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Recent developments and applications of LAMMPS for granular media

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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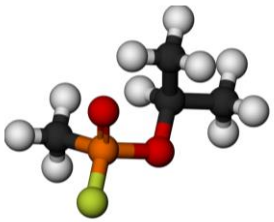
What is ‘granular’?

Molecular dynamics

vs.



Atoms (or small groups of atoms)

Particle length scale ~ atomic

System length scale >> particle length scale

Point particles → position, velocity

```
atom_style atomic, full,…
fix nve/nvt/npt,…
```

Long-range, conservative interactions

```
pair_style lj/cut
```

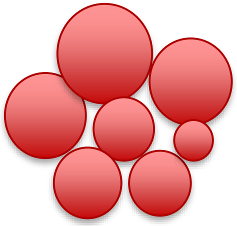
Thermal, often equilibrium

```
fix nvt
```

Representative sample, boundaries often periodic

```
boundary ppp
```

Granular



Macroscopic grains

Particle length scale >> atomic

System length scale >> particle length scale

Finite particles → position, velocity, orientation, angular velocity

```
atom_style sphere,
fix nve/sphere
```

Short-range, complex, dissipative interactions

```
pair_style gran/hooke/history
```

Athermal, non-equilibrium

```
fix nve/sphere, fix gravity
```

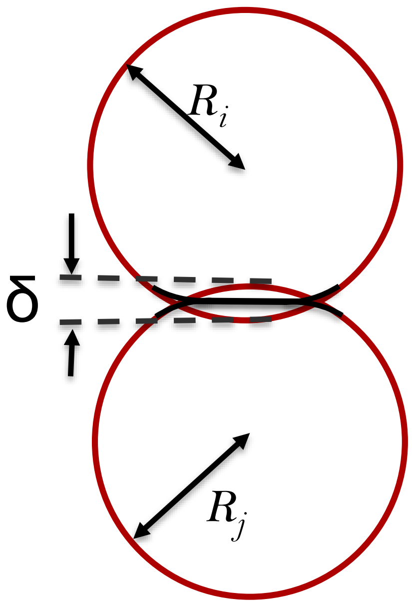
Often ‘full system’, boundaries complex, particles added/removed

```
boundary fff, fix pour,
fix wall/gran, ….
```

Granular models: more details

`pair gran/hertz:`

Analytical Hertz solution (1882 for normal contact force:



$$\delta = R_i + R_j - \|\mathbf{r}_i - \mathbf{r}_j\| > 0$$

$$\mathbf{F}_n = k_n \sqrt{R}\delta^{3/2}\mathbf{n} - \sqrt{R\delta} m \gamma_n \mathbf{v}_n$$

Dissipative term;
Many damping models

What about oblique contact/tangential force?
→ friction, with option of accumulated shear

`pair gran/hertz/history`

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

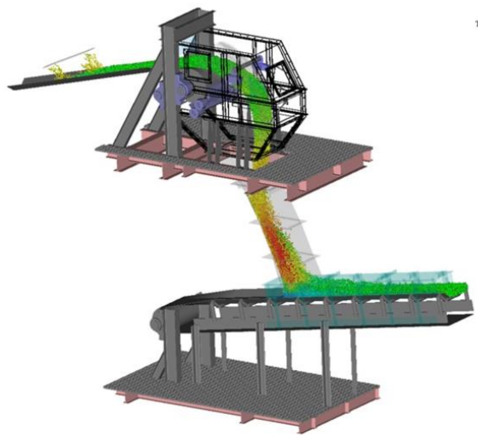
Needs to account for rotating frame of reference

$$\boldsymbol{v}_{tR} = \boldsymbol{v}_t - (R_i \boldsymbol{\Omega}_i + R_j \boldsymbol{\Omega}_j) \times \boldsymbol{n}$$

$$\|\boldsymbol{F}_S\| \leq \mu_S \|\boldsymbol{F}_n\|$$

Larger world of granular simulations: discrete element method (DEM)

