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Examining the smooth and nonsmooth DEM approaches to granular matter

M. Servin, C. Lacoursière, D. Wang, K. Bodin

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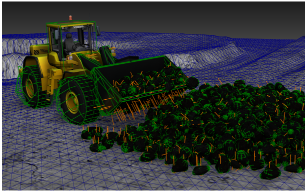
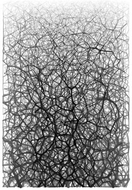
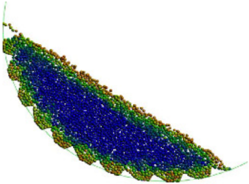
When choose *smooth* or *nonsmooth* DEM?

Motivation

- DEM important tool in R&D involving granular matter
- Major challenge: reduce computing time

Example: Machine and 1K rigid bodies in realtime

Example: 80K spheres in 1:100 of realtime

Theory

- Smooth DEM (DEM)
- Nonsmooth DEM (NDEM)
- Computational scaling

Discrete Element Method (DEM)

Rigid rotational particles
Hertz spring-and-dashpot

$$f_n^i = k_n \left[g_i^{3/2} + c g_i^{1/2} \dot{g}^i \right] n^i$$

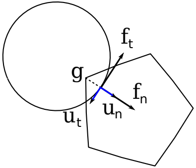
$$f_t^i = \mathrm{proj}_{\mu |f_n|} \left(f_t^{i-1} - h k_t u_t^i \right)$$

Integration of *smooth* ODEs

$$(x^i, v^i) \rightarrow (x^{i+1}, v^{i+1})$$

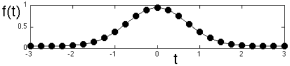
time-step

$$h \lesssim \sqrt{m/k}$$



Hertz

Cundall & Strack (1979)



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Nonsmooth Discrete Element Method (NDEM)

References: Moreau (1988), Jean (1999), Radjai (2009)

- Large time-step → impact, stick-slip → nonsmooth dynamics
- Constraints and complementarity conditions $g \geqslant 0$
- Auxiliary variable λ (impulse/multiplier) $f \rightarrow f + G^T\lambda$
- Dynamics constrained by the Signorini-Coulumb law

$$(x^i, v^i) \rightarrow \begin{cases} (x^{i+1}, v^{i+1}, \lambda^{i+1}) \\ \text{law}_{SC}[v^{i+1}, \lambda^{i+1}] = \text{true} \end{cases}$$

$$\mathbf{f}_n \geqslant 0, \quad \mathbf{u}_n \geqslant 0, \quad \mathbf{f}_n \cdot \mathbf{u}_n = 0$$

$$\mu|\mathbf{f}_n| \geqslant |\mathbf{f}_t|, \quad |\mathbf{u}_t|(\mu|\mathbf{f}_n| - |\mathbf{f}_t|), \quad \mathbf{f}_t^T \mathbf{u}_t = -|\mathbf{f}_t||\mathbf{u}_t|$$

Several alternatives to solve for (v^{i+1}, λ^{i+1})

- Blocked nonsmooth projected Gauss-Seidel
- Direct, iterative and hybrid split-solvers for *mixed linear complementarity problem* (MLCP)

$$Hz + b = w_+ - w_-$$
$$0 \leqslant z - l \perp w_+ \geqslant 0$$
$$0 \leqslant u - z \perp w_- \geqslant 0$$

$$H = \begin{bmatrix} M & -\bar{G}_t^T & -\bar{G}_n^T \\ \bar{G}_t & \Gamma & 0 \\ \bar{G}_n & 0 & \Sigma \end{bmatrix}, \quad z = \begin{bmatrix} v^{i+1} \\ \lambda_t^{i+1} \\ \lambda_n^{i+1} \end{bmatrix}, b = \begin{bmatrix} -Mv_{free} \\ 0 \\ \frac{4}{h}\Upsilon\bar{g} - \Upsilon\bar{G}_n v_i \end{bmatrix}$$

- problem size $\dim(H) = (3N_p + 3N_c) \times (3N_p + 3N_c)$

Reference: Lacoursière (2007) - the SPOOK stepper

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Nonlinear NDEM

Nonlinear contact constraints are derived from smooth DEM for Hertz spring potentials

$$U_n = \frac{1}{2}\varepsilon_n^{-1}\bar{g}^2 \quad , \qquad \mathcal{R}_n = \frac{1}{2}\gamma_n^{-1}(\bar{G}_n v)^2$$

$$\bar{g} = g^{\alpha} \quad , \quad \bar{G}_n = \alpha g^{\alpha-1}[n, -n] \quad , \quad \alpha = 5/4$$

Regularization and stabilization terms

$$\Gamma = \frac{\gamma_t}{h} \; , \; \Sigma = \frac{4}{h^2}\frac{\varepsilon_n}{1 + 4\frac{\tau_n}{h}} \; , \; \Upsilon = \frac{1}{1 + 4\frac{\tau_n}{h}}$$

$$\varepsilon_n^{-1} = \alpha k_n \; , \; \gamma_n^{-1} = k_n c/\alpha$$

Standard NDEM limit

Standard nonsmooth DEM follows in the infinitely stiff limit

$$\alpha = 1$$

$$\varepsilon, \gamma \to 0 \ , \ \tau \to \infty \quad \Rightarrow \quad \Gamma, \Sigma, \Upsilon \to 0$$

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Standard smooth DEM limit

Smooth DEM follows in the limit of $h \to 0$ with $\varepsilon, \gamma, \tau$ fix

$$\Sigma \to \frac{\varepsilon_n}{\tau_n h}, \quad \Upsilon \to \frac{h}{4\tau_n}$$

and the MLCP simplifies to

$$Mv^{i+1} = Mv^i - \bar{G}_n^T \lambda_n - \bar{G}_t^T \lambda_t =$$

$$Mv^i - \bar{G}_n^T \left[-\tfrac{\tau h}{\varepsilon} \bar{G}_n v^{i+1} - \tfrac{\tau h}{\varepsilon \tau} \bar{g} \right] - h\,\mathrm{proj}_{\mu |f_n|}(\bar{G}_t^T \left[-\gamma^{-1} \bar{G}_t v^i \right])$$

$$= Mv^i + h \underbrace{k_n \left[g^{3/2} + c g^{1/2} \dot{g} \right] n}_{f_n} + h \underbrace{\mathrm{proj}_{\mu |f_n|} \left(-k_t v_t^i \right)}_{f_t}$$

Computational scaling: DEM versus NDEM

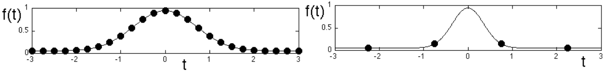
Example:

$d = 0.01$ m, $m = 10^{-3}$ kg, $k = 10^{-8}$ N/m, $v_n = 0.1$ m/s

Different time-step size for DEM and NDEM

$$h_{\mathrm{DEM}} \leqslant \sqrt{m/k} \sim 10^{-5} \text{ s}$$

$$h_{\mathrm{NDEM}} \leqslant \min\left(\frac{d}{v_n}, \sqrt{\frac{d}{g_{\mathrm{acc}}}}\right) \sim \min\left(10^{-1.5}, 10^{-2}\right) \text{ s}$$



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Computational scaling: DEM versus NDEM

For spherical particles of similar size

$$\frac{t_{\mathsf{NDEM}}}{t_{\mathsf{DEM}}} \sim \underbrace{\sqrt{\frac{\max\left(\frac{1}{2}mv_n^2, mgd\right)}{\frac{1}{2}kd^2}}}_{\text{time-step effect}} \; \underbrace{\frac{\Omega(N_p)}{N_p}}_{\text{solver scaling}}$$

Example:

$d = 0.01$ m, $m = 10^{-3}$ kg, $k = 10^8$ N/m, $v_n = 0.1$ m/s

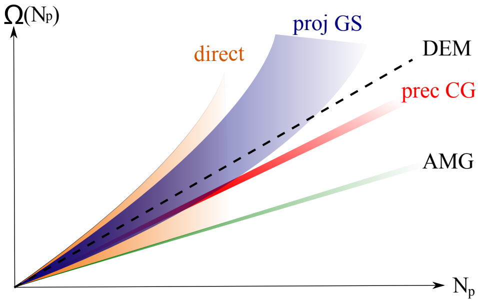
$\Omega(N_p) \sim \mathcal{O}(N_p)$

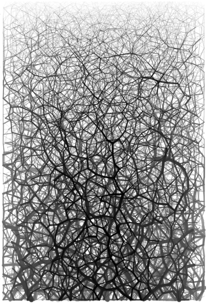
$\frac{t_{\mathsf{NDEM}}}{t_{\mathsf{DEM}}} \sim 10^{-4}$ $\Rightarrow$ NDEM 10^4 times faster!?

Computational scaling of NDEM

Theoretical limits for $\Omega(N_p)$ in solving MLCP

solver	**1D**	**2D**	**3D**
projected Guass-Seidel	$\mathcal{O}(N_p^3)$	$\mathcal{O}(N_p^{2.5})$	$\mathcal{O}(N_p^2)$
direct sparse	$\mathcal{O}(N_p)$	$\mathcal{O}(N_p^{1.5})$	$\mathcal{O}(N_p^2)$
preconditioned CG	$\mathcal{O}(N_p)$	$\mathcal{O}(N_p)$	$\mathcal{O}(N_p)$
algebraic multigrid	$\mathcal{O}(N_p)$	$\mathcal{O}(N_p)$	$\mathcal{O}(N_p)$





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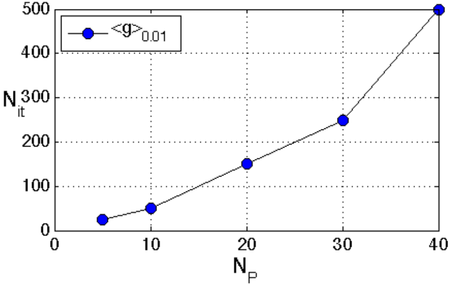
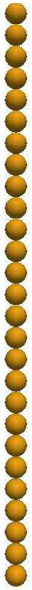
Results - 1D column

N_{it} iterations with projected GS solver

Overlap error $< g >_{0.01} = 0.01d$, $d = 0.01$ m, $h = 0.01$ s





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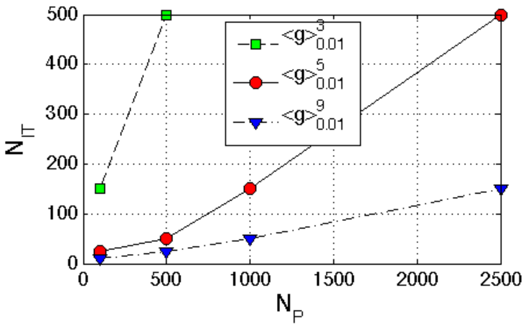
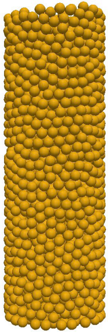
Results - 3D column

N_{it} iterations with projected GS solver

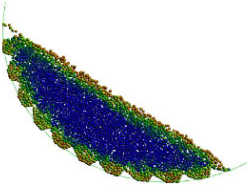
Overlap error $< g >_{0.01} = 0.01d$, $d = 0.01$ m, $h = 0.01$ s





Column diameter
$\Phi = \{3d, 9d, 15d\}$

Results - 3D rotating drum

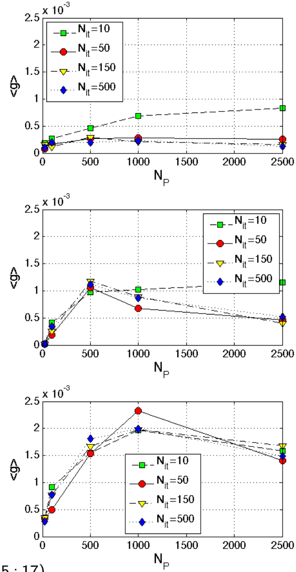


$$D = 0.8 \text{ m}, \ d = 0.01 \text{ m}, \ L = 7d$$

$$\text{Froude number } Fr = \omega\sqrt{\frac{D}{2g}}$$

ω rad/s	Fr
0.12	0.02
0.62	0.1
2.5	0.5

Strongly sub-linear scaling



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Conclusions

- NDEM much faster than DEM in some regimes
- Regularization can be mapped to Hertz contact model
- GS solver scales badly with system size (height)
- Few iterations are sufficient in flowing systems (sublinear)

Future

- Parallelization
- preconditioned CG
- Algebraic/geometric multigrid

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