Sandia National Laboratories

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Discrete element modeling of damage and fracture

PRESENTED BY

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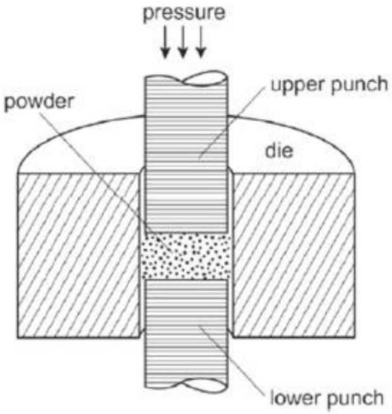
SAND2019-######

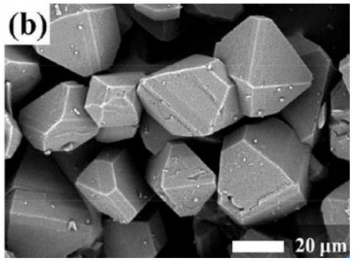
Motivation: extreme deformation and fragmentation

Sea ice dynamics for climate modeling

Powder compaction for energetic materials



Rojek et al, Comp. Part. Mech. (2016)



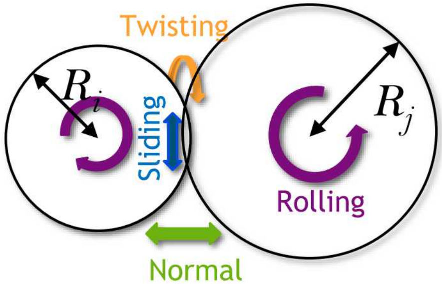
Yang et al, Cryst Growth & Design (2018)

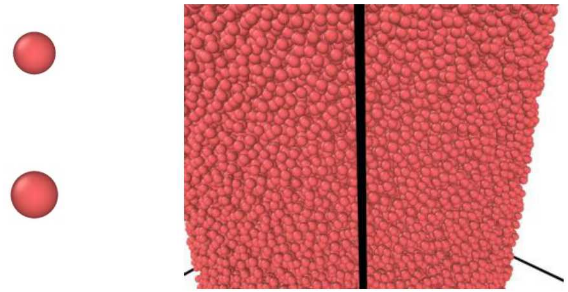
- Mesh-based methods: expensive for evolving topology
- Mesh-free methods: not well-suited for interfaces
- DEM: naturally suited for granular systems, what about deformation/fracture?

Discrete element method (DEM)

- Molecular-dynamics like method, elements are rigid individual particles
- Explicitly integrate $\mathbf{F}_i = m_i\mathbf{a}_i$, $\tau_i = L_i\boldsymbol{\omega}_i$; $i = 1,\ldots,N$, $\mathbf{F}_i = \mathbf{F}_i(\mathbf{r}_1, \mathbf{r}_2,\ldots, \mathbf{r}_N)$

Contact





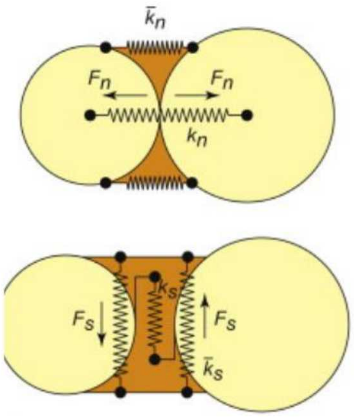
Normal: $\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 4\pi\gamma R\right)\boldsymbol{n} - \eta_n \boldsymbol{v}_R \cdot \boldsymbol{n}$

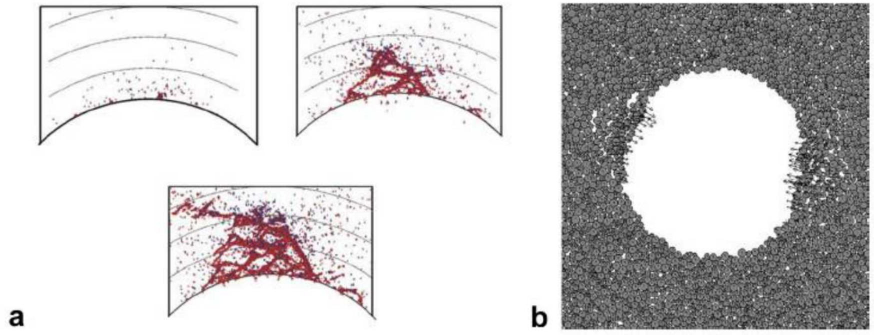
Sliding: $\boldsymbol{F}_S = -k_S \int_{t0}^{t} \boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau - \eta_T \boldsymbol{v}_{tR}$

$$\|\mathbf{F}_s\| \leq \mu_s \|\mathbf{F}_N\|$$

...