Traditional uses in geomechanics, mining industry, particle technologies



From EDEM youtube channel

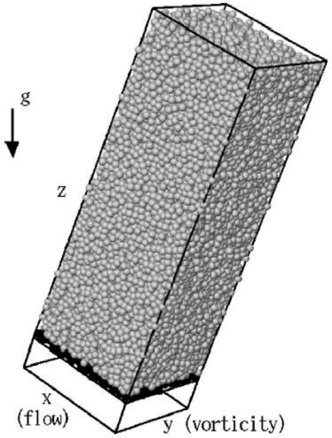
Many DEM codes: EDEM, Yade, PFC 2D/3D, Esys-Particle, <u>LIGGGHTS</u>

Granular simulations in LAMMPS

- LAMMPS: used for seminal work in granular physics simulations (Grest, Silbert, Landry, others, ca. 2000)

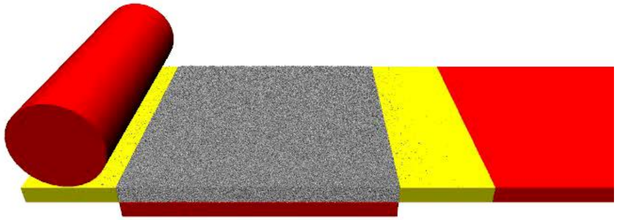
- Historically: granular physics
  - spheres (often monodisperse)
  - simple contact potentials, w/ friction
  - simple geometries (periodic packings, flow down inclined plane,…)

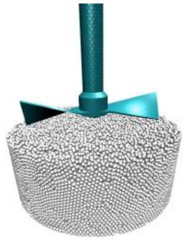
    → glass beads



Silbert et al, PRE 2001

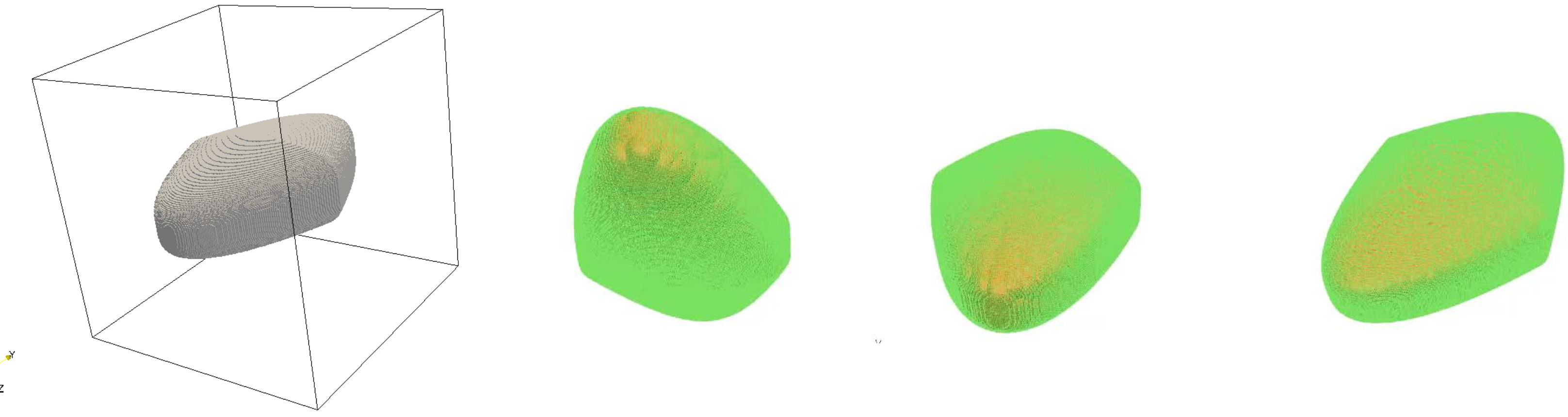
- More recent: engineering applications
  - Non-spherical particles
  - More realistic, complex contact potentials (e.g. cohesion, rolling/twisting friction)
  - Complex geometries





Recent capability: arbitrary particle shapes via overlapping spheres

- Algorithms to pack a shape represented on a voxel grid (3D image) optimally with overlapping spheres (pre-processing, external to LAMMPS):



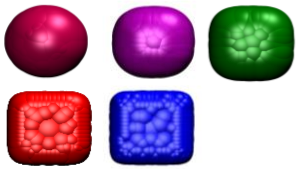
Original shape   N=200 spheres   N=500   N=2000

