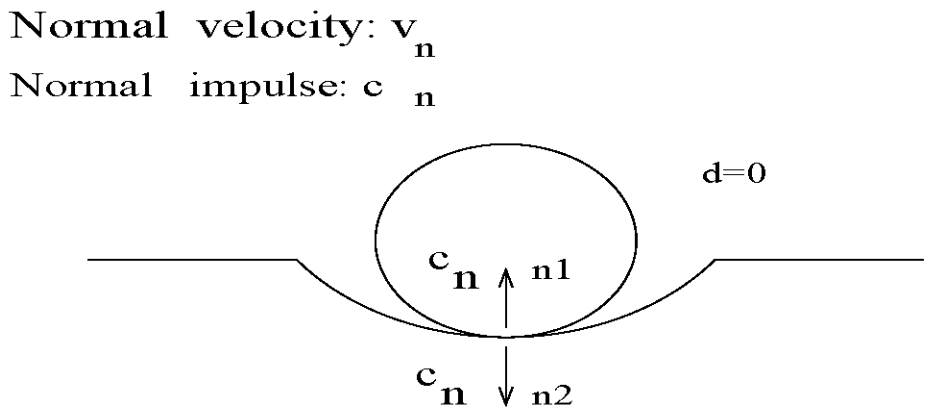
A fuel pebble (60 mm diameter, with a graphite outer shell) contains 11,000 fuel microspheres.

A fuel microsphere (0.9 mm diameter).



Model Requirement and Notation

- MBD system : generalized positions q and velocities v. Dynamic parameters: mass $M(q)$ (positive definite), external force $k(t,q,v)$.
- Non interpenetration constraints: $\Phi^{(j)}(q) \geq 0,\ 1 \leq j \leq n_{total}$ and compressive contact forces at a contact.
- Joint (bilateral) constraints: $\Theta^{(i)}(q) = 0,\ 1 \leq i \leq m$.
- Frictional Constraints: Coulomb friction, for friction coefficients $\mu^{(j)}$.
- Dynamical Constraints: Newton laws, conservation of impulse at collision.



Contact Model

- Contact configuration described by the (generalized) distance function $d = \Phi(q)$, which is defined for some values of the interpenetration. Feasible set: $\Phi(q) \geq 0$.
- Contact forces are compressive, $c_n \geq 0$.
- Contact forces act only when the contact constraint is exactly satisfied, or

$\Phi(q)$ is complementary to c_n or $\Phi(q)c_n = 0$, or $\Phi(q) \perp c_n$.

Friction Model

- Tangent space generators: $\widehat{D}(q) = \left[\widehat{d}_1(q), \widehat{d}_2(q)\right]$, tangent force multipliers: $\beta \in R^2$, tangent force $D(q)\beta$.
- Conic constraints: $||\beta|| \leq \mu c_n$, where μ is the friction coefficient.
- Max Dissipation Constraints: $\beta = \text{argmin}_{||\widehat{\beta}|| \leq \mu c_n} v^T \widehat{D}(q) \widehat{\beta}$.
- v_T, the tangential velocity, satisfies $|v_T| = \lambda = -v^T \widehat{D}(q) \frac{\beta}{||\beta||}$. λ is the Lagrange multiplier of the conic constraint.
- Discretized Constraints: The set $\widehat{D}(q)\beta$ where $||\beta|| \leq \mu c_n$ is approximated by a polygonal convex subset: $D(q)\tilde{\beta}$, $\tilde{\beta} \geq 0$, $\left|\left|\tilde{\beta}\right|\right|_1 \leq \mu c_n$. Here $D(q) = [d_1(q), d_2(q), \ldots, d_m(q)]$.

For simplicity, we denote $\tilde{\beta}$ the vector of force multipliers by β.

Defining the friction cone

For one contact:

$$\begin{aligned} FC^{(j)}(q) &= \Big\{ c_n^{(j)} n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \Big| \\ &\quad c_n^{(j)} \geq 0, \sqrt{\left(\beta_1^{(j)}\right)^2 + \left(\beta_2^{(j)}\right)^2} \leq \mu^{(j)} c_n^{(j)} \Big\}. \end{aligned}$$

The total friction cone:

$$\begin{aligned} FC(q) &= \Big\{ \textstyle\sum_{j=1,2,\ldots,p} c_n^{(j)} n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \Big| \\ &\quad \sqrt{\left(\beta_1^{(j)}\right)^2 + \left(\beta_2^{(j)}\right)^2} \leq \mu^{(j)} c_n^{(j)}, \\ &\quad c_n^{(j)} \geq 0 \perp \Phi^{(j)}(q) = 0, j = 1, 2, \ldots, p \Big\}. \end{aligned}$$

