

**Optimization-based simulation for nonsmooth dynamics.  
Applications to the Pebble Bed Reactor**

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Grenoble, July 8, 2005**

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## Constraint methods for Nonsmooth Rigid Body Dynamics ...

- ... do not regularize nonsmoothness so do not suffer from the associated type of instability, but they are typically solving a more complex problem, a variational inequality, LCP, NCP.
- Nonsmooth dynamics due to contact, collision, and friction.
- Simulate-detect-restart (a.k.a. event-driven, hard particle) both in acceleration formulation (Baraff 1993), (Pang et al. 1995), (Glocker and Pfeiffer, 1992, partially elastic), and velocity-impulse formulation (Anitescu, Potra 1997, partially elastic).
- Fixed time step, NCP (Moreau et al. \*\*\*, Jean 1999, Stewart and Trinkle, 1995) and LCP (Anitescu and Hart, 2004, Stewart \*\*\*) ... to mention a few references.

## How does one solve the subproblem ?

- In the work of Moreau, Jean et al., by Gauss-Seidell iteration following velocity elimination. Works well for many reported situations, but theoretical complexity and guaranteed completion unclear.
- In (Baraff, Anitescu et al., Stewart et al.), by Lemke's method, that has finite termination following velocity elimination.

### Issues we pursue

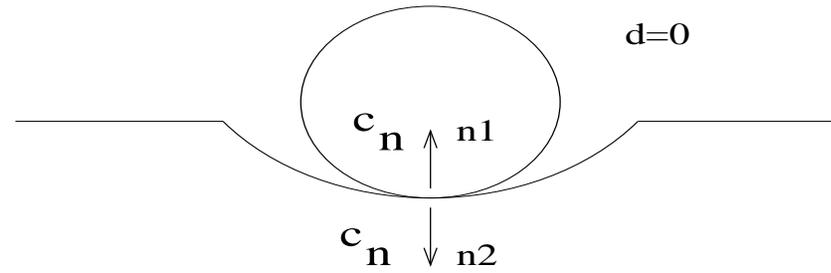
- What can we say about the complexity of solving the LCP?
- Can we define schemes that retain good convergence properties but have a reasonable complexity?

## Outline

1. Contact and Friction Models and original LCP impulse velocity time stepping scheme.
2. Convexity of the Solution Set.
3. Modified LCP-scheme. Equivalence of the subproblem to the QP.
4. Convergence of the QP scheme to the solution of MDI.
5. Initial application to the pebble bed reactor.

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

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

## Coulomb Friction Model

- Tangent space generators:  $\hat{D}(q) = [\hat{d}_1(q), \hat{d}_2(q)]$ , tangent force multipliers:  $\beta \in R^2$ , tangent force  $D(q)\beta$ .
- Conic constraints:  $\|\beta\| \leq \mu c_n$ , where  $\mu$  is the friction coefficient.
- Max Dissipation Constraints:  $\beta = \operatorname{argmin}_{\|\hat{\beta}\| \leq \mu c_n} v^T \hat{D}(q) \hat{\beta}$ .

Polyhedral approximation:

$$\left\{ \hat{D}(q)\beta \mid \|\beta\| \leq \mu c_n \right\} \approx \left\{ D(q)\tilde{\beta} \mid \tilde{\beta} \geq 0, \|\tilde{\beta}\|_1 \leq \mu c_n \right\},$$

where  $D(q) = [d_1(q), d_2(q), \dots, d_m(q)]$ .

## Strong Form — DSEC

$$M(q) \frac{d^2 q}{dt^2} - \sum_{i=1}^m \nu^{(i)} c_v^{(i)} - \sum_{j=1}^p \left( n^{(j)}(q) c_n^{(j)} + D^{(j)}(q) \beta^{(j)} \right) = k(t, q, \frac{dq}{dt})$$

$$\Theta^{(i)}(q) = 0, \quad i = 1 \dots m$$

$$\Phi^{(j)}(q) \geq 0, \quad \text{compl. to} \quad c_n^{(j)} \geq 0, \quad j = 1 \dots p$$

$$\beta = \operatorname{argmin}_{\widehat{\beta}^{(j)}} v^T D(q)^{(j)} \widehat{\beta}^{(j)} \quad \text{subject to} \quad \left\| \widehat{\beta}^{(j)} \right\|_1 \leq \mu^{(j)} c_n^{(j)}, \quad j = 1 \dots p$$

$M(q)$  : the PD mass matrix,  $k(t, q, v)$  : external force,  $\Theta^{(i)}(q)$  : joint constraints.

- It is known that these problems do not have a classical solution even in 2 dimensions, where the discretized cone coincides with the total cone:  
**Painleve's paradox – no strong solutions**– justification for impulse-velocity time stepping.
- In addition, time-stepping needs one less derivative.

