Modeling & simulation of granulation system using nonsmooth discrete element method

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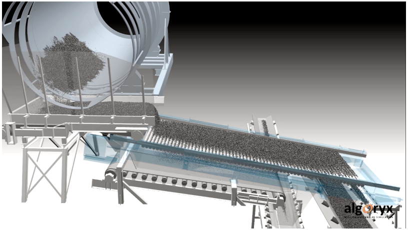
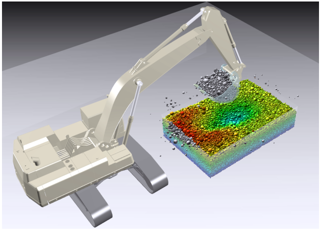
Motivating examples



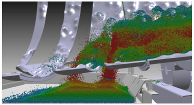


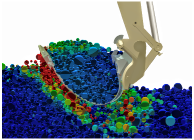
Challenges

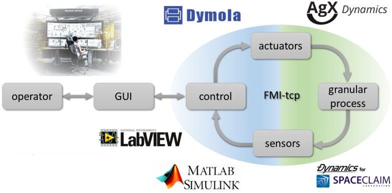
- number of particles: $1 - 100$ M
- disparate time-scales: $10^{-6} - 10^{3}$ s
- model validity
- multidomain
- interoperability

Solutions

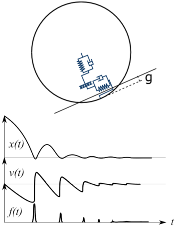
- validated model for iron ore green pellet model as a nonsmooth discrete element method (NDEM)
- computational acceleration
- distributed modular co-simulation

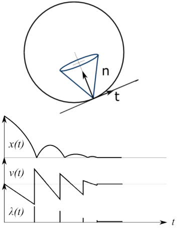


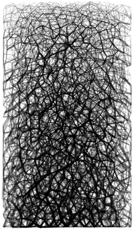




Nonsmooth discrete element method (NDEM)







Smooth DEM	**Nonsmooth DEM**
smooth trajectories	velocity discontinuities
smooth forces	constraints, impulses & inequalities
small time-step	large time-step (implicit)
explicit integrator	QP or MLCP solve

Nonsmooth contact dynamics (Moreau [6], Jean [3], Acary [1], Servin [8])

NDEM - equations of motion

Multibody system $(\mathbf{q}, \dot{\mathbf{q}})$ on descriptor form $(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, \bar{\boldsymbol{\lambda}})$

$$\mathbf{M}\ddot{\mathbf{q}} + \dot{\mathbf{M}}\dot{\mathbf{q}} - \mathbf{G}(\mathbf{q})^T\boldsymbol{\lambda} - \bar{\mathbf{G}}(\mathbf{q})^T\bar{\boldsymbol{\lambda}} = \mathbf{f}_e \quad (1)$$

$$\varepsilon\boldsymbol{\lambda} + \mathbf{g}(\mathbf{q}) = 0 \quad (2)$$

$$\gamma\bar{\boldsymbol{\lambda}} + \bar{\mathbf{G}}(\mathbf{q})\dot{\mathbf{q}} = \boldsymbol{w}(t) \quad (3)$$

constraints $\mathbf{g}(\mathbf{q}) = 0$, $\bar{\mathbf{G}}(\mathbf{q})\dot{\mathbf{q}} = \boldsymbol{w}(t)$ - regularization ε, γ.

Contacts: Hertz, Newton impact, Coulomb, rolling resistance

$$\mathbf{G}_n\boldsymbol{\lambda}_n \sim k_n\left[g_i^{3/2} + c g_i^{1/2}\dot{g}\right]\mathbf{n}\ , \quad \mathbf{G}_n\dot{\mathbf{q}}^+ = -e\mathbf{G}_n\dot{\mathbf{q}}^-$$

$$|\bar{\mathbf{G}}_t\bar{\boldsymbol{\lambda}}_t| \leqslant \mu_s|\mathbf{G}_n\boldsymbol{\lambda}_n|\ , \quad |\bar{\mathbf{G}}_r\bar{\boldsymbol{\lambda}}_t| \leqslant \mu_r|\mathbf{G}_n\boldsymbol{\lambda}_n|$$