We have

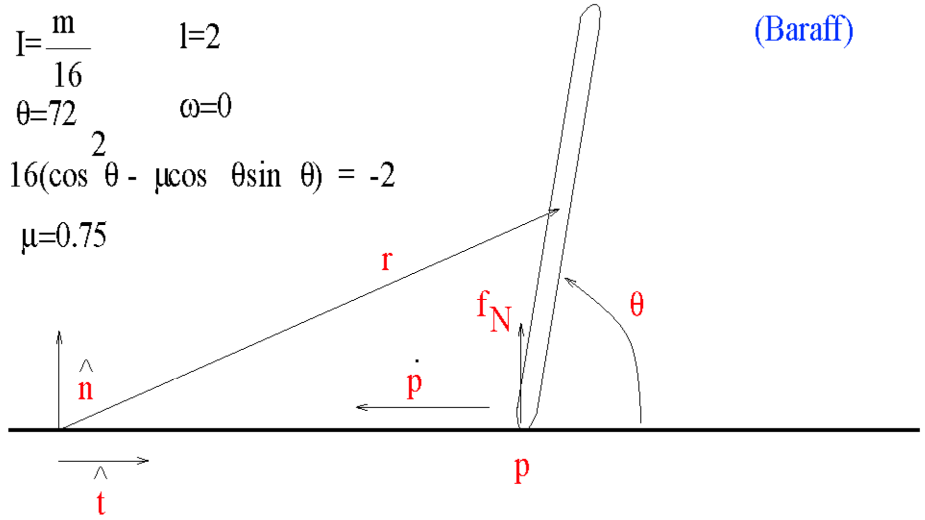
$$FC(q) = \sum_{j=1,2,\ldots,p,\ \Phi^{(j)}(q)=0} FC^{(j)}(q).$$

Nonsmooth dynamics

- Contact, dynamics, friction for rigid bodies. Applicable to granular media, structural analysis, robotics …
- Differential problem with equilibrium constraints – DPEC.

$$
\begin{aligned}
M\frac{dv}{dt} &= \sum_{j=1,2,..,p}\left(c_n^{(j)}n^{(j)}+\beta_1^{(j)}t_1^{(j)}+\beta_2^{(j)}t_2^{(j)}\right)+f_c(q,v)+k(t,q,v)\\
\frac{dq}{dt} &= v\\
c_n^{(j)} &\geq 0 \quad \perp \quad \Phi^{(j)}(q)\geq 0,\; j=1,2,\ldots,p\\
\left(\beta_1^{(j)},\beta_2^{(j)}\right) &= \operatorname{argmin}_{\mu^{(j)}c_n^{(j)}\geq\sqrt{\left(\beta_1^{(j)}+\beta_2^{(j)}\right)^2}} \qquad j=1,2,\ldots,p\\
&\quad \left[\left(v^Tt_1^{(j)}\right)t_1^{(j)}+\left(v^Tt_2^{(j)}\right)t_2^{(j)}\right]^T\left(\beta_1t_1^{(j)}+\beta_2t_2^{(j)}\right).
\end{aligned}
$$

Painleve Paradox—no strong solutions



$$p = r - \frac{l}{2}\begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix}$$

Constraint: $\hat{n}p \geq 0$ (defined everywhere).

$$\hat{n}\ddot{p} = -g + f_N\left(\frac{1}{m} + \frac{l}{2I}\left(\cos^2(\theta) - \mu\sin(\theta)\cos(\theta)\right)\right)$$

$$\hat{n}\ddot{p}_a = -g - \frac{f_N}{m}$$

Painleve Paradox: No classical solutions!

Measure differential inclusion—first step

$$
\begin{aligned}
M\frac{dv}{dt} &= f_C(q,v) + k(q,v) + \rho \\
\frac{dq}{dt} &= v. \\
\rho &= \sum_{j=1}^{p} \rho^{(j)}(t). \\
\rho^{(j)}(t) &\in FC^{(j)}(q(t)) \\
\Phi^{(j)}(q) &\geq 0, \\
\left|\left|\rho^{(j)}\right|\right| \Phi^{(j)}(q) &= 0, \quad j = 1, 2, \ldots, p.
\end{aligned}
$$

However, we cannot expect even that the velocity is continuous!. So we must consider a weaker form of differential relationship

Measure differential inclusion – second step

We must now assign a meaning to

$$M\frac{dv}{dt} - f_c(q,v) - k(t,q,v) \in FC(q).$$

Definition If ν is a measure and $K(\cdot)$ is a convex-set valued mapping, we say that v satisfies the differential inclusions

$$\frac{dv}{dt} \in K(t)$$

if, for all continuous $\phi \geq 0$ with compact support, not identically 0, we have that

$$\frac{\int \phi(t)\nu(dt)}{\int \phi(t)dt} \in \bigcup_{\tau:\phi(\tau)\neq 0} K(\tau).$$

Weak solution for NRMD

Find $q(\cdot), v(\cdot)$ such that

1. $v(0)$ is a function of bounded variation (but may be discontinuous).
2. $q(\cdot)$ is a continuous, locally Lipschits function that satisfies

$$q(t) = q(0) + \int_0^t v(\tau) d\tau$$

3. The measure $dv(t)$, which exists due to v being a bounded variation function, must satisfy, (where $f_c(q, v)$ is the Coriolis and Centripetal Force)

$$\frac{d(Mv)}{dt} - k(t, v) - f_c(q, v) \in FC(q(t))$$

4. $\Phi^{(j)}(q) \geq 0, \forall j = 1, 2, \ldots, p.$

Optimization-based simulation of nonsmooth dynamics.