■: unknowns

## LCP Fixed time step scheme

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

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

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

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

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

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

**Result, A & H, 2004:** The LCP is solvable, the geometrical constraint infeasibility is bounded above by  $O(h^2)$  and stabilized, (as opposed to  $O(h)$ ), and the numerical velocities sequence is uniformly bounded.

## Solving the LCP, $h=0.05$ , PATH (Lemke)

Problem	Bodies	Initial Contacts	$\mu$	Average CPU time (s)
1	10	21	0.2	0.04
2	10	21	0.8	0.03
3	21	52	0.2	0.28
4	21	52	0.8	0.20
5	36	93	0.2	0.81
6	36	93	0.8	0.82
7	55	146	0.2	2.10
8	55	146	0.8	2.07
9	210	574	0.0	0.80
10	210	574	0.2	174.29
11	210	574	0.8	MAXIT

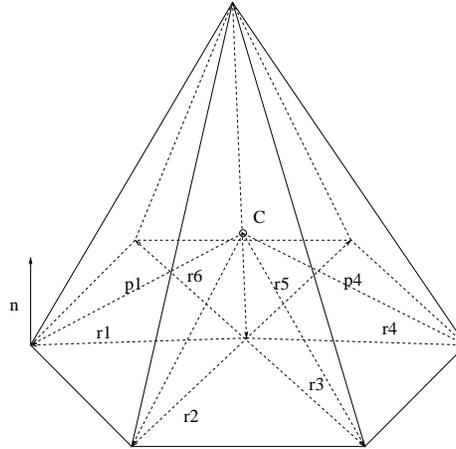
## Solving the LCP ...

- ... with Lemke's method does not seem to scale well.
- Interior Point methods have not been proven to work in general for problems for which the solution set is not convex, as is the case for frictionless problems.
- Is the solution set of the complementarity problem convex? From practical experience, this is the key property that separates “hard” problems from “easy” problems.

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## Nonconvex solution set



Force Balance:

$$\sum_{j=1}^6 c_n^{(j)} n^{(j)} - hmg \begin{pmatrix} n \\ \mathbf{0}_3 \end{pmatrix} = 0.$$

$$\mu c_n^{(j)} \geq 0 \quad \perp \quad \lambda^{(j)} \geq 0, \quad j = 1, 2, \dots, 6.$$

## Nonconvex solution set

The following solutions

1.  $c_n^{(1)} = c_n^{(3)} = c_n^{(5)} = \frac{hmg}{3}$ ,  $c_n^{(2)} = c_n^{(4)} = c_n^{(6)} = 0$ ,  
 $\lambda^{(1)} = \lambda^{(3)} = \lambda^{(5)} = 0$ ,  $\lambda^{(2)} = \lambda^{(4)} = \lambda^{(6)} = 1$ ,
2.  $c_n^{(1)} = c_n^{(3)} = c_n^{(5)} = 0$ ,  $c_n^{(2)} = c_n^{(4)} = c_n^{(6)} = \frac{hmg}{3}$ ,  
 $\lambda^{(1)} = \lambda^{(3)} = \lambda^{(5)} = 1$ ,  $\lambda^{(2)} = \lambda^{(4)} = \lambda^{(6)} = 0$ .

The average of these solutions satisfies  $c_n^{(j)} = \frac{hmg}{6}$ ,  $\lambda^{(j)} = \frac{1}{2}$ , for  $j = 1, 2, \dots, 6$ , which violate

$$\mu c_n^{(j)} \geq 0 \perp \lambda^{(j)} \geq 0, \quad j = 1, 2, \dots, 6,$$

The average of these solutions, **that both induce  $v = 0$** , violates,

$$\beta_1^{(2)} \geq 0 \perp \lambda^{(2)} \geq 0.$$

For any  $\mu > 0$  the LCP matrix is no  $P^*$  matrix, polynomiality unlikely.

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## The convex relaxation

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

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

The LCP is actually equivalent to a QP—but is the method any good? A fixed point iteration approach based on the above was proved to converge for small  $\mu$  and pointed friction cone ( MA and G.D.Hart, (2004b)).

## Equivalent, Strongly Convex, Quadratic Program

$$\begin{aligned} v^{(l+1)} &= \operatorname{argmin}_{\hat{v}} \quad \frac{1}{2} \hat{v}^T M \hat{v} + k^{(l)T} \hat{v} \\ &\text{subject to} \quad \gamma \frac{1}{h} \Phi^{(j)}(q^{(l)}) + \nabla \Phi^{(j)T} \hat{v} + \mu^{(j)} d_k^{(j)T} \hat{v} \geq 0, \\ &\quad j \in \mathcal{A}(q^{(l)}, \epsilon), \quad k = 1, 2, \dots, m^{(j)}, \end{aligned} \tag{1}$$

