Complementarity Models for Rolling and Plasticity

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1. DVI MODELS, STATE OF RESEARCH

Nonsmooth contact dynamics—what is it?

- Differential problem with variational inequality constraints – DVI

Newton Equations

Non-Penetration Constraints

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

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

Generalized Velocities

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

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

Friction Model

- Truly, a Differential Problem with Equilibrium Constraint

Granular materials: abstraction: DVI

- Differential variational inequalities Mixture of differential equations and variational inequalities.

$$\begin{array}{rcl} y' & = & f(t, y(t), x(t)) \\ x(t) & \in & SOL(K; F(t, y(t), \cdot)) \\ y(0) & = & y_0 \end{array}$$

$$x \in SOL(K; F(t, y, \cdot) \Leftrightarrow (\tilde{x} - x)^T F(t, y, x) \geq 0, \forall \tilde{x} \in K$$

- Target Methodology (only hope for stability): time-stepping schemes.

$$\begin{array}{rcl} y^{h,(i+1)} & = & y^{h,i} + h\tilde{f}\left(\tilde{t}^{h,(i+1)}, \theta_1 y^{h,i} + (1-\theta_1) y^{h,(i+1)}, x^{h,(i+1)}\right) \\ x^{h,(i+1)} & \in & SOL(K; \tilde{F}(\tilde{t}^{h,(i+1)}, \theta_2 y^{h,i} + (1-\theta_2) y^{h,(i+1)}, \cdot)) \\ y(0) & = & y_0. \end{array}$$

Smoothing/regularization/DEM

- Recall, DVI (for C=R+)

$$\dot{x} = f\left(t, x(t), u(t)\right);$$
$$u \geq 0 \perp F\left(t, x(t), u(t)\right) \geq 0$$

- Smoothing

$$\dot{x} = f\left(t, x(t), u(t)\right);$$
$$u_i \; F_i\left(t, x(t), u(t)\right) = \varepsilon, \quad i = 1, 2, \ldots n_u$$

- Followed by forward Euler. Easy to implement!!

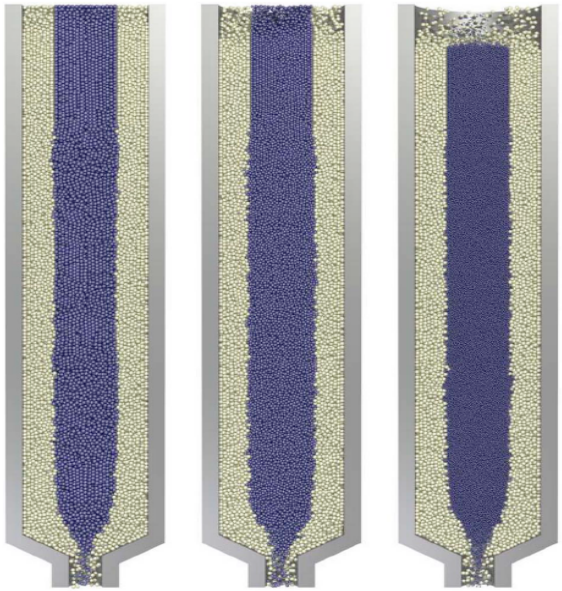
$$u_i^n \; F_i\left(t^{n-1}, x^{n-1}, u^{n-1}\right) = \varepsilon, \quad i = 1, 2, \ldots n_u$$
$$x^{n+1} = x^n + hf\left(t^n, x^n, u^n\right);$$

- Compare with the complexity of time-stepping
- Which is faster?

$$x^{n+1} = x^n + hf\left(t^{n+1}, x^{n+1}, u^{n+1}\right);$$
$$u^{n+1} \geq 0 \perp F\left(t^{n+1}, x^{n+1}, u^{n+1}\right) \geq 0$$

Simulating the PBR nuclear reactor

- Generation IV nuclear reactor with continuously moving fuel.
- Previous attempts: DEM methods on supercomputers at Sandia Labs regularization)
- 40 seconds of simulation for 440,000 pebbles needs 1 week on 64 processors dedicated cluster (Rycroft et al.)