Bonded

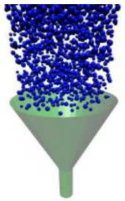


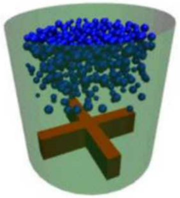


Lisjak and Grasselli, J Rock Mech Geotech Eng. 2014

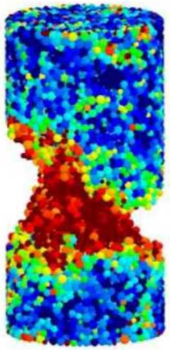
DEM scope

- Well-established for (coarse) granular materials
  → challenges remain with contact model calibration

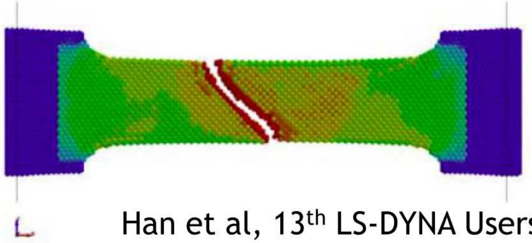




- Bonded DEM: natural choice for discontinuous materials: cementitious materials (concrete, geomaterials), particulate composites, etc.



- What about homogeneous materials?



Han et al, 13th LS-DYNA Users Conference

Bonded DEM for continuum mechanics

Challenges:

- Bond/contact model takes the place of a constitutive model:

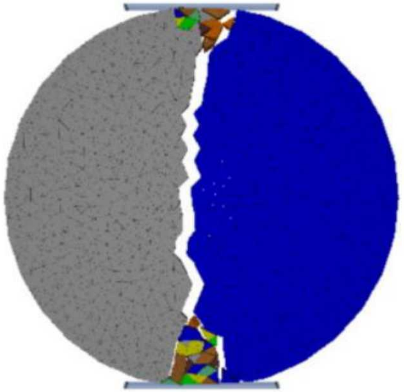
$$\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 4\pi\gamma R\right)\boldsymbol{n} \; -\eta_n \boldsymbol{v}_R \cdot \boldsymbol{n}$$

$$\boldsymbol{F}_S = -k_S \int_{t0}^{t} \boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau - \eta_T \boldsymbol{v}_{tR}$$

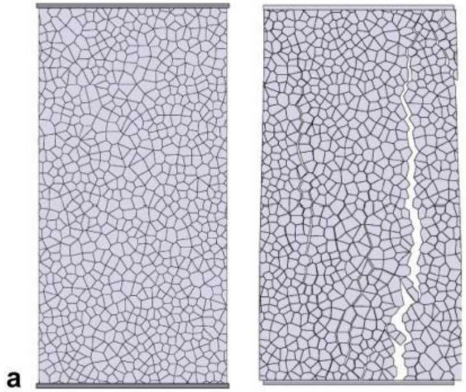
$$\|\mathbf{F}_s\| \leq \mu_s \|\mathbf{F}_N\|$$

- Difficult to parametrize: material property → bond parameters?

- Mesh resolution, element size/shape distribution can affect bond parametrization



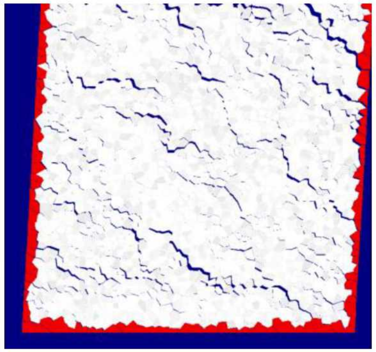
Galindo-Torres et al, Comp Phys Comm 2012



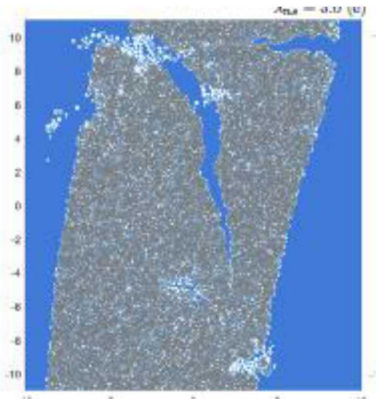
Lisjak and Grasselli, J Rock Mech Geotech Eng. 2014

Bonded DEM for modeling sea ice mechanics

- Sea ice covers ~5% of global surface: dynamics have a significant impact on climate
- Current continuum sea ice models lose validity at high resolution
- Sea ice as a granular 2D material?



