SAND2022-XXXXX

SAND2022-14228C

Sandia National Laboratories

Exceptional service in the national interest

Modeling powder compaction with peridynamics

Stewart Silling

SOCIETY OF ENGINEERING SCIENCE ANNUAL TECHNICAL MEETING

October 17, 2022

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

What this talk will cover

- Modeling the deformation, contact, and failure of grains
- Discrete elements as peridynamic material points
    - High stress powder compaction

Powder compaction

- Many things are manufactured by compressing powders.
- Typically want high, uniform density and low residual stress.

Image: Alchemist-hp

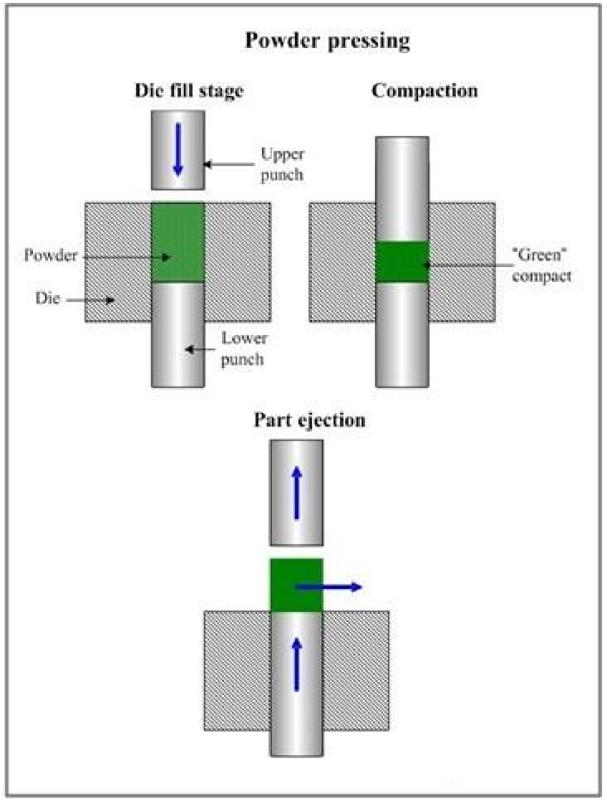


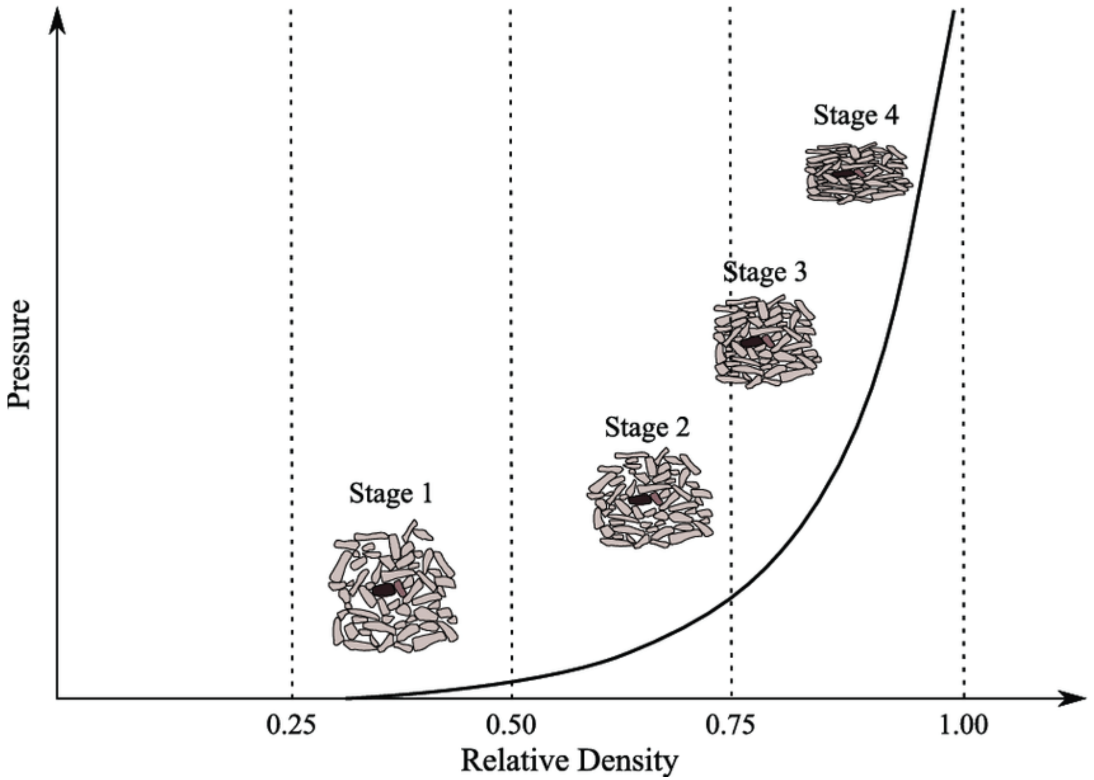
Image: https://blogmech.com/methods-of-compacting-powder-metallurgy/

