Iterative Methods for DVIs Appearing in time-stepping for Multibody Dynamics

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1. TIME-STEPPING SCHEMES AND THEIR RELAXATION

Nonsmooth contact dynamics—what is it?

- Differential problem with variational inequality constraints – DVI

Newton Equations

Non-Penetration Constraints

$$M\frac{dv}{dt} = \sum_{j=1,2,\ldots,p}\left(c_n^{(j)}n^{(j)} + \beta_1^{(j)}t_1^{(j)} + \beta_2^{(j)}t_2^{(j)}\right) + f_c(q,v) + k(t,q,v)$$

$$\frac{dq}{dt} = \Gamma(q)v$$

Generalized Velocities

$$c_n^{(j)} \geq 0 \perp \Phi^{(j)}(q) \geq 0, \quad j = 1,2,\ldots,p$$

$$\left(\beta_1^{(j)},\beta_2^{(j)}\right) = \operatorname{argmin}_{\mu^{(j)}c_n^{(j)} \geq \sqrt{\left(\beta_1^{(j)}+\beta_2^{(j)}\right)^2}}\left[\left(v^T t_1^{(j)}\right)\beta_1 + \left(v^T t_2^{(j)}\right)\beta_2\right]$$

Friction Model

- Truly, a Differential Problem with Equilibrium Constraints

Time stepping scheme -- original

- A measure differential inclusion solution can be obtained by time-stepping (Stewart, 1998, Anitescu 2006)

$$M(\boldsymbol{v}^{(l+1)} - \boldsymbol{v}^{l}) = \sum_{i \in \mathcal{A}(q^{(l)}, \epsilon)} (\gamma_n^i \boldsymbol{D}_n^i + \gamma_u^i \boldsymbol{D}_u^i + \gamma_v^i \boldsymbol{D}_v^i) + \sum_{i \in \mathcal{G}_\mathcal{B}} (\gamma_b^i \nabla \Psi^i) + h \boldsymbol{f}_t(t^{(l)}, \boldsymbol{q}^{(l)}, \boldsymbol{v}^{(l)})$$

Speeds

Reaction impulses

Forces

$$0 = \frac{1}{h}\Psi^i(\boldsymbol{q}^{(l)}) + \nabla \Psi^{i^T} \boldsymbol{v}^{(l+1)} + \frac{\partial \Psi^i}{\partial t}, \quad i \in \mathcal{G}_\mathcal{B}$$

Bilateral constraint equations

Constraint Stabilization

$$0 \le \frac{1}{h}\Phi^i(\boldsymbol{q}^{(l)}) + \nabla \Phi^{i^T} \boldsymbol{v}^{(l+1)}$$

Contact constraint equations

$$\perp \quad \gamma_n^i \ge 0, \; i \in \mathcal{A}(q^{(l)}, \epsilon)$$

COMPLEMENTARITY!

$$(\gamma_u^i, \gamma_v^i) = \operatorname{argmin}_{\mu^i \gamma_n^i \ge \sqrt{(\gamma_u^i)^2 + (\gamma_v^i)^2}} \quad i \in \mathcal{A}(q^{(l)}, \epsilon)$$

$$\left[\boldsymbol{v}^T (\gamma_u \boldsymbol{D}_u^i + \gamma_v \boldsymbol{D}_v^i)\right]$$

Coulomb 3D friction model

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

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Pause: Constraint Stabilization

- Compared to original scheme

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

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

- Allows fixed time steps for plastic collisions.
- How do we know it is achieved? Infeasibility is one order better than accuracy (O(h^2))

Time Stepping -- Convex Relaxation

- A modification (relaxation, to get convex QP with conic constraints):

$$M(\boldsymbol{v}^{(l+1)} - \boldsymbol{v}^{l}) = \sum_{i \in \mathcal{A}(q^{(l)}, \epsilon)} (\gamma_n^i \boldsymbol{D}_n^i + \gamma_u^i \boldsymbol{D}_u^i + \gamma_v^i \boldsymbol{D}_v^i) +$$

$$+ \sum_{i \in \mathcal{G}_{\mathcal{B}}} (\gamma_b^i \nabla \Psi^i) + h \boldsymbol{f}_t(t^{(l)}, \boldsymbol{q}^{(l)}, \boldsymbol{v}^{(l)})$$

$$0 = \frac{1}{h} \Psi^i(\boldsymbol{q}^{(l)}) + \nabla {\Psi^i}^T \boldsymbol{v}^{(l+1)} + \frac{\partial \Psi^i}{\partial t}, \quad i \in \mathcal{G}_{\mathcal{B}}$$

$$0 \leq \frac{1}{h} \Phi^i(\boldsymbol{q}^{(l)}) + \nabla {\Phi^i}^T \boldsymbol{v}^{(l+1)} - \mu^i \sqrt{(\boldsymbol{D}_u^{i,T} \boldsymbol{v})^2 + (\boldsymbol{D}_v^{i,T} \boldsymbol{v})^2}$$

$$\perp \quad \gamma_n^i \geq 0, \; i \in \mathcal{A}(q^{(l)}, \epsilon)$$

$$(\gamma_u^i, \gamma_v^i) = \operatorname{argmin}_{\mu^i \gamma_n^i \geq \sqrt{(\gamma_u^i)^2 + (\gamma_v^i)^2}} \quad i \in \mathcal{A}(q^{(l)}, \epsilon)$$

$$[\boldsymbol{v}^T (\gamma_u \boldsymbol{D}_u^i + \gamma_v \boldsymbol{D}_v^i)]$$

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

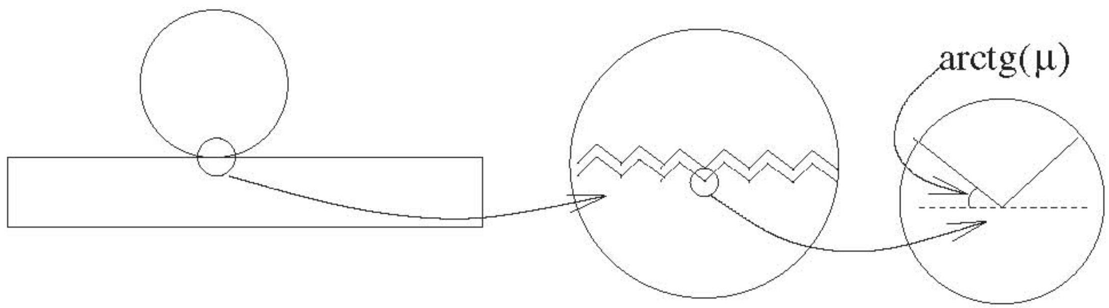
(For small μ and/or small speeds, almost no one-step differences from the Coulomb theory)

But In any case, converges to same MDI as unrelaxed scheme.

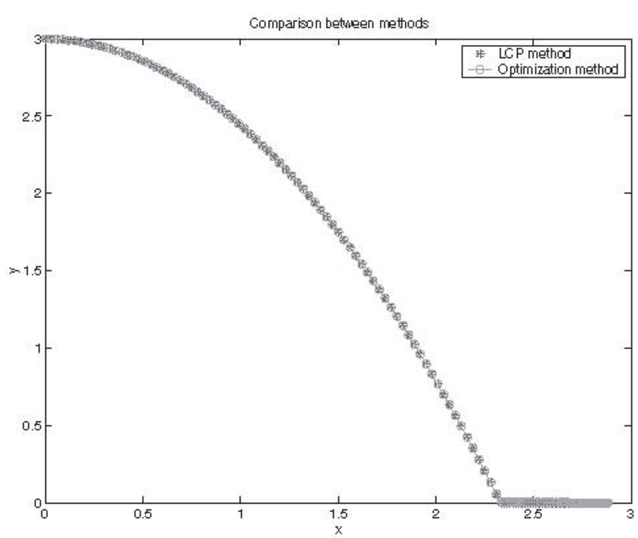
[see M.Anitescu, "Optimization Based Simulation of Nonsmooth Rigid Body Dynamics"]

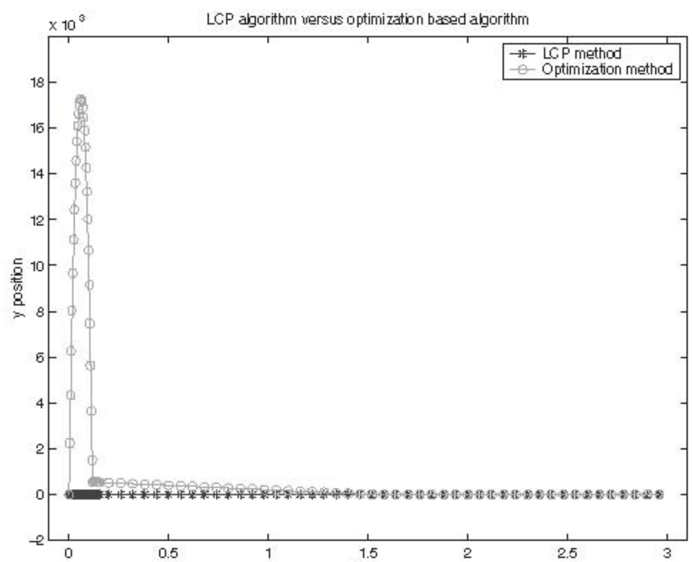
What is physical meaning of the relaxation?

- Origin



- Behavior





Further insight.

- The key is the combination between relaxation and constraint stabilization.

$$0 \leq \frac{1}{h}\Phi^{(j)}\left(q^{(l)}\right)+\nabla_q\Phi^{(j)}\left(q^{(l)}\right)v^{(l+1)}-\mu^{(j)}\sqrt{\left(D_u^{l,t}v\right)^2+\left(D_v^{l,t}v\right)^2}$$

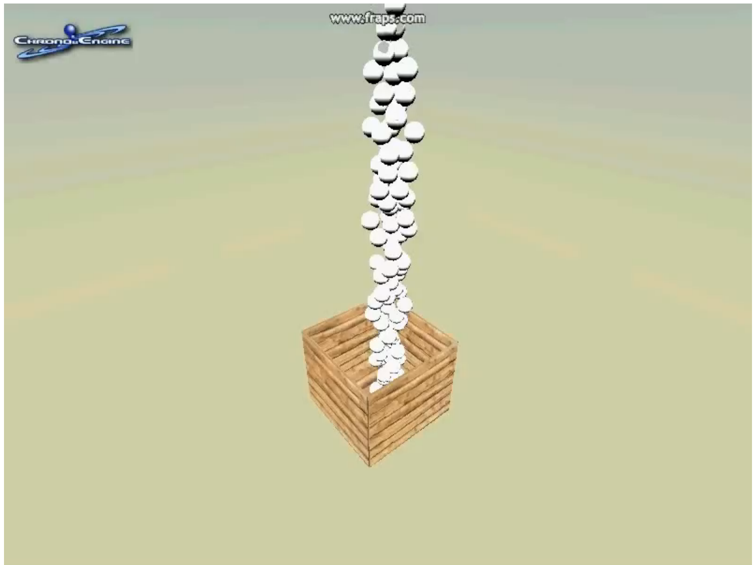
- If the time step is smaller than the variation in velocity then the gap function settles at

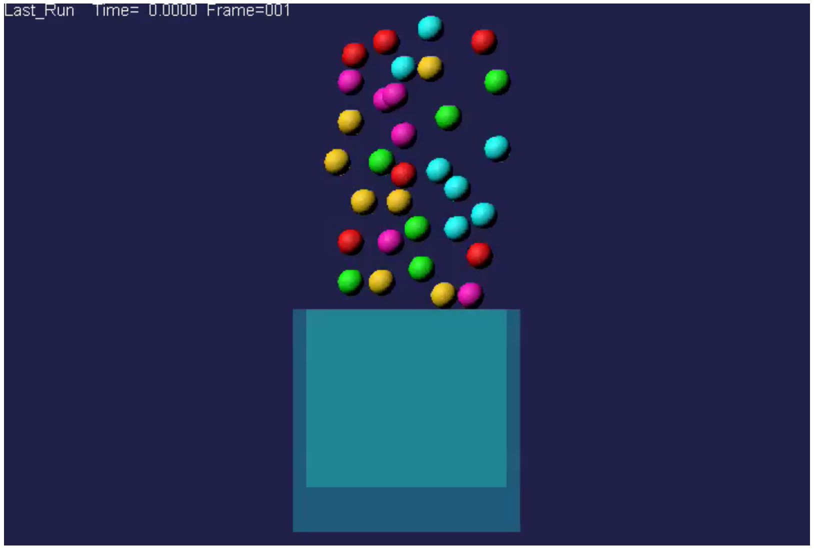
$$0 \approx \frac{1}{h}\Phi^{(j)}\left(q^{(l)}\right)-\mu^{(j)}\sqrt{\left(D_u^{l,t}v\right)^2+\left(D_v^{l,t}v\right)^2}$$

- So the solution is the same as the original scheme for a slightly perturbed gap function…..

Comparing with penalty methods: Applying ADAMS to granular flow

- ADAMS is the workhorse of engineering dynamics.
- ADAMS/View Procedure for simulating.
- Spheres: diameter of 60 mm and a weight of 0.882 kg.
- Forces:smoothing with stiffness of 1E5, force exponent of 2.2, damping coefficient of 10.0, and a penetration depth of 0.1





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ADAMS versus ChronoEngine *

* From Madsen et al.

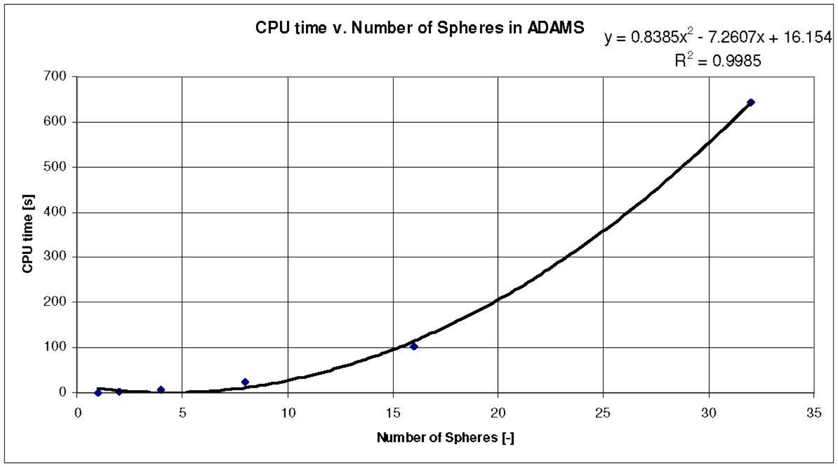
Table 1: Number of rigid bodies v. CPU time in ADAMS

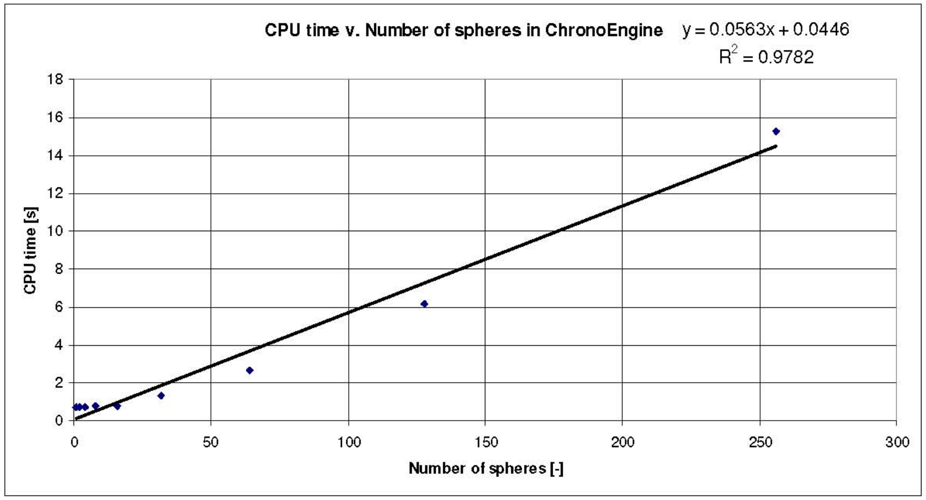
Number of Spheres	Max Number of Mutual Contacts [-]	CPU time (seconds)
1	1	0.41
2	3	3.3
4	14	7.75
8	44	25.36
16	152	102.78
32	560	644.4

The following graph shows the nonlinear increase in the CPU time as the number of colliding bodies increases.