Define the following time-stepping scheme

$$v^{(l+1)} = \begin{bmatrix} \text{argmin}_{\hat{v}} & \frac{1}{2}\hat{v}^T M \hat{v} + k^{(l)^T} \hat{v} & \\ \text{subject to} & \nabla\Phi^{(j)^T} \hat{v} - \mu^{(j)} \sqrt{\left(t_1^{(j)^T} \hat{v}\right)^2 + \left(t_2^{(j)^T} \hat{v}\right)^2} & \\ & + \frac{1}{h}\Phi^{(j)}(q^{(l)}) & \geq 0 \\ & j \in A(q^{(l)}, \varepsilon), \quad k = 1, 2, \ldots, m^{(j)} & \end{bmatrix}$$

$$A(q^{(l)}, \varepsilon) = \left\{ j \mid \Phi^{(j)}(q^{(l)}) \leq \varepsilon \right\}$$

$$q^{(l+1)} = q^l + h v^{l+1}$$

Result

H1 The functions $n^{(j)}(q), t_1^{(j)}(q), t_2^{(j)}(q)$ are smooth and globally Lipschitz, and they are bounded in the 2-norm.

H2 The mass matrix M is positive definite.

H3 The external force increases at most linearly with the velocity and position.

H4 The uniform pointed friction cone assumption holds.

Then there exists a subsequence $h_k \rightarrow 0$ where

- $q^{h_k}(\cdot) \rightarrow q(\cdot)$ uniformly.
- $v^{h_k}(\cdot) \rightarrow v(\cdot)$ pointwise a.e.
- $dv^{h_k}(\cdot) \rightarrow dv(\cdot)$ weak * as Borel measures. in [0,T], and every such subsequence converges to a solution $(q(\cdot), v(\cdot))$ of MDI. Here q^{h_k} and v^{h_k} is produced by the relaxed algorithm.

How we got here (I)

Euler method, half-explicit in velocities, linearization for constraints.
Maximum dissipation principle enforced through optimality conditions.

$$M(v^{l+1} - v^{(l)}) - \sum_{i=1}^{m} \nu^{(i)} c_\nu^{(i)} - \sum_{j \in \mathcal{A}} \left(n^{(j)} c_n^{(j)} + D^{(j)} \beta^{(j)} \right) = hk$$

$$\nu^{(i)^T} v^{l+1} = -\gamma \frac{\Theta^{(i)}}{h}, \qquad i = 1, 2, \ldots, m$$

$$\rho^{(j)} = n^{(j)^T} v^{l+1} \geq -\gamma \frac{\Phi^{(j)}(q)}{h}, \quad \textbf{compl. to} \quad c_n^{(j)} \geq 0, \quad j \in \mathcal{A}$$

$$\sigma^{(j)} = \lambda^{(j)} e^{(j)} + D^{(j)T} v^{l+1} \geq 0, \quad \textbf{compl. to} \quad \beta^{(j)} \geq 0, \quad j \in \mathcal{A}$$

$$\zeta^{(j)} = \mu^{(j)} c_n^{(j)} - e^{(j)^T} \beta^{(j)} \geq 0, \quad \textbf{compl. to} \quad \lambda^{(j)} \geq 0, \quad j \in \mathcal{A}.$$

Here $\nu^{(\mathbf{i})} = \nabla \boldsymbol{\Theta}^{(\mathbf{i})}$, $n^{(j)} = \nabla \Phi^{(j)}$. h is the time step. The set $\mathcal{A}$ consists of the active constraints. Stewart and Trinkle, 1996, MA and Potra,1997:
Scheme has a solution although the classical formulation doesn't!

How we got here (II)—in the limit of faces of cone approx to infinity

Define $\Theta^{(l)} = -Mv^{(l)} - hk^{(l)}$. We solve the following LCP

$$\begin{bmatrix} M & -\tilde{\nu} & -\tilde{n} & -\tilde{D} & 0 \\ \tilde{\nu}^T & 0 & 0 & 0 & 0 \\ \tilde{n}^T & 0 & 0 & 0 & -\tilde{\mu} \\ \tilde{D}^T & 0 & 0 & 0 & \tilde{E} \\ 0 & 0 & \tilde{\mu} & -\tilde{E}^T & 0 \end{bmatrix} \begin{bmatrix} v^{(l+1)} \\ \tilde{c}_\nu \\ \tilde{c}_n \\ \tilde{\beta} \\ \tilde{\lambda} \end{bmatrix} + \begin{bmatrix} \Theta^{(l)} \\ \Upsilon \\ \Delta \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \tilde{\rho} \\ \tilde{\sigma} \\ \tilde{\zeta} \end{bmatrix}$$