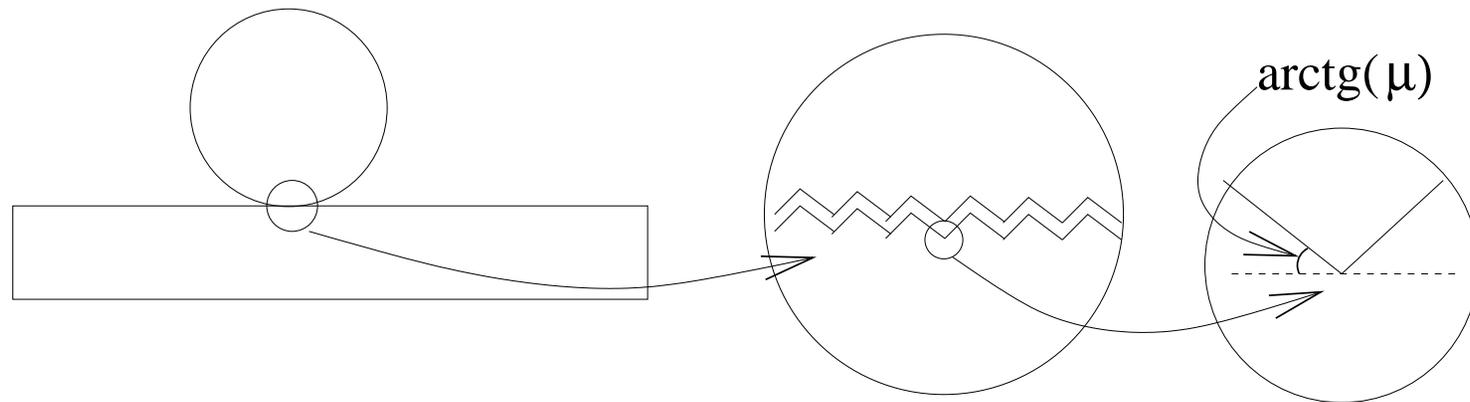
For the case without equality constraints.

## The extension to circular cone

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

- The scheme has the same stability properties, and uses the **original** friction cone.
- Quadratic Programs with Conical constraints, for which software **does** exist.
- The problem can be extended to accommodate a **dynamical** friction coefficients.

## Microscopic interpretation



- It is “almost” as if we integrate with the exact reaction given by frictionless asperities, mitigated by the proximity modification.
- The term  $\gamma \frac{\Phi}{h}$  acts as a controller, and keeps a nonzero gap to accommodate the nonzero tangential velocity.

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## Defining the friction cone (no joints)

The total friction cone:

$$FC(q) = \left\{ \sum_{j=1,2,\dots,p} c_n^{(j)} n^{(j)} + \beta_1^{(j)} t_1^{(j)} + \beta_2^{(j)} t_2^{(j)} \mid \sqrt{\left(\beta_1^{(j)}\right)^2 + \left(\beta_2^{(j)}\right)^2} \leq \mu^{(j)} c_n^{(j)}, c_n^{(j)} \geq 0 \perp \Phi^{(j)}(q) = 0, j = 1, 2, \dots, p \right\}.$$

We have

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

**Pointed friction cone:** if  $0 \in FC(q)$  can be realized only by

$$\tilde{c}_n = \tilde{\beta}_1 = \tilde{\beta}_2 = 0.$$

## Continuous formulation in terms of friction cone

$$M \frac{dv}{dt} = f_C(q, v) + k(q, v) + \rho$$

$$\frac{dq}{dt} = v.$$

$$\rho = \sum_{j=1}^p \rho^{(j)}(t).$$

$$\rho^{(j)}(t) \in FC^{(j)}(q(t))$$

$$\Phi^{(j)}(q) \geq 0,$$

$$\|\rho^{(j)}\| \Phi^{(j)}(q) = 0, \quad j = 1, 2, \dots, p.$$

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

## Measure Differential Inclusions

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

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

## Weaker formulation for NRMD

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

1.  $v(\cdot)$  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.  $\Phi^{(j)}(q) \geq 0, \forall j = 1, 2, \dots, p.$

## Regularity Conditions: Friction cone assumptions

Define  $\epsilon$  cone

$${}^\epsilon \widehat{FC}(q) = \sum_{\Phi^{(j)}(q) \leq \epsilon} FC^{(j)}(q).$$

Uniformly pointed friction cone assumption:  $\exists K_\epsilon, K_\epsilon^*$ , and  $t(q, \epsilon) \in {}^\epsilon \widehat{FC}(q)$  and  $v(q, \epsilon) \in {}^\epsilon \widehat{FC}^*(q)$ , such that,  $\forall q \in R^n$ , and  $\forall \epsilon \in [0, \bar{\epsilon}]$ , we have that

- $t(q, \epsilon)^T w \geq K_\epsilon \|t(q, \epsilon)\| \|w\|, \forall w \in {}^\epsilon \widehat{FC}(q).$
- $n^{(j)T} v(q, \epsilon) \geq \mu \sqrt{t_1^{(j)T} v(q, \epsilon) + t_2^{(j)T} v(q, \epsilon)} + K_\epsilon^* \|v(q, \epsilon)\|,$   
 $j = 1, 2, \dots, p.$