Table 2: Number of rigid bodies v. CPU time in ChronoEngine

Number of Spheres	Max Number of Mutual Contacts [-]	CPU time (seconds)
1	1	0.70
2	3	0.73
4	14	0.73
8	44	0.76
16	152	0.82
32	560	1.32
64	2144	2.65
128	8384	6.17
256	33152	15.30





Conclusion 1: Often, time stepping is more promising,

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2. CONE COMPLEMENTARITY TIME STEPPING

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Cone complementarity

- Aiming at a more compact formulation:

$$\boldsymbol{b}_{\mathcal{A}} = \left\{\frac{1}{h}\Phi^{i_1}, 0, 0, \frac{1}{h}\Phi^{i_2}, 0, 0, \ldots, \frac{1}{h}\Phi^{i_{n_{\mathcal{A}}}}, 0, 0\right\}$$

$$\boldsymbol{\gamma}_{\mathcal{A}} = \left\{\gamma_n^{i_1}, \gamma_u^{i_1}, \gamma_v^{i_1}, \gamma_n^{i_2}, \gamma_u^{i_2}, \gamma_v^{i_2}, \ldots, \gamma_n^{i_{n_{\mathcal{A}}}}, \gamma_u^{i_{n_{\mathcal{A}}}}, \gamma_v^{i_{n_{\mathcal{A}}}}\right\}$$

$$\boldsymbol{b}_{\mathcal{B}} = \left\{\frac{1}{h}\Psi^1 + \frac{\partial \Psi^1}{\partial t}, \frac{1}{h}\Psi^2 + \frac{\partial \Psi^2}{\partial t}, \ldots, \frac{1}{h}\Psi^{n_{\mathcal{B}}} + \frac{\partial \Psi^{n_{\mathcal{B}}}}{\partial t}\right\}$$

$$\boldsymbol{\gamma}_{\mathcal{B}} = \left\{\gamma_b^1, \gamma_b^2, \ldots, \gamma_b^{n_{\mathcal{B}}}\right\}$$

$$D_{\mathcal{A}} = \left[D^{i_1} | D^{i_2} | \ldots | D^{i_{n_{\mathcal{A}}}}\right], \quad i \in \mathcal{A}(\boldsymbol{q}^l, \epsilon) \qquad D^i = \left[\boldsymbol{D}_n^i | \boldsymbol{D}_u^i | \boldsymbol{D}_v^i\right]$$

- $D_{\mathcal{B}} = \left[\nabla\Psi^{i_1} | \nabla\Psi^{i_2} | \ldots | \nabla\Psi^{i_{n_{\mathcal{B}}}}\right], \quad i \in \mathcal{G}_{\mathcal{B}}$

$$\boldsymbol{b}_{\mathcal{E}} \in \mathbb{R}^{n_{\mathcal{E}}} = \{\boldsymbol{b}_{\mathcal{A}}, \boldsymbol{b}_{\mathcal{B}}\}$$

$$\boldsymbol{\gamma}_{\mathcal{E}} \in \mathbb{R}^{n_{\mathcal{E}}} = \{\boldsymbol{\gamma}_{\mathcal{A}}, \boldsymbol{\gamma}_{\mathcal{B}}\}$$

$$D_{\mathcal{E}} = [D_{\mathcal{A}} | D_{\mathcal{B}}]$$

Cone complementarity

- Also define:

$$\tilde{\boldsymbol{k}}^{(l)} = M\boldsymbol{v}^{(l)} + h\boldsymbol{f}_t(t^{(l)}, \boldsymbol{q}^{(l)}, \boldsymbol{v}^{(l)})$$

$$N = D_{\mathcal{E}}^T M^{-1} D_{\mathcal{E}}$$

$$\boldsymbol{r} = D_{\mathcal{E}}^T M^{-1} \tilde{\boldsymbol{k}} + \boldsymbol{b}_{\mathcal{E}}$$

- Then:

$$\begin{aligned}
M(\boldsymbol{v}^{(l+1)} - \boldsymbol{v}^{l}) &= \sum_{i \in \mathcal{A}(q^{(l)},\epsilon)} (\gamma_n^i \boldsymbol{D}_n^i + \gamma_u^i \boldsymbol{D}_u^i + \gamma_v^i \boldsymbol{D}_v^i) + \\
&\quad + \sum_{i \in \mathcal{G}_{\mathcal{B}}} (\gamma_b^i \nabla \Psi^i) + h\boldsymbol{f}_t(t^{(l)}, \boldsymbol{q}^{(l)}, \boldsymbol{v}^{(l)}) \\
0 &= \frac{1}{h}\Psi^i(\boldsymbol{q}^{(l)}) + \nabla {\Psi^i}^T \boldsymbol{v}^{(l+1)} + \frac{\partial \Psi^i}{\partial t}, \quad i \in \mathcal{G}_{\mathcal{B}} \\
0 &\le \frac{1}{h}\Phi^i(\boldsymbol{q}^{(l)}) + \nabla {\Phi^i}^T \boldsymbol{v}^{(l+1)} \\
&\perp \quad \gamma_n^i \ge 0, \; i \in \mathcal{A}(q^{(l)}, \epsilon) \\
(\gamma_u^i, \gamma_v^i) &= \mathrm{argmin}_{\mu^i \gamma_n^i \ge \sqrt{(\gamma_u^i)^2 + (\gamma_v^i)^2}} \quad i \in \mathcal{A}(q^{(l)}, \epsilon) \\
&\quad [\boldsymbol{v}^T (\gamma_u \boldsymbol{D}_u^i + \gamma_v \boldsymbol{D}_v^i)]
\end{aligned}$$

becomes..

$$(N\boldsymbol{\gamma}_{\mathcal{E}} + \boldsymbol{r}) \in -\Upsilon^{\circ} \quad \perp \quad \boldsymbol{\gamma}_{\mathcal{E}} \in \Upsilon$$

This is a CCP,
CONE COMPLEMENTARITY PROBLEM

Cone Complementarity Problems and Stationary Iterative Methods

- The resulting cone complementarity problem

$$(N\boldsymbol{\gamma}_{\mathcal{E}} + \boldsymbol{r}) \in -\Upsilon^{\circ} \quad \perp \quad \boldsymbol{\gamma}_{\mathcal{E}} \in \Upsilon \quad \equiv \min_{\gamma_{\mathcal{E}}} \frac{1}{2}\gamma_{\mathcal{E}} N \gamma_{\mathcal{E}} + r^T \gamma_{\mathcal{E}}$$

- One method: use a fixed-point iteration

$$\boldsymbol{\gamma}^{r+1} = \lambda \Pi_{\Upsilon}\left(\boldsymbol{\gamma}^{r} - \omega B^{r}\left(N\boldsymbol{\gamma}^{r} + \boldsymbol{r} + K^{r}\left(\boldsymbol{\gamma}^{r+1} - \boldsymbol{\gamma}^{r}\right)\right)\right) + (1-\lambda)\,\boldsymbol{\gamma}^{r}$$

- Covers SOR, GS, Jacobi
- Solves it really as a CCP (even if it is an OP)
- Using projector onto cone (or a set …)

$$B^{r} = \begin{bmatrix} \eta_1 I_{n_1} & 0 & \cdots & 0 \\ 0 & \eta_2 I_{n_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \eta_{n_k} I_{n_{n_k}} \end{bmatrix}$$

$$N^T = \begin{bmatrix} 0 & K_{12} & K_{13} & \cdots & K_{1n_k} \\ 0 & 0 & K_{23} & \cdots & K_{2n_k} \\ 0 & 0 & 0 & \cdots & K_{3n_k} \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & 0 & & 0 \end{bmatrix}$$

$$\Pi_{\Upsilon} : \mathbb{R}^{n_{\mathcal{E}}} \longrightarrow \mathbb{R}^{n_{\mathcal{E}}}$$

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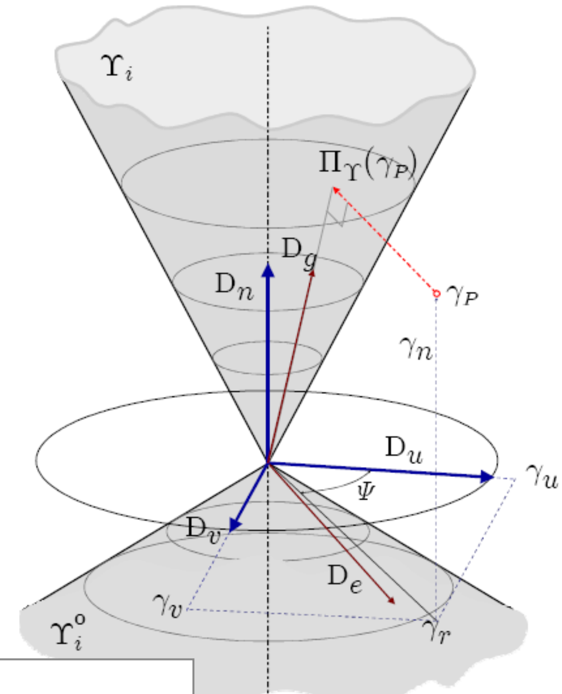
The projection operator is easy and separable

- *For each frictional contact constraint:*

$$\Pi_\Upsilon = \left\{ \Pi_{\Upsilon_1}(\gamma_1)^T, \ldots \Pi_{\Upsilon_{n_\mathcal{A}}}(\boldsymbol{\gamma}^{n_\mathcal{A}})^T, \Pi_b^1(\gamma_b^1), \ldots, \Pi_b^{n_\mathcal{B}}(\gamma_b^{n_\mathcal{B}}) \right\}^T$$



- *For each bilateral constraint, simply do nothing.*
- The complete operator:

$$\forall i \in \mathcal{A}(\boldsymbol{q}^{(l)}, \epsilon)$$

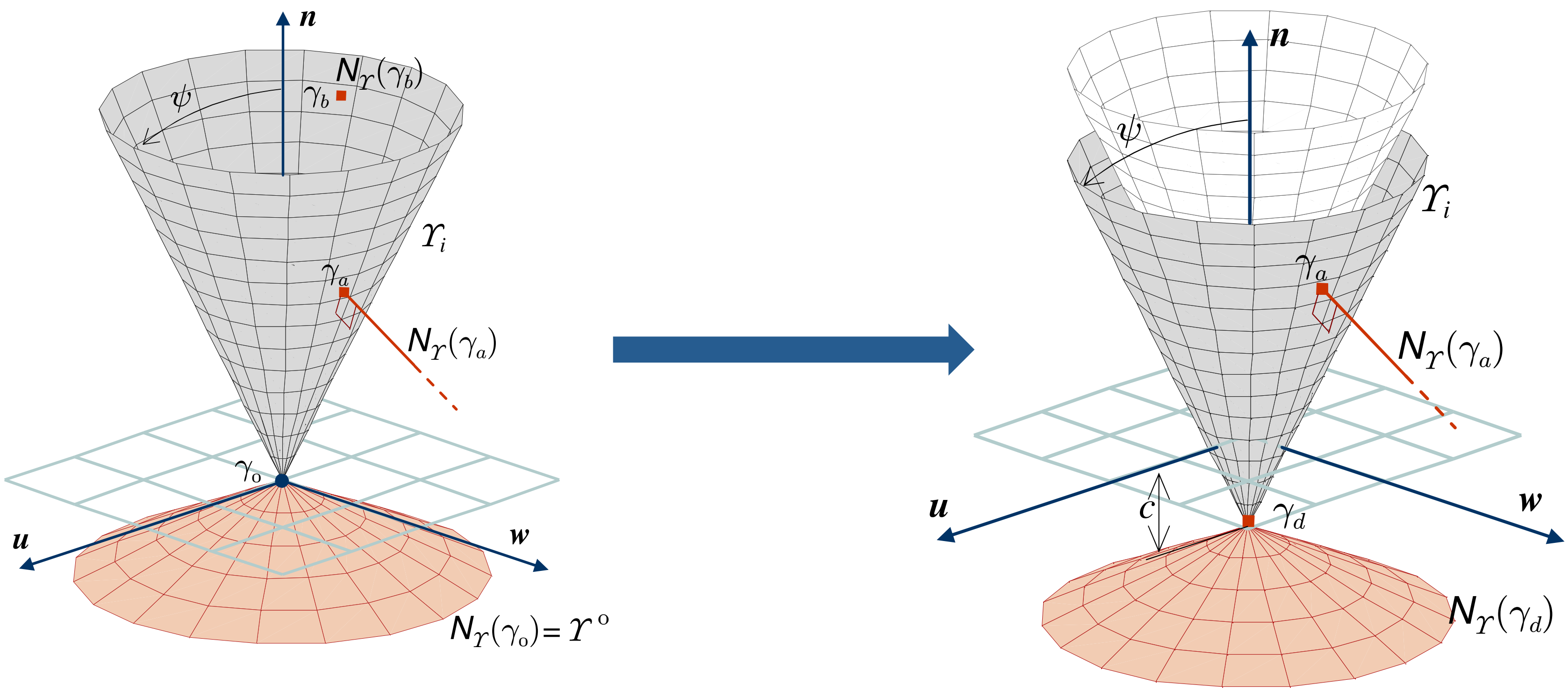
$\gamma_r < \mu_i \gamma_n$	$\Pi_i = \boldsymbol{\gamma}_i$
$\gamma_r < -\frac{1}{\mu_i}\gamma_n$	$\Pi_i = \{0, 0, 0\}$
$\gamma_r > \mu_i \gamma_n \wedge \gamma_r > -\frac{1}{\mu_i}\gamma_n$	$\Pi_{i,n} = \frac{\gamma_r \mu_i + \gamma_n}{\mu_i^2 + 1}$
	$\Pi_{i,u} = \gamma_u \frac{\mu_i \Pi_{i,n}}{\gamma_r}$
	$\Pi_{i,v} = \gamma_v \frac{\mu_i \Pi_{i,n}}{\gamma_r}$

Finding other Interesting Behaviors by Modeling the Force Constraint Set

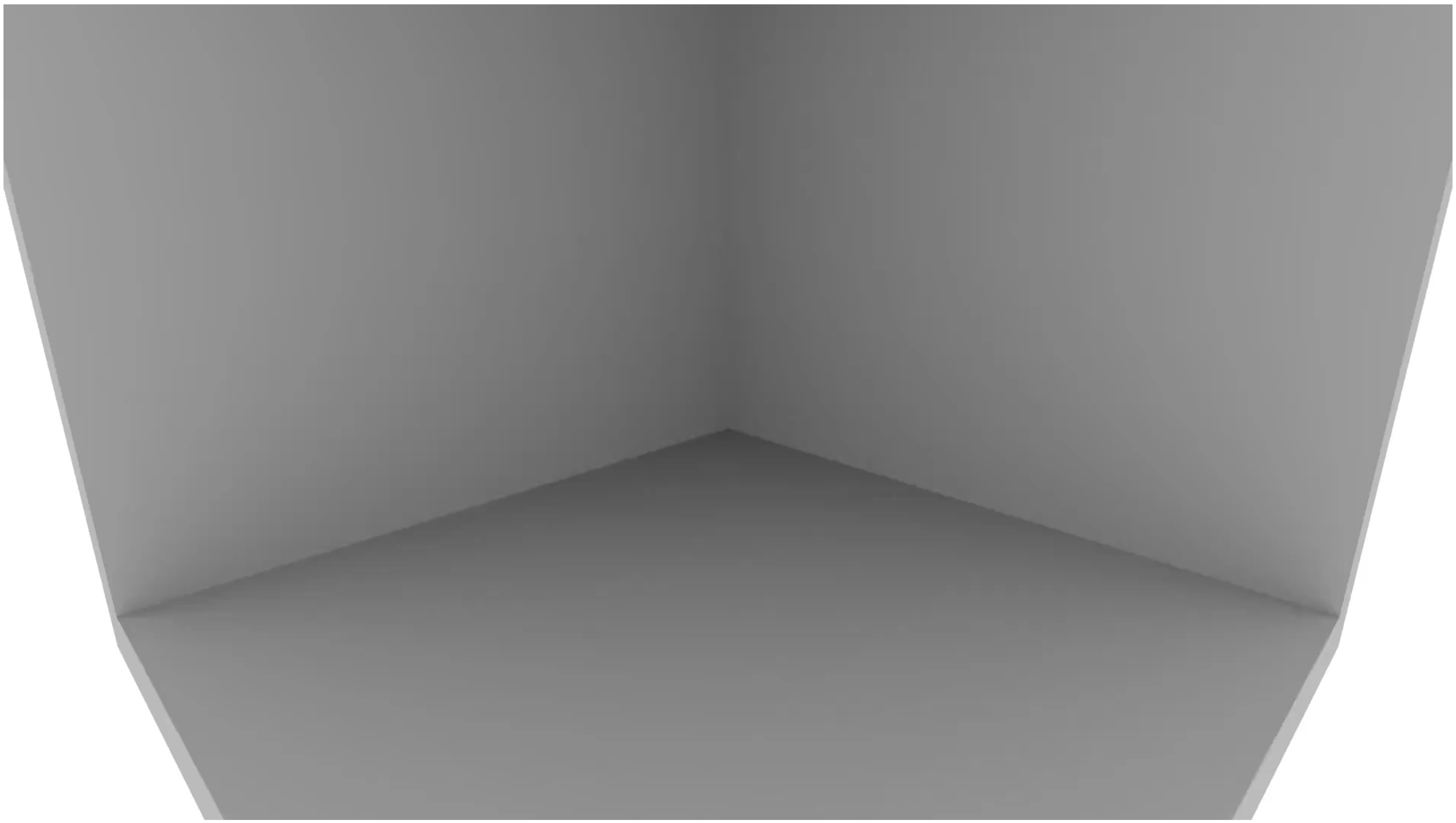
- For computational reasons, we like the relaxation: it leads to solving convex optimization at each step.
- It seems to be easy to solve any time I can have a force constraint set that I can project easily onto. This implicitly (by duality) constrains the motion.
- This allows me to explore other sets and simulate other behaviors.

Example: Friction and Cohesion in 3D by playing around with Yield surfaces

- Shift the Coulomb cone downward and make it an associative yield surface.



Cohesive Particle Flow Simulation (cohesive foam)



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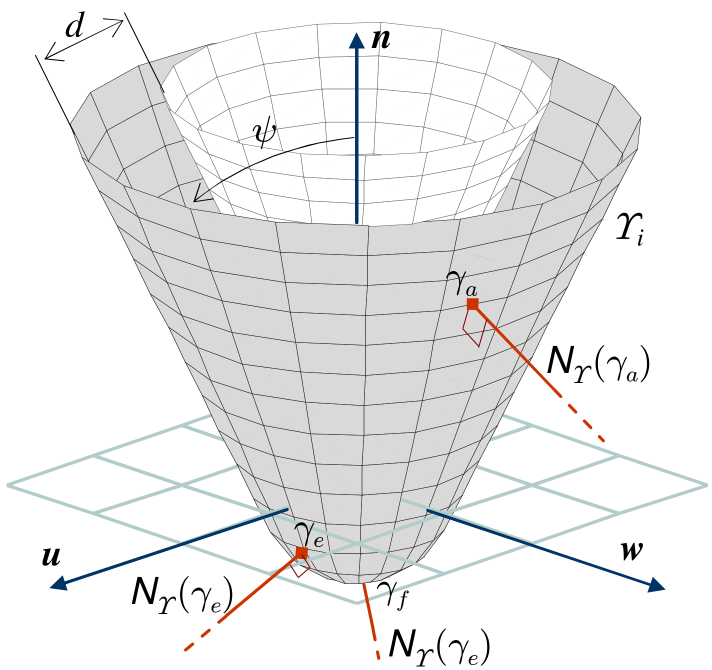
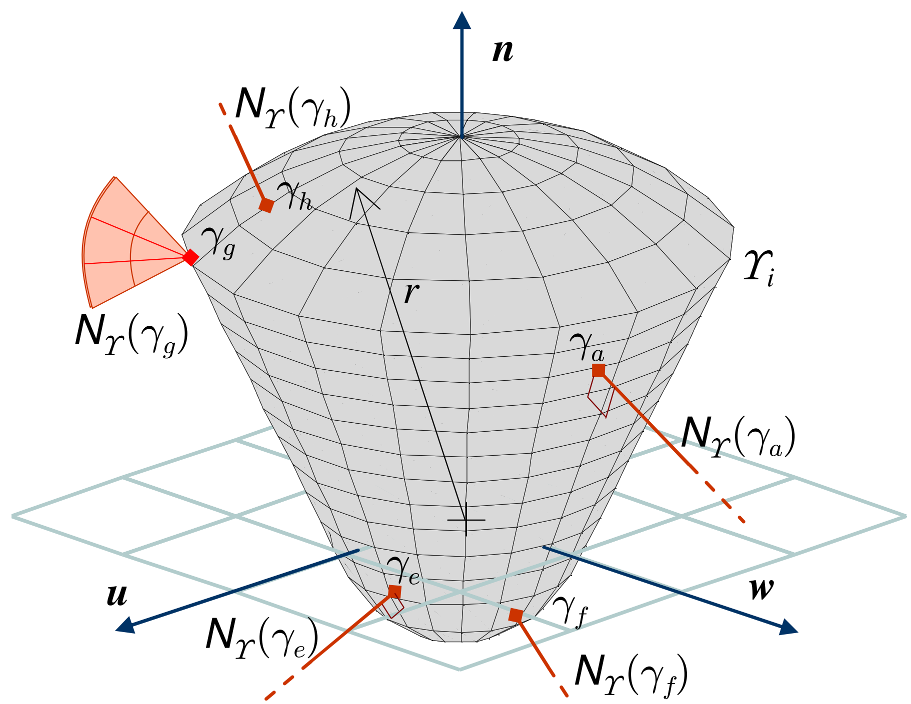
Also can model similarly ….