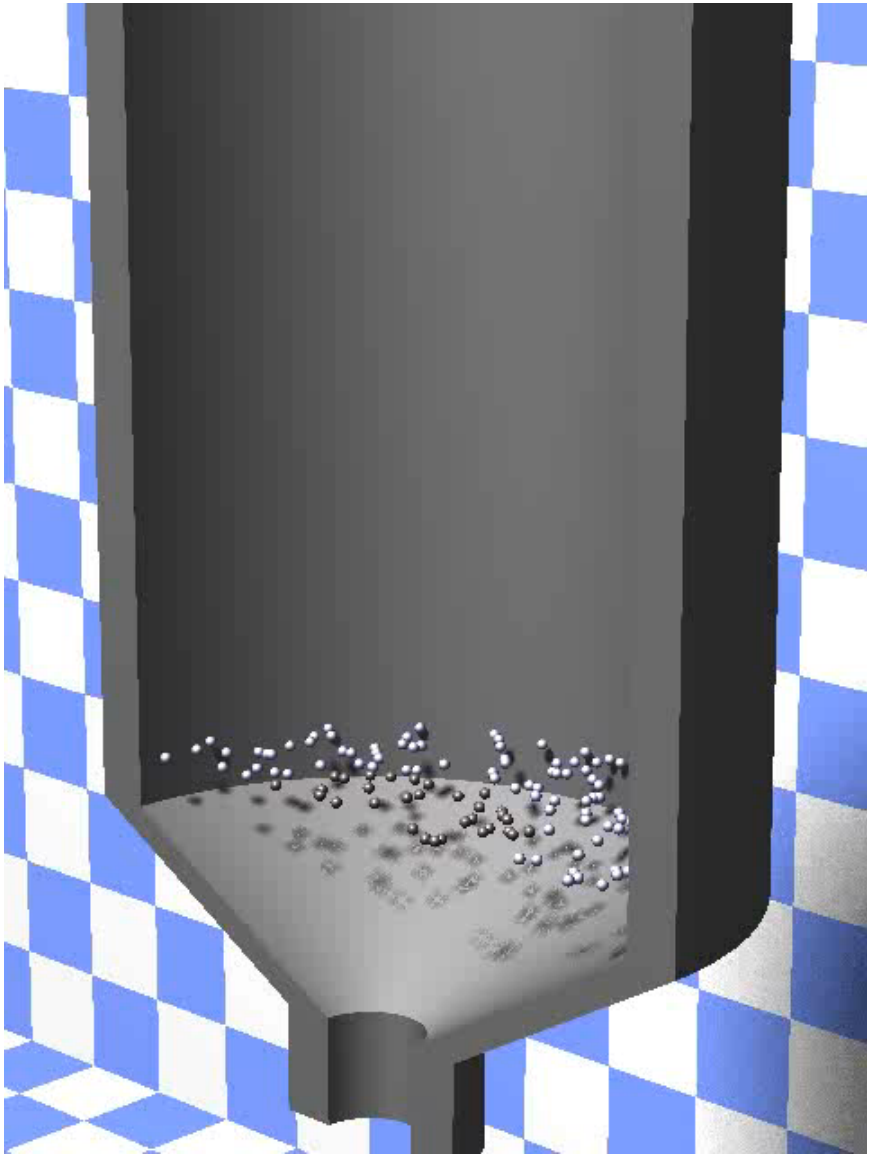


model a frictionless wall, $\mu_w = 0.0$. For the current simulations we set $k_t = \frac{2}{7} k_n$ and choose $k_n = 2 \times 10^5\ gm/d$. While this is significantly less than would be realistic for graphite pebbles, where we expect $k_n > 10^{10}\ gm/d$, such a spring constant would be prohibitively computationally expensive, as the time step scales as $\delta t \propto k_n^{-1/2}$ for collisions to be modeled effectively. Previous simulations have shown that

Simulations with DEM. Bazant et al. (MIT and Sandia laboratories).

Simulating the PBR nuclear reactor

- 160’000 Uranium-Graphite spheres, 600’000 contacts on average
- Two millions of primal variables, six millions of dual variables
- *1 CPU day on a single processor…*
- We estimate 3CPU days, compare with 150 CPU days for DEM !!!



An iterative method

- Convexification opens the path to high performance computing.
- How to efficiently solve the Cone Complementarity Problem for large-scale systems?

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

- Our method: use a fixed-point iteration (Gauss-Seidel-Jacobi)

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

- with matrices:
- ..and a non-extensive separable projection operator onto feasible set