Powder compaction

- Loose powder is poured into a die, compressed by a ram.
- As it is compressed…
  - Void space is crushed out.
  - Particles deform and may fracture.
  - Friction can be important.

Stages of powder compaction

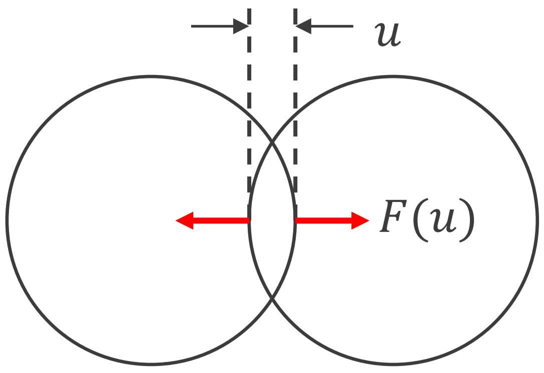
Image: H. Yi et al., 2018, KONA Powder and Particle Journal



Modeling regimes

- Low stress: Discrete elements are very effective.
  - Each grain has 3-6 degrees of freedom.
  - Usually assume pair interactions.
  - Non-spherical grains add complexity.
- High stress: Need a more detailed model of grains.
  - Need nonlinear 3D model.
  - Need contact forces.
  - Not practical to model more than a few hundr