- Plasticity
- Nonassociative plasticity (which results no longer in an optimization equivalent problem!!)
- Spinning/Rolling Friction

Modeling plasticity

- The yield surface give by Coulomb needs to be modified as no infinite reaction is now allowed (crushing)





The model

- Separate elastic and plastic displacement:

$$\mathbf{y}^i = \mathbf{y}_E^i + \mathbf{y}_P^i$$

- The elastic part of the force allows to compute the force at the contact if the plastic part of the displacement is known.

$$\widehat{\gamma}_{\mathcal{A}}^i = -K^i \left(\mathbf{y}^i - \mathbf{y}_P^i\right)$$

- Except, of course, the plastic part is NOT known***. But now we use the associated plasticity hypothesis to constrain the plastic displacement evolution with a variational inequality.***

$$\dot{\mathbf{y}}_P^i \in -\mathcal{N}_{\widehat{\Upsilon}^i}(\widehat{\gamma}_{\mathcal{A}}^i) \quad ; \quad \widehat{\gamma}_{\mathcal{A}}^i \in \widehat{\Upsilon}^i$$

- Mathematically, it is the same idea with normal velocity at the contact; EXCEPT that the containing set is no longer a cone, proper (it can be a shifted cone, or just some convex set. So we can time-step and close it.

Nonassociative plasticity

- However, not all plasticity is associative.
- How do we do things in the nonassociative case?
- Extension

$$\gamma_{\mathcal{E}} \in \Upsilon, \; N\gamma_{\mathcal{E}} + \mathbf{r} \in -H^{-1}\mathcal{N}_{\Upsilon}(\gamma_{\mathcal{E}}),$$

- H is positive definite and symmetric, but N is only symmetric psd.
- Do we have existence? – yes
- Non reducible to an optimization problem.

Modeling Rolling/Spinning

- The reaction cone:

$$\mathcal{Z}^i = \left\{ \gamma \in \mathbb{R}^6 \mid \mu^i \gamma_n \geq \sqrt{\gamma_u^2 + \gamma_w^2}, \rho^i \gamma_n \geq \sqrt{\tau_u^2 + \tau_w^2}, \sigma^i \gamma_n \geq |\tau_n| \right\}$$

- Define total cone (inclusive of bilateral constraints) and its polar:

$$\Upsilon = \left(\times_{i \in \mathcal{G}_\mathcal{A}} \mathcal{Z}^i \right) \times \left(\times_{i \in \mathcal{G}_\mathcal{B}} \mathcal{B}^i \right)$$
$$\Upsilon^\circ = \left(\times_{i \in \mathcal{G}_\mathcal{A}} \mathcal{Z}^{i^\circ} \right) \times \left(\times_{i \in \mathcal{G}_\mathcal{B}} \mathcal{B}^{i^\circ} \right)$$

- Using the virtually identical sequence of time stepping, notations and relaxation we obtain the cone complementarity problem.

$$(N \boldsymbol{\gamma}_\mathcal{S} + \boldsymbol{r}) \in -\Upsilon^\circ \quad \perp \quad \boldsymbol{\gamma}_\mathcal{S} \in \Upsilon.$$

3. ITERATIVE METHODS

Iterative Methods

- Stationary iterative methods (we presented before Gauss-Jacobi, Gauss-Seidel, SOR)
- Iterative Methods we did not apply before
  - Gradient Projected Minimum Residual (GPMINRES) [FRICTIONLESS]
  - Modified Proportioning with Reduced Gradient Projection (MPRGP) [FRICTIONLESS]
  - Accelerated Projected Gradient Descent (APGD)
  - Preconditioned Spectral Projected Gradients with Fallback (P-SPG-FB)
- Primal-Dual Interior Point (PD-IP) (at the moment, single processor only, difficult for our platform parallel, GPU)

GP-MINRES

ALGORITHM GPMINRES($\mathbf{N}$, $\mathbf{r}$, τ, η_1, η_2, N_{max}, M_{max})

$\gamma^{(0)} := \mathbf{0}_{nc}$
for $k := 0$ **to** N_{max}
    $\mathbf{y}^{(0)} = \gamma^{(k)}$
    while agressively changing active set and reducing cost function
        $\mathbf{y}^{(j+1)} = P[\mathbf{y}^{(j)} - \alpha_j \nabla q(\mathbf{y}^{(j)})]$
        $j = j + 1$
    endwhile
    $\gamma^{(k)} := \mathbf{y}^{(j)}$
    Determine active set $\mathcal{A}(\gamma^{(k)})$ and $\mathbf{Z}_k$ and $\mathbf{r}_k$
    $\mathbf{w}_0 = \mathbf{0}_{m_k}$
    for $j := 0$ **to** M_{max}
        MINRES step: $\mathbf{w}^{(j)} \rightarrow \mathbf{w}^{(j+1)}$
        $j = j + 1$
        if slughish convergence
            break
    enfor
    Set $\bar{\mathbf{w}}_k := \mathbf{w}^{(j)}$
    Get $\gamma^{(k+1)} \rightarrow$ backtracking line-search with direction $\mathbf{d}_k = \mathbf{Z}_k \bar{\mathbf{w}}_k$
    if $\|\nabla_\Omega q(\gamma^{(k+1)})\|_\infty < \tau$
        break
enfor
return Value at time step t_{l+1}, $\gamma^{l+1} := \gamma^{(k+1)}$.

Line search

MINRES is used as opposed to CG since many matrices are Only PSD, and MINRES was Observed to be more robust.

Based on work of Jorge Moré (1991)

Nesterov's Accelerated Projected Gradient Descent

ALGORITHM NAPG($N, r, t \leq \frac{1}{\lambda_{max}(N)}, \tau, N_{max}$)

$\gamma_0 = 0_{n_c}$

$\hat{\gamma}_0 = 1_{n_c}$

$y_0 = \gamma_0$

$\theta_0 = 1$

for $k := 0$ **to** N_{max}

  $g = N y_k - r$

  $\gamma_{k+1} = \Pi_{\mathcal{K}}\left(y_k - tg\right)$

  $\theta_{k+1} = \frac{-\theta_k^2 + \theta_k \sqrt{\theta_k^2 + 4}}{2}$

  $\beta_{k+1} = \theta_k \frac{1-\theta_k}{\theta_k^2 + \theta_{k+1}}$

  $y_{k+1} = \gamma_{k+1} + \beta_{k+1}\left(\gamma_{k+1} - \gamma_k\right)$

  $\epsilon = \epsilon\left(\gamma_{k+1}\right)$

  if $\epsilon < \tau$

    break

  endif

endfor

return Value at time step t_{l+1}, $\gamma^{l+1} := \hat{\gamma}$.

Preconditioned Spectral Projected Gradients with Fallback (Birgin et al. 99), bounds only

ALGORITHM P-SPG-FB($\mathbf{N}$, $\mathbf{r}$, $\mathbf{x}_0$, $\mathcal{K}$, $\mathbf{P} \mapsto \mathbf{x}$)

$\mathbf{x}_0 := \Pi_{\mathcal{K}}(\mathbf{x}_0)$, $\mathbf{x}_{FB} = \mathbf{x}_0$, $\hat{\alpha}_0 \in [\alpha_{min}, \alpha_{max}]$
$\mathbf{g}_0 := \mathbf{N}\mathbf{x}_0 + \mathbf{r}$, $f(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^T\mathbf{N}\mathbf{x}_0 + \mathbf{x}_0^T\mathbf{r}$, $w_0 = 10^{29}$
for $j := 0$ **to** N_{max}
    $\mathbf{p}_j = \mathbf{P}^{-1}\mathbf{g}_j$
    $\mathbf{d}_j = \Pi_{\mathcal{K}}(\mathbf{x}_j - \hat{\alpha}_j\mathbf{p}_j) - \mathbf{x}_j$
    if $\langle \mathbf{d}_j, \mathbf{g}_j \rangle \geq 0$
        $\mathbf{d}_j = \Pi_{\mathcal{K}}(\mathbf{x}_j - \hat{\alpha}_j\mathbf{g}_j) - \mathbf{x}_j$
    $\lambda := 1$
    while line search
        $\mathbf{x}_{j+1} := \mathbf{x}_j + \lambda\mathbf{d}_j$
        $\mathbf{g}_{j+1} := \mathbf{N}\mathbf{x}_{j+1} + \mathbf{r}$
        $f(\mathbf{x}_{j+1}) = \frac{1}{2}\mathbf{x}_{j+1}^T\mathbf{N}\mathbf{x}_{j+1} + \mathbf{x}_{j+1}^T\mathbf{r}$
        if $f(\mathbf{x}_{j+1}) > \max_{i=0,..,\min(j,N_{GLL})} f(\mathbf{x}_{j-i}) + \gamma\lambda\langle \mathbf{d}_j, \mathbf{g}_j \rangle$
            define $\lambda_{\text{new}} \in [\sigma_{\text{min}}\lambda, \sigma_{\text{max}}\lambda]$ and repeat line search
        else
            terminate line search
    $\mathbf{s}_j = \mathbf{x}_{j+1} - \mathbf{x}_j$
    $\mathbf{y}_j = \mathbf{g}_{j+1} - \mathbf{g}_j$
    if j is odd
        $\hat{\alpha}_{j+1} = \frac{\langle \mathbf{s}_j, \mathbf{P}\mathbf{s}_j \rangle}{\langle \mathbf{s}_j, \mathbf{y}_j \rangle}$
    else
        $\hat{\alpha}_{j+1} = \frac{\langle \mathbf{s}_j, \mathbf{y}_j \rangle}{\langle \mathbf{y}_j, \mathbf{P}^{-1}\mathbf{y}_j \rangle}$
    $\hat{\alpha}_{j+1} = \min(\alpha_{\text{max}}, \max(\alpha_{\text{min}}, \hat{\alpha}_{j+1}))$
    $w_{j+1} = \|[\mathbf{x}_{j+1} - \Pi_{\mathcal{K}}(\mathbf{x}_{j+1} - \tau_g\mathbf{g}_{j+1})]/\tau_g\|_2 = \|\epsilon\|_2$
    if $w_{j+1} \leq \min_{k=0,..,j} w_k$
        $\mathbf{x}_{FB} = \mathbf{x}_{j+1}$
return $\mathbf{x}_{FB}$

Attempt Preconditioning (we use diagonal) Grippo et al. 86

Nonomonotone line search

One of the many step choice rules, we observed it has more smoothness

Accept Best KKT point so far as FB

Modified Proportioning with Reduced Gradient Projection (MPRGP), Dostal and Schoberl, 05, bound constraints only

ALGORITHM KUCERA$(\mathbf{N}, \mathbf{r}, \mathbf{x}^0, \mathcal{K}, \Gamma > 0, \tilde{\alpha} \in (0, \|\mathbf{N}\|^{-1}], \epsilon > 0)$

$k = 0$
$\mathbf{g} = \mathbf{N}\mathbf{x}^0 + \mathbf{r}$
$\mathbf{p} = \phi(\mathbf{x}^0)$
while $\|\tilde{\mathbf{g}}(\mathbf{x}^k)\| > \epsilon$
  if $\tilde{\beta}(\mathbf{x}^k)^T \mathbf{g}(\mathbf{x}^k) \leq \Gamma^2 \tilde{\phi}(\mathbf{x}^k)^T \mathbf{g}(\mathbf{x}^k)$
    $\alpha_{cg} = \mathbf{g}^T\mathbf{p}/\mathbf{p}^T\mathbf{N}\mathbf{p}$
    $\alpha_f = min(\alpha_{f,i})$ where $\alpha_{f,i} = \begin{cases} \mathbf{x}_i/\mathbf{p}_i, & \text{if } \mathbf{p}_i > 0 \\ \infty, & \text{if } \mathbf{p}_i \leq 0 \end{cases}$
    if $\alpha_{cg} < \alpha_f$
      $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_{cg}\mathbf{p}$
      $\mathbf{g} = \mathbf{g} - \alpha_{cg}\mathbf{N}\mathbf{p}$
      $\gamma = \phi(\mathbf{x}^{k+1})^T\mathbf{N}\mathbf{p}/\mathbf{p}^T\mathbf{A}\mathbf{p}$
      $\mathbf{p} = \phi(\mathbf{x}^{k+1}) - \gamma\mathbf{p}$
    else
      $\mathbf{x}^{k+1/2} = \mathbf{x}^k - \alpha_f\mathbf{p}$
      $\mathbf{x}^{k+1} = \mathbf{x}^{k+1/2} - \tilde{\alpha}\tilde{\phi}(\mathbf{x}^{k+1/2})$
      $\mathbf{g} = \mathbf{N}\mathbf{x}^{k+1} + \mathbf{r}$
      $\mathbf{p} = \phi(\mathbf{x}^{k+1})$
  else
    $\mathbf{x}^{k+1} = \mathbf{x}^k - \tilde{\alpha}\tilde{\beta}(\mathbf{x}^k)$
    $\mathbf{g} = \mathbf{N}\mathbf{x}^{k+1} + \mathbf{r}$
    $\mathbf{p} = \phi(\mathbf{x}^{k+1})$
  $k = k + 1$
return $\mathbf{x}^k$

Boundary Effects < Descent Effects?

Do CG as much as possible.

Expansion Step

Proportioning Step

Interior Point

ALGORITHM PD-IP($f_0, f_1, \ldots, f_m, \mu \geq 1, \epsilon$)

(1) **while** $||\boldsymbol{r}_t(\boldsymbol{x}, \boldsymbol{\lambda})||_2 > \epsilon$

(2) Compute $t = \frac{\mu m}{\hat{\eta}}$

(3) Compute search direction $[\Delta \boldsymbol{x}^T \; \Delta \boldsymbol{\lambda}^T]^T$

(4) Compute step length $s > 0$ via line search

(5) Update: $\boldsymbol{x} = \boldsymbol{x} + s\Delta\boldsymbol{x}, \boldsymbol{\lambda} = \boldsymbol{\lambda} + s\Delta\boldsymbol{\lambda}$

(6) **endwhile**

(7) **return** Solution $\boldsymbol{x}^\star = \boldsymbol{x}, \boldsymbol{\lambda}^\star = \boldsymbol{\lambda}$

$$\begin{bmatrix} \nabla^2 f_0(\boldsymbol{x}) + \sum_{i=1}^{m} \boldsymbol{\lambda}_i \nabla^2 \boldsymbol{f}_i(\boldsymbol{x}) & \nabla \boldsymbol{f}(\boldsymbol{x})^T \\ -diag(\boldsymbol{\lambda}) \nabla \boldsymbol{f}(\boldsymbol{x}) & -diag(\boldsymbol{f}(\boldsymbol{x})) \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{x} \\ \Delta \boldsymbol{\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla f_0(\boldsymbol{x}) + \nabla \boldsymbol{f}(\boldsymbol{x})^T \boldsymbol{\lambda} \\ -diag(\boldsymbol{\lambda}) \boldsymbol{f}(\boldsymbol{x}) - \frac{1}{t}\mathbf{1} \end{bmatrix}$$

How well do they perform?