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

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

$K^T =$

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

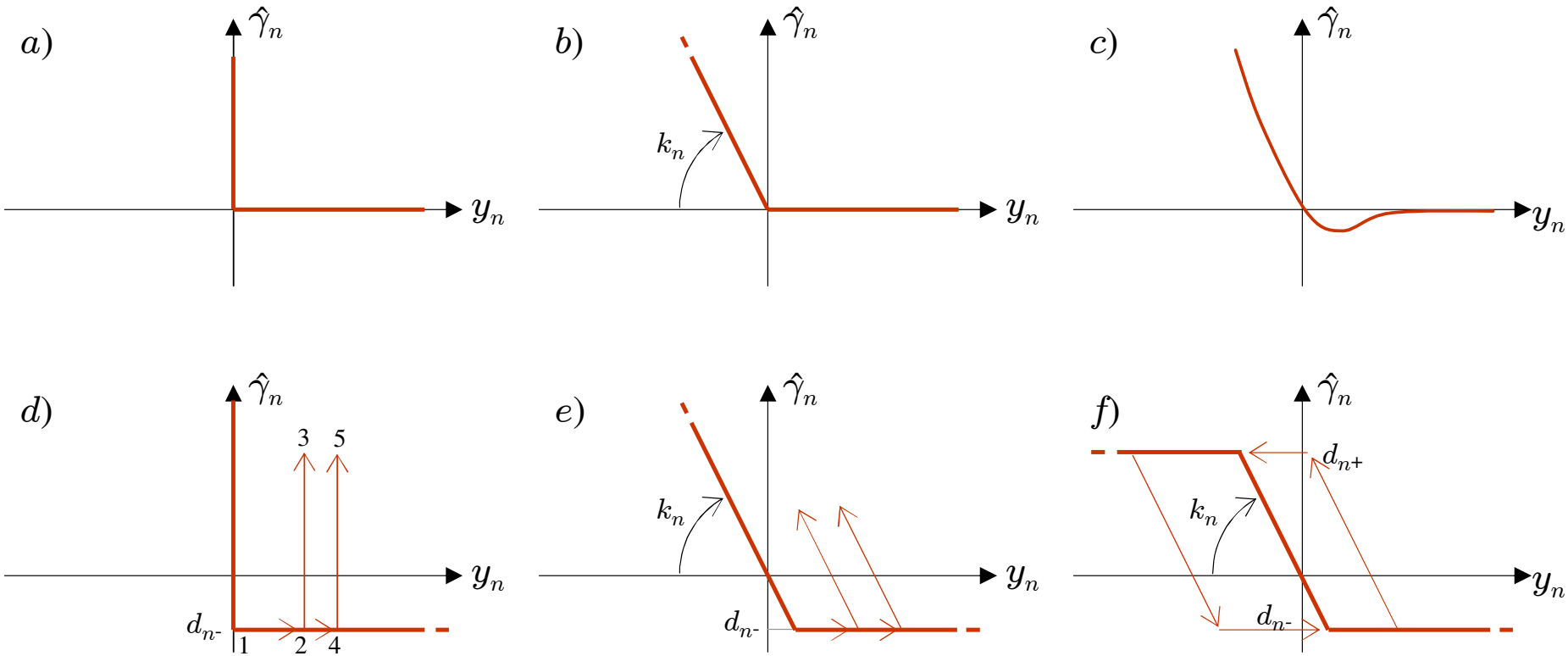
2. Plasticity Models

Need for plasticity models

- This is a very important effect in materials.
- It is also true for granular materials where it is about phenomena of cohesion, friction, compliance and plasticization.
- Think of the effect of water bridges and cohesion in powders such as appear in medication.

Type of plasticity models in 1D.

- Plasticity elicits a different constitutive law compared to rigid contact



- Force-displacement relationship at a contact a) Rigid b) Compliant c) Nonlinear d) cohesion e) Cohesion + Compliance f) Cohesion + Compliance + plastic

The yield surface.

- Standard rigid contact 1-a can be turned to cohesive one by the transformation:

$$\hat{\gamma}_n \geq 0 \quad \Rightarrow \hat{\gamma}_n \in \left[d_n, \infty \right] = \Upsilon$$

- In addition, rule in 1-d satisfies (at contact):