## The new convergence result with convex subproblems

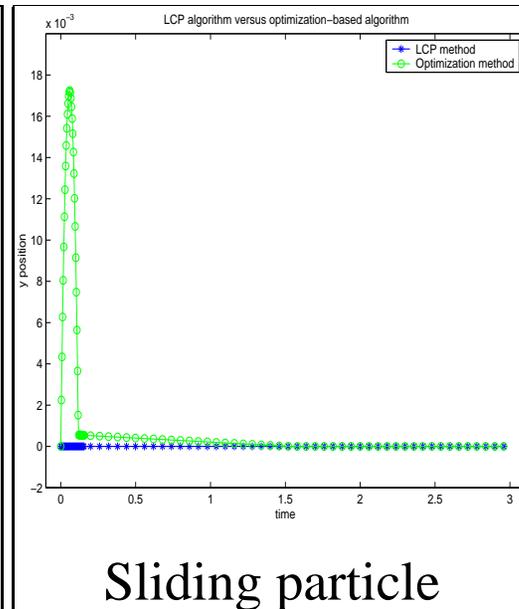
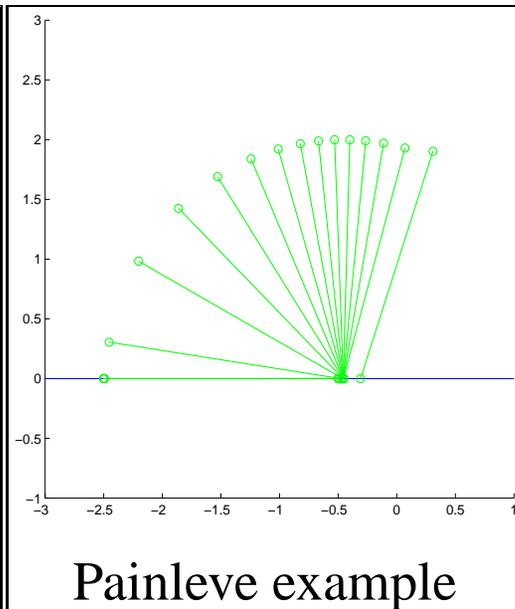
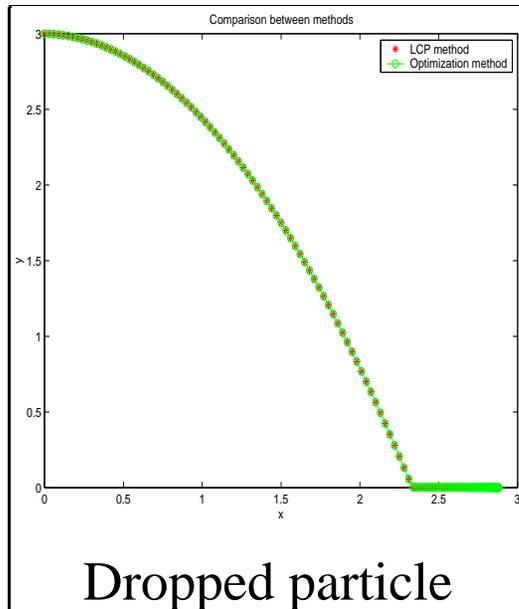
- H1 The functions  $n^{(j)}(q), t_1^{(j)}(q), t_2^{(j)}(q)$  are smooth and globally Lipschitz, and they are bounded in the 2-norm.
- H2 The mass matrix  $M$  is positive definite.
- H3 The external force increases at most linearly with the velocity and position.
- H4 The uniform pointed friction cone 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.

## The convergence result

- Mimics the similar result for the original scheme (Stewart,(1998)), including decrease of energy ...
- ... but says nothing of the Coulomb Law.
- In a regime with small tangential velocity it can be show that the difference of the two schemes is small.
- In some sense, it is the natural integration procedure based on the microscopic modeling of friction with a large time step.
- We used the QP approach for the simulation of size-based segregation of granular matter, 270 bodies with time steps of 100 ms, for 50 seconds. We implemented a fixed time step restitution model, described in (Anitescu, 2004). Granular matter still an unsolved mystery, insofar continuum model.



$$h_k = \frac{0.1}{2^k}, \mu = 0.3$$

$$h_k = \frac{0.1}{2^k}, \mu = 0.75$$

k	$h_k$	$\ y_{QP} - y_{LCP}\ _2$
0	5.6314784e-02	
1	1.7416198e-02	
2	6.7389905e-03	
3	2.1011170e-03	
4	7.6112319e-04	
5	2.6647317e-04	
6	9.2498029e-05	
7	3.2649217e-05	

k	$h_k$	$\ y_{QP} - y_{LCP}\ _2$
0	1.5736018e+000	
1	7.2176724e-001	
2	1.4580267e-001	
3	9.2969637e-002	
4	5.5543025e-003	
5	4.3982975e-003	
6	3.7537593e-003	
7	3.7007014e-004	