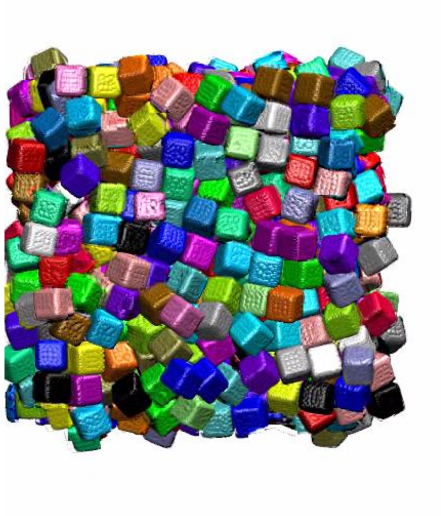
- Aggregates move as rigid bodies
- Interactions are pairwise sums of sphere-sphere granular interactions

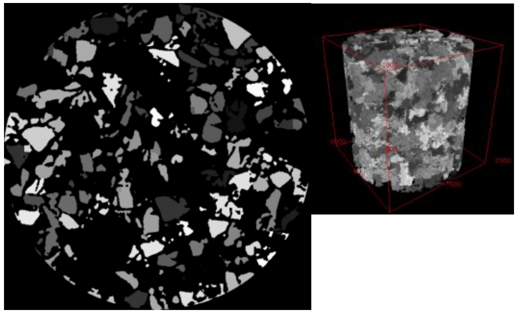
Credits: Leo Silbert, K Michael Salerno, Steve Plimpton

Arbitrary shape particles

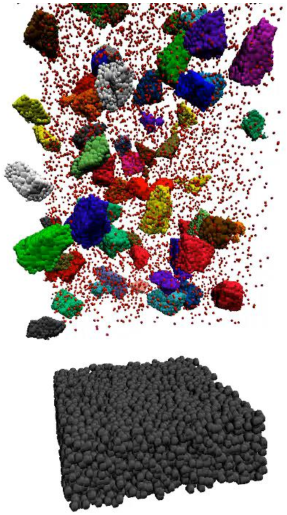
```
molecule mymol shape1.data shape2.data
fix 1 all rigid/small molecule mol mymol infile moi
fix 2 all pour 1000 1 1234 mol mymol rigid 1
```







MicroCT, courtesy Emilee Reinholz

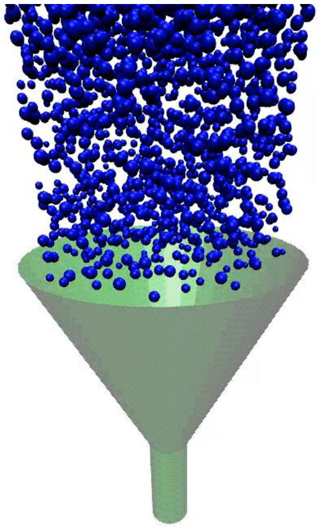


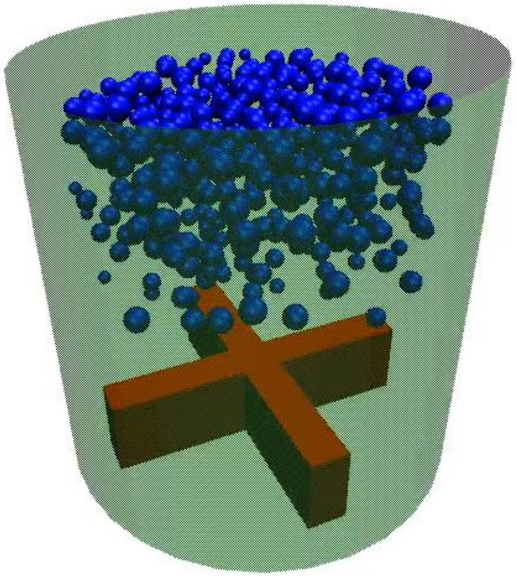
Study effect of shape on granular packing and rheology (Salerno et al, in prep)

Study effects of particle shape/size on battery electrode microstructure

Credits: Leo Silbert, K Michael Salerno, Steve Plimpton

Recent capability: complex boundaries for granular





```
region conereg cone z 0 0 5 20 10 30 open 1 open 2
...
fix 2 all wall/gran/region hertz/history &
   ${kn} ${kt} ${gamma_n} ${gamma_t} ${coeffFric} 1 region conereg
```