$$\begin{bmatrix} \tilde{c}_n \\ \tilde{\beta} \\ \tilde{\lambda} \end{bmatrix}^T \begin{bmatrix} \tilde{\rho} \\ \tilde{\sigma} \\ \tilde{\zeta} \end{bmatrix} = 0, \qquad \begin{bmatrix} \tilde{c}_n \\ \tilde{\beta} \\ \tilde{\lambda} \end{bmatrix} \geq 0, \qquad \begin{bmatrix} \tilde{\rho} \\ \tilde{\sigma} \\ \tilde{\zeta} \end{bmatrix} \geq 0.$$

The LCP is actually equivalent to a strongly convex QP.

Why to do the conic constrained problems?

- Since it is much more compact, fewer constraints
- Most users report improvement over polyhedral cones without proof of convergence for Gauss-Seidell.

Optimality conditions for problems with cone constraints, Polar cones.

MRBD – Conic formulation.

We now define the cones

$$\Lambda^i = \left\{x, y, z \in \mathbb{R}^3 | x \geq \mu^i \sqrt{y^2 + z^2}\right\}, \quad \mathcal{FC}^i = \left\{x, y, z \in \mathbb{R}^3 | \mu^i x \geq \sqrt{y^2 + z^2}\right\}.$$

$\tilde{u} \in \Lambda^i$ and $\tilde{w} \in \mathcal{FC}^i$ imply that $\tilde{u}^T \tilde{w} \geq 0$ **Why ?**

Use notation:

$$n^i \leftrightarrow D_n, \quad d^i_{1,2},\ t^i_{1,2} \leftrightarrow D_u, D_v, \quad \tilde{f}^l \leftrightarrow \tilde{k}^l$$

$$\begin{array}{rcl} v^{l+1} & = & \arg\min_v \frac{1}{2} v^T M v + v^T \tilde{f}^{(l)} \\ \text{subject to} & & \left(\frac{1}{h}\Phi^i(q^{(l)}) + \nabla\Phi^{i^T} v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)}\right) \in -\mathcal{FC}^{i\circ}, \\ & & i \in \mathcal{A}(q^{(l)}, \epsilon) \end{array} \tag{1}$$

Optimality conditions – Conic complementarity problem

$$
\begin{array}{rcl}
v^{l+1} & = & \arg\min_v \frac{1}{2} v^T M v + v^T \tilde{f}^{(l)} \\
\text{subject to} & & \left(\frac{1}{h} \Phi^i(q^{(l)}) + \nabla {\Phi^i}^T v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)} \right) \in -\mathcal{FC}^{i\circ}, \\
& & i \in \mathcal{A}(q^{(l)}, \epsilon)
\end{array} \tag{1}
$$

$$
\begin{array}{rcl}
M v^{(l+1)} & = & \tilde{f}^{(l)} + \sum_{i \in \mathcal{A}(q^{(l)},\epsilon)} \left(\gamma_n^i D_n^i + \gamma_u^i D_u^i + \gamma_v^i D_v^i \right), \\
i \in \mathcal{A}(q^{(l)}, \epsilon) & & \left(\frac{1}{h} \Phi^i(q^{(l)}) + \nabla {\Phi^i}^T v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)} \right) \\
& & \in -\mathcal{FC}^{i\circ} \perp (\gamma_n^i, \gamma_u^i, \gamma_v^i) \in \mathcal{FC}^i.
\end{array} \tag{1}
$$

Why ?

Abstract form—preliminaries.

$$
\begin{aligned}
b \in \mathbb{R}^{3n_{\mathcal{A}}} &= \left(\tfrac{1}{h}\Phi^{i_1}(q^{(l)}), 0, 0, \tfrac{1}{h}\Phi^{i_2}(q^{(l)}), 0, 0, \ldots, \tfrac{1}{h}\Phi^{i_{n_{\mathcal{A}}}}(q^{(l)}), 0, 0\right) \\
r \in \mathbb{R}^{3n_{\mathcal{A}}} &= \Big(\tfrac{1}{h}\Phi^{i_1}(q^{(l)}) + D_n^{i_1^T} M^{-1}\tilde{k}, D_u^{i_1^T} M^{-1}\tilde{k}, D_v^{i_1^T} M^{-1}\tilde{k}, \\
&\quad \tfrac{1}{h}\Phi^{i_2}(q^{(l)}) + D_n^{i_2^T} M^{-1}\tilde{k}, D_u^{i_2^T} M^{-1}\tilde{k}, D_v^{i_2^T} M^{-1}\tilde{k}, \\
&\quad \ldots, \tfrac{1}{h}\Phi^{i_{n_{\mathcal{A}}}}(q^{(l)}) + D_n^{i_{n_{\mathcal{A}}}^T} M^{-1}\tilde{k}, D_u^{i_{n_{\mathcal{A}}}^T} M^{-1}\tilde{k}, D_v^{i_{n_{\mathcal{A}}}^T} M^{-1}\tilde{k}\Big) \\
\gamma \in \mathbb{R}^{3n_{\mathcal{A}}} &= \left(\gamma_n^{i_1}, \gamma_u^{i_1}, \gamma_v^{i_1}, \gamma_n^{i_2}, \gamma_u^{i_2}, \gamma_v^{i_2}, \ldots, \gamma_n^{i_{n_{\mathcal{A}}}}, \gamma_u^{i_{n_{\mathcal{A}}}}, \gamma_v^{i_{n_{\mathcal{A}}}}\right)
\end{aligned}
\tag{1}
$$