NDEM - numerical integration

Linearized varational time stepper SPOOK (Lacoursière [4, 5])

$$\mathbf{q}_{n+1} = \mathbf{q}_n + \Delta t \dot{\mathbf{q}}_{n+1} \tag{4}$$

$$\underbrace{\begin{bmatrix} \mathbf{M} & -\mathbf{G}^T & -\bar{\mathbf{G}}^T \\ \mathbf{G} & \mathbf{\Sigma} & 0 \\ \bar{\mathbf{G}} & 0 & \bar{\mathbf{\Sigma}} \end{bmatrix}}_{\mathbf{H}} \underbrace{\begin{pmatrix} \dot{\mathbf{q}}_{n+1} \\ \boldsymbol{\lambda} \\ \bar{\boldsymbol{\lambda}} \end{pmatrix}}_{\mathbf{z}} = \underbrace{\begin{pmatrix} \mathbf{M}\dot{\mathbf{q}}_n + \Delta t \mathbf{f}_n \\ -\frac{4}{\Delta t}\Upsilon \mathbf{g} + \Upsilon \mathbf{G} \dot{\mathbf{q}}_n \\ \boldsymbol{\omega}_n \end{pmatrix}}_{-\mathbf{r}} \tag{5}$$

Diagonal regularization and stabilization matrices

$$\mathbf{\Sigma} = \frac{4}{\Delta t^2}\,\mathrm{diag}\left(\frac{\varepsilon_i}{1 + 4\frac{\tau_i}{\Delta t}}\right)$$

$$\bar{\mathbf{\Sigma}} = \frac{1}{\Delta t}\,\mathrm{diag}\left(\gamma_i\right)$$

$$\Upsilon = \mathrm{diag}\left(\frac{1}{1 + 4\frac{\tau_i}{\Delta t}}\right)$$

Constraint potential and dissipation

$$U = \tfrac{1}{2}\mathbf{g}^T \varepsilon^{-1} \mathbf{g}$$

$$R = \tfrac{1}{2}(\bar{\mathbf{G}}\mathbf{v})^T \gamma^{-1} \bar{\mathbf{G}}\mathbf{v}$$

Nonsmooth MBD - MLCP

Including frictional contacts, impacts, joint and motor limits lead to limits and complementarity conditions on the solution variables

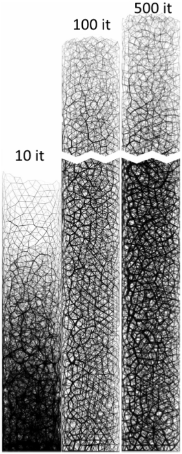
$$
\begin{aligned}
\mathbf{H}\boldsymbol{z} + \mathbf{r} &= \boldsymbol{w}_+ - \boldsymbol{w}_- \\
0 \leqslant \boldsymbol{w}_+ &\perp \boldsymbol{z} - \mathbf{l} \geqslant 0 \\
0 \leqslant \boldsymbol{w}_- &\perp \mathbf{u} - \boldsymbol{z} \geqslant 0
\end{aligned}
\tag{6}
$$

The problem transforms from linear system to a mixed linear complementarity condition (MLCP)

Nonsmooth MBD - Projected Gauss-Seidel solver

Algorithm 2 NDEM simulation with PGS solver

initial state: $(\mathbf{x}_0, \mathbf{v}_0)$
for $i = 0, 1, 2, \ldots, t/\Delta t$ **do**
  contact detection
  compute $\mathbf{g}, \mathbf{G}, \mathbf{\Sigma}, \mathbf{D}$
  impact stage PGS solve $\mathbf{v}_i \rightarrow (\mathbf{v}_i^+, \boldsymbol{\lambda}_i^+)$
  compute $\mathbf{q}_\mathrm{n} = -(4/\Delta t)\mathbf{\Upsilon}_\mathrm{n}\mathbf{g}_\mathrm{n} + \mathbf{\Upsilon}_\mathrm{n}\mathbf{G}_\mathrm{n}\mathbf{v}_i^+$
  pre-step $\mathbf{v} = \mathbf{v}_i^+ + \Delta t \mathbf{M}^{-1}\mathbf{f}_\mathrm{ext}$
  for $k = 1, \ldots, N_\mathrm{it}$ and **while** *criteria*$(\mathbf{r})$ **do**
    for each contact $\alpha = 0, 1, \ldots, N_\mathrm{c} - 1$ **do**
      for each constraint n of contact α **do**
        $\mathbf{r}_{n,k}^{(\alpha)} = -\mathbf{q}_{n,k}^{(\alpha)} + \mathbf{G}_n^{(\alpha)}\mathbf{v}$
        $\boldsymbol{\lambda}_{n,k}^{(\alpha)} = \boldsymbol{\lambda}_{n,k-1}^{(\alpha)} + \mathbf{D}_{n,(\alpha)}^{-1}\mathbf{r}_{n,k}^{(\alpha)}$
        $\boldsymbol{\lambda}_{n,k}^{(\alpha)} \leftarrow \mathrm{proj}_{\mathcal{C}_\mu}(\boldsymbol{\lambda}_k^{(\alpha)})$
        $\Delta\boldsymbol{\lambda}_{n,k}^{(\alpha)} = \boldsymbol{\lambda}_{n,k}^{(\alpha)} - \boldsymbol{\lambda}_{n,k-1}^{(\alpha)}$
        $\mathbf{v} = \mathbf{v} + \mathbf{M}^{-1}\mathbf{G}_{n,(\alpha)}^T \Delta\boldsymbol{\lambda}_{n,k}^{(\alpha)}$
      end for
    end for
  end for
  $\mathbf{v}_{i+1} = \mathbf{v}$
  $\mathbf{x}_{i+1} = \mathbf{x}_i + \Delta t \mathbf{v}_{i+1}$
end for