Residual Measures

$$r_1 = ||\boldsymbol{f}_1||_\infty, \boldsymbol{f}_1 = \left[\ldots, min\left(\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)_{i,n}, 0\right), \ldots\right]^T \in \mathbb{R}^{N_c}$$

$$r_2 = ||\boldsymbol{f}_2||_\infty, \boldsymbol{f}_2 = \left[\ldots, \gamma_{i,n}\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)_{i,n}, \gamma_{i,u}\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)_{i,u}, \gamma_{i,v}\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)_{i,v}, \ldots\right]^T \in \mathbb{R}^{3N_c}$$

$$r_3 = ||\boldsymbol{f}_3||_\infty, \boldsymbol{f}_3 = \left[\ldots, \boldsymbol{\gamma}_i^T\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)_i, \ldots\right]^T \in \mathbb{R}^{N_c}$$

$$r_4 = ||\boldsymbol{f}_4||_2, \boldsymbol{f}_4 = \frac{1}{g_d}\left(\boldsymbol{\gamma} - \Pi_{\mathcal{K}}\left(\boldsymbol{\gamma} - g_d\left(\boldsymbol{N\gamma}+\boldsymbol{r}\right)\right)\right) \in \mathbb{R}^{3N_c}$$

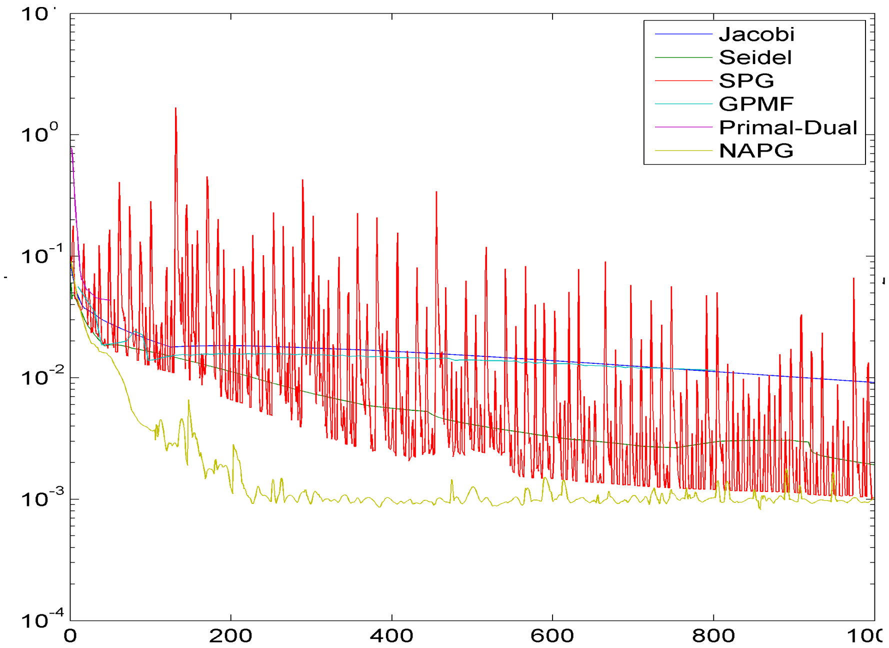
Feasibility

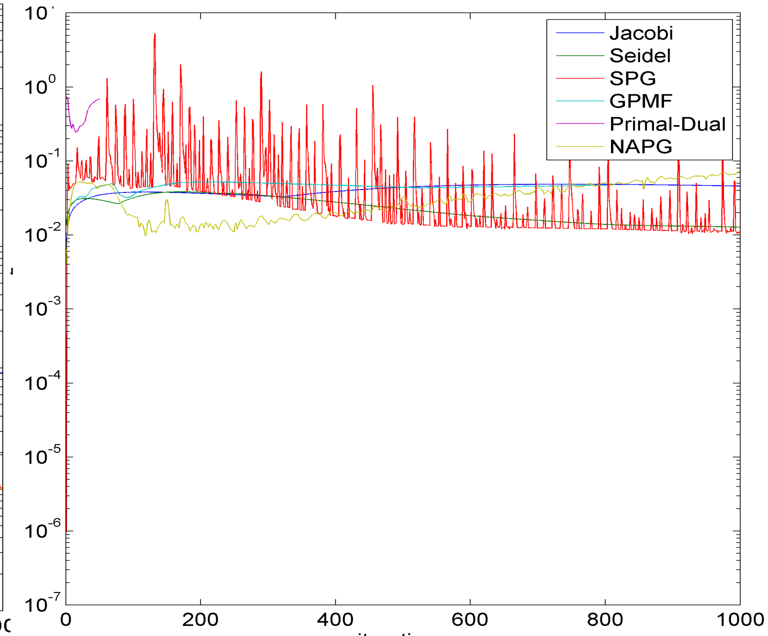
Complementarity 1

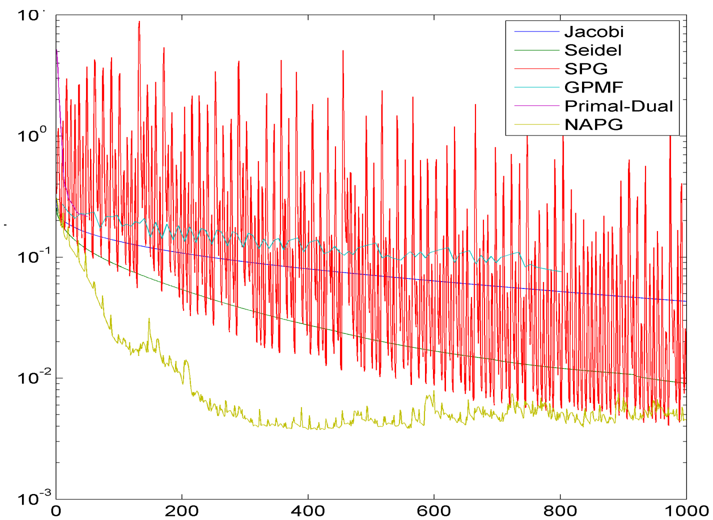
Complementarity 2,
=Com 1 for
Frictionless

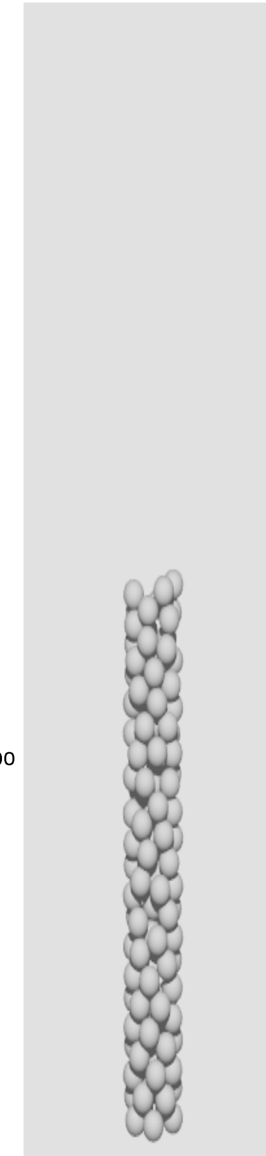
Optimality

Residuals: 128 Body Problem







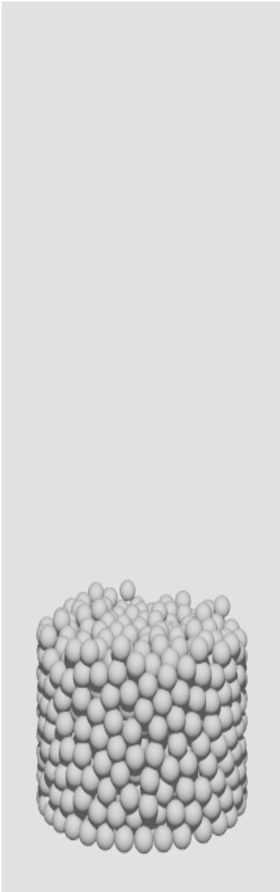


- IP is the best (duh) but GPU hard

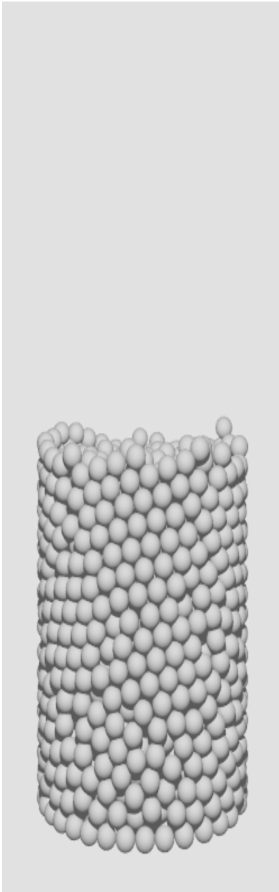
Among iterative:

- APGD is the best, followed by spectral
- APGD is easily the best at low iteration counts

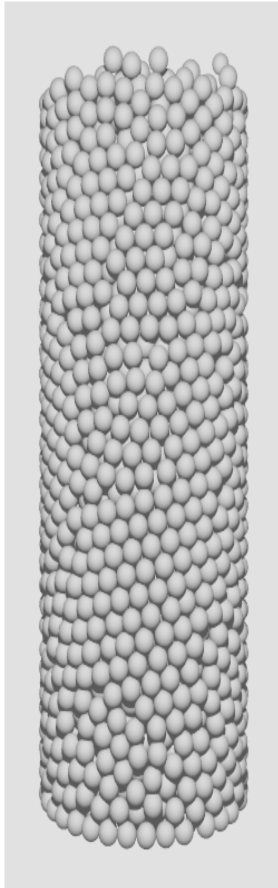
Single Step Tests



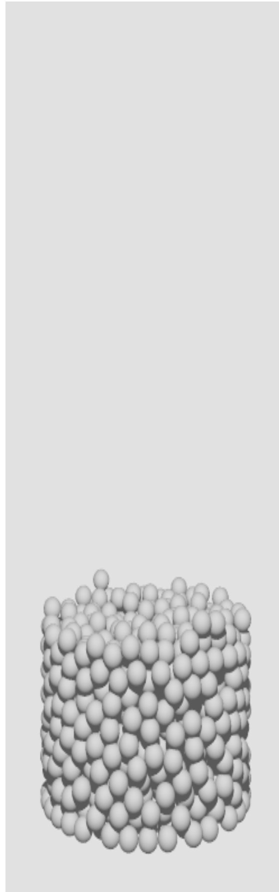
1,000
bodies
μ=0



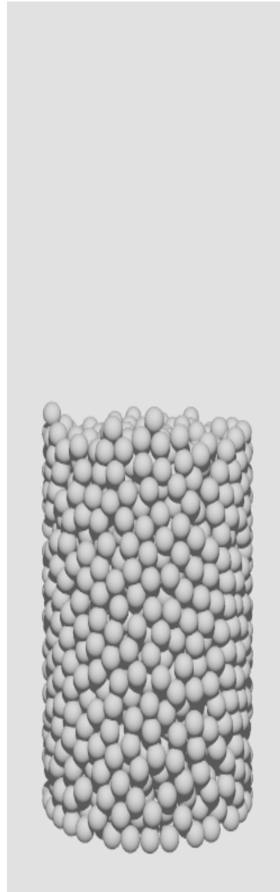
2,000
bodies
μ=0



4,000
bodies
μ=0

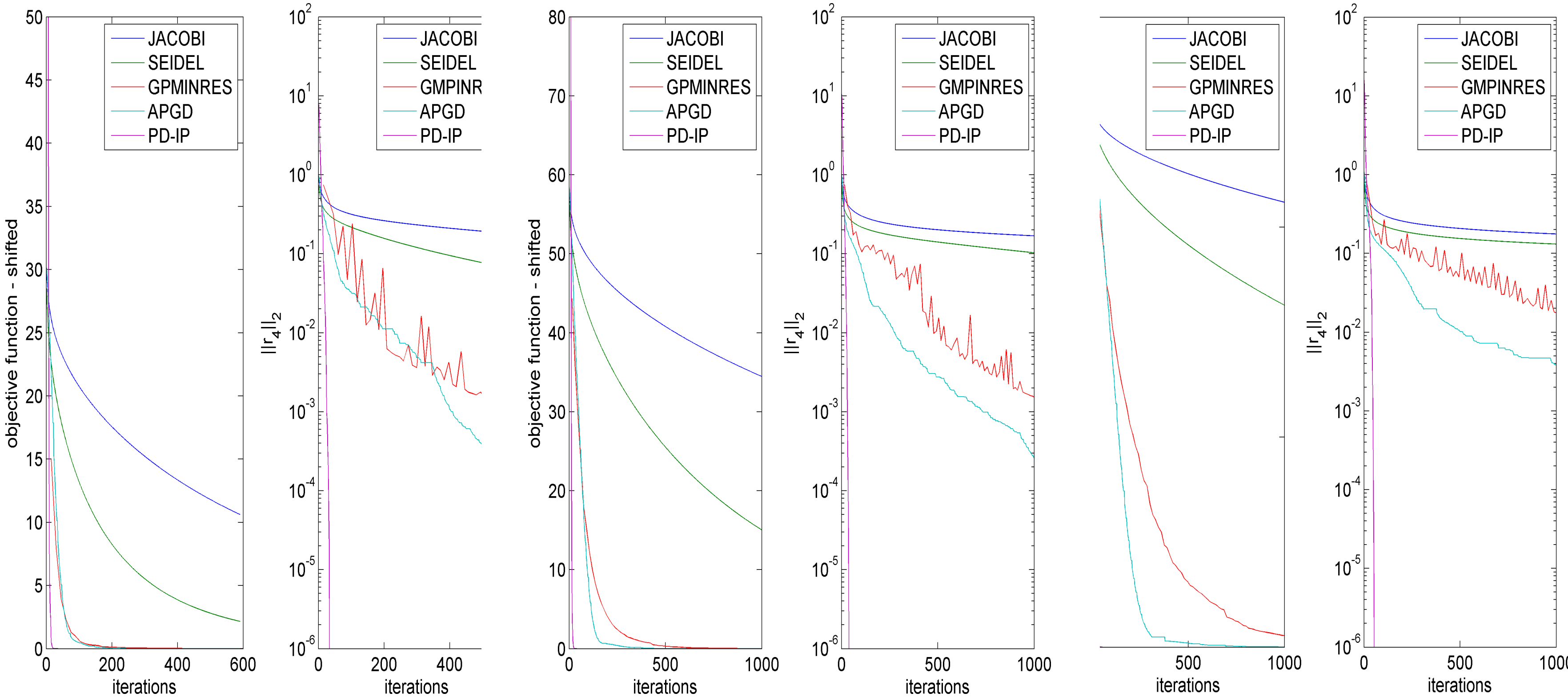


1,000
bodies
μ=0.25



2,000
bodies
μ=0.25

Single Step Tests: Frictionless (obj and opt)