and the following matrices

$$
\begin{aligned}
D^i &= \left[D_n^i, D_u^i, D_v^i\right], i \in \mathcal{A}(q^{(l)}, \epsilon), \\
D &= \left[D^{i_1}, D^{i_2}, \ldots, D^{i_{n_{\mathcal{A}}}}\right], \quad N = D^T M^{-1} D.
\end{aligned}
\tag{2}
$$

Abstract form

$$(CCP) \quad (N\gamma + r)^{i} \in -\mathcal{FC}^{i\circ} \perp \gamma^{i} \in \mathcal{FC}^{i}, i = 1, 2, \ldots, n_{\mathcal{A}}. \tag{1}$$

- Note that it includes linear complementarity problems, if the cones are products of R^+
- It can also be seen as the optimality conditions of a problem with cone-constrained variables (problems with bound constraints in the case above)

Convex cones facts and prelims

Assume that we have a set of closed convex cones $\Upsilon^i \subset \mathbb{R}^{n_i}$, where the index takes the values $i = 1, 2, \ldots, n_k$. We consider the Cartesian product of such cones $\Upsilon = \bigoplus_{i=1}^{n_k} \Upsilon^i$, which we assume is a cone in $\mathbb{R}^{n_c}$, that is, that the sum of the dimensions of the element cones satisfies $n_c = \sum_{i=1}^{n_k} n_i$.

$\Pi_C(y)$ the projection of the vector $y \in \mathbb{R}^m$ onto the convex cone C.

Polar cone: $C^\circ = \{x \in \mathbb{R}^m | \langle x, y\rangle \leq 0, \ \forall y \in C\}$.

Properties of cones (Lemarechal)

P1 $\|\Pi_C(y_1) - \Pi_C(y_2)\|^2 \leq \langle \Pi_C(y_1) - \Pi_C(y_2), y_1 - y_2 \rangle, \quad \forall y_1, y_2 \in \mathbb{R}^m$

P2 $x = \Pi_C(y) \Leftrightarrow x \in C, \ y - x \in C^\circ, \ \langle x, y - x\rangle = 0$

P3 $\Pi_\Upsilon(x) = (\Pi_{\Upsilon^1}(x_1), \Pi_{\Upsilon^2}(x_2), \ldots, \Pi_{\Upsilon^{n_k}}(x_{n_k}))$

P4 $\Upsilon^\circ = \bigoplus_{i=1}^{n_k} \Upsilon^{i,\circ}$

*Gauss * Algorithm*

Theorem Solution of (CCP) iff fixed point of

$$x^{r+1} = \lambda \Pi_{\Upsilon} \left(x^r - \omega B^r \left(N x^r + r + K^r \left(x^{r+1} - x^r \right) \right) \right) + (1-\lambda) x^r, \quad r = 0, 1, 2, \ldots, \tag{1}$$

where $0 < \lambda \leq 1, \quad \omega > 0.$

$$B^r = \begin{pmatrix} \eta_1 I_{n_1} & 0 & \cdots & 0 \\ 0 & \eta_2 I_{n_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \eta_{n_k} I_{n_{n_k}} \end{pmatrix}, \quad L^r = \begin{pmatrix} 0 & K_{12} & K_{13} & \cdots & K_{1n_k} \\ 0 & 0 & K_{23} & \cdots & K_{2n_k} \\ 0 & 0 & 0 & \cdots & K_{3n_k} \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & 0 & & 0 \end{pmatrix}, \tag{1}$$

where $\eta_i > 0, \quad i = 1, 2, \ldots, n_k,\ I_{n_i} \in \mathbb{R}^{n_i \times n_i},\ K_{ij} \in \mathbb{R}^{n_i \times n_j},\ 1 \leq i < j \leq n_k,$ and we have either that $K^r = L^r$, or that $K^r = L^{rT}$.

$K^r = 0$: Gauss Jacobi, $K^r = L^{rT}$, Gauss Seidel

Assumptions about the algorithm

A1 The matrix N of the problem (CCP) is symmetric and positive semi-definite.