This talk will discuss a multipoint interaction model



Basic discrete element pair interaction

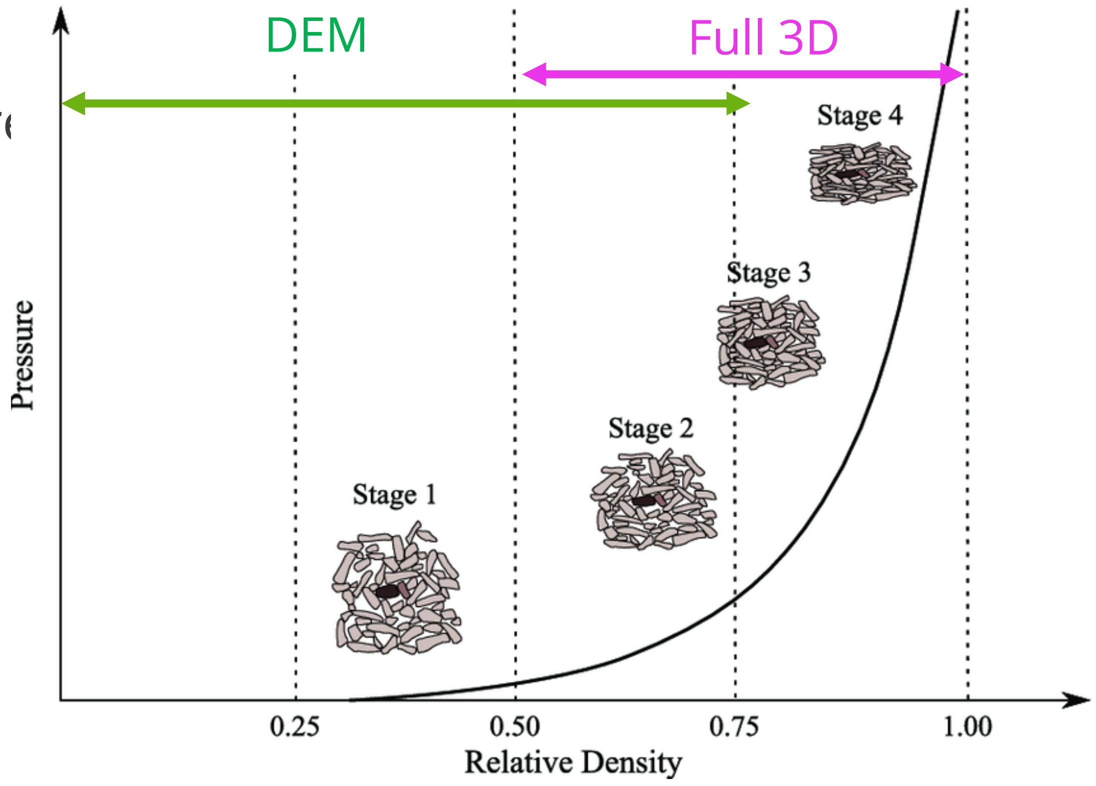
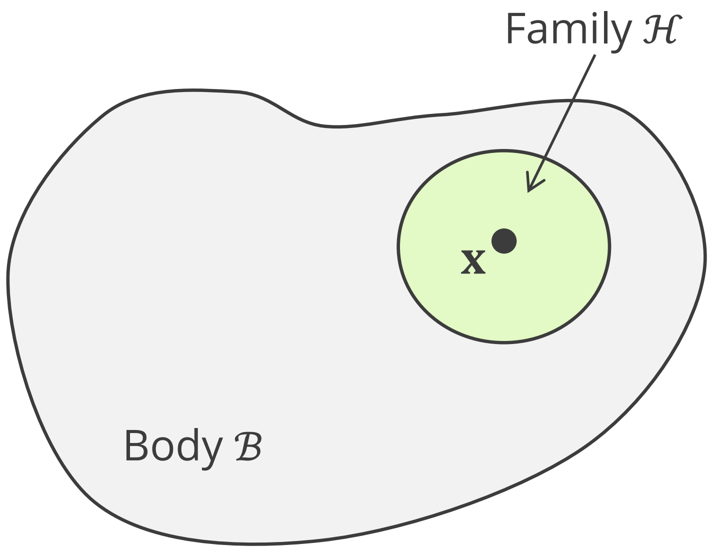
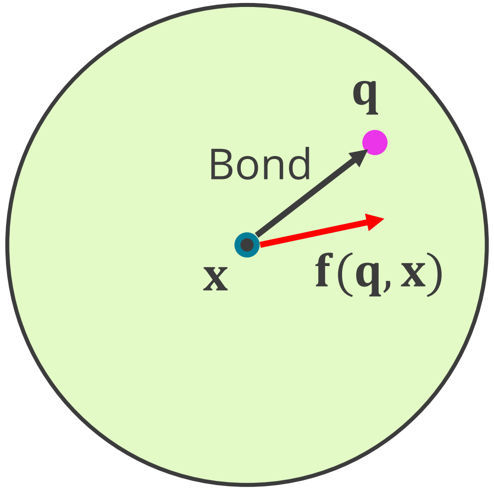


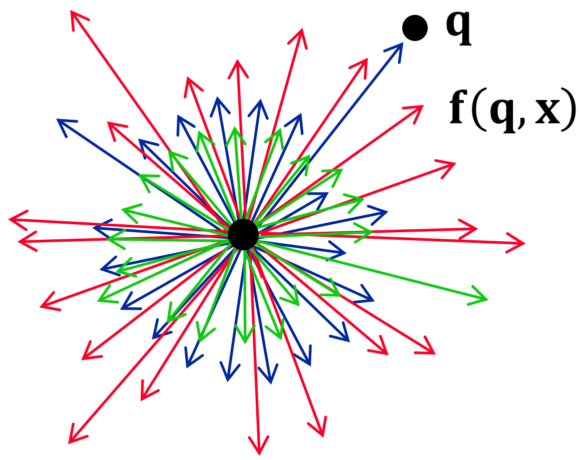
Image: H. Yi et al., 2018, KONA Powder and Particle Journal