Number of iterations v.s. particles and error tolerance

$$N_\mathrm{it} \sim 0.1 \cdot N_\mathrm{p}^z / \mathcal{E}$$

Nonsmooth MBD - Projected Gauss-Seidel solver

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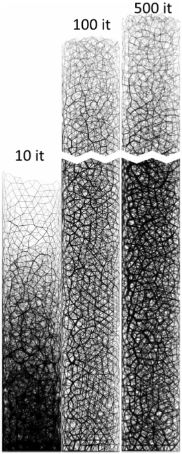
$$\mathbf{v} = \mathbf{v} + \mathbf{M}^{-1}\mathbf{G}_{n,(\alpha)}^T\Delta\boldsymbol{\lambda}_{n,k}^{(\alpha)}$$

  $\mathbf{v}_{i+1} = \mathbf{v}$
  $\mathbf{x}_{i+1} = \mathbf{x}_i + \Delta t \mathbf{v}_{i+1}$
end for



Number of iterations v.s. particles and error tolerance

$$\mathrm{N_{it}} \sim 0.1 \cdot \mathrm{N_p^{z}}/\mathcal{E}$$

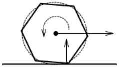
NDEM model for iron ore green pellets

Contacts: Hertz, Newton impact, Coulomb, rolling resistance

$$\mathbf{G}_n\boldsymbol{\lambda}_n \sim k_n(E, d)\left[g_i^{3/2} + c g_i^{1/2}\dot{g}\right]\mathbf{n} \quad , \qquad \text{if } \mathbf{G}_n\dot{\mathbf{q}} \leqslant v_{\text{imp}}$$

$$\mathbf{G}_n\dot{\mathbf{q}}^+ = -e\mathbf{G}_n\dot{\mathbf{q}}^- \quad , \qquad \text{if } \mathbf{G}_n\dot{\mathbf{q}} > v_{\text{imp}}$$

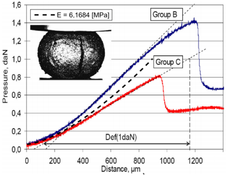
$$|\bar{\mathbf{G}}_t\bar{\boldsymbol{\lambda}}_t| \leqslant \mu_s|\mathbf{G}_n\boldsymbol{\lambda}_n| \ , \quad |\bar{\mathbf{G}}_r\bar{\boldsymbol{\lambda}}_t| \leqslant \mu_r|\mathbf{G}_n\boldsymbol{\lambda}_n|$$

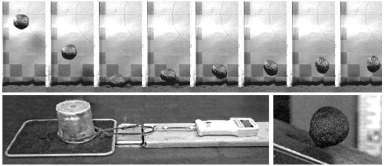


Variable size and mass - fines and moisture

Rate equations for coalesence, layering and breakage

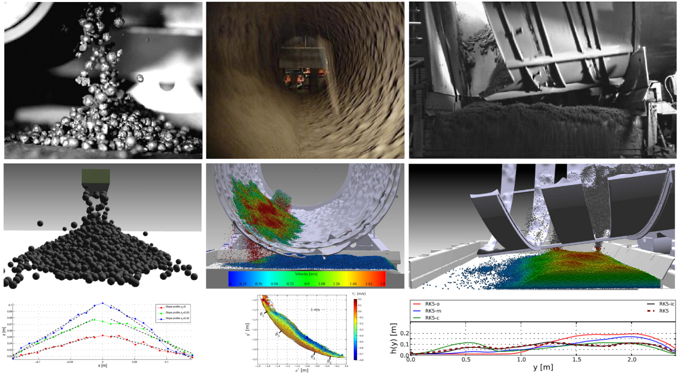
Parametrization





ρ	$3700\ \mathrm{kg/m^3}$	mass density
d	$2 - 20$ mm	diameter
E	6.2 ± 0.7 MPa	Young's modulus
c	1 ± 0.1 mm/s	viscous damping
e	0.18 ± 0.04	coefficient of restitution
μ_s	0.91 ± 0.04	surface friction coefficient
μ_r	0.32 ± 0.02	rolling resistance coefficient