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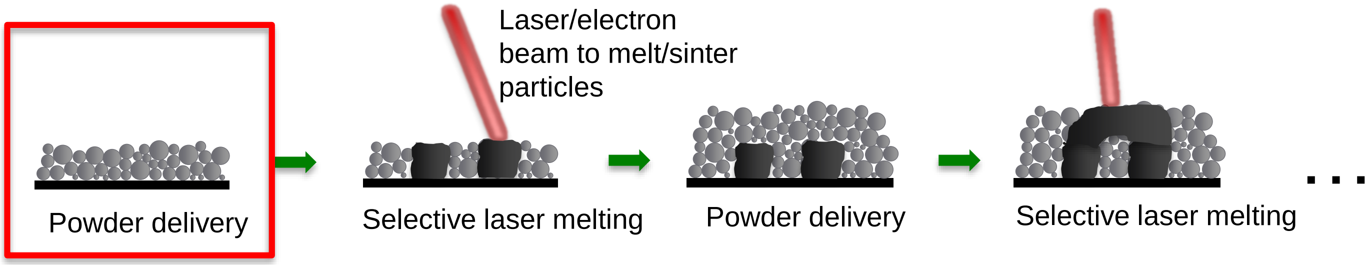
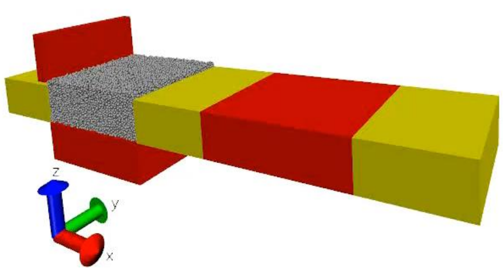
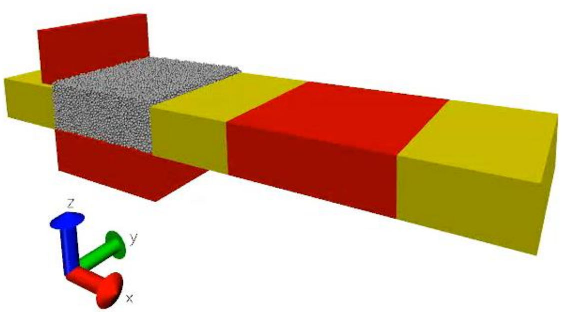
Application: additive manufacturing

Layer-by-layer powder bed fusion processes (e.g. SLM/SLS):

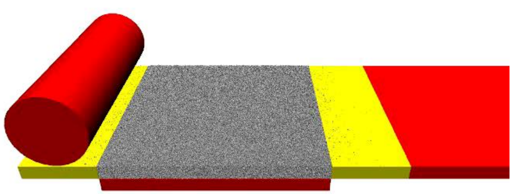




Very high cohesion
Moderate friction



No cohesion
Moderate rolling and sliding friction

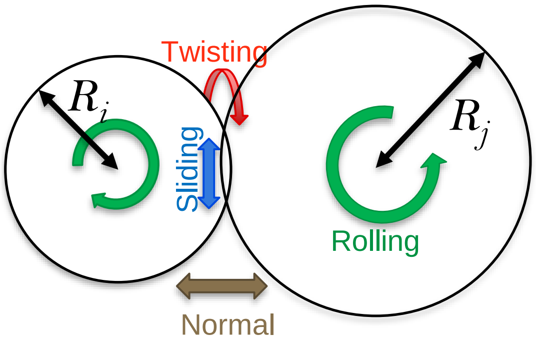


No cohesion
Moderate sliding friction
No rolling/twisting friction

Coming attractions

1.) Granular pair styles with **cohesion**, **rolling** friction, **twisting** friction:

```
pair gran/dmt/rolling, pair gran/jkr/rolling
```



Cohesion (DMT):