Peridynamics: What it is

- It is a generalization of the theory of solid mechanics that allows for discontinuities and long-range interactions.
- Each material point $\mathbf{x}$ interacts with neighbors $\mathbf{q}$ within a cutoff distance δ (the ***horizon***).







Bond forces

- $\mathbf{f}$ is the bond force density (N/m^6).
- Equlibrium:

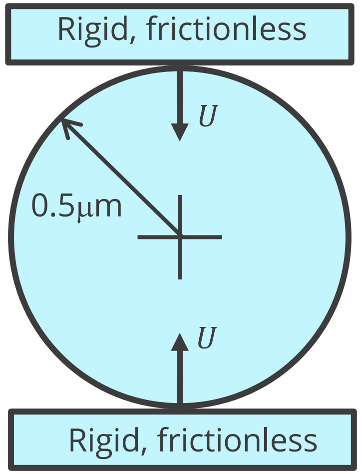
$$\int_{\mathcal{H}} \mathbf{f}(\mathbf{q},\mathbf{x})d\mathbf{q} + \mathbf{b}(\mathbf{x}) = 0$$

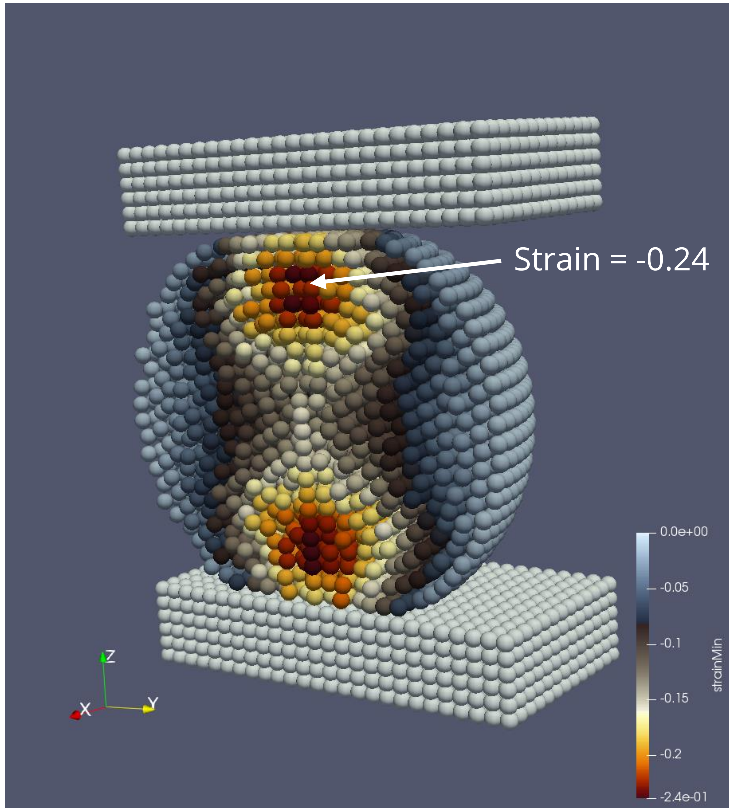
Peridynamics for granular media

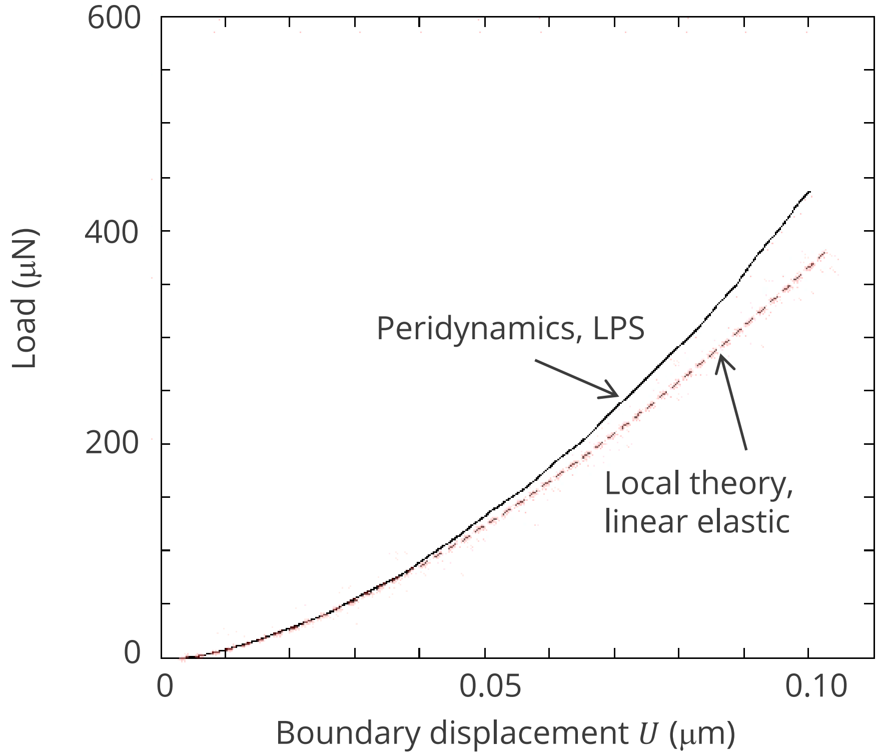
- Irregular shapes
  - Jha, P.K., Desai, P.S., Bhattacharya, D. and Lipton, R., 2021. Journal of the Mechanics and Physics of Solids, 151, p.104376.
  - Bhattacharya, D. and Lipton, R.P., 2021. arXiv preprint arXiv:2108.07212.
  - Zhu, F. and Zhao, J., 2021. Powder Technology, 378, pp.455-467.
- Shock compression (2D)
  - Lammi, C.J. and Vogler, T.J., 2012. In AIP Conference Proceedings (Vol. 1426, No. 1, pp. 1467-1470). American Institute of Physics.
  - Behzadinasab, M., Vogler, T.J., Peterson, A.M., Rahman, R. and Foster, J.T., 2018. Journal of Dynamic Behavior of Materials, 4(4), pp.529-542.
- Brittle single grains
  - Zhu, F. and Zhao, J., 2019. Géotechnique, 69(6), pp.526-540.
- Rheological behavior of large numbers of grains
  - Xu, T. and Jin, Y.C., 2021. Journal of Fluid Mechanics, 917.