Hopkins, 1994



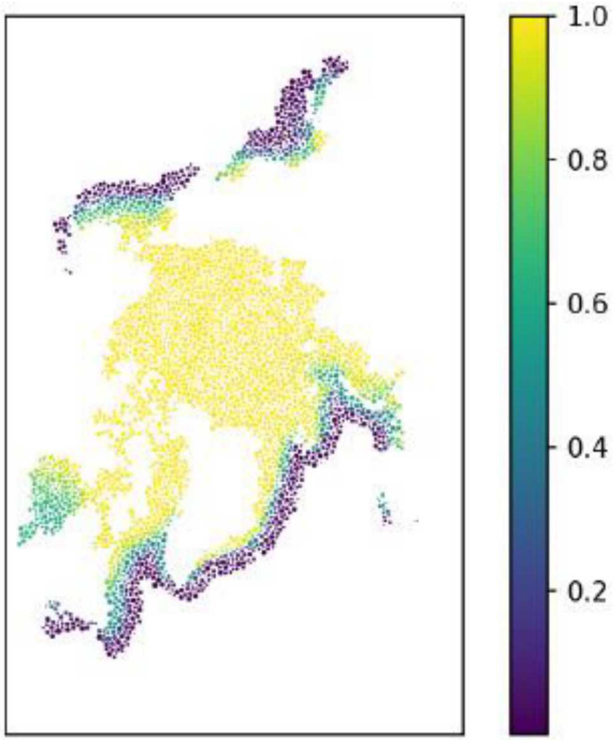
Herman, Geosci Model Dev, 2016

SciDAC Scientific Discovery through Advanced Computing

SciDAC funded project, LANL (PI: Turner) + SNL

Bonded DEM for modeling sea ice mechanics

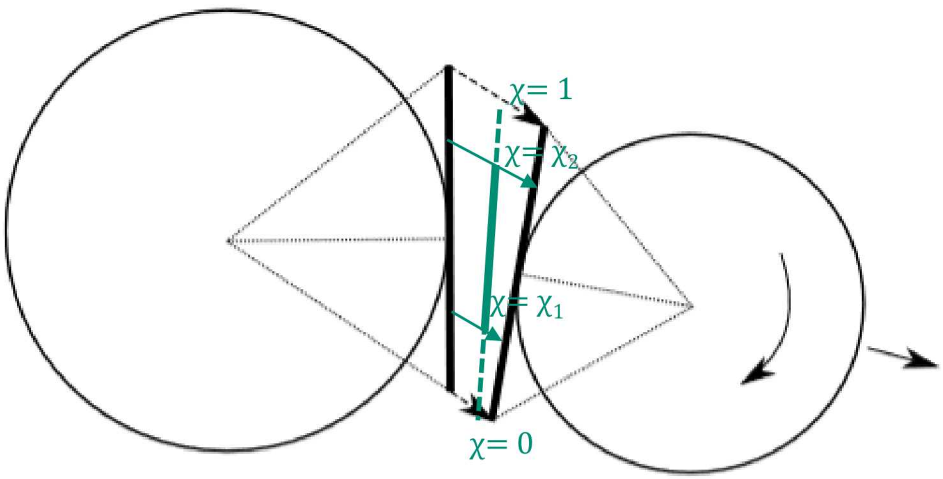
- Goal: simulate global scale, 100+ years
- Circular elements instead of polygonal, interpolate quantities to grid
- Elements phenomenological, *not* individual floes
  - Fewer elements, lower stiffness
- Coupled to ocean, air currents, thermodynamics



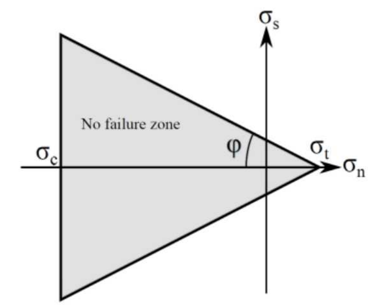
Ice concentration

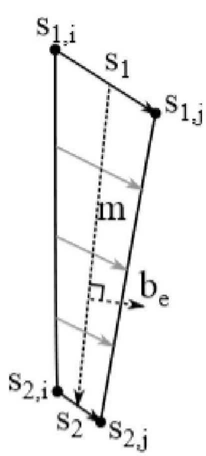
Bonded DEM for modeling sea ice mechanics