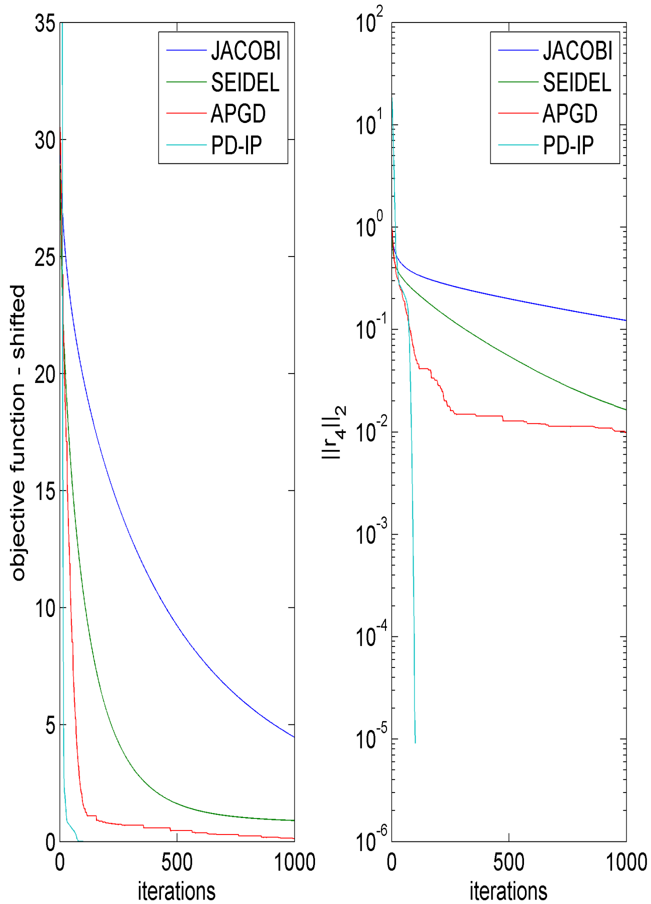
1,000 Bodies
4,192 Contacts

2,000 Bodies
8,622 Contacts

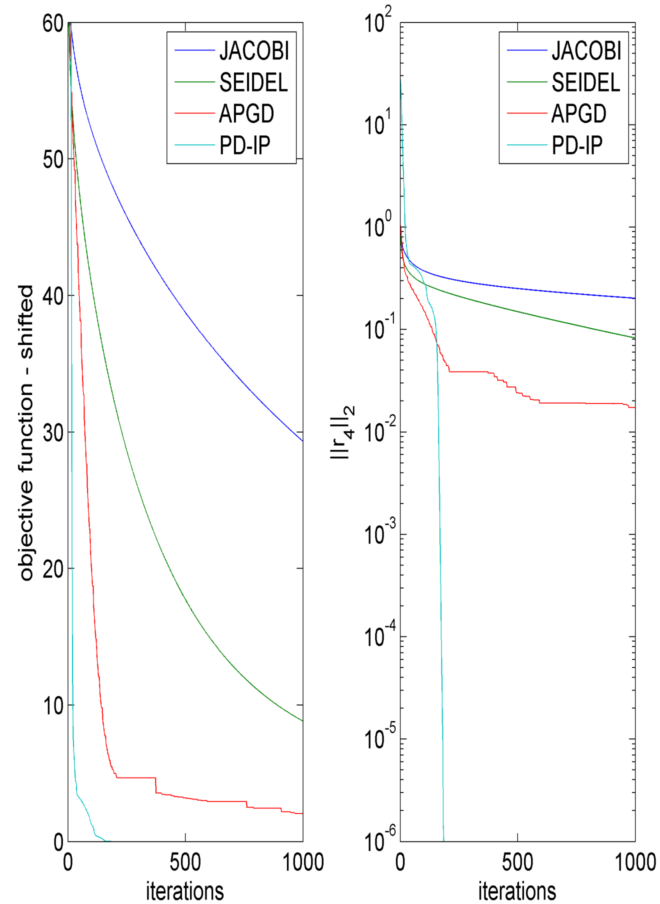
4,000 Bodies
17,510
Contacts

•Among iterative, APGD again best. So we did not expand MRGP and SGP to friction

Single Step Tests: Frictional, APGD much better than stationary iterations



1,000 Bodies
3,872 Contacts



2,000 Bodies
7,931 Contacts

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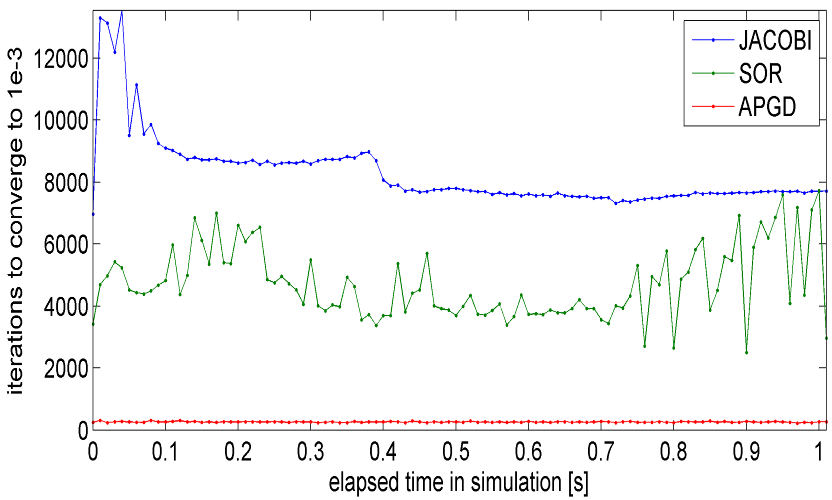
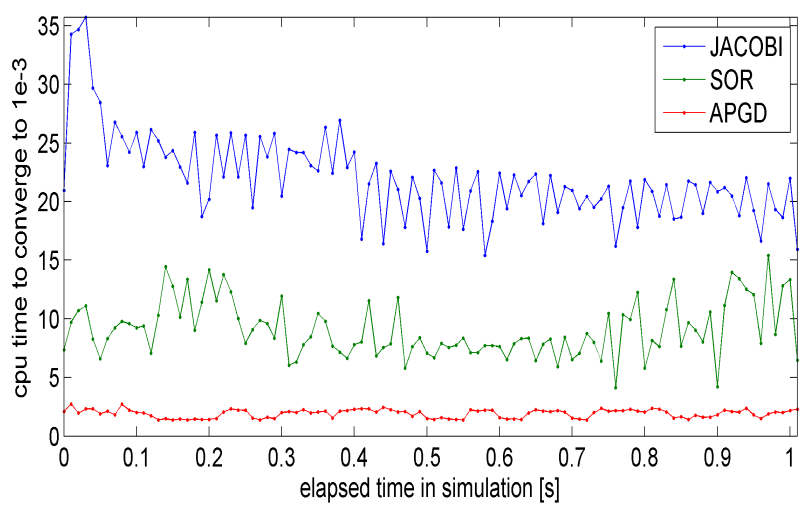
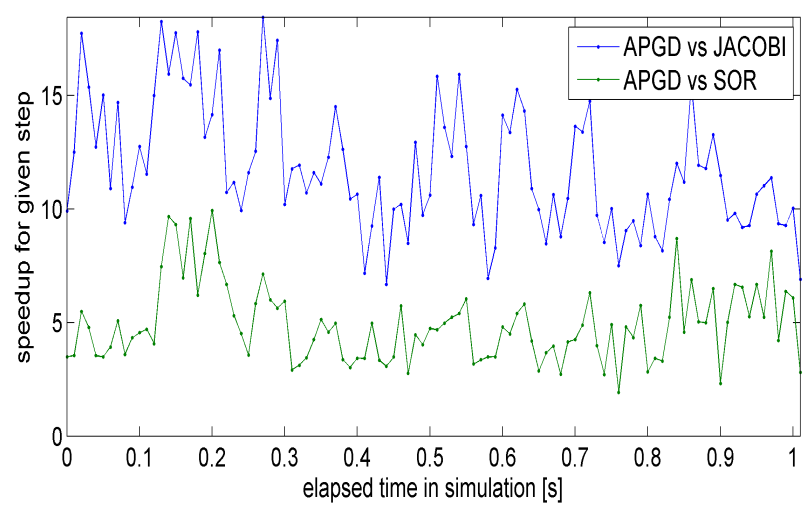
Simulation Tests: 1,000 Settled Spheres



1,000 Bodies	3,752 Contacts	
Method	Comp. Time [s]	Speedup
JACOBI	2,243.6	11.43
SOR	927.6	4.72
APGD	196.3	1

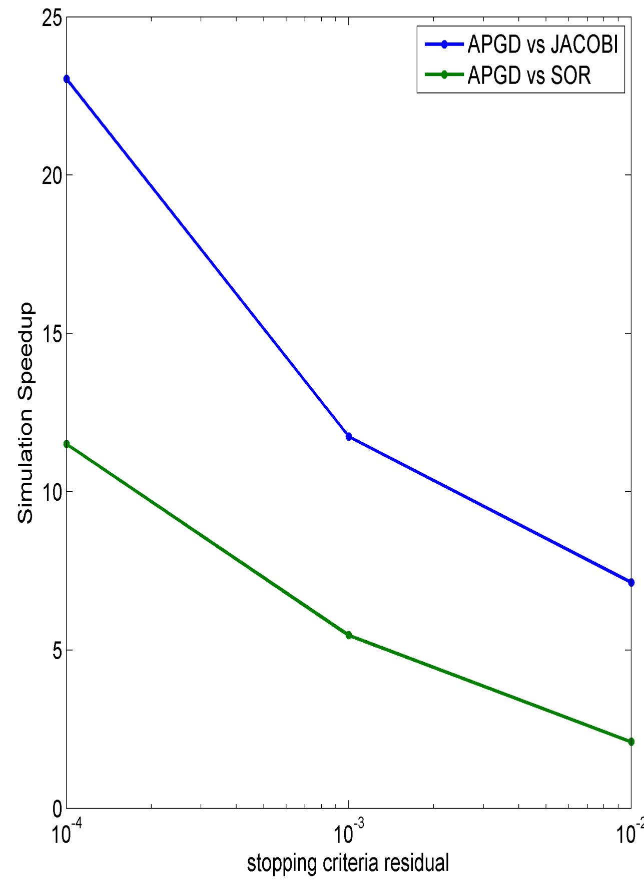




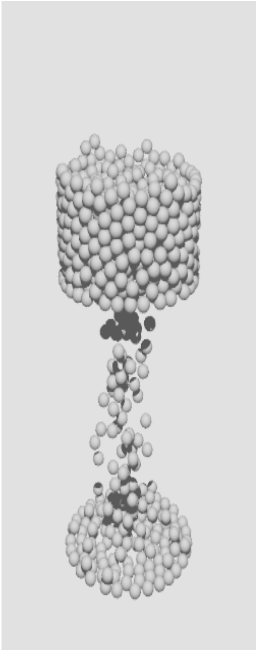
Simulation Tests: Settled Spheres

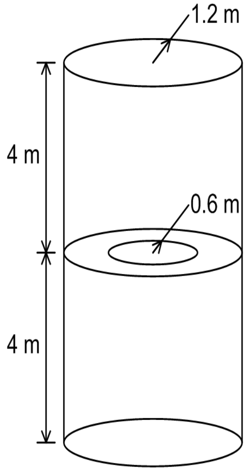
2,000 Bodies 7,678 Contacts		
Method	Comp. Time [s]	Speedup
JACOBI	9,311.4	14.73
SOR	5,047.1	7.99
APGD	632.0	1

4,000 Bodies 15,653 Contacts		
Method	Comp. Time [s]	Speedup
JACOBI	26,592.3	9.40
SOR	25,147.6	8.89
APGD	2,829.2	1

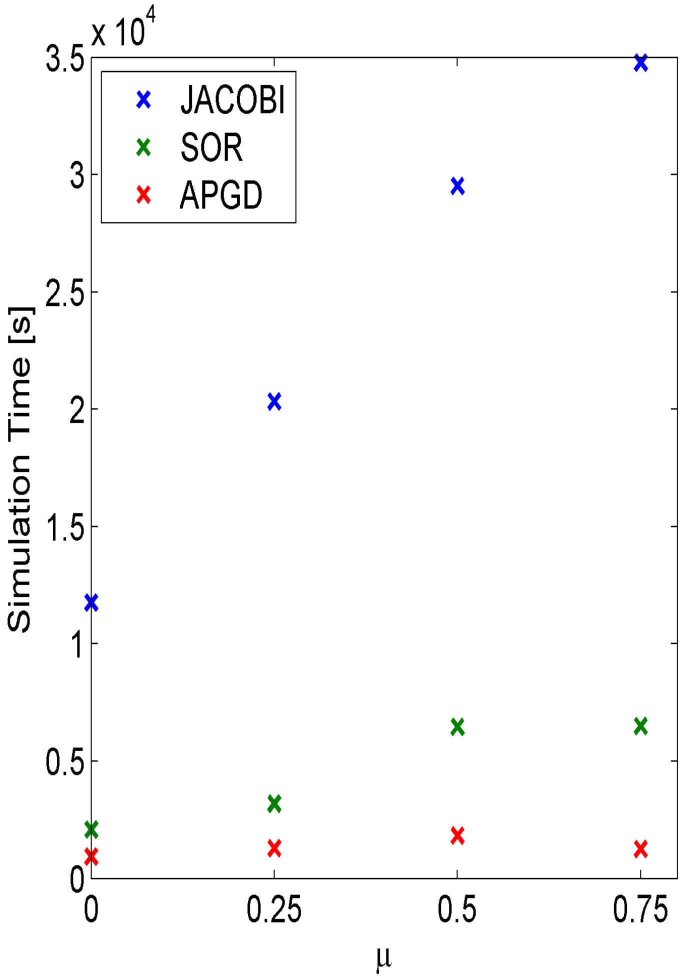


Simulation Tests: Flowing Spheres





5 second long flow simulation with 1,000 bodies		
Method	Comp. Time [s]	Speedup
JACOBI	49,356.4	20.54
SOR	11,580.1	4.82
APGD	2,403.3	1



SUMMARY OF SIMULATIONS

- APGD is a great improvement over the other algorithms we considered.
- We implemented in OpenMP/GPU + MPI for multiGPU.
- We ran it for >10M particles ~ 30-40M variables.
- We can solve some industrial strength problems.

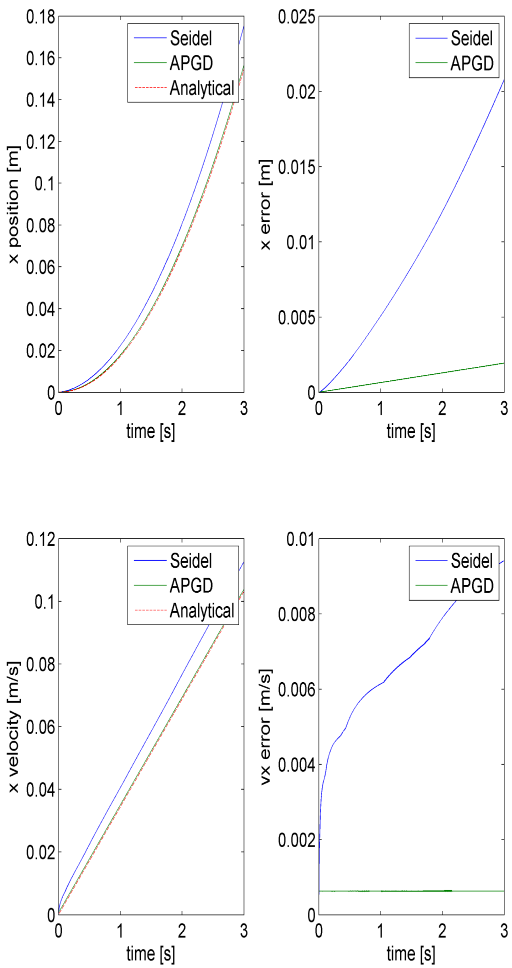
4. VALIDATION

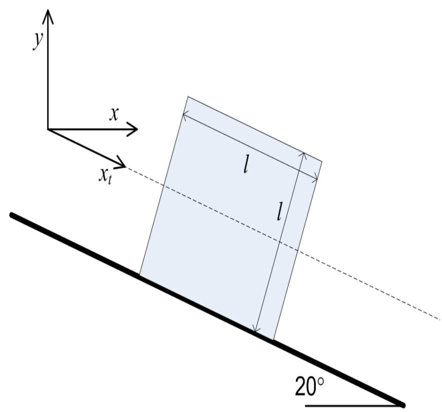
Do we really need validation … ? Yes

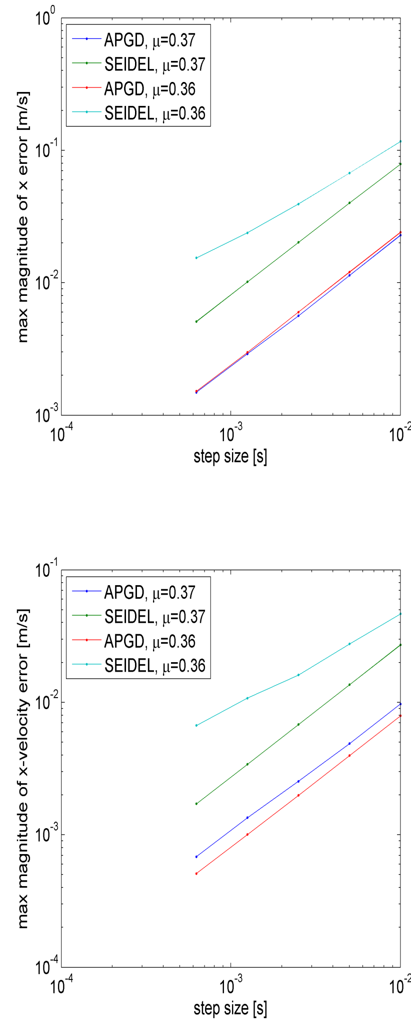
- We approximated the distributed/microscopic body model with a “macroscopic” rigid one
- We approximated the resulting nonconvex LCP with a convex one
- We solve the resulting solutions approximately.
- For many time steps.

- We have many chances to get the wrong result.