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

$$\delta_N = a^2/R$$

Rolling friction:

$$\tau_i = -\tau_j = R\mathbf{n} \times \mathbf{F}_R$$

$$\boldsymbol{F}_R = -k_R \int_{t_0}^{t} \boldsymbol{v}_L(\tau)\mathrm{d}\tau - \eta_R \boldsymbol{v}_L$$

$$\|\boldsymbol{F}_R\| \leq \mu_R \|\boldsymbol{F}_n\|$$

$$\boldsymbol{v}_L = -R(\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_j) \times \boldsymbol{n}$$

gran/hertz/history,
high friction

gran/dmt/rolling
Moderate cohesion,
rolling friction

gran/dmt/rolling
High cohesion, moderate
rolling friction

Coming attractions

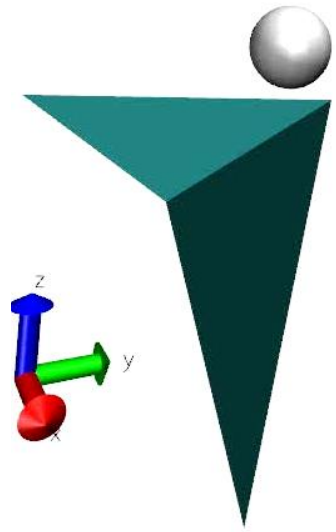
2.) Triangulated surfaces, sphere-triangle and sphere-line interactions

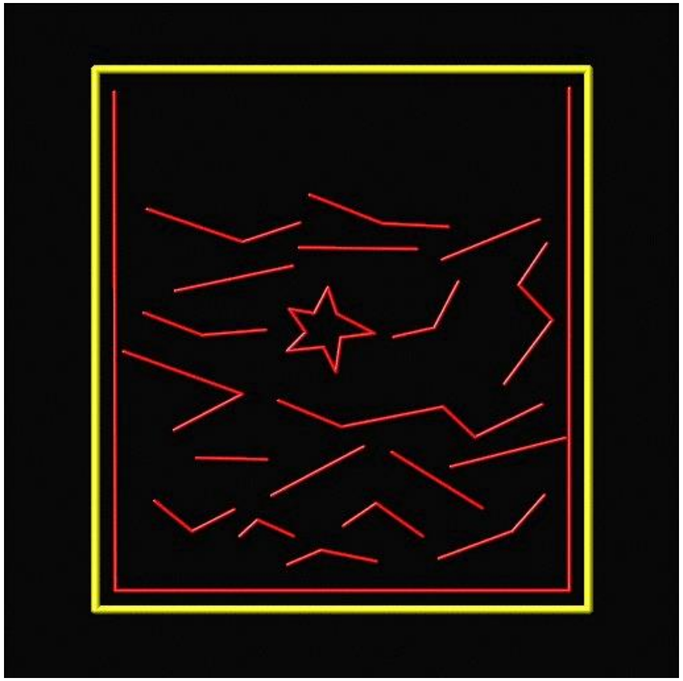
```
pair_style tri/gran/hooke/history
pair_style line/gran/hooke/history
```

Triangles/lines treated as particles, distributed across procs → ideal when $L_{tri} \sim L_{sphere}$, $N_{tri} >> 1$

```
fix surface/global
```

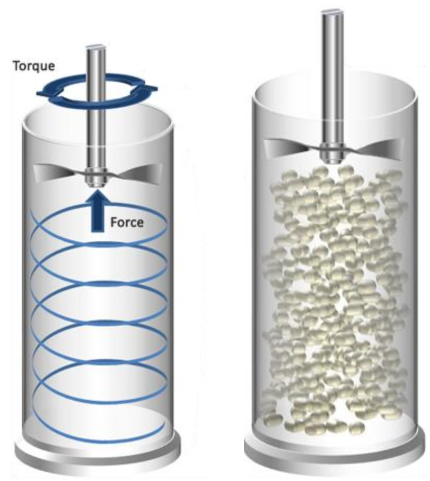
Triangles/lines belong to fix, each proc owns all tris/lines → ideal when $L_{tri} >> L_{sphere}$, N_{tri} small

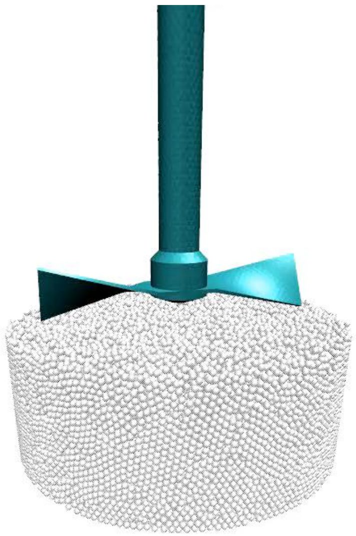




Application: powder rheology

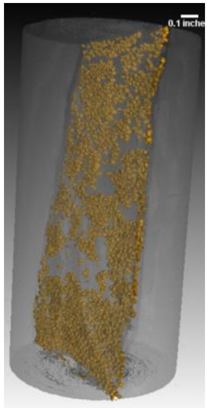
- Goal: calibrate DEM parameters based on powder dynamics experiments
- Freeman Technology FT4 rheometer: annular shear; measure force/torque for various impeller motions



