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).

- silicon carbide
- porous buffer
- pyrocarbon
- UO₂ kernel
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.
Normal velocity: \( v_n \)
Normal impulse: \( c_n \)

**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

\[ \Phi(q) \text{ is complementary to } c_n \text{ or } \Phi(q)c_n = 0, \text{ or } \Phi(q) \perp c_n. \]
Friction Model

- Tangent space generators: \( \hat{D}(q) = \begin{bmatrix} \hat{d}_1(q), \hat{d}_2(q) \end{bmatrix} \), tangent force multipliers: \( \beta \in \mathbb{R}^2 \), tangent force \( D(q) \beta \).
- Conic constraints: \( ||\beta|| \leq \mu c_n \), where \( \mu \) is the friction coefficient.
- Max Dissipation Constraints: \( \beta = \arg\min_{||\tilde{\beta}|| \leq \mu c_n} v^T \hat{D}(q) \tilde{\beta} \).
- \( v_T \), the tangential velocity, satisfies \( |v_T| = \lambda = -v^T \hat{D}(q) \frac{\beta}{||\beta||} \). \( \lambda \) is the Lagrange multiplier of the conic constraint.
- Discretized Constraints: The set \( \hat{D}(q) \beta \) where \( ||\beta|| \leq \mu c_n \) is approximated by a polygonal convex subset: \( D(q) \tilde{\beta}, \tilde{\beta} \geq 0, \|\tilde{\beta}\|_1 \leq \mu c_n \). 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 \( \beta \).
Defining the friction cone

For one contact:
\[
FC^{(j)}(q) = \left\{ c_n^{(j)} n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \right| \right. \\
\left. c_n^{(j)} \geq 0, \sqrt{\left(\beta_1^{(j)}\right)^2 + \left(\beta_2^{(j)}\right)^2} \leq \mu^{(j)} c_n^{(j)} \right\}.
\]

The total friction cone:
\[
FC(q) = \left\{ \sum_{j=1,2,\ldots,p} c_n^{(j)} n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \right| \right. \\
\left. \sqrt{\left(\beta_1^{(j)}\right)^2 + \left(\beta_2^{(j)}\right)^2} \leq \mu^{(j)} c_n^{(j)} \right. \\
\left. c_n^{(j)} \geq 0 \perp \Phi^{(j)}(q) = 0, j = 1, 2, \ldots, p \right\}.
\]

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.

\[
\begin{align*}
M \frac{dv}{dt} &= \sum_{j=1,2,\ldots,p} \left( c^{(j)}_n n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \right) + f_c(q,v) + k(t,q,v) \\
\frac{dq}{dt} &= v \\
c^{(j)}_n &\geq 0 \quad \Phi^{(j)}(q) \geq 0, \ j = 1,2,\ldots,p \\
\left( \beta_1^{(j)}, \beta_2^{(j)} \right) &= \arg\min_{\mu^{(j)} c^{(j)}_n \geq \sqrt{\left( \beta_1^{(j)} \right)^2 + \left( \beta_2^{(j)} \right)^2}} j = 1,2,\ldots,p \\
\left[ \left( v^T t_1^{(j)} \right) t_1^{(j)} + \left( v^T t_2^{(j)} \right) t_2^{(j)} \right]^T \left( \beta_1 t_1^{(j)} + \beta_2 t_2^{(j)} \right).
\end{align*}
\]
Painleve Paradox—no strong solutions

\[
\begin{align*}
I &= \frac{m}{16} \\
\theta &= \frac{72}{2} \\
\omega &= 0 \\
16(\cos \theta - \mu \cos \theta \sin \theta) &= -2 \\
\mu &= 0.75
\end{align*}
\]

(Baraff)

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

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

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

\[
\hat{n}\dddot{p}_a = -g - \frac{f_N}{m}
\]

Painleve Paradox: No classical solutions!
Measure differential inclusion—first step

\[ M \frac{dv}{dt} = f_C(q, v) + k(q, v) + \rho \]
\[ \frac{dq}{dt} = v. \]
\[ \rho = \sum_{j=1}^{p} \rho^{(j)}(t). \]
\[ \rho^{(j)}(t) \in FC^{(j)}(q(t)) \]
\[ \Phi^{(j)}(q) \geq 0, \]
\[ \|\rho^{(j)}\| \Phi^{(j)}(q) = 0, \quad j = 1, 2, \ldots, p. \]