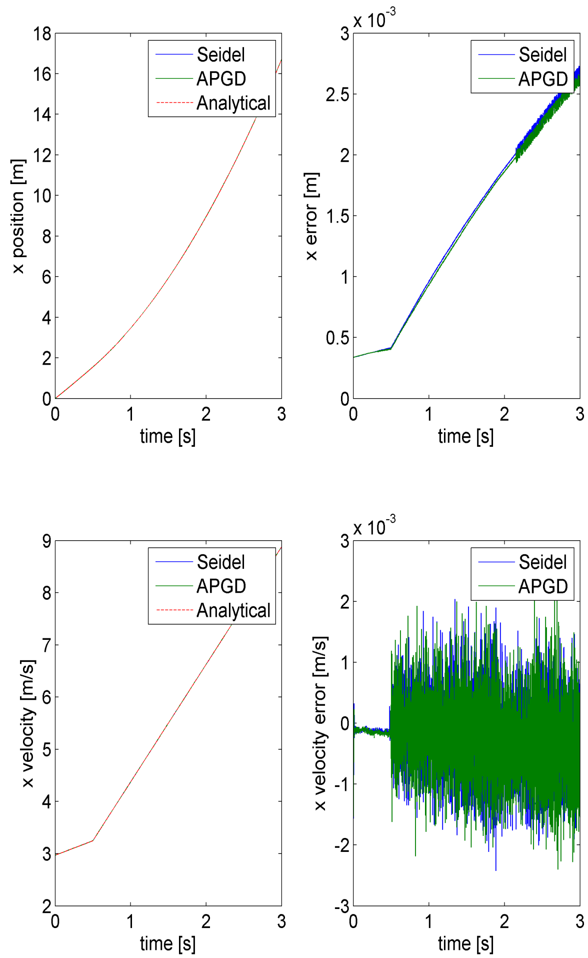
Analytical Validation: Sliding

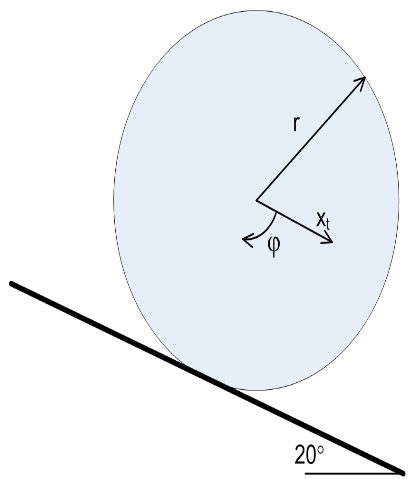


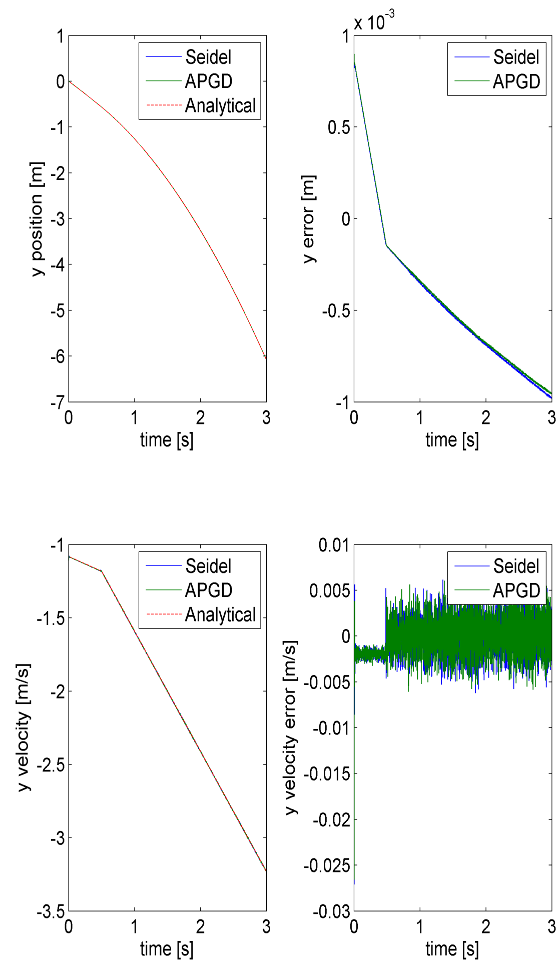




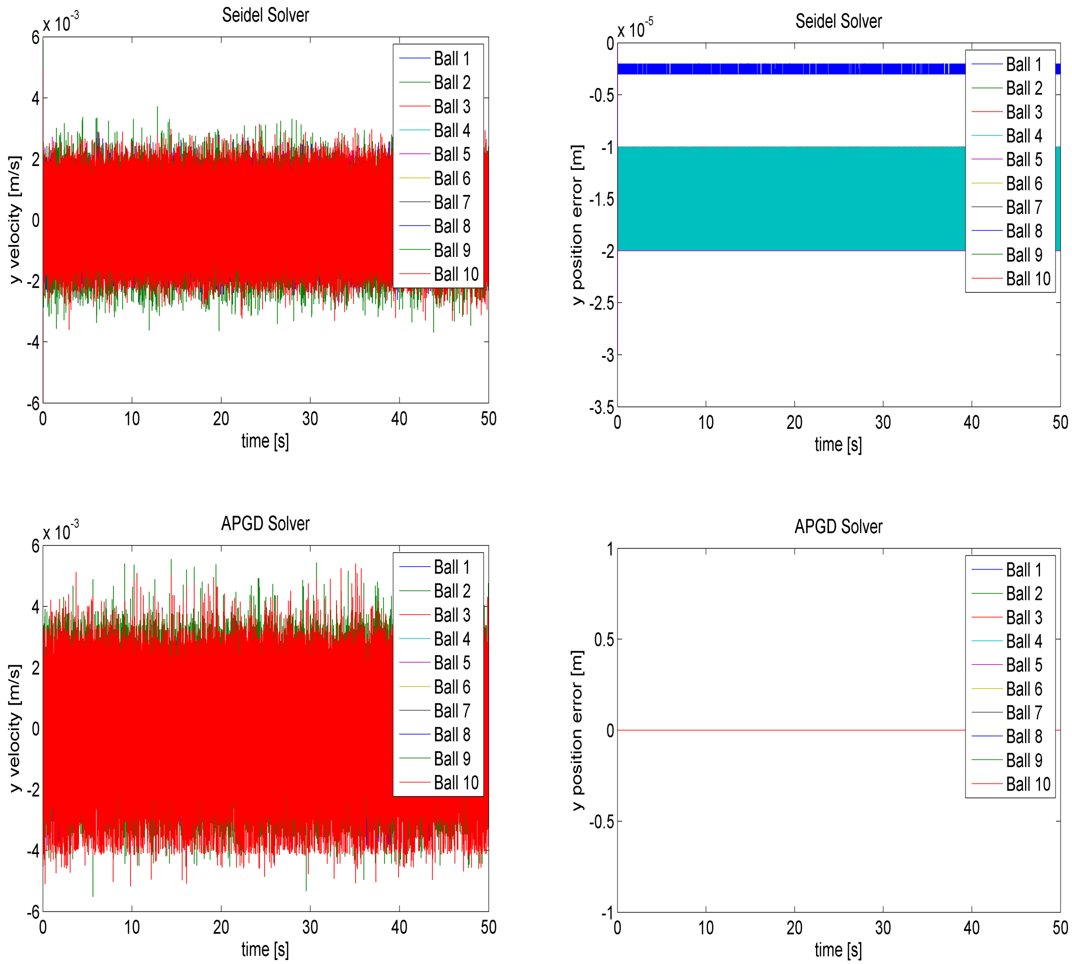
Analytical Validation: Rolling

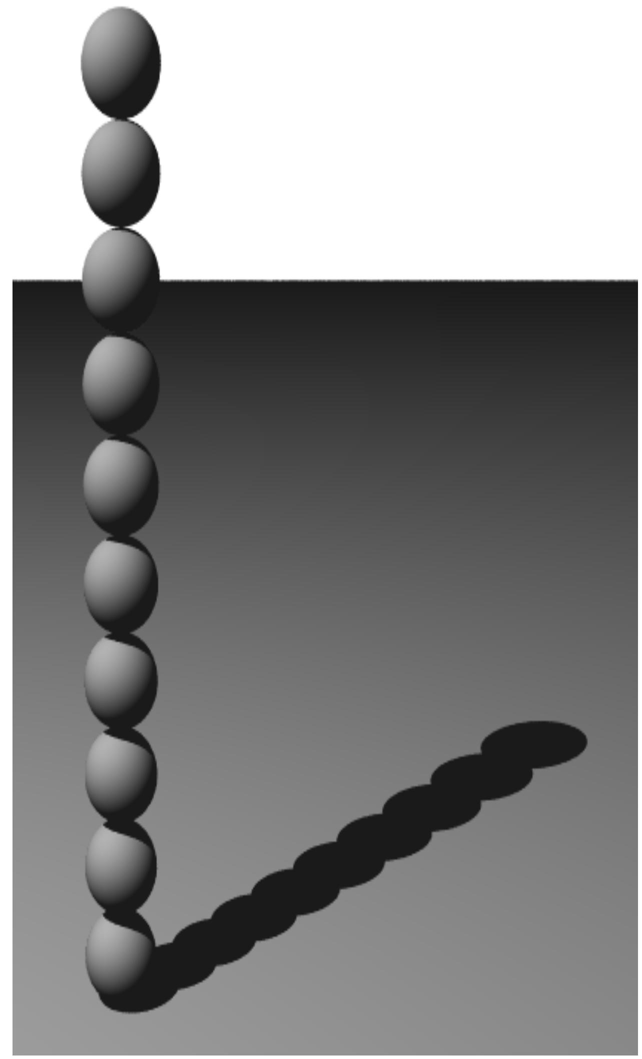






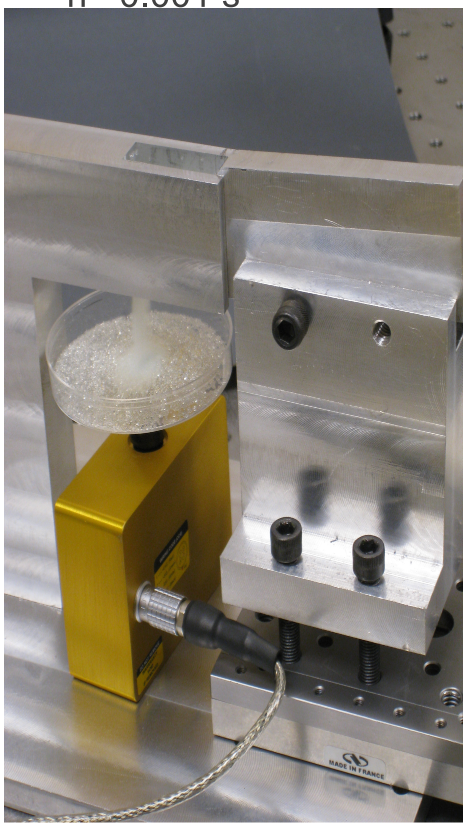
Analytical Validation: Stacking

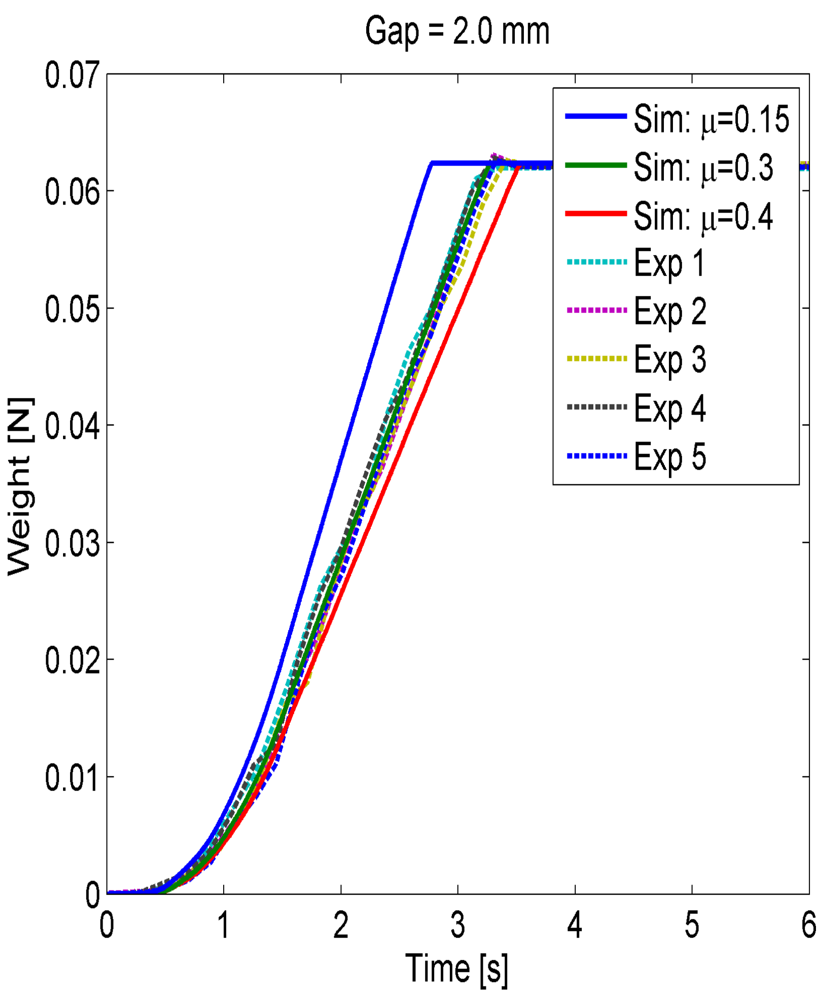


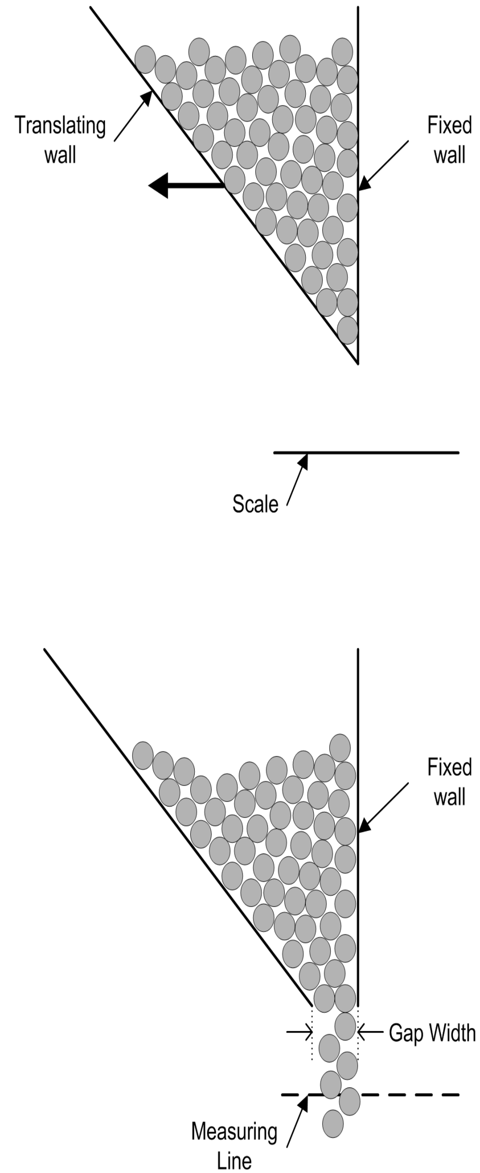


Experimental Validation: Mass Flow Rate

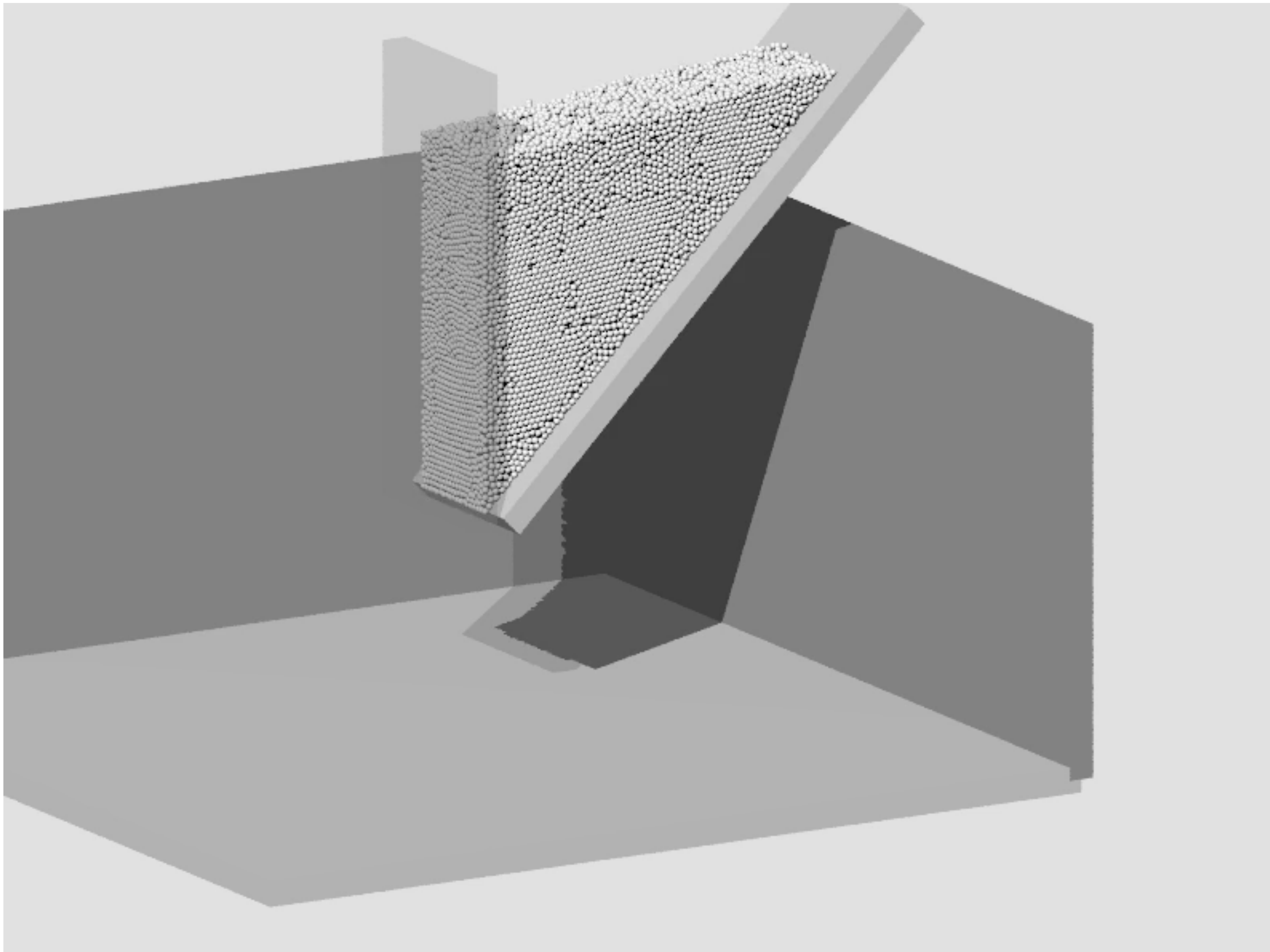
- 39,000 spherical bodies
- d=500 μm
- ρ=2.5 g/cm^3
- h= 0.001 s