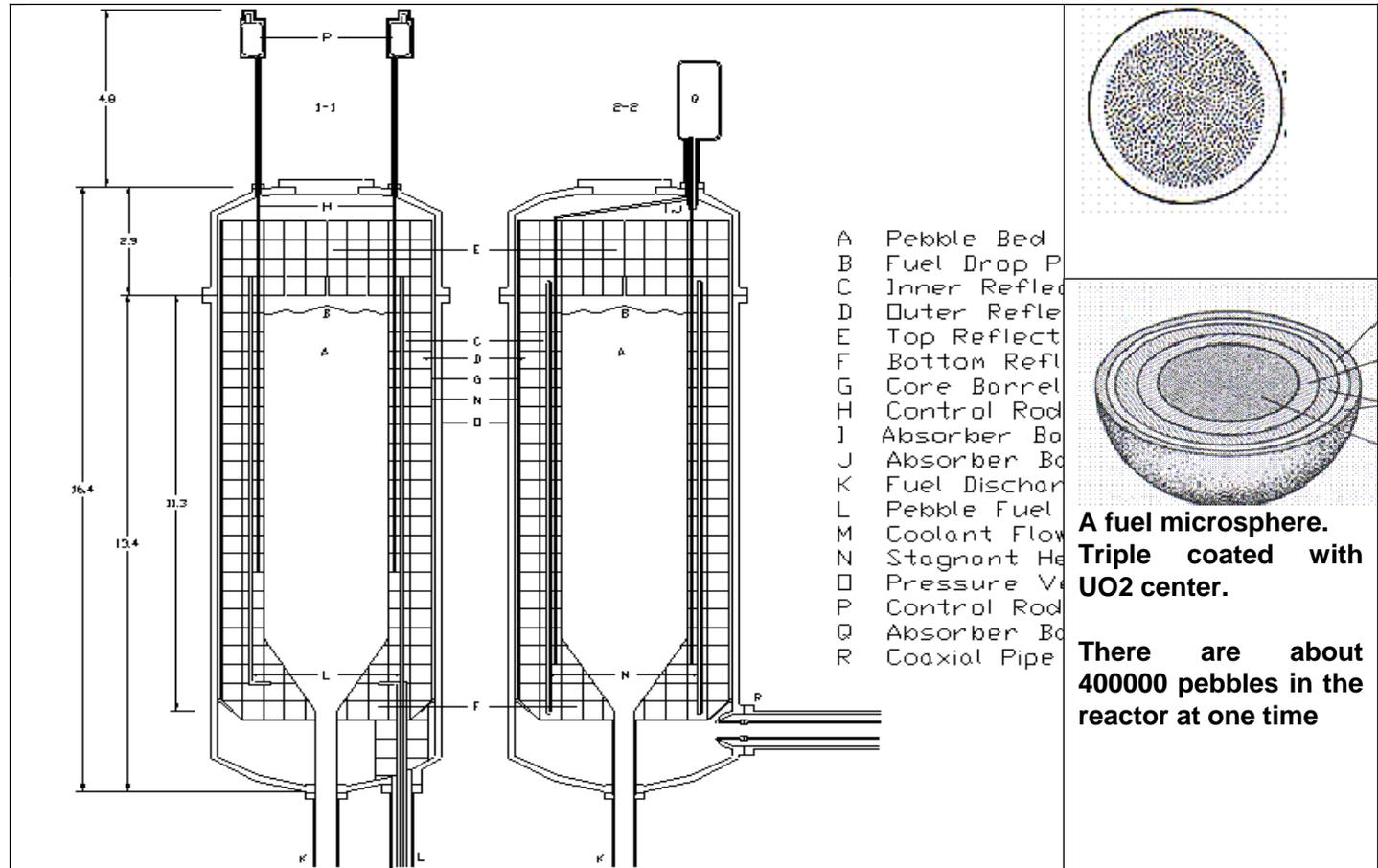
No convergence, but  
small absolute error.

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## The pebble bed nuclear reactor

- One of the great hopes of achieving low maintenance passively safe reactors.
- The fuel consists of tennis-ball-size pebbles filled with  $UO_2$ ,
- The fuel is in continuous motion and the fuel pebbles are either recycled or replaced.
- Cooled with helium through the inter-pebble voids.
- Prototype to be completed by 2015 by INL.
- Initial simulation of loading with Bogdan Gavrea, UMBC.



## Current Status

- We have implemented our scheme in three dimensions.
- For solving the quadratic program, we have used an interior-point approach **OOQP** and one active set method **BQPD**.
- Both take about 20 hrs CPU time for 2000 pebbles.
- The bottleneck is **hot starting** for interior point and **insufficient memory** for the active set method, though the latter is very efficient at high density of pebbles.
- We are currently investigating projected gradient approaches.