Validation



Test	Quantity	Observation	Simulation
Pile shape	θ_r	$34 \pm 3\ ^\circ$	$36 \pm 2\ ^\circ$
Drum flow	θ_r'	$35 \pm 5\ ^\circ$	$34 \pm 2\ ^\circ$
	v_{tr}	0.20 ± 0.03 m/s	0.22 ± 0.02 m/s
	v_s	1.31 ± 0.06 m/s	1.27 ± 0.09 m/s
	v_{sz}	0.58 ± 0.05 m/s	0.49 ± 0.03 m/s
	$v_{s\perp}$	1.18 ± 0.07 m/s	1.17 ± 0.09 m/s

Computational acceleration

Computational time for simulation of t_{real} seconds

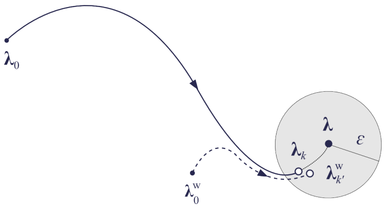
$$t_{comp} = t_{real} \cdot \frac{1}{\Delta t} \cdot \underbrace{K_{cpu} \cdot \alpha\, N_p \cdot N_{it}}_{\text{PGS}} \cdot \frac{1}{N_{cpu}} \tag{7}$$

DEM: $\Delta t = 0.02$ ms, $N_{it} = 1$ $\Longleftrightarrow$ NDEM: $\Delta t = 5$ ms, $N_{it} = 250$

where $K_{cpu} \sim 10^{-6}$ s - time for one force update.

techniques	**speed-up**
parallelization	$N_{cpu} < N_{cpu}^{sat}$
warm starting	$2 - 5$
model reduction	$1 -$ "∞"

Warm starting



Reach the solution faster by warm starting the PGS based on

model:

$\lambda_{n,0}^{(\alpha)} = \frac{5}{4} k_n g_{n(\alpha)}^{5/4}$

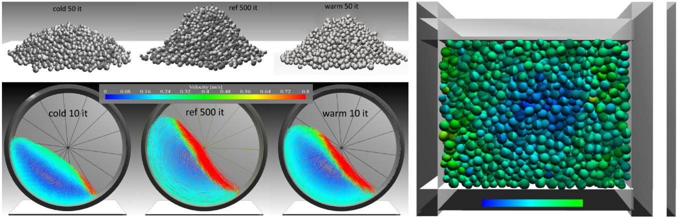
$\boldsymbol{\lambda}_{t,0} = \mathrm{proj}_{\mathcal{C}_\mu}[\gamma_t^{-1}(\mathbf{G}_t \boldsymbol{v})^T \mathbf{G}_t]$

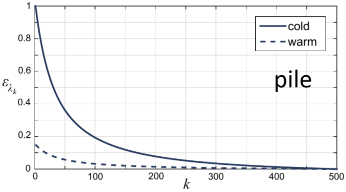
history:

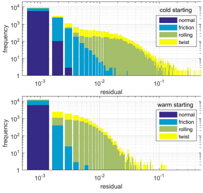
$\boldsymbol{\lambda}_0(t) = \beta \boldsymbol{\lambda}_{N_{it}}(t - \Delta t)$

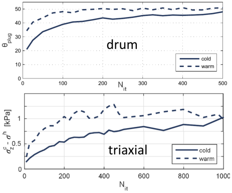
Apply to velocity also $\boldsymbol{v}_0 = \mathbf{M}^{-1}\mathbf{p} + \mathbf{M}^{-1}\mathbf{G}^T\boldsymbol{\lambda}_0$

Warm starting







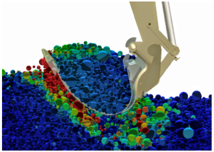


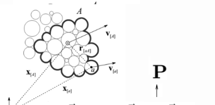
2 - 5 times speed-up for history based warm starting
friction and rolling resistance is most improved
marginal speedup by model based warm starting