Adaptation of contact model developed by Hopkins (J Geophys Res 1996):



$$\sigma_n(\chi) = k_n \vec{s}(\chi) \cdot \vec{b}_e$$
$$\sigma_s(\chi) = k_s \vec{s}(\chi) \cdot \vec{m}_e$$

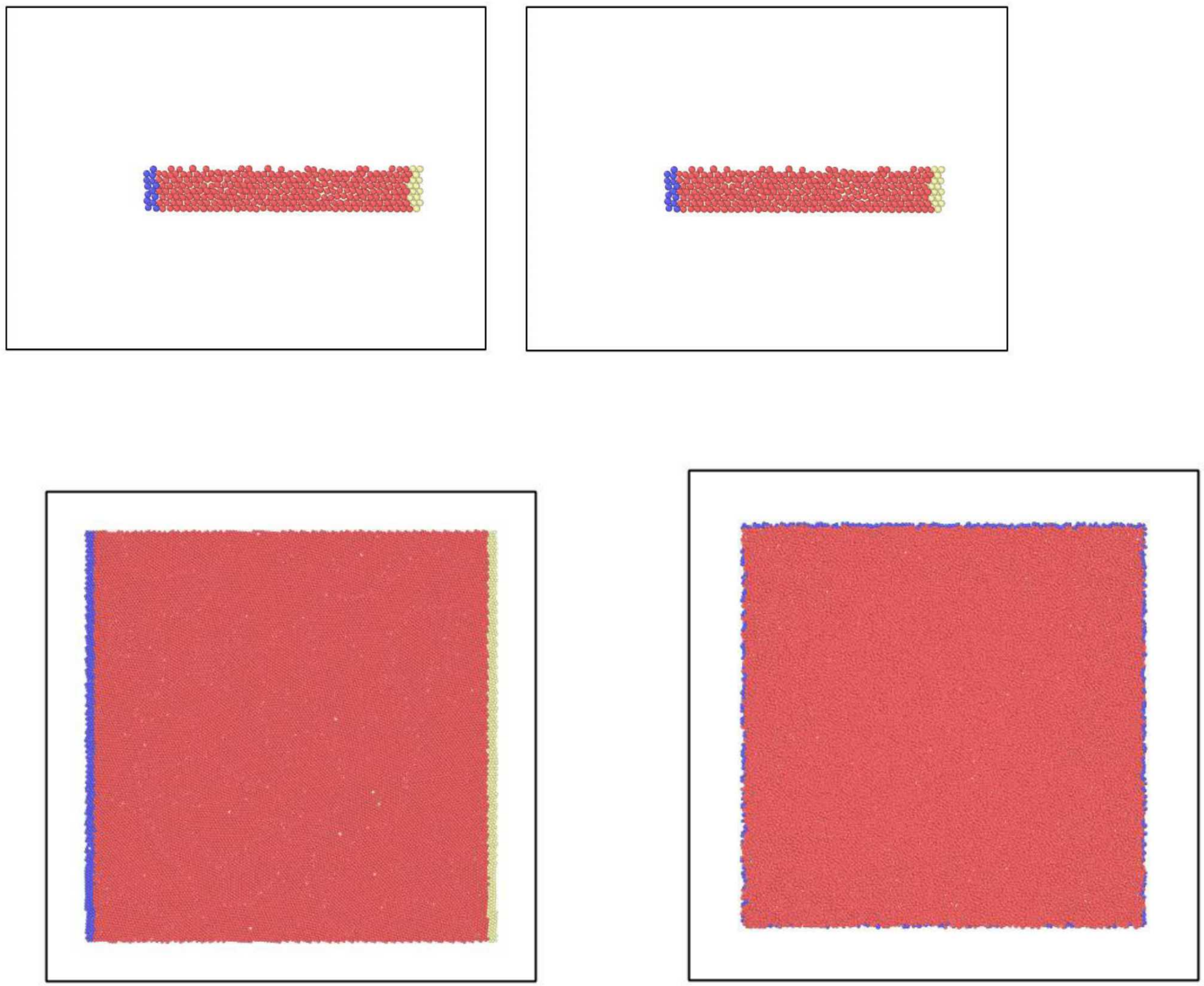




$$\vec{F}_n = \left(hL \int_{\chi_1}^{\chi_2} \sigma_n(\chi) \mathrm{d}\chi \right) \vec{b}_e$$
$$\vec{F}_s = \left(hL \int_{\chi_1}^{\chi_2} \sigma_s(\chi) \mathrm{d}\chi \right) \vec{m}_e$$