## Primal hot starting active-set methods

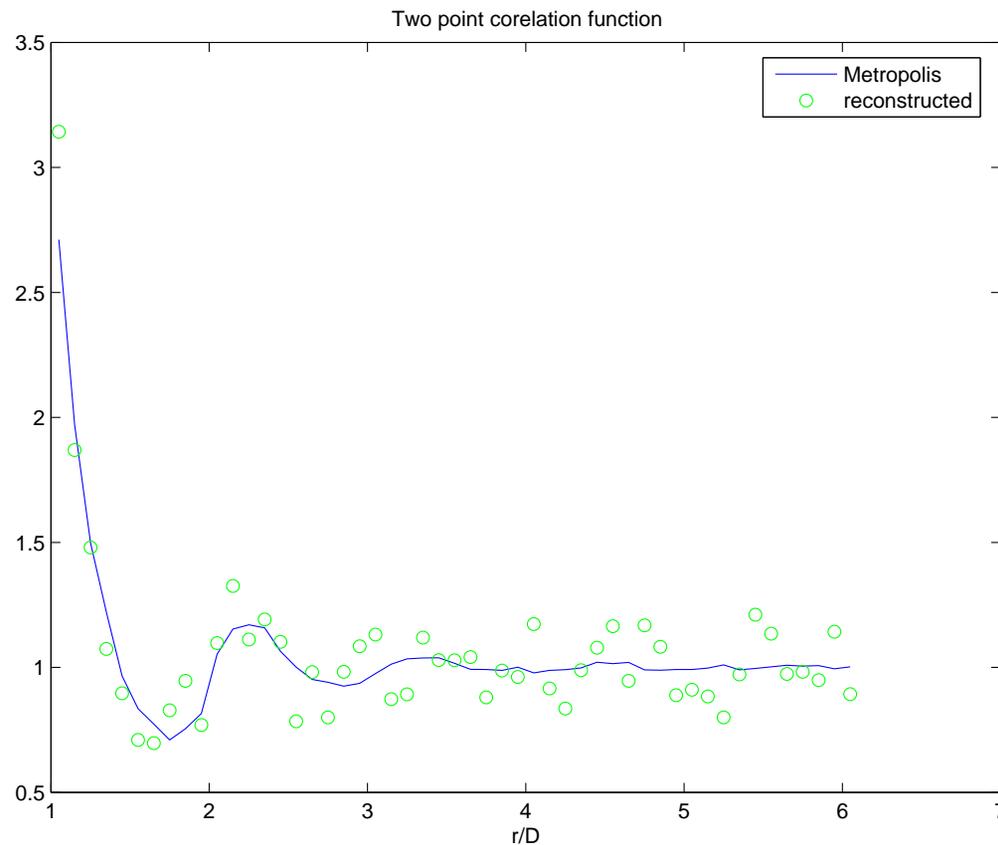
$$\begin{aligned}
 v^{(l+1)} &= \operatorname{argmin}_{\hat{v}, \zeta} \quad \frac{1}{2} \hat{v}^T M \hat{v} + k^{(l)T} \hat{v} + C \sum_{j=1}^p \zeta^{(j)} \\
 \text{subject to} \quad &\zeta_j + \frac{1}{h} \Phi^{(j)}(q^{(l)}) + \nabla \Phi^{(j)T} \hat{v} + \mu^{(j)} d_k^{(j)T} \hat{v} \geq 0, \\
 &j \in \mathcal{A}(q^{(l)}, \epsilon), \quad k = 1, 2, \dots, m^{(j)}, \\
 &\zeta^{(j)} \geq 0, \quad j = 1, 2, \dots, p.
 \end{aligned}$$

$$C \geq \max_{j=1,2,\dots,p} c_n^{(j)} \implies \zeta_j = 0, \quad j = 1, 2, \dots, p,$$

We use  $C = \max\{20mg, 5 \max_{j=1,2,\dots,p} c_n^{(j),(l)}\}$ , always worked.