Adaptive model reduction

Substitute rigid bodies for particle regions co-moving rigidly

The reduced system is a sub-space projection of the full system





$$\vec{x}_{[a]} = \vec{x}_{[A]} + \vec{r}_{[aA]}$$

$$\begin{array}{rcll} \mathbf{M}\ddot{\mathbf{x}} & = & \mathbf{f}_{\text{ext}} + \mathbf{G}^{\mathrm{T}}\boldsymbol{\lambda} & \mathbf{x} \in \mathbb{R}^{n} \\ \varepsilon\boldsymbol{\lambda} + \eta\mathbf{g}(\mathbf{x}) + \tau\mathbf{G}\dot{\mathbf{x}} & = & 0 & \boldsymbol{\lambda} \in \mathbb{R}^{m} \end{array}$$

$$\begin{array}{rcll} \mathbf{x} & \approx & \mathbf{P}\tilde{\mathbf{x}} & \mathbf{P} \in \mathbb{R}^{n\times\tilde{n}} \\ \boldsymbol{\lambda} & \approx & \mathbf{Q}\tilde{\boldsymbol{\lambda}} & \mathbf{Q} \in \mathbb{R}^{m\times\tilde{m}} \\ & & & \tilde{n},\tilde{m} \ll n,m \end{array}$$

$$\begin{array}{rcll} \tilde{\mathbf{M}}\ddot{\tilde{\mathbf{x}}} & = & \tilde{\mathbf{f}}_{\text{ext}} + \tilde{\mathbf{G}}^{\mathrm{T}}\tilde{\boldsymbol{\lambda}} & \tilde{\mathbf{x}} \in \mathbb{R}^{\tilde{n}} \\ \varepsilon\tilde{\boldsymbol{\lambda}} + \eta\tilde{\mathbf{g}}(\tilde{\mathbf{x}}) + \tau\tilde{\mathbf{G}}\dot{\tilde{\mathbf{x}}} & = & 0 & \tilde{\boldsymbol{\lambda}} \in \mathbb{R}^{\tilde{m}} \end{array}$$

$$\tilde{\mathbf{M}} = \mathbf{P}\mathbf{M}\mathbf{P}^{T},\ \tilde{\mathbf{f}}_{\text{ext}} = \mathbf{P}\mathbf{f}_{\text{ext}},\ \tilde{\mathbf{G}} = \mathbf{Q}^{T}\mathbf{G}\mathbf{P},\ \tilde{\lambda} = \mathbf{Q}\boldsymbol{\lambda},\ \tilde{\mathbf{g}} = \mathbf{Q}\mathbf{g}$$

Dramatic speed-up if $\tilde{n}, \tilde{m} \ll n, m$ by reduction of equations

The tricky part is when and where to split

Adaptive model reduction

Model approximation error - orthogonal decomposition

$$\mathcal{E}(t) = \mathbf{x}(t) - \mathbf{P}\tilde{\mathbf{x}}(t) \qquad \mathcal{E}(t) = \mathcal{E}_\perp(t) + \mathcal{E}_\parallel(t)$$

$$\begin{aligned}
\mathcal{E}_\perp(t) &= \left[\mathbf{1} - \mathbf{P}\mathbf{P}^T\right]\mathbf{x}(t) \\
\mathcal{E}_\parallel(t) &= \mathbf{P}\left[\mathbf{P}^T\mathbf{x}(t) - \tilde{\mathbf{x}}(t)\right]
\end{aligned}$$

Error evolution - deviation from rigid rigid motion

$$\boxed{\ddot{\mathcal{E}}_\perp = \underline{\mathbf{M}}^{-1}\left[\underline{\mathbf{f}}_e - \frac{\eta}{\varepsilon}\underline{\mathbf{G}}^T\mathbf{g} - \frac{\tau}{\varepsilon}\underline{\mathbf{G}}^T\underline{\mathbf{G}}\dot{\mathbf{x}}\right]}$$

$$\underline{\mathbf{M}} = \mathbf{P}_\perp\mathbf{M}\mathbf{P}_\perp^T,\ \underline{\mathbf{f}}_{\mathrm{ext}} = \mathbf{P}_\perp\mathbf{f}_{\mathrm{ext}} \text{ and } \underline{\mathbf{G}} = \mathbf{G}\mathbf{P}_\perp$$