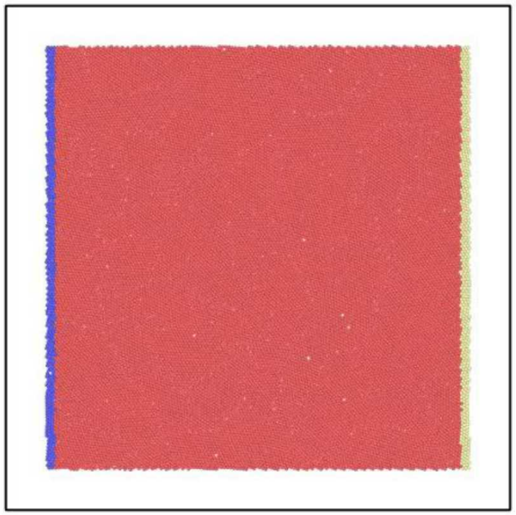
$$N = hL \int_{\chi_1}^{\chi_2} \vec{r}(\chi) \times \left(\sigma_n \vec{b}_e + \sigma_t \vec{m}_e \right) \mathrm{d}\chi$$

Illustration of Hopkins contact model

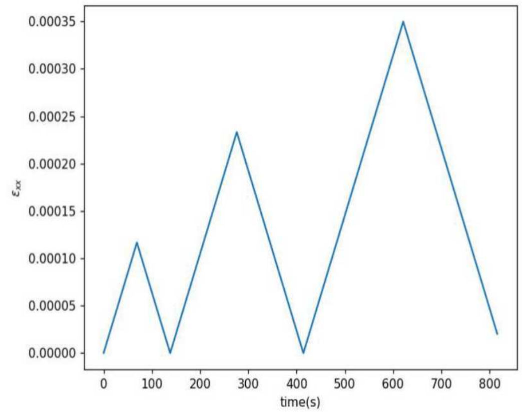


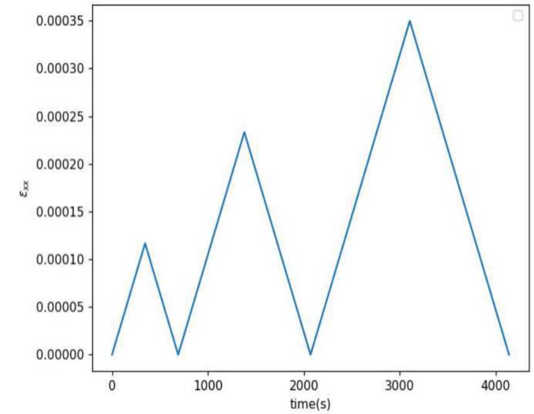
Bonded DEM for sea ice mechanics: preliminary results

Uniaxial tension
(well beyond yield):