## What are we hoping to accomplish

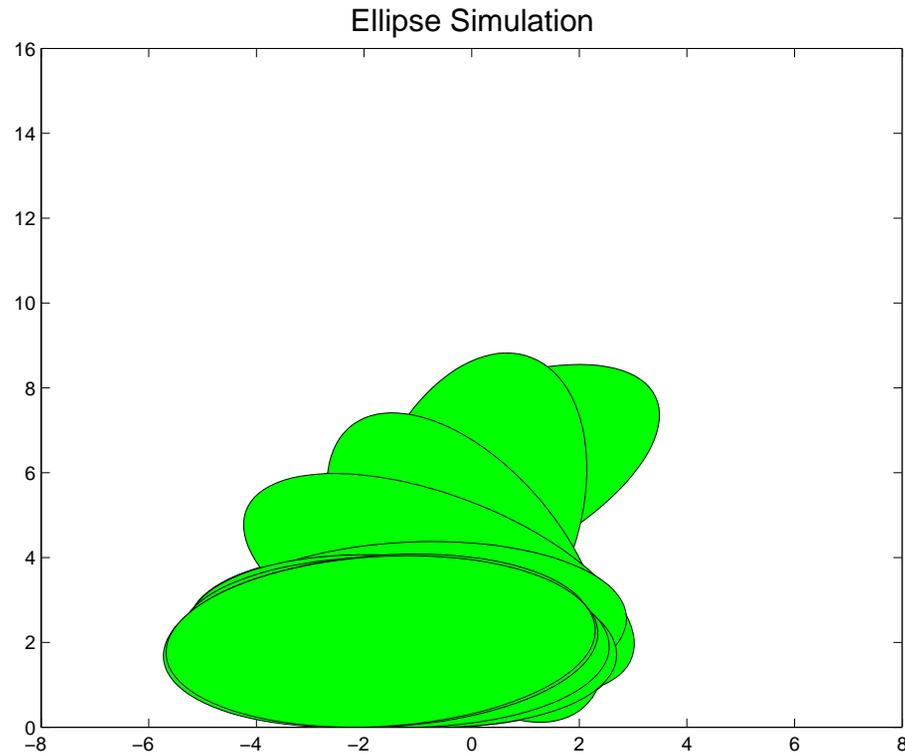
To determine the steady-state statistics of the pebble distribution, including the two-point correlation function (2D equilibrium, with Gun Srijutongsiri).



## Conclusions and remarks

- We have shown that we find solutions to measure differential inclusions by solving quadratic programs, as opposed to LCP with possible nonconvex solution set.
- There remain quite a few challenges (the most important of which is computational efficiency in solving the subproblem), but the large number of applications that can be impacted are worth the investigation in these areas.
- Work is in progress for the simulation of the fuel behavior in the pebble bed reactor.

## Elliptic body simulation

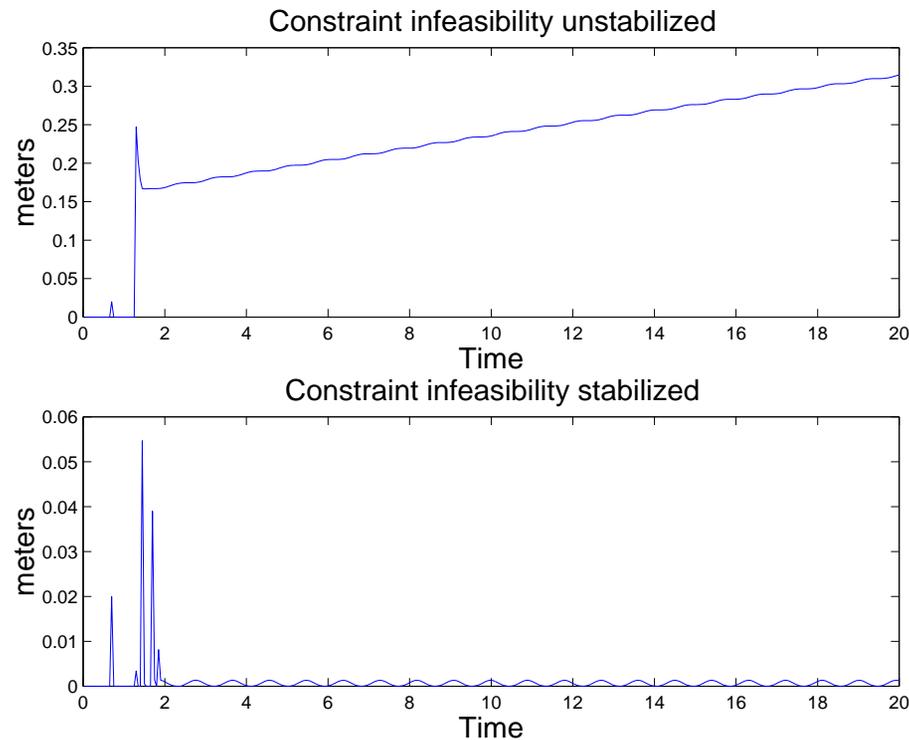


We present ten frames of the simulation of an elliptic body that is dropped on the table. There is an initial angular velocity of 3, the body has axes 4 and 8 and is dropped from a height of 8.

## In Progress

- Trapezoidal scheme, though fixed time-stepping property is lost.
- Nonsmooth bodies with *fixed* time step.
- Using projected gradient type approaches to accelerate the solution of the quadratic program.

## Infeasibility behavior unstabilized versus stabilized method



We see that drift becomes catastrophic for the unstabilized method, whereas remains in a narrow range for the stabilized method.

**Constraint stabilization is accomplished!**

## Constraint Stabilization

- Despite the fact that we have the term  $\frac{1}{h}$  the scheme is still stable (for  $h$  fixed but arbitrary).
- For solvability, we need a stronger condition, **pointed friction cone assumption**, though weaker than linear independence of constraints.
- Note that in the case of DAE, even the postprocessing method (Ascher, 1998) needs one additional linear system (with same matrix).
- The method was implemented in **GraspIt!**, a dynamical grasp simulation tool by Andrew Miller at Columbia.
- The scheme can be modified to include partial elasticity and seems to work fine, though we did not prove the same stability results (MA, (2003)).