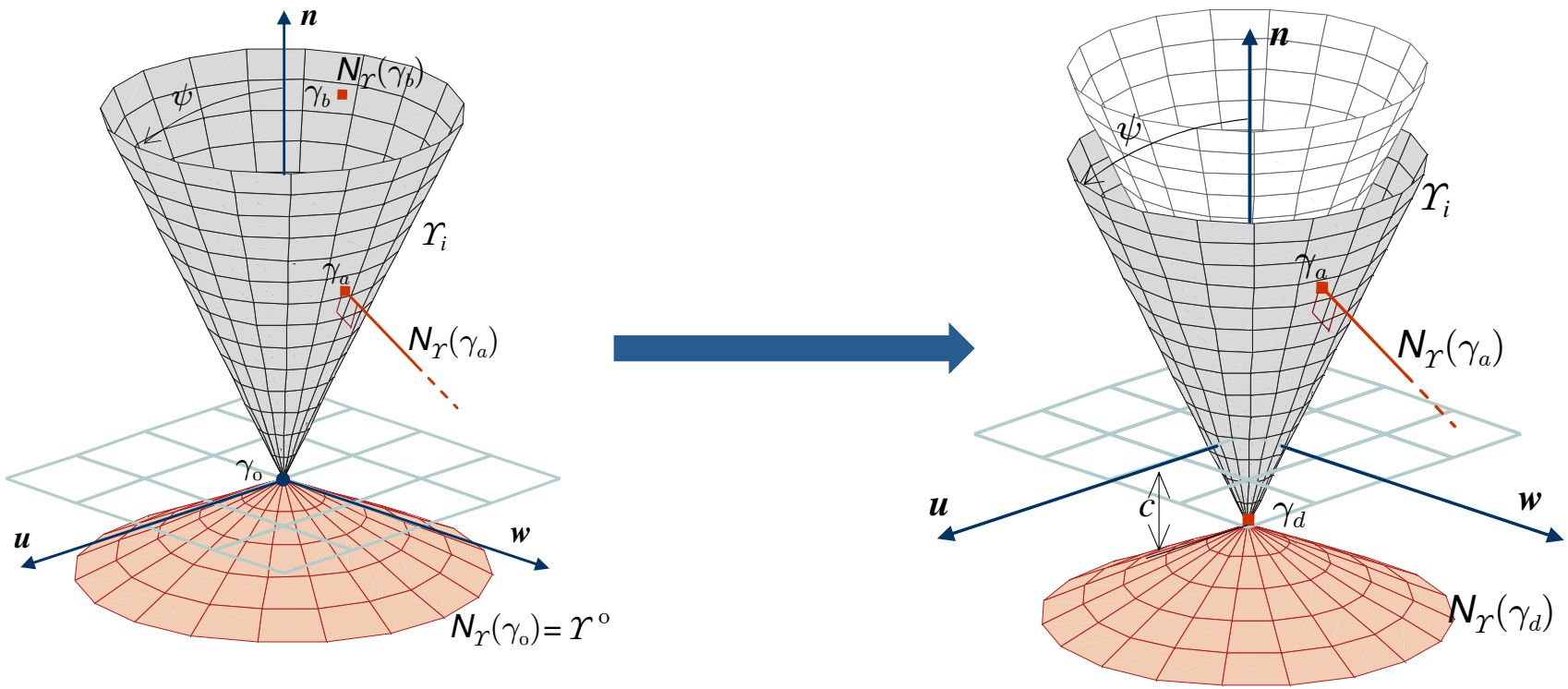
$$\Delta y_n \in -\mathcal{N}_{\Upsilon}\left(\hat{\gamma}_n \right)$$

- In this context Υ is called the yield surface.

- The displacement is normal at the Yield surface, such constitutive rules are called associative.

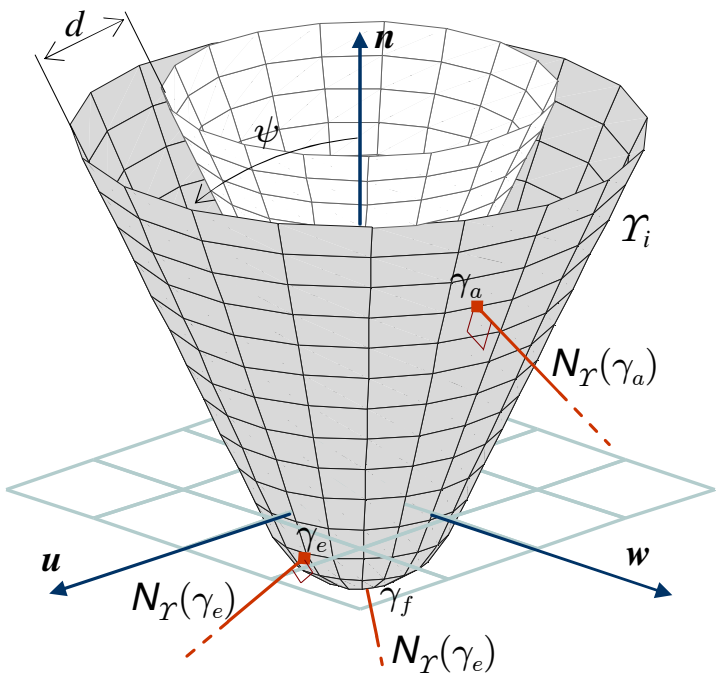
Example: Friction and Cohesion in 3D by playing around with Yield surfaces