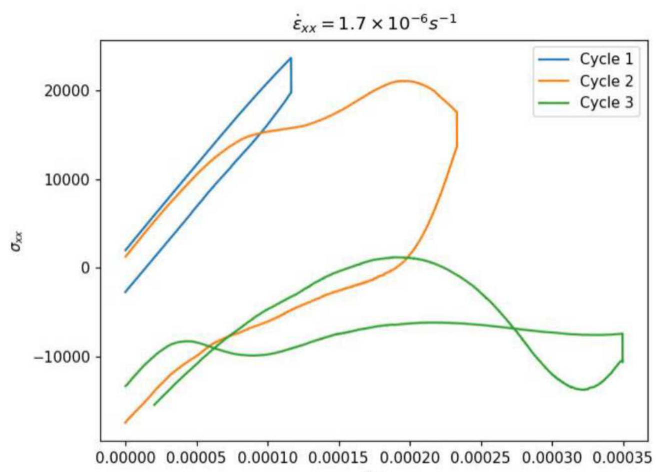


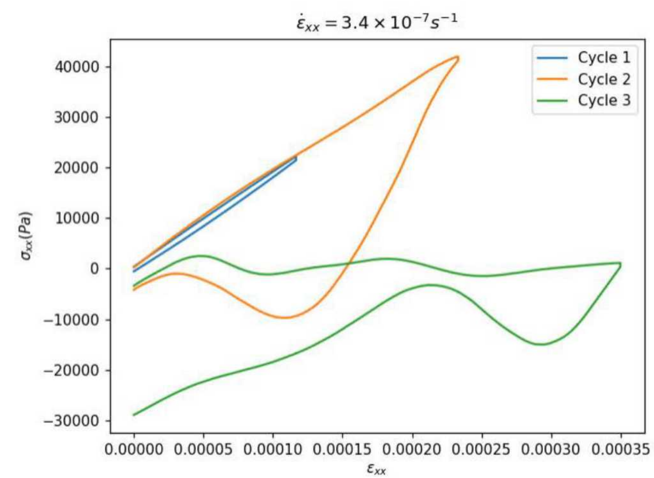
Imposed motion (strain control):



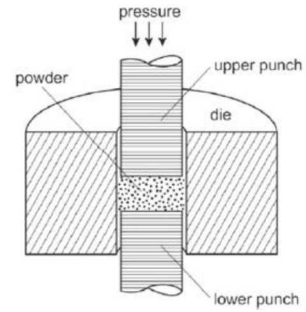


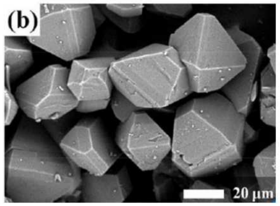
Measured response





Powder compaction (Sandia LDRD, PI Lechman)



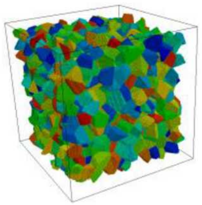


Yang et al, Cryst Growth & Design (2018)

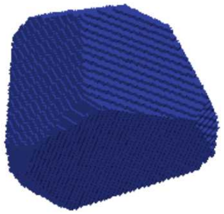
Goal: produce realistic mesostructures of powder compacts

First step: loose powder packing

Voronoi tesslation



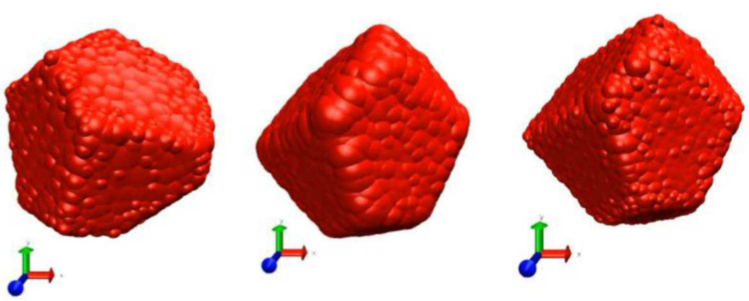
Single particle (voxelated representation)



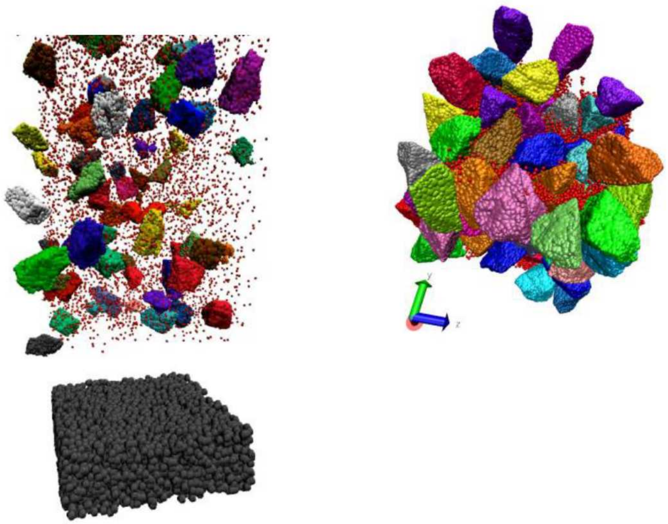
Overlapping spheres representation

d_{min} is the smallest sphere diameter allowed,

N_S is the number of spheres



DEM simulations to generate loose packings



Conclusions

- DEM is a natural choice for direct simulation of granular/discontinuous/cementitious materials

- Phenomenological extension to broader class of materials is being investigated
  - Challenges with calibration and verification of bond/contact model
  - Mesh and geometry dependence remains a challenge
  - Key advantages: easily captures fragmentation and subsequent dynamics

- Hybrid methods (e.g. DEM + FEM/peridynamics)?

- Damage evaluation: bulk response, but also statistics of damage spatial distribution