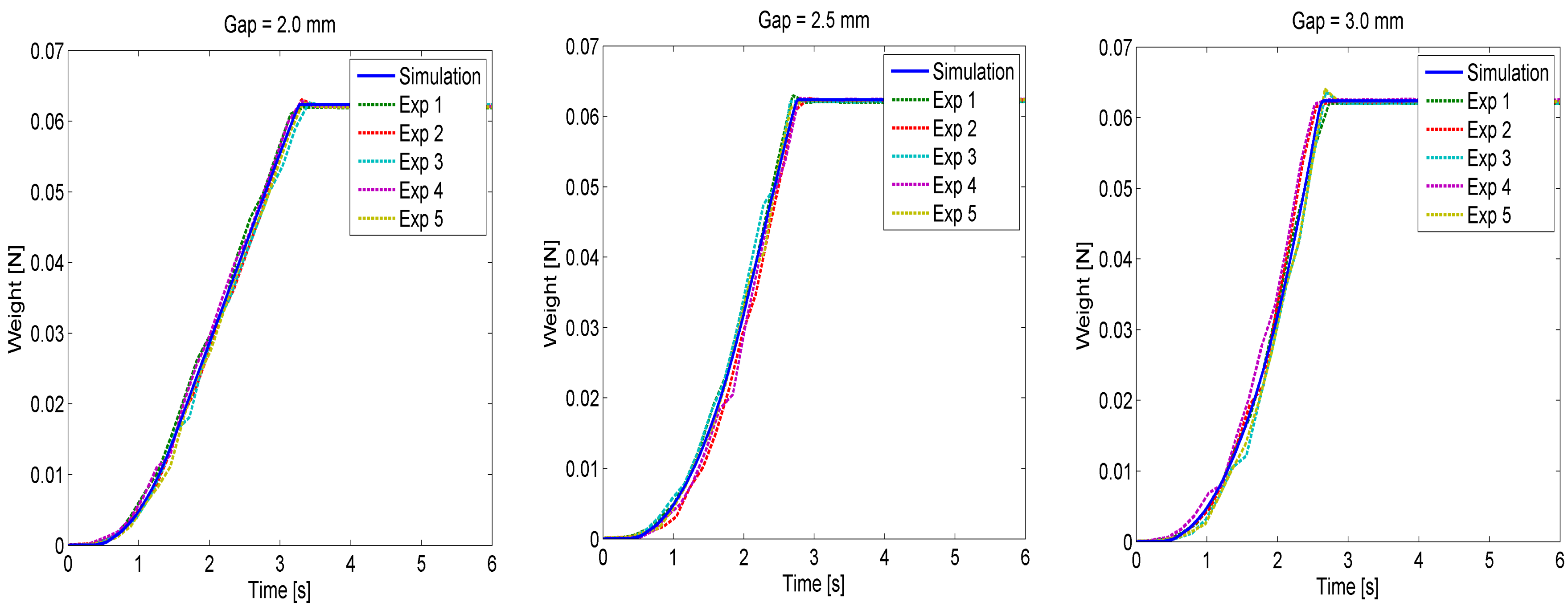




Experimental Validation: Mass Flow Rate

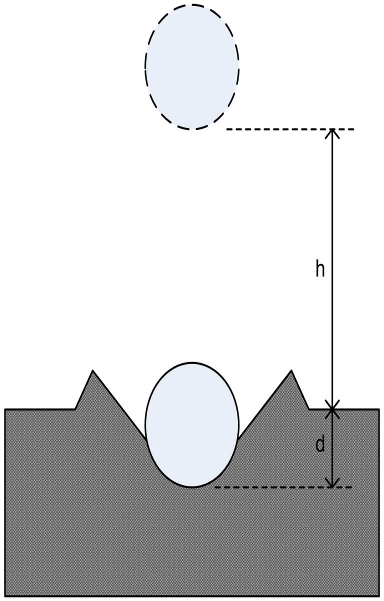


Experimental Validation: Varying Gap; Mass Flow Rate

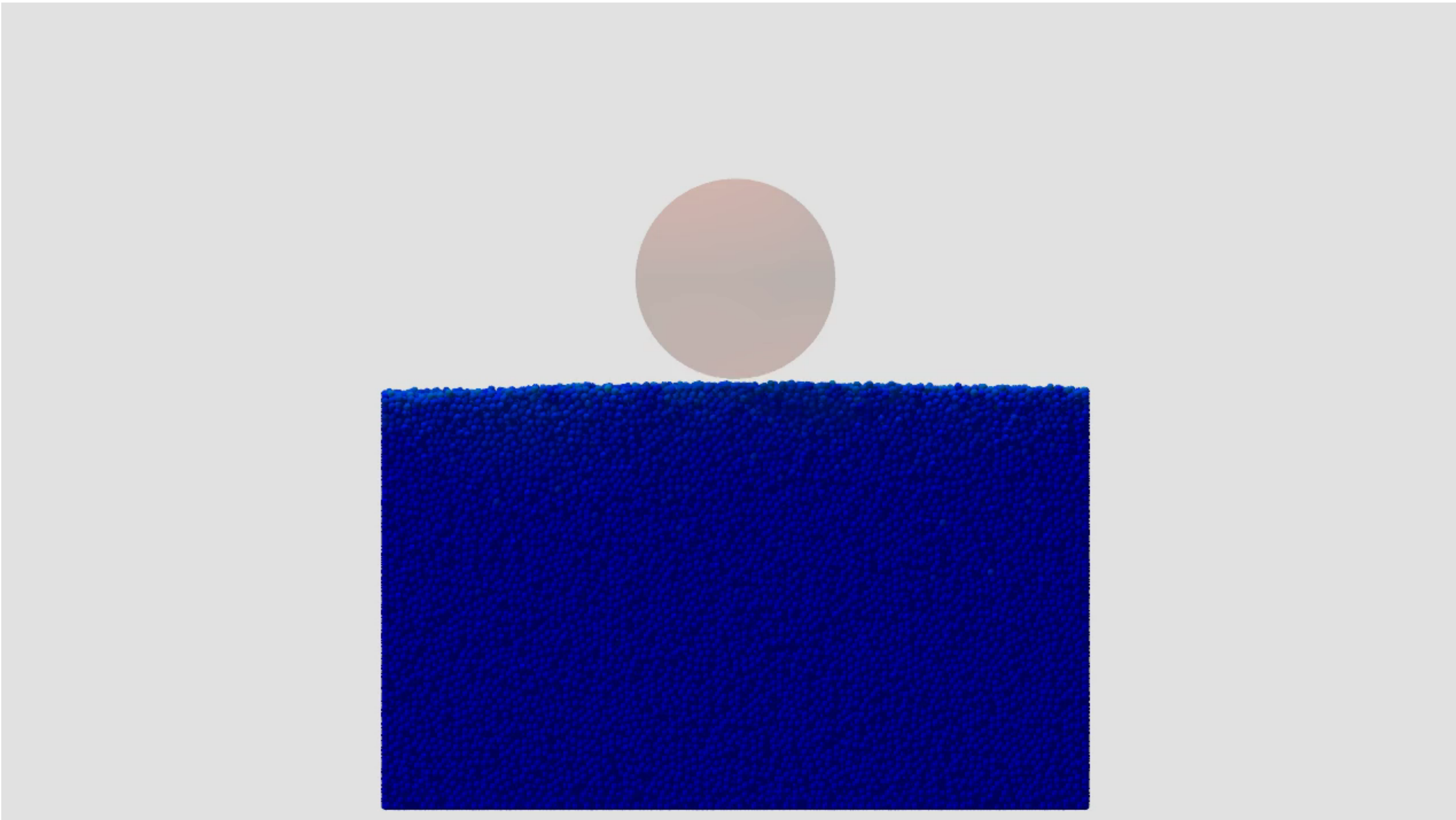


Experimental Validation: Impact into Granular Material

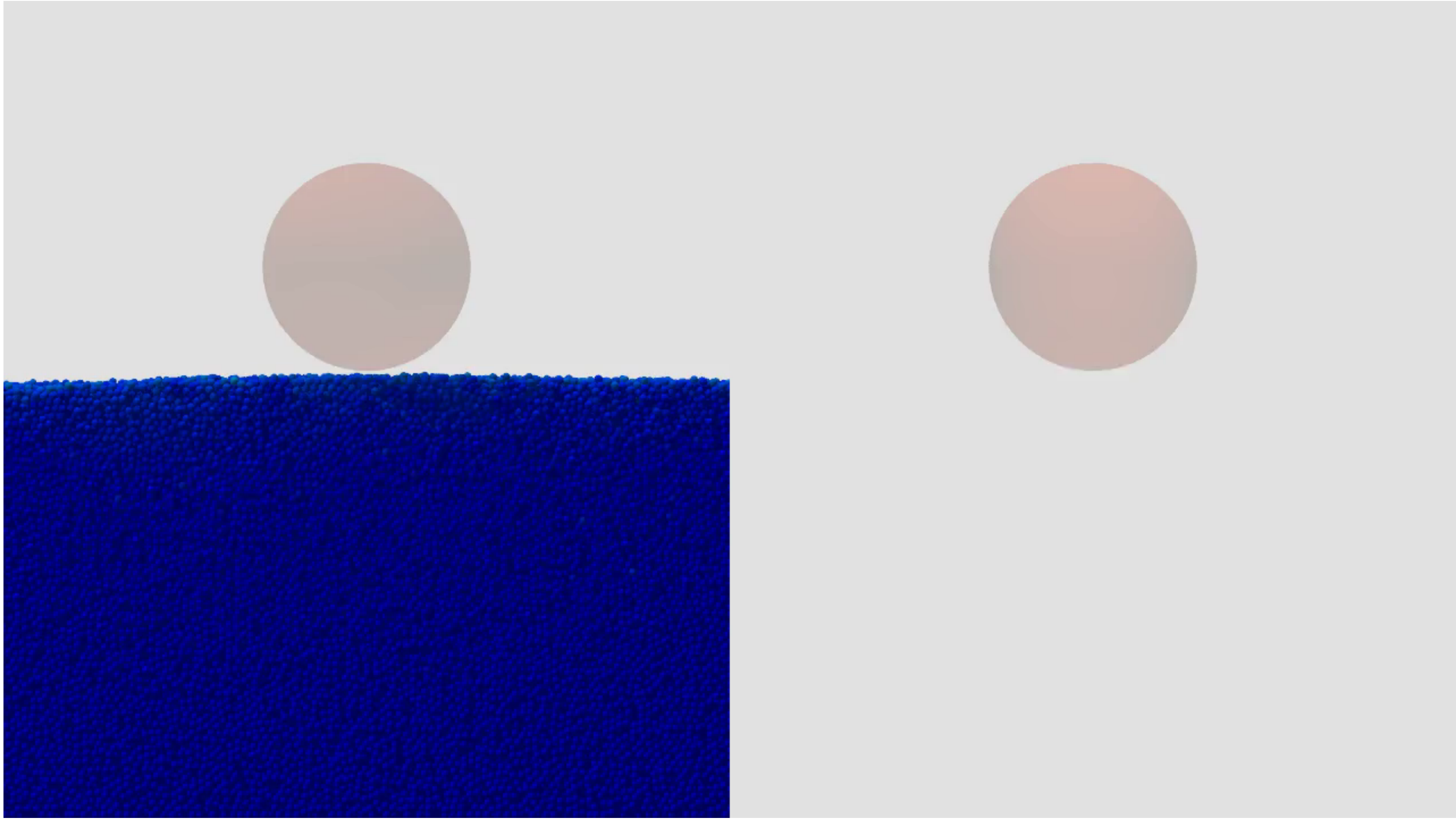
- Experiment:
  - Carried out by Durian Research Group (Physics, U Penn)
  - Measured penetration of spherical projectiles into loose non-cohesive granular media
  - Parameters: ρ_b, D_b, h, ρ_g, μ
- Simulations:
  - Used DVI formulation, APGD solver
  - 500,400 granular particles of 1 mm diameter
  - ρ_g =1.51 g/cm3, D_b=2.54 cm, μ=0.3
  - h={5,10,20} cm, ρ_b={0.28,0.7,2.2} g/cm_3



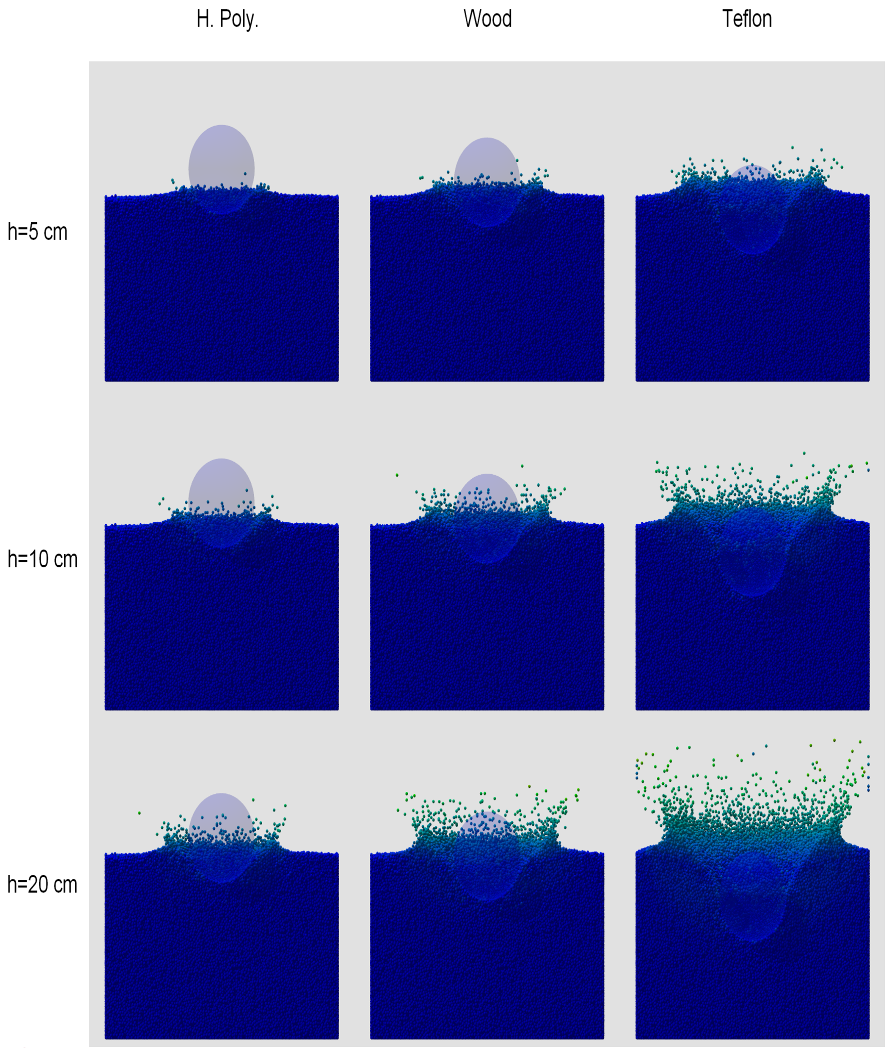
Experimental validation: splatter h=10 cm, ρ_b=2.2 g/cm^3

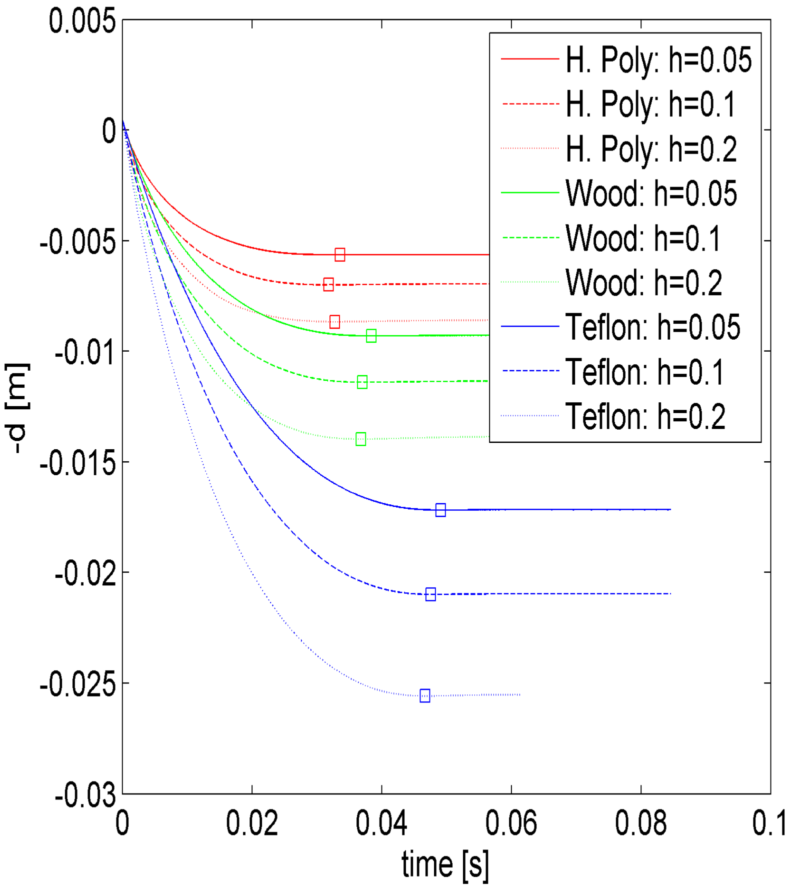


Splatter with Force Depiction. Upscaling this looks scary

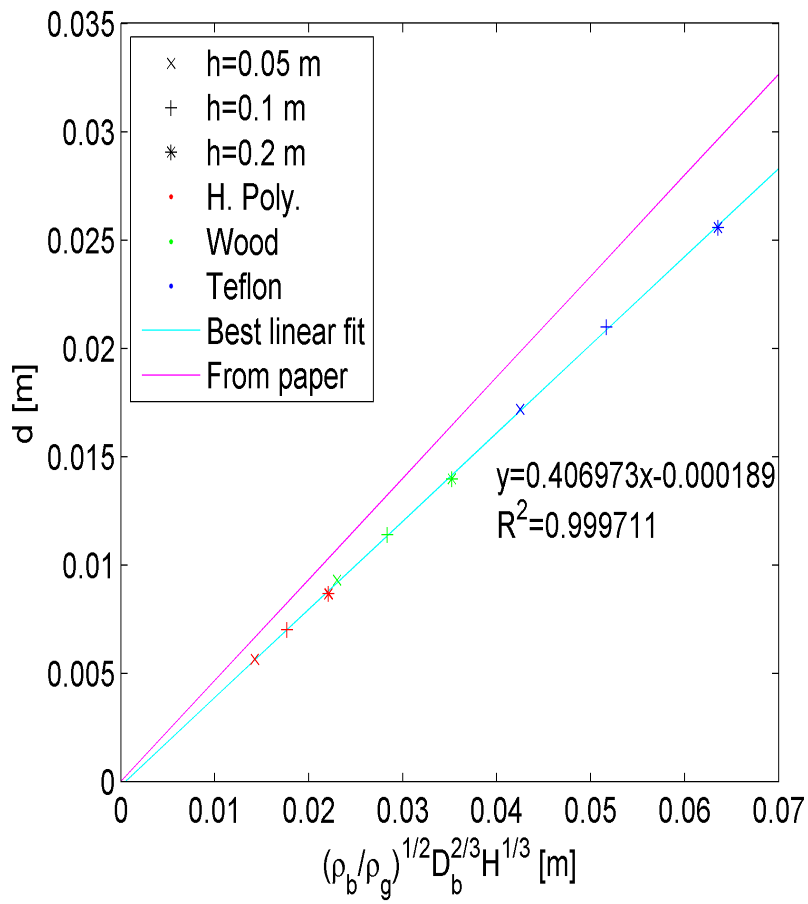


Deepest Penetration





Penetration and Scaling



Experimental Scaling:

$$d = \frac{0.14}{\mu}\left(\frac{\rho_b}{\rho_g}\right)^{1/2} D_b^{2/3} H^{1/3}$$

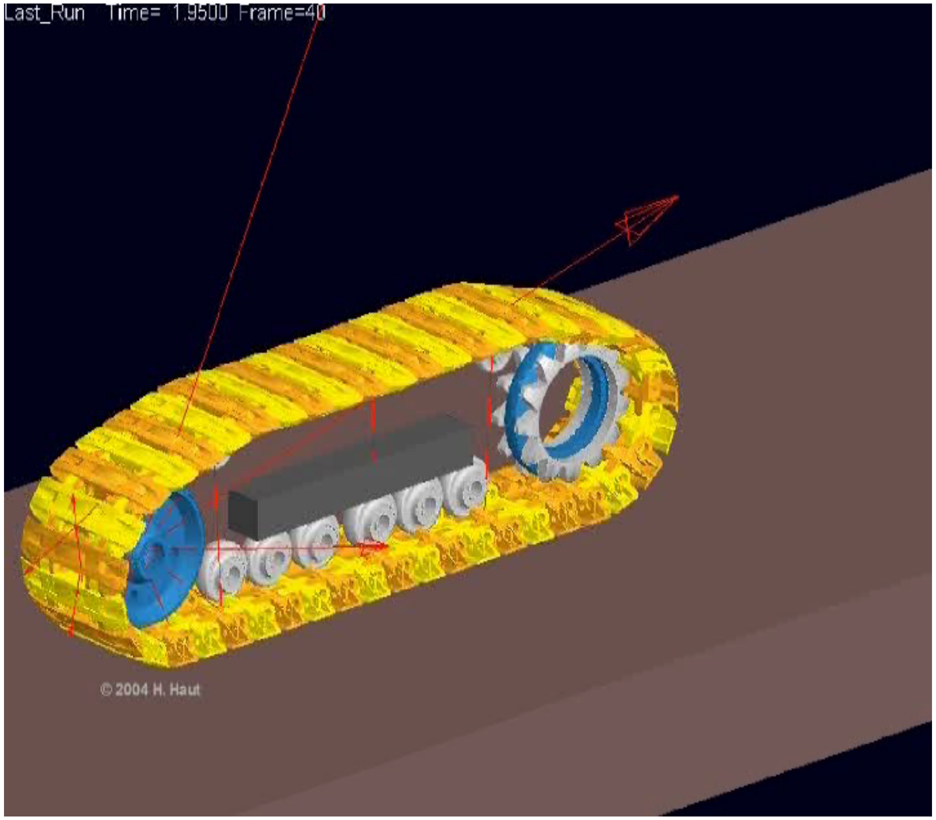
Simulation Scaling:

$$d = \frac{0.1221}{\mu}\left(\frac{\rho_b}{\rho_g}\right)^{1/2} D_b^{2/3} H^{1/3}$$