Single grain modeling with peridynamics

- Linear peridynamic solid (LPS)
- Hertzian contact

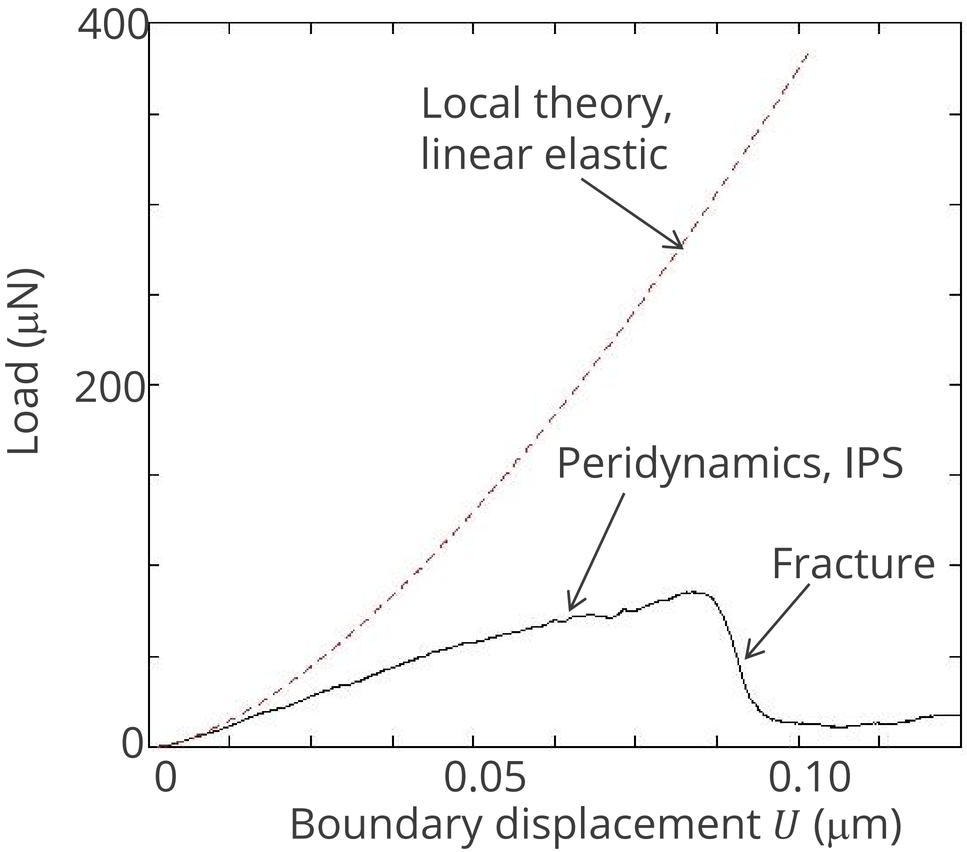


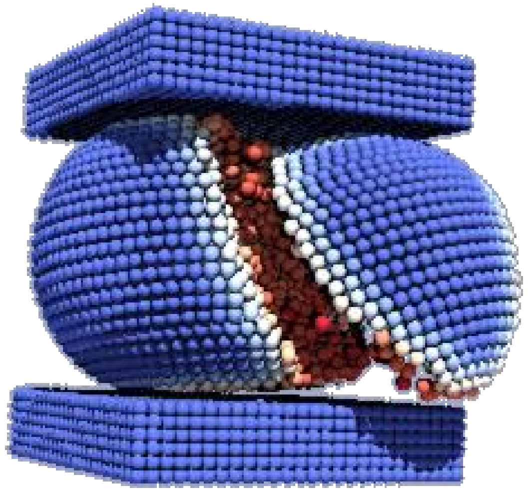




Single grain peridynamic modeling

- Inelastic state-based material model

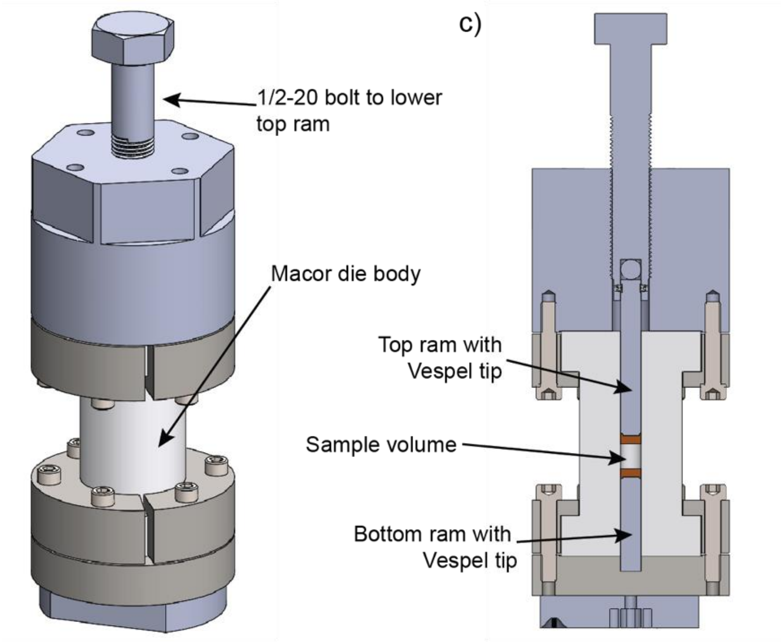