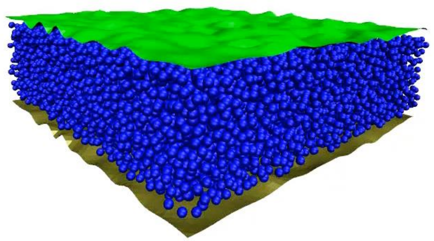


Application: geosciences

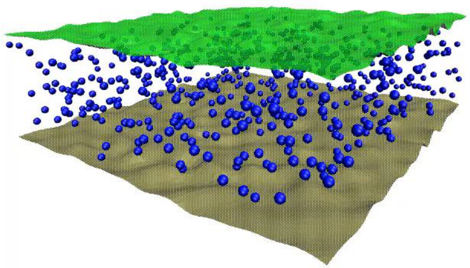
- Hydraulic fracturing ("fracking") involves fracturing rock with high-pressure fluid
- Fractures are kept open with proppant particles
- Various proppant packing strategies:



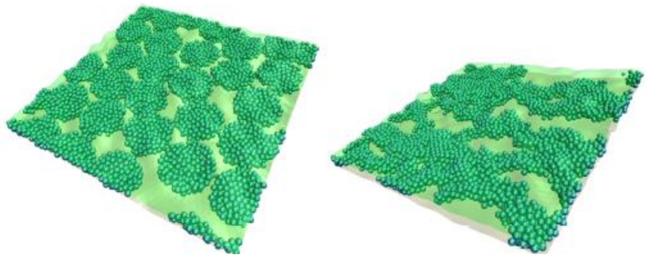
Conventional:
multi-layered, homogeneous



Partial monolayer



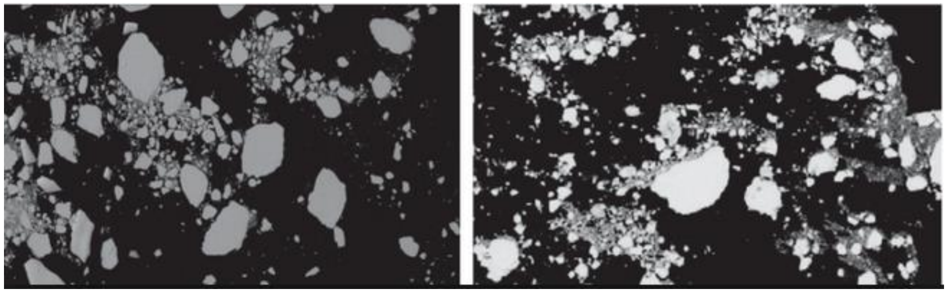
Heterogeneous, multi-layered
(e.g. Schlumberger HiWAY)[1]

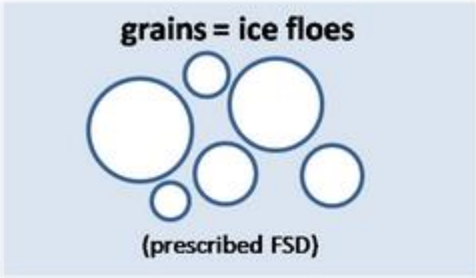


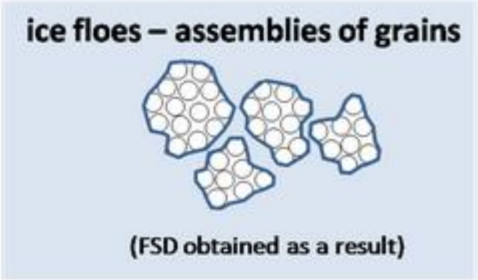
→ Use DEM to <u>artificially</u> generate pack structures, study interplay of **mechanical stability** and **pack permeability**

Application: climate modeling

Sea ice: 2D granular material?







Herman, Geosci Model Dev., 2016

xhi-xlo ~ 

Time scale: ~100 years

QUESTIONS?