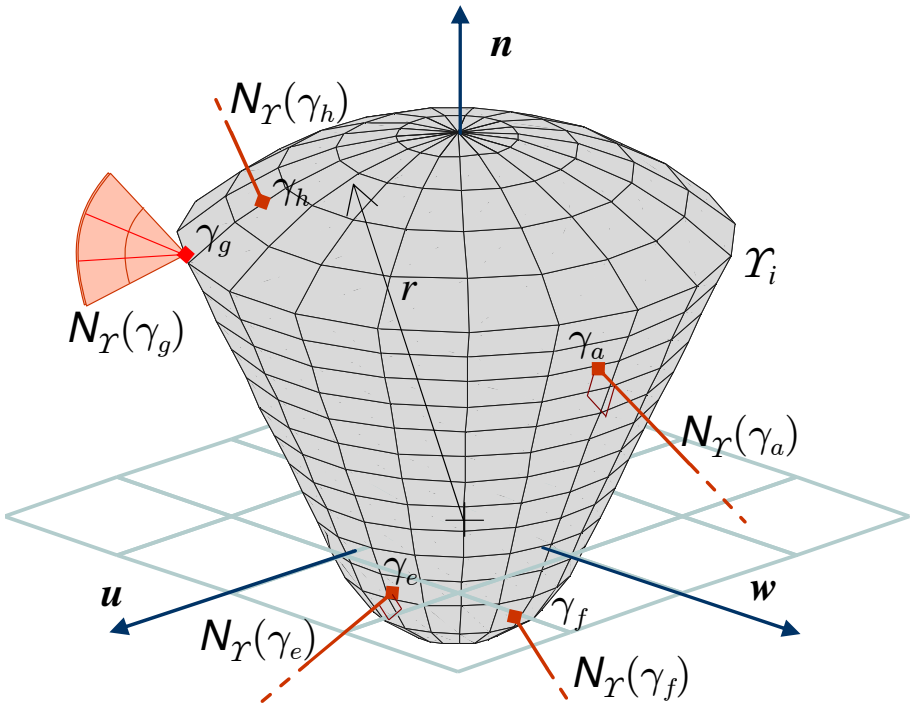
- Shift the Coulomb cone downward and make it an associative yield surface.



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.

Time-stepping

- After some notation

$$\dot{\mathbf{y}}_P^i = D^{i^T}\mathbf{v}^{l+1} + \left(h^2 K^i\right)^{-1}\gamma_{\mathcal{A}}^{i,l+1} - \frac{1}{h}\left(\mathbf{y}^{i,l} - \mathbf{y}_P^{i,l}\right) \quad \in -\mathcal{N}_{\Upsilon^i}(\gamma_{\mathcal{A}}^i)$$

- After this is solved, all we have to do is to solve the plasticity displacement

$$\mathbf{y}_P^{i,l+1} = \mathbf{y}_P^{i,l} + h\dot{\mathbf{y}}_P^i$$

- Use the velocity update

$$\mathbf{v}^{l+1} = \mathbf{v}^l + M^{-1}\sum_{i\in\mathcal{G}_{\mathcal{A}}} D^i\gamma_{\mathcal{A}}^{i,l+1} + hM^{-1}\mathbf{f}(\mathbf{q},\mathbf{v},t)$$

- Replace in the plasticity velocity equation; to obtain the variational inequality

$$\dot{\mathbf{y}}_P = D_{\mathcal{E}}{}^T M D_{\mathcal{E}}\gamma_{\mathcal{E}}^{l+1} + D_{\mathcal{E}}{}^T\left(\mathbf{v}^l + hM^{-1}\mathbf{f}(\mathbf{q},\mathbf{v},t)\right) - E_{\mathcal{E}}\gamma_{\mathcal{E}}^{l+1} - \mathbf{c} \quad \in -\mathcal{N}_{\Upsilon}(\widehat{\gamma}_{\mathcal{E}})$$

- Over the cartesian product of cones: $\Upsilon = \underset{i\in\mathcal{G}_{\mathcal{A}}}{\times}\Upsilon^i$

Damping and VI

- We can similarly accommodate damping

$$\widehat{\gamma}_{\mathcal{A}}^{i} = -K^{i}\left(\mathbf{y}^{i} - \mathbf{y}_{P}^{i}\right) - R^{i}\left(\dot{\mathbf{y}}^{i} - \dot{\mathbf{y}}_{P}^{i}\right)$$
$$\dot{\mathbf{y}}_{P}^{i} \in -\mathcal{N}_{\widehat{\Upsilon}^{i}}(\widehat{\gamma}_{\mathcal{A}}^{i}) \quad ; \quad \widehat{\gamma}_{\mathcal{A}}^{i} \in \widehat{\Upsilon}^{i}$$

- And obtain the VI

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

- Where

$$N \equiv \left[D_{\mathcal{E}}{}^{T} M D_{\mathcal{E}} - E_{\mathcal{E}}\right]$$
$$\mathbf{r} \equiv D_{\mathcal{E}}{}^{T}\left(\mathbf{v}^{l} + hM^{-1}\mathbf{f}(\mathbf{q},\mathbf{v},t)\right) - \mathbf{c}$$