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 \( \nu \) is a measure and \( K(\cdot) \) is a convex-set valued mapping, we say that \( \nu \) 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 Lipschitz 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

\[ v^{(l+1)} = \begin{bmatrix}
\argmin_{v} & \frac{1}{2} \hat{v}^T M \hat{v} + k^{(l)^T} \hat{v} \\
\text{subject to} & \nabla \Phi^{(j)^T} \hat{v} - \mu^{(j)} \sqrt{(t_{1}^{(j)^T} \hat{v})^2 + (t_{2}^{(j)^T} \hat{v})^2} \\
& + \frac{1}{h} \Phi^{(j)}(q^{(l)}) \\
& j \in A(q^{(l)}, \varepsilon), \ k = 1, 2, \ldots, m^{(j)} \end{bmatrix} \geq 0 \]

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

\[ q^{(l+1)} = q^{l} + hv^{l+1} \]
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 \( h_k \to 0 \) where

- \( q^{h_k}(\cdot) \to q(\cdot) \) uniformly.
- \( v^{h_k}(\cdot) \to v(\cdot) \) pointwise a.e.
- \( dv^{h_k}(\cdot) \to dv(\cdot) \) 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.

\[ M(v^{l+1} - v^{(l)}) - \sum_{i=1}^{m} \nu^{(i)} c^{(i)} - \sum_{j \in A} (n^{(j)} c^{(j)} + D^{(j)} \beta^{(j)}) = hk \]

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

\[ \rho^{(j)} = n^{(j)^T} v^{l+1} \geq -\gamma \frac{\Phi^{(j)}(q)}{h}, \quad \text{compl. to} \quad c^{(j)} \geq 0, \quad j \in A \]

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

\[ \zeta^{(j)} = \mu^{(j)} c^{(j)} - e^{(j)^T} \beta^{(j)} \geq 0, \quad \text{compl. to} \quad \lambda^{(j)} \geq 0, \quad j \in A. \]

Here \( \nu^{(i)} = \nabla \Theta^{(i)}, n^{(j)} = \nabla \Phi^{(j)} \). \( h \) is the time step. The set \( A \) 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

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

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

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

\[ \Lambda^i = \{ x, y, z \in \mathbb{R}^3 | x \geq \mu^i \sqrt{y^2 + z^2} \} \],

\[ \mathcal{FC}^i = \{ x, y, z \in \mathbb{R}^3 | \mu^i x \geq \sqrt{y^2 + z^2} \} . \]

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

Use notation:

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

\[ v^{l+1} = \arg \min_v \frac{1}{2} v^T M v + v^T \tilde{f}^{(l)} \]

subject to

\[ \left( \frac{1}{h} \Phi^i(q^{(l)}) + \nabla \Phi^i_T v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)} \right) \in -\mathcal{FC}^{i \circ}, \]

\[ i \in A(q^{(l)}, \epsilon) \]

(1)
Optimality conditions – Conic complementarity problem

\[ v^{l+1} = \arg \min_v \frac{1}{2} v^T M v + v^T \tilde{f}^{(l)} \]

subject to

\[ \left( \frac{1}{h} \Phi^i(q^{(l)}) + \nabla \Phi^i v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)} \right) \in - \mathcal{FC}^i, \]

\[ i \in A(q^{(l)}, \epsilon) \]

\( (1) \)

\[ M v^{(l+1)} = \tilde{f}^{(l)} + \sum_{i \in A(q^{(l)}, \epsilon)} \left( \gamma_n^i D_n^i + \gamma_u^i D_u^i + \gamma_v^i D_v^i \right), \]

\[ i \in A(q^{(l)}, \epsilon) \]

\[ \left( \frac{1}{h} \Phi^i(q^{(l)}) + \nabla \Phi^i v^{(l+1)}, D_u^T v^{(l+1)}, D_v^T v^{(l+1)} \right) \in - \mathcal{FC}^i \]

\[ \perp \left( \gamma_n^i, \gamma_u^i, \gamma_v^i \right) \in \mathcal{FC}^i. \]

Why?
Abstract form—preliminaries.

\[ b \in \mathbb{R}^{3n_\mathcal{A}} = \begin{pmatrix} \frac{1}{\hbar} \Phi_1^{i_1}(q^{(l)}), 0, 0, \frac{1}{\hbar} \Phi_2^{i_2}(q^{(l)}), 0, 0, \ldots, \frac{1}{\hbar} \Phi_n^{i_n}(q^{(l)}), 0, 0 \end{pmatrix}, \]