A2 There exists a positive number, $\alpha > 0$ such that, at any iteration r, $r = 0, 1, 2, \ldots,$ we have that $B^r \succ \alpha I$

A3 There exists a positive number, $\beta > 0$ such that, at any iteration r, $r = 0, 1, 2, \ldots,$ we have that $(x^{r+1} - x^r)^T \left((\lambda \omega B^r)^{-1} + K^r - \frac{N}{2} \right) (x^{r+1} - x^r) \geq \beta \left\| x^{r+1} - x^r \right\|^2$.,

(so $\lambda\omega$ needs to be sufficiently small; but theory works with λ and ω changed at every iteration, but bounded away from 0 and this is a computable test, as long as α and β are fixed. Any obvious test would work after a FINITE number of iterations)

Theory

$$
(OC) \quad \begin{array}{lll} \min & f(x) = \frac{1}{2} x^T N x + r^T x & \\ s.t. & x_i \in \Upsilon^i, & i = 1, 2, \ldots, n_k. \end{array}
$$

Theorem Assume that $x^0 \in \Upsilon$ and that the sequences of matrices B^r and K^r are bounded. Then we have that

$$
f(x^{r+1}) - f(x^r) \le -\beta \left\| x^{r+1} - x^r \right\|^2
$$

for any iteration index r, and any accumulation point of the sequence x^r is a solution of (CCP).

Corollary Assume that the friction cone of the configuration is pointed (that is, there does not exist a choice of reaction forces whose net effect is zero). If the relevant parameters satisfy assumptions A2 and A3, then the algorithm produces a bounded sequence, and any accumulation point results in the same velocity solution

Gauss-Seidell optimized version (in terms of storage)

1. For $i = 1, 2, \ldots, n_{\mathcal{A}}$ compute the $m \times 3$ matrices $s^i = M^{-1} D^i$ and 3×3 matrices $g^i = D^{i,T} s^i$.

2. For $i = 1, 2, \ldots, n_{\mathcal{A}}$, compute $\eta_i = \frac{3}{\mathrm{Trace}(g^i)}$.

3. If warm starting with some initial guess γ^*, initialize reactions as $\gamma^0 = \gamma^*$, otherwise $\gamma^0 = 0$.

4. Initialize speeds: $v = \sum_{i=1}^{n_{\mathcal{A}}} s^i \gamma^{i0} + M^{-1} \tilde{k}$.

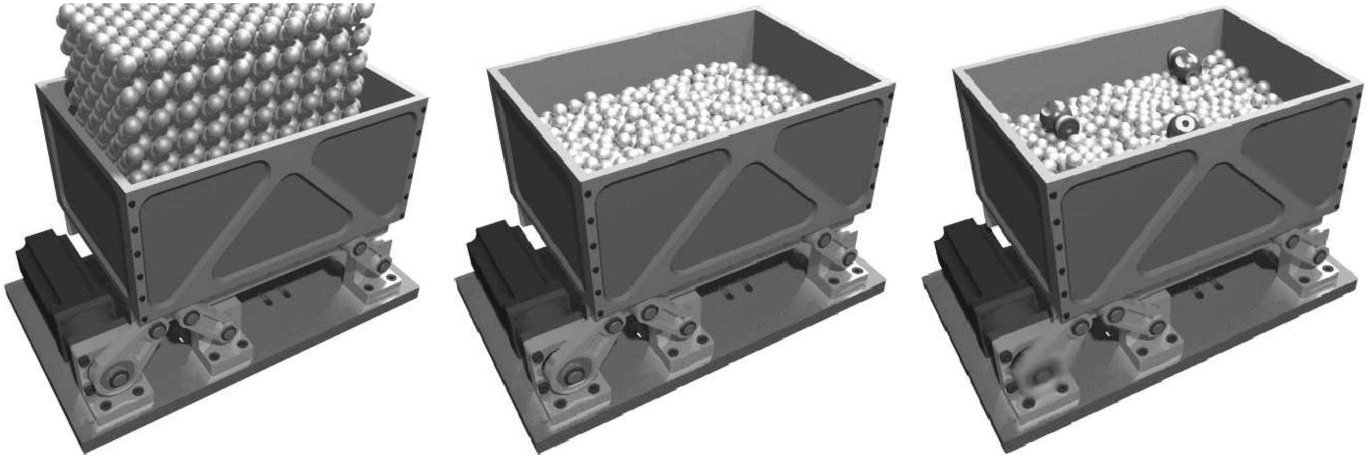
5. For $i = 1, 2, \ldots n_{\mathcal{A}}$, perform the updates
   $\delta^{ir} = \left(\gamma^{ir} - \omega \eta_i \left(D^{i,T} v^r + b^i\right)\right);$
   $\gamma^{i,r+1} = \lambda \Pi_{\Upsilon} \left(\delta^{ir}\right) + (1 - \lambda) \gamma^{ir} \;;$
   $\Delta \gamma^{i,r+1} = \gamma^{i,r+1} - \gamma^{ir} \;;$
   $v := v + {s^i}^T \Delta \gamma^{i,r+1}.$

6. Repeat the loop 5 in reverse order, if symmetric updates are desired.

7. $r := r + 1$. Repeat from 5 until convergence, or until $r > r_{max}$.