- And

$$E_{\mathcal{E}} = diag\left[E_i\right]; \quad E_i = -\left(h^2 K_i + hR_i\right) \prec 0$$

$$\mathbf{c}^{i} = \left(h^{2}K^{i} + hR^{i}\right)^{-1}\left(\gamma_{\mathcal{A}}^{i,l} + hR^{i}(\dot{\mathbf{y}}^{l} - \dot{\mathbf{y}}_{P}^{l})\right)$$

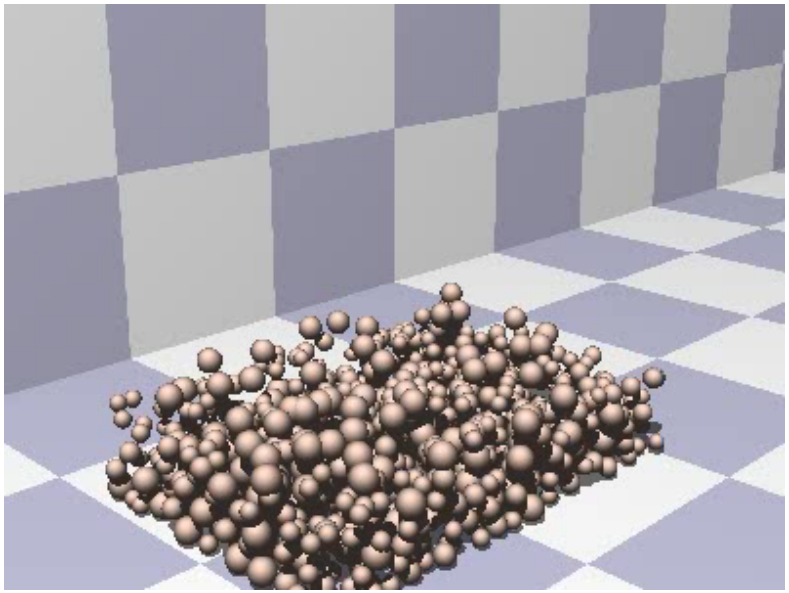
- Once we compute new contact impulse, we compute velocity, and update position, and iterate.

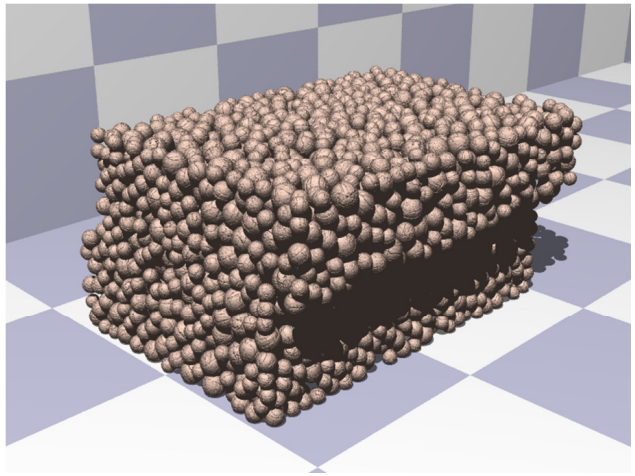
How do we solve it:

- There is no need to change the PGS algorithm as the matrix N is still symmetric positive definite.
- Only the projection over more complex sets needs to be implemented, but the problem and the algorithm have the same abstraction; that is.
- We are expending the proof to the general case of convex sets, we do not expect problems.

Numerical Experiments

- Compaction and shear test of a granular media.
- Advanced cases of earth-moving machines (bulldozzers, vehicles) need such things to understand soil reaction.
- Configuration: soil sample put in 0.1m x 0.1 mx0.2 m,
- Top part is pulled by a “drawer” after a mass is dropped on top; shear force is measured and compared with experiment.



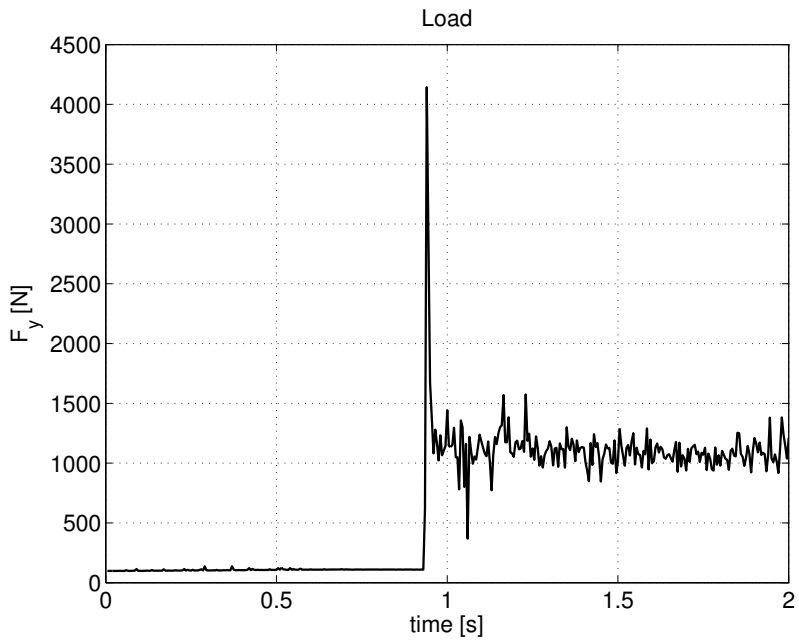


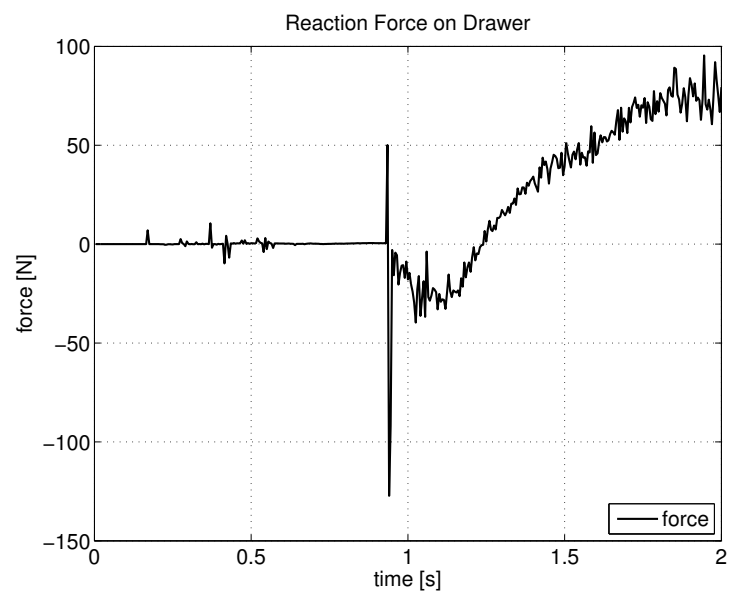
Results.

- Configuration: Getting parameters is hard; Normal and tangentia compliances are 0:910e-7 m/N and damping coefficient is = 0.1. Sphere distribution.

Number	Density	Diameter	Friction
90	1700 kg/m^3	0.020 m	0.5
630	1700 kg/m^3	0.010 m	0.5

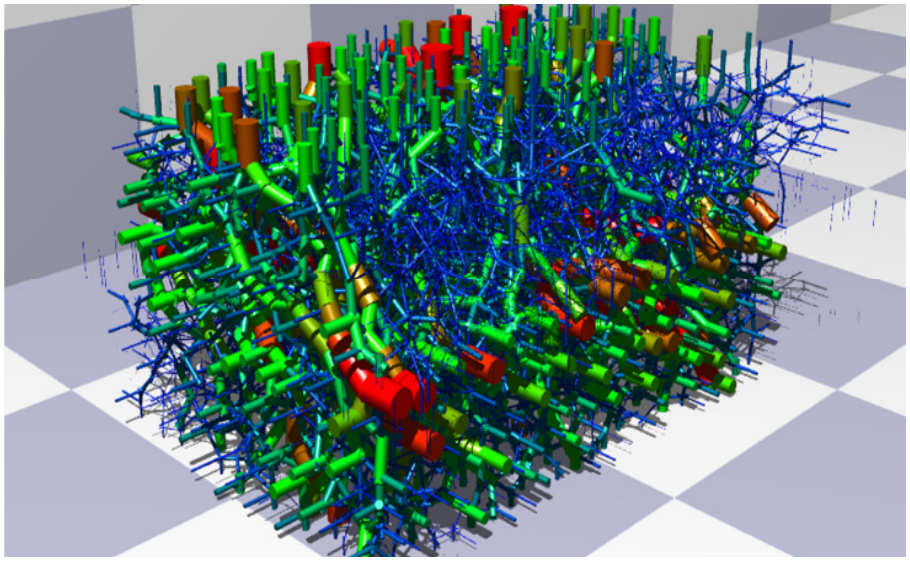
- Evolution of the shear force and vertical force. These will be measured from experiments. Note spike in forces – including shear! When load is dropped (probably some lock-in before it relaxes and pushes on the drawe)

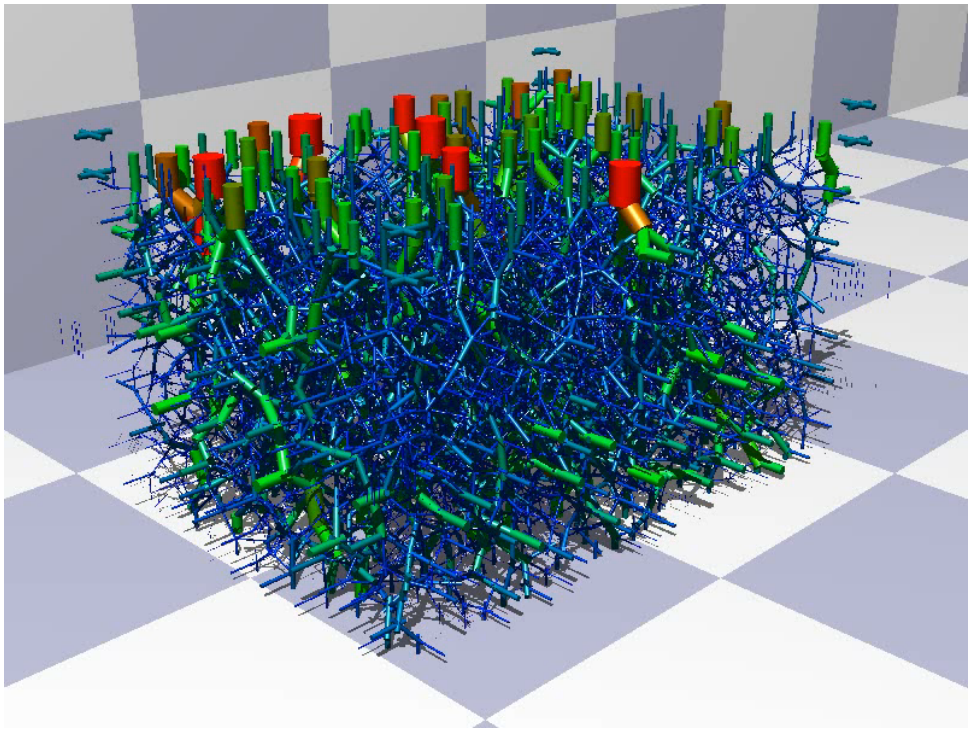




The advantage of a simulator is that we can have a deeper understanding of the forces.

- Evolution of the contact network. Note the “rolling” behavior.
- Calibration and experiments are in progress.





Nonassociative plasticity

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

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

- H is positive definite and symmetric, but N is only symmetric.
- Do we have existence?

Existence for non-associative plasticity

- Consider the eigendecomposition of H $H = Q^T D Q$
- We then have that the nonassociative plasticity problem is equivalent to: the following problem over a rotated cone:

$$\eta_\varepsilon \in Q\Upsilon,\ D\left(\widetilde{N}\eta_\varepsilon + \widetilde{\mathbf{r}}\right) \in -\mathcal{N}_{Q\Upsilon}(\eta_\varepsilon).$$

Definition 2. *We say that a matrix $T \in \mathbb{R}^{n\times n}$ has the R_0 property with respect to the cone $\mathcal{K}$ if and only if*

$$u \in \mathcal{K}, Tu \in \mathcal{K}^*, \max_{i=1,2,\ldots,n} u_i(Tu)_i \leq 0 \Rightarrow u = 0$$

Proposition 1. *Assume N is symmetric positive semidefinite. Then,*

(i) The matrix $D\tilde{N}$ has the P_0 property.

(ii) If the matrix N satisfies $\gamma^T N\gamma > 0$ for every $0 \neq \gamma \in \Upsilon$, then $D\widetilde{N}$ has the R_0 property with respect to the cone $Q\Upsilon$.

Existence result

- We use results from Kong, Tuncel and Xiu to obtain:

Theorem 1. *Assume that the CCP problem (43) has a problem with symmetric semidefinite N and does not result in nontrivial internal forces, that is,*

$$\gamma \in \Upsilon, N\gamma = 0 \Rightarrow \gamma = 0.$$

Then the skewed complementarity problem modeling non-associative plastic flow (52) has a nonempty and bounded solution set.

- In addition, we can solve the problem by continuation:

$$D\widetilde{N}\eta + \widetilde{r}(1-\alpha) + \alpha\widetilde{r}_0 + \alpha\nabla I_{Q\Upsilon}(\eta) = 0$$

- P_0 guarantees the path exists; R_0 that it accumulates to a solution.
- What to do about stationary iterations: unclear

To do

- Lots and lots of things.
- Extend the nonassociative plasticity to general compact convex sets
- Extend projected iteration to the general convex sets and nonassociative plasticity
- Simulations for cohesion and plasticity.
- Do physical experiments to compare; choose the right parameters.