13.7% Difference

5. OTHER REAL AND FUN APPS

Tires/tracks



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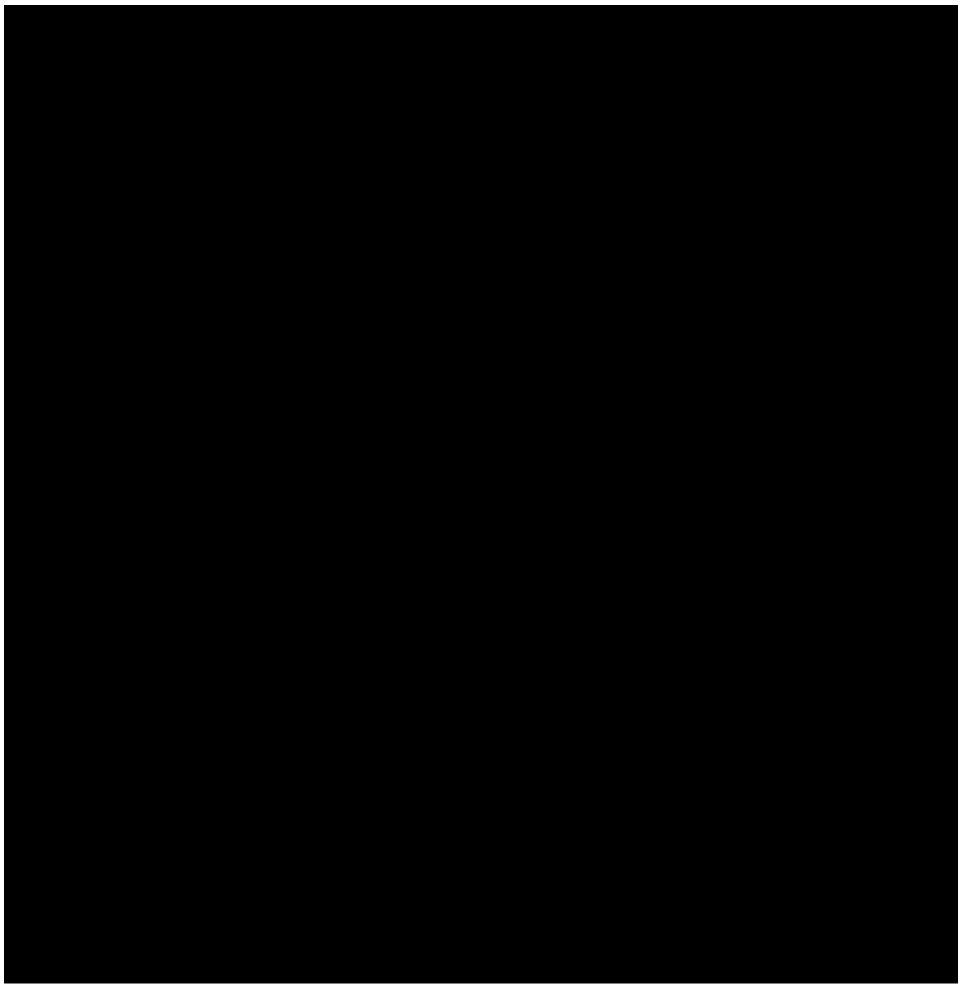
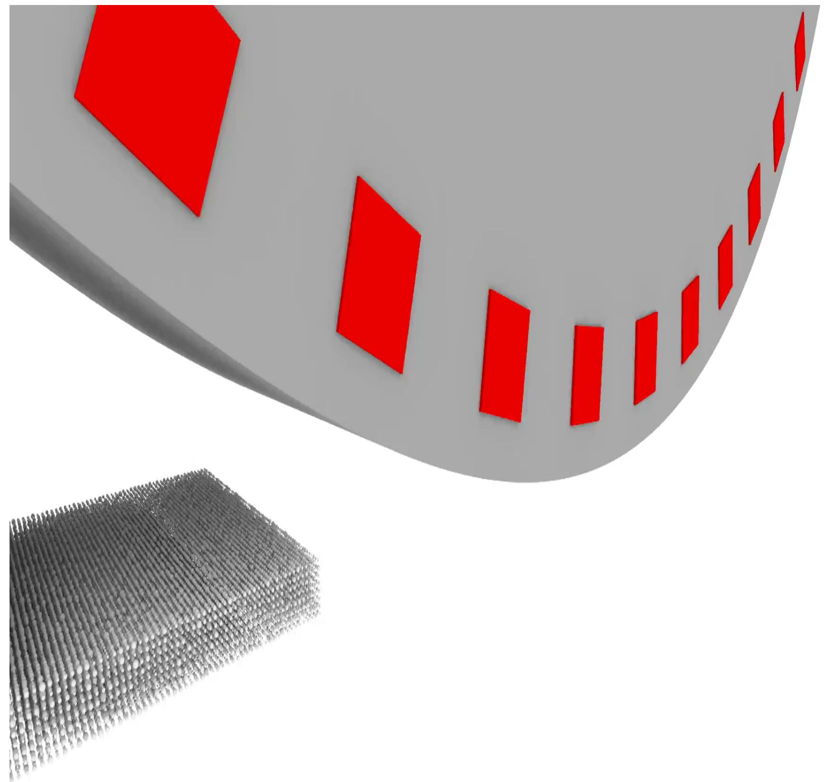
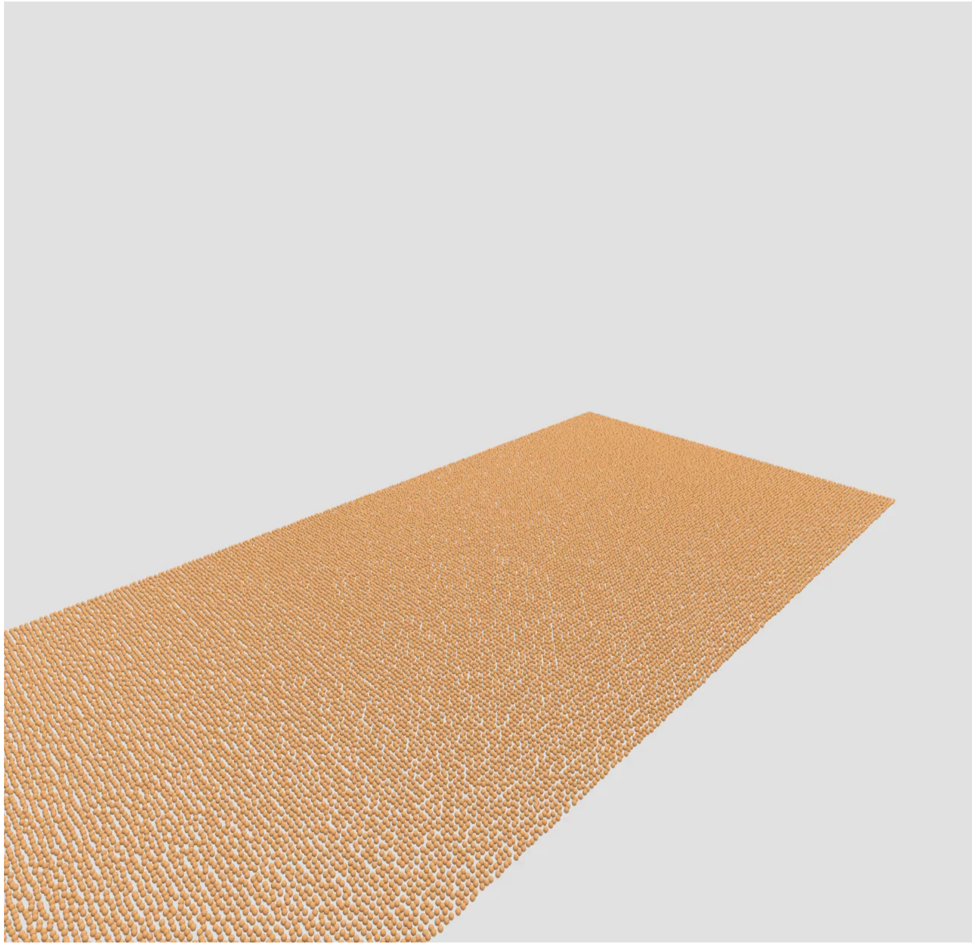
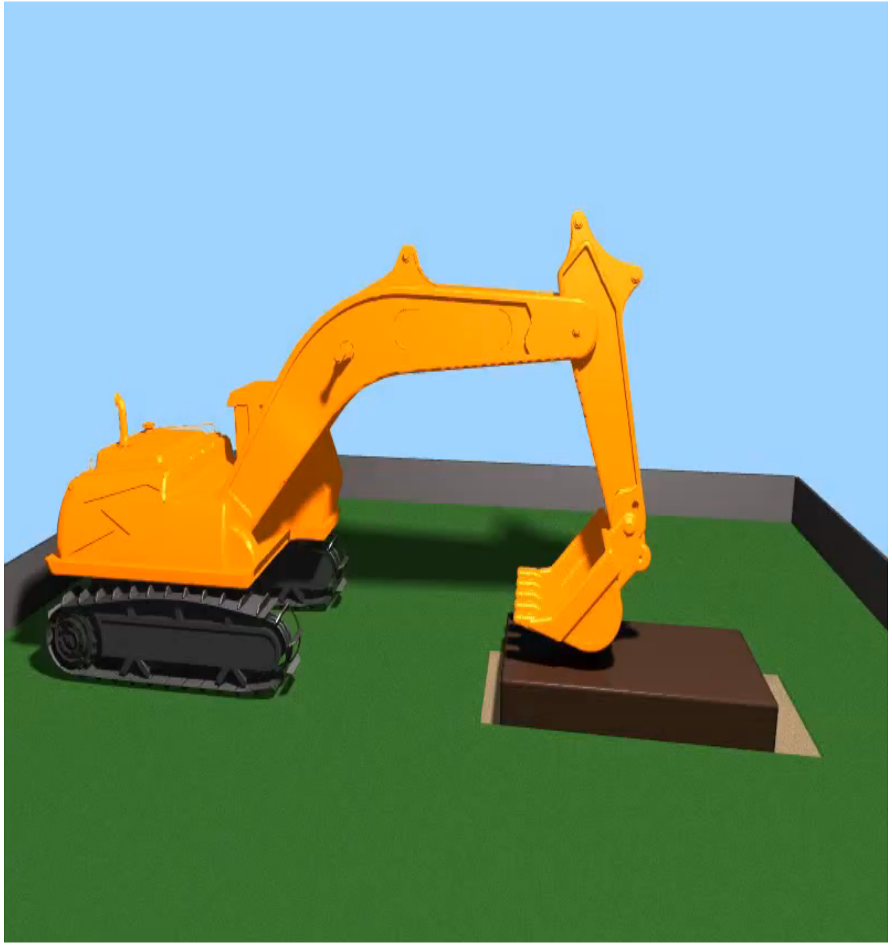
Powder/Material Processing



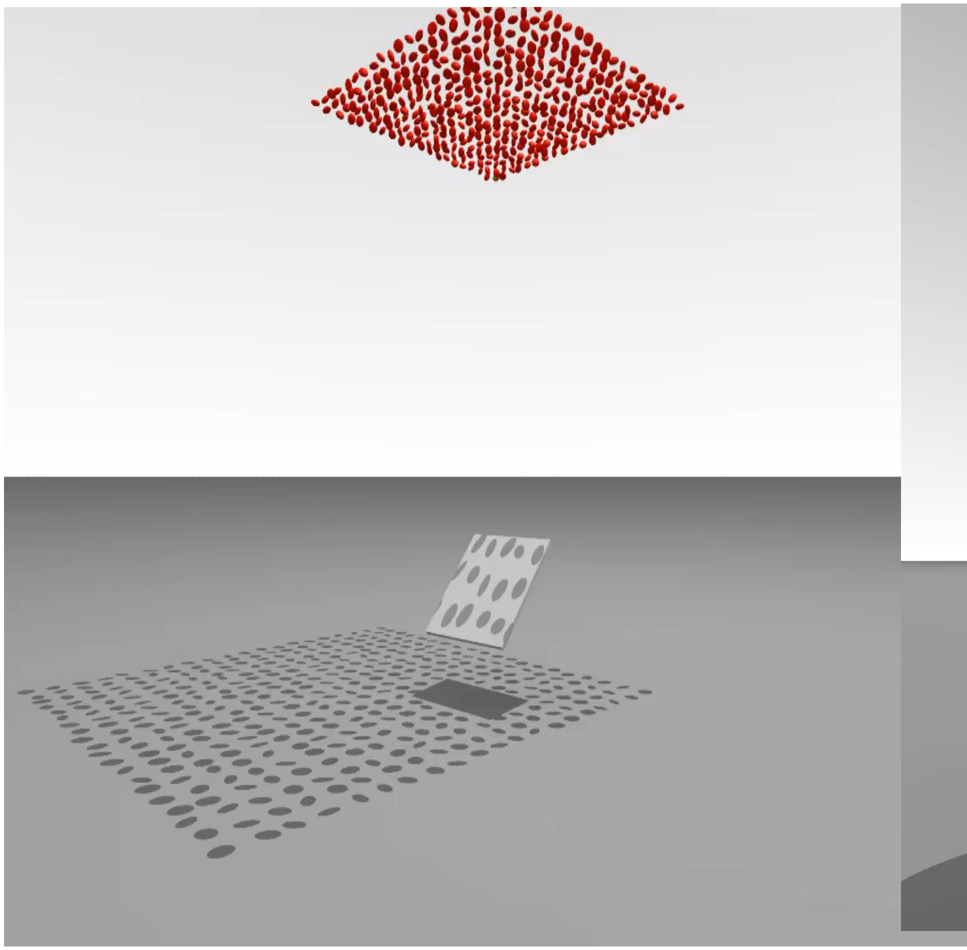


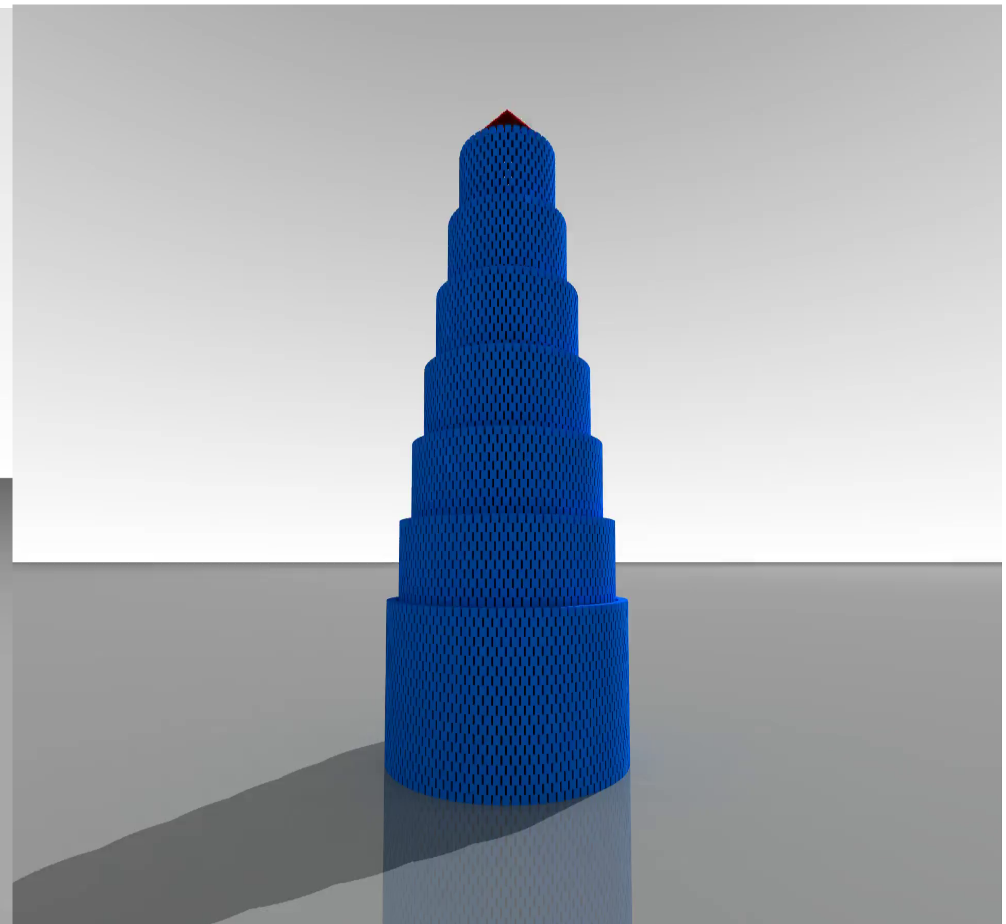
Vehicles





Fun





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Summary

- Specific Contributions
  - Developed new numerical methods for the DVI formulation which demonstrate improved convergence
    - Developed Gradient-Projected Minimum Residual (GPMINRES) method for frictionless problems
    - Developed Accelerated Projected Gradient Descent (APGD) method for frictional problems
    - Implemented APGD to run in parallel with OpenMP or GPU programming
    - Demonstrated potential of Interior Point methods for future work
  - APGD works unexpectedly well.
- Validation:
  - Validated APGD against analytical solutions for simple scenarios
  - Validated APGD against experimental data for two complex scenarios
- Reference: Toby Heyn, Mihai Anitescu, Alessandro Tasora3, Dan Negrut . “Using Krylov Subspace and Spectral Methods for Solving Complementarity Problems in Many-Body Contact Dynamics Simulation", *International Journal for Numerical Methods in Engineering*, Volume 95, Issue 7, pages 541–561, 17 August 2013.