Numerical Results: Example 1: Size-based segregation

- 300-1500 bodies
- omega=lambda=1
- Time step=0.01
- 20-80 iterations



Example 1 (II): Convergence

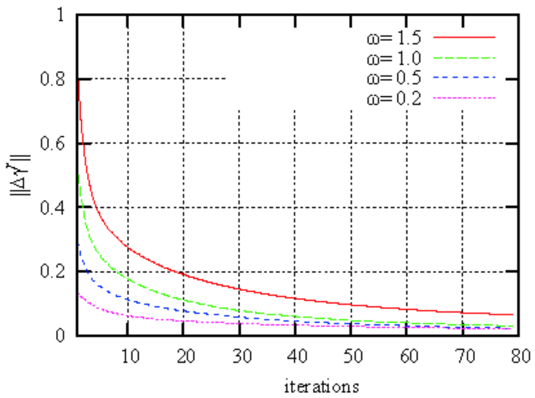


Fig. 3 Convergence of $\Delta\gamma^r$ for varying ω, for a sample time step in the 300-sphere benchmark.

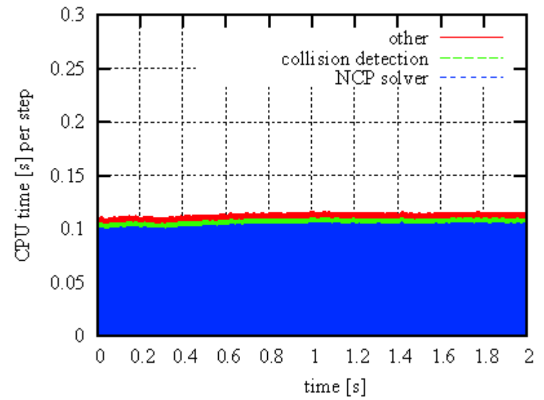


Fig. 4 CPU time for each step in a 1000-body simulation, split into CCP fraction, collision detection fraction, and other.

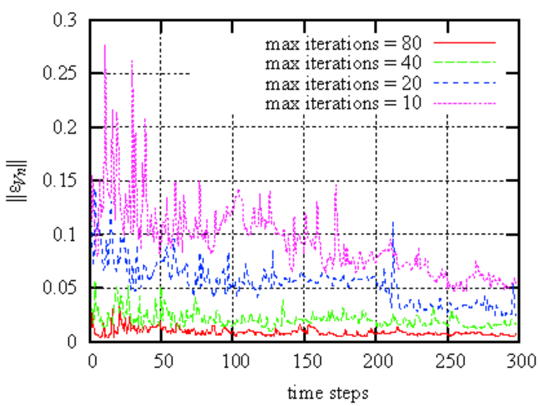


Fig. 5 Maximum speed violation in constraints, for the 300-sphere benchmark.

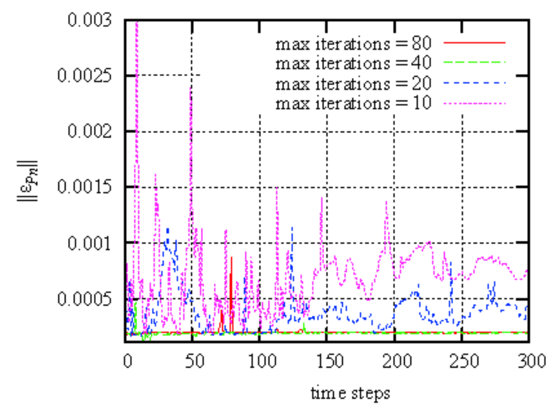


Fig. 6 Maximum penetration error in constraints, for the 300-sphere benchmark.

Example 1 (III): Scalability

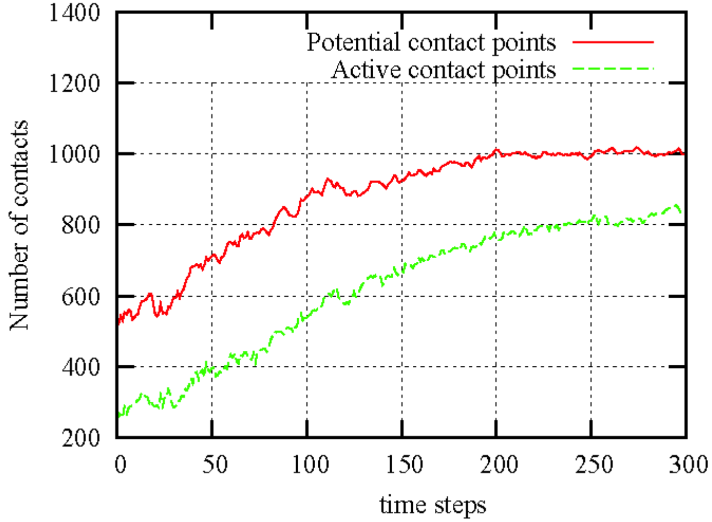


Fig. 7 Number of contact constraints, increasing while pouring spheres in the shaker.

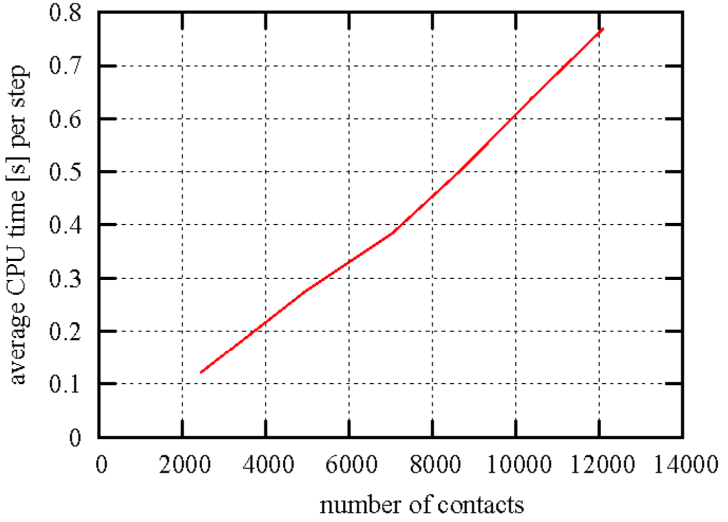
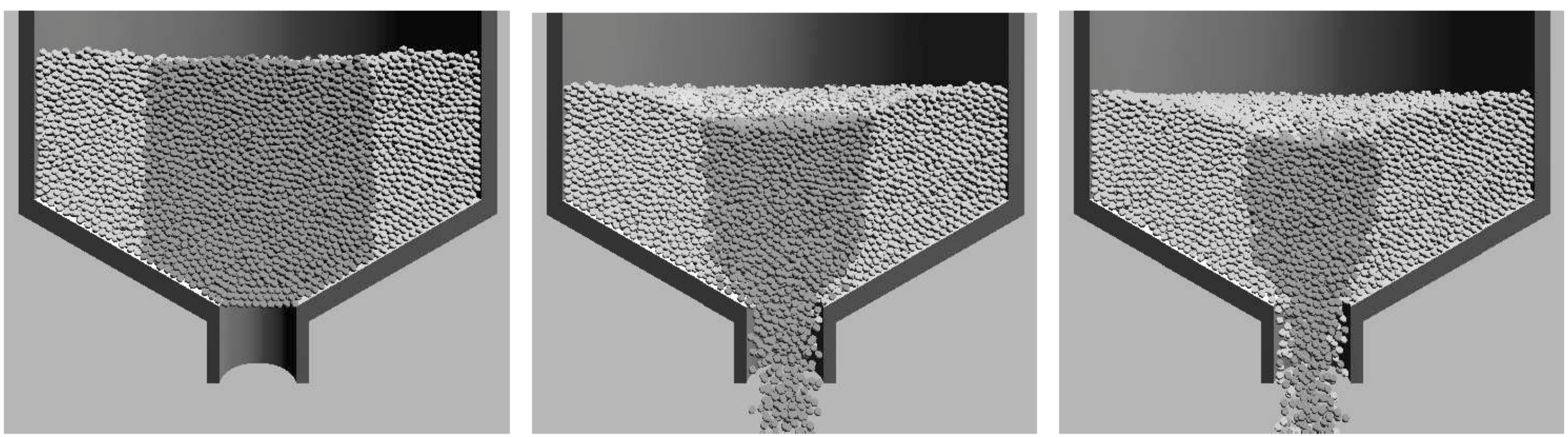


Fig. 8 Average CPU time used to compute a step of simulation, as a function of the number of contacts.

Example 2: Nuclear reactor "Loading"

- Currently time is in weeks of CPU for 30000 on 64 proc cluster for 10 seconds of simulations, though not quite same configuration
- Our simulations up to 30000 spheres on a laptop—memory limited by broad phase collision.
- More than 140000 contact points and 420000 unknowns.
- 140 iterations
- It takes about 2hr of CPU (Windows).



Conclusion Iterative methods for NRMD Simulations

- Time-stepping methods: Different from hard particle, since they do not necessarily stop at collisions, and do not suffer from the strong time step limitation of penalty (spring and dashpot) approaches.
- Problems with conic constraints substantially reduce the size of the problem with the tradeoff of a more mathematically complex constraint.
- Our “Gauss Seidell” works well for up to ~1/2 mil vars and promises to scale.
- TO do: parallelism. Theory is nonetheless readily available block GJ with GS blocks is covered by our method.
- TO do: very high accuracy. Preconditioning? Multigrid?