\[ r \in \mathbb{R}^{3n_\mathcal{A}} = \begin{pmatrix} \frac{1}{\hbar} \Phi_1^{i_1}(q^{(l)}) + D_n^{i_1} M^{-1} \tilde{k}, D_u^{i_1} M^{-1} \tilde{k}, D_v^{i_1} M^{-1} \tilde{k}, \\
\frac{1}{\hbar} \Phi_2^{i_2}(q^{(l)}) + D_n^{i_2} M^{-1} \tilde{k}, D_u^{i_2} M^{-1} \tilde{k}, D_v^{i_2} M^{-1} \tilde{k}, \\
\ldots, \frac{1}{\hbar} \Phi_n^{i_n}(q^{(l)}) + D_n^{i_n} M^{-1} \tilde{k}, D_u^{i_n} M^{-1} \tilde{k}, D_v^{i_n} M^{-1} \tilde{k} \end{pmatrix}, \]

\[ \gamma \in \mathbb{R}^{3n_\mathcal{A}} = \begin{pmatrix} \gamma_1^{i_1}, \gamma_1^{i_1}, \gamma_1^{i_1}, \gamma_2^{i_2}, \gamma_2^{i_2}, \gamma_2^{i_2}, \ldots, \gamma_n^{i_n}, \gamma_n^{i_n}, \gamma_n^{i_n} \end{pmatrix}. \]

and the following matrices

\[ D^i = \begin{bmatrix} D_n^i, D_u^i, D_v^i \end{bmatrix}, i \in \mathcal{A}(q^{(l)}, \epsilon), \]

\[ D = \begin{bmatrix} D_1^i, D_2^i, \ldots, D_{n_\mathcal{A}}^i \end{bmatrix}, \quad N = D^T M^{-1} D. \]
Abstract form

\[(CCP) \quad (N\gamma + r)^i \in -\mathcal{F}C^i \quad \perp \gamma^i \in \mathcal{F}C^i, \quad i = 1, 2, \ldots, n_A. \quad (1)\]

- Note that it includes linear complementarity problems, if the cones are products of $\mathbb{R}^+$
- 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 $\mathcal{Y}^i \subset \mathbb{R}^{n_i}$, where the index takes the values $i = 1, 2, \ldots, n_k$. We consider the Cartesian product of such cones $\mathcal{Y} = \bigoplus_{i=1}^{n_k} \mathcal{Y}^i$, 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: $C^\circ = \{ x \in \mathbb{R}^m \mid \langle x, y \rangle \leq 0, \forall y \in C \}$.

Properties of cones (Lemarechal)

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

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

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

P4 $\mathcal{Y}^\circ = \bigoplus_{i=1}^{n_k} \mathcal{Y}_i^\circ$
**Gauss * Algorithm**

**Theorem** Solution of (CCP) iff fixed point of

\[
x^{r+1} = \lambda \Pi_{\gamma} \left( x^r - \omega B^r \left( N x^r + r + K^r (x^{r+1} - x^r) \right) \right) + (1 - \lambda) x^r,
\]

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

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

where \( \eta_i > 0, \quad i = 1, 2, \ldots, n_k, \quad I_{n_i} \in \mathbb{R}^{n_i \times n_i}, \quad K_{ij} \in \mathbb{R}^{n_i \times n_j}, \quad 1 \leq i < j \leq n_k, \)

and we have either that \( K^r = L^r, \) or that \( K^r = L^r^T. \)

\( K^r = 0: \) Gauss Jacobi, \( K^r = L^r^T, \) 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 $(x^{r+1} - x^r)^T \left( (\lambda \omega B^r)^{-1} + K^r - \frac{N}{2} \right) (x^{r+1} - x^r) \geq \beta \| x^{r+1} - x^r \|^2$,

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

\[(OC) \quad \min_{s.t.} \quad f(x) = \frac{1}{2} x^T N x + r^T x \quad x_i \in \mathcal{Y}^i, \quad i = 1, 2, \ldots, n_k.\]

**Theorem** Assume that \( x^0 \in \mathcal{Y} \) and that the sequences of matrices \( B^r \) and \( K^r \) are bounded. Then we have that

\[
f(x^{r+1}) - f(x^r) \leq -\beta \|x^{r+1} - x^r\|^2
\]

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

2. For $i = 1, 2, \ldots, n_A$, compute $\eta_i = \frac{3}{\text{Trace}(g^i)}$.

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

4. Initialize speeds: $v = \sum_{i=1}^{n_A} s^i \gamma^{i0} + M^{-1}\dot{k}$.

5. For $i = 1, 2, \ldots n_A$, perform the updates
   
   $\delta^{ir} = (\gamma^{ir} - \omega \eta_i (D^{i,T}v^r + b^i))$;
   
   $\gamma^{i,r+1} = \lambda \Pi^{(i)} (\delta^{ir}) + (1 - \lambda)\gamma^{ir}$;
   
   $\Delta\gamma^{i,r+1} = \gamma^{i,r+1} - \gamma^{ir}$;
   
   $v := v + s^{iT} \Delta\gamma^{i,r+1}$.

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

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