## Related Research

- Time stepping methods of this type originate with the work of **Moreau**, early 70's, though most (all?) of those developments are NLCPs, not guaranteed to be solvable, expressed in language of projections. **The key here: work with optimality conditions (S & T 96).**
- Other LCP approaches use accelerations as primary variables (**Glocker and Pfeiffer, (1992), Baraff(1993), Pang and Trinkle, (1996)**). They need the existence of a strong solution, and an extra derivative of the data, but work well in many applications.
- Piecewise differential algebraic equation approaches (DAE) (**Haug et al., 1988**), create difficult nonlinear systems and can get stuck at points of inconsistency.
- Differential variational inequalities (DAVINCI).

## About convergence of the scheme

- For this class of time stepping methods, Stewart (1998) proved convergence to a Measure Differential Inclusion MDI as  $h \rightarrow 0$ , and satisfaction of the Coulomb Friction law for one contact, or several contacts at points of continuity of the velocity.
- Note that one has to accommodate discontinuous velocity due to Painleve paradoxes and collisions, though the strong form contains  $\frac{dv}{dt}$ .
- We use a similar technique for proving convergence of our convex relaxation method.

## Can the LCP approach be extended for

- Stiff systems ?
- Constraint stabilization?
- Fixed time step ?
- Efficient computation of the subproblems?

while preserving the linearity, the solvability and the stability?

The “numerical analysis” of LCP time-stepping schemes is done by exploiting the the stability of the solution of LCP with respect to perturbations, as an extension to DAE approaches. We describe the results.

## Acommodating stiffness

Define

$$\widehat{M} = \left[ M \left( q^{(n)} \right) - h^2 \nabla_q k \left( q^{(n)}, v^{(n)} \right) - h \nabla_v k \left( q^{(n)}, v^{(n)} \right) \right],$$
$$\widehat{k} = k \left( q^{(n)}, v^{(n)} \right) - \nabla_v k \left( q^{(n)}, v^{(n)} \right) v^{(n)}$$

and replace  $\widehat{M} \rightarrow M$ , in the LCP matrix and  $\widehat{k} \rightarrow k$  in the right hand side (linear implicit approach). **Then**

- If the external force is linear spring and damper, resulting problem is solvable LCP and the scheme is unconditionally stable. **MA & FP, 2002,**
- Can extend to nonlinear spring and damper with small modifications.

## Constraint stabilization: Linearization method

Projection methods are expensive. Our solution: enforce geometrical constraints by linearization.

$$\nabla\Phi(q^{(l)})^T v^{(l+1)} \geq 0 \implies \Phi^{(j)}(q^{(l)}) + \gamma h_l \nabla\Phi(q^{(l)})^T v^{(l+1)} \geq 0.$$

$$\nabla\Theta(q^{(l)})^T v^{(l+1)} = 0 \implies \Theta^{(j)}(q^{(l)}) + \gamma h_l \nabla\Theta(q^{(l)})^T v^{(l+1)} = 0.$$

Here  $\gamma \in (0, 1]$ .  $\gamma = 1$  corresponds to exact linearization.

## Is the LCP solvable?

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

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

Yes, with Lemke, if  $M$  is positive definite, MA & FP, 1997. In addition collision with compression-decompression can be modeled by LCP with the same matrix and are also solvable.

## Energy Properties (Stability)

### Assumptions

- The Mass matrix  $M$  is constant.
- The collisions do not increase the kinetic energy.
- The number of collisions is finite.
- The external force is inertial + at most linear growth:  
 $k(t, v, q) = f_c(q, v) + k_1(t, v, q)$ , where  $v^T f_c(q, v) = 0$ ,  
 $\|k_1(t, q, v)\| \leq A(1 + \|q\| + \|v\|)$ .

Then  $v^{(l),h}$  is uniformly bounded.

## Time-stepping, the linear complementarity problem (LCP)

Euler method, half-explicit in velocities, linearization for constraints.

Maximum dissipation principle enforced through optimality conditions.

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

$$\nu^{(i)T} v^{l+1} = 0, \quad i = 1, 2, \dots, m$$

$$\rho^{(j)} = n^{(j)T} v^{l+1} \geq 0, \quad \text{compl. to } c_n^{(j)} \geq 0, \quad j \in \mathcal{A}$$

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

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

$\nu^{(i)} = \nabla \Theta^{(i)}$ ,  $n^{(j)} = \nabla \Phi^{(j)}$ ,  $h$ : time step,  $\mathcal{A}$ : active constraints.

Stewart and Trinkle, 1996 (LCP) **MA** and Potra, 1997 (solvable LCP).

We use the same notation for impulses that replace forces. ■: unknowns

MIHAI