$$\mathbf{P}_\perp \equiv \mathbf{1} - \mathbf{P}\mathbf{P}^T$$

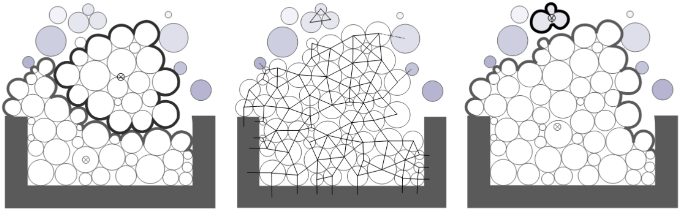
Adaptive model reduction

Merge conditions - rigid co-motion and force balance

$$-v_{\mathcal{E}}^{-} < \underline{\mathbf{G}}\dot{\underline{\mathbf{x}}} < v_{\mathcal{E}}^{+}$$
$$-a_{\mathcal{E}}^{-} < \underline{\mathbf{G}}\ddot{\underline{\mathbf{x}}} < a_{\mathcal{E}}^{+}$$

$$\frac{\left|\underline{\mathbf{f}}_{\mathrm{e}} - \frac{\eta}{\varepsilon}\underline{\mathbf{G}}^T\mathbf{g}\right|}{|\underline{\mathbf{f}}_{\mathrm{e}}| + \left|\frac{\eta}{\varepsilon}\underline{\mathbf{G}}^T\mathbf{g}\right|} \leq f_{\mathcal{E}}$$

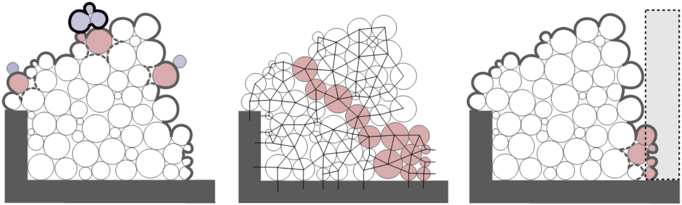
Merge process



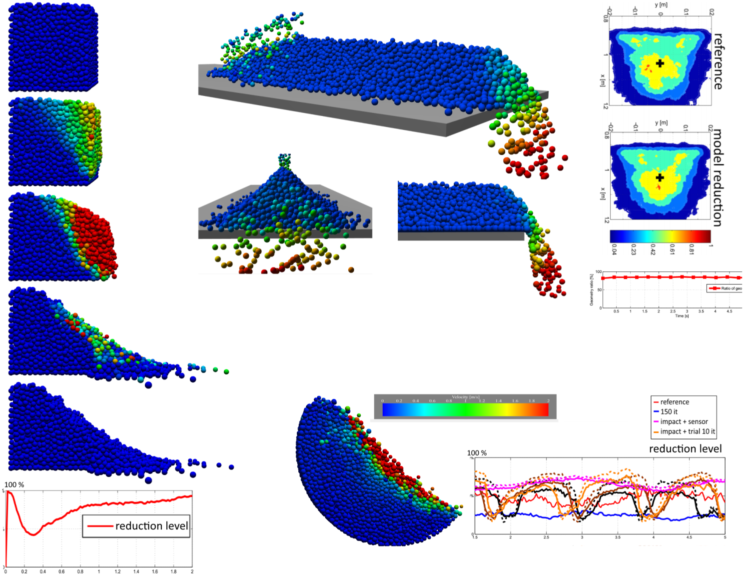
Adaptive model reduction

Refinement prediction methods

- contact split
- trial solve split
- sensor split

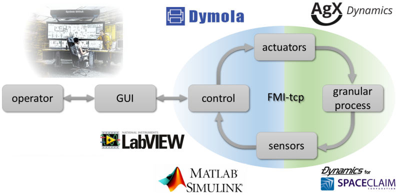


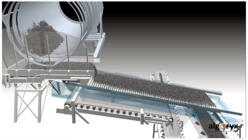
Adaptive model reduction

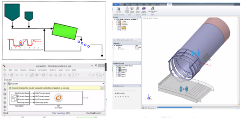


Interoperability

Connecting: NDEM + CAD + control software + hardware







Distributed modular co-simulation (FMI-TCP)

- Functional Mockup Interface - www.fmi-standard.org
- Master-slave over web (TCP)

introduction
NDEM
validation
acceleration
interoperability
conclusions

Summary and conclusions

Summary

- validated NDEM model for iron ore green pellets
- computational speed-up: $(10) \times (2 - 5) \times (1 - "\infty")$
- distributed modular co-simulation

Conclusions

- Particulate simulation of granulation systems is in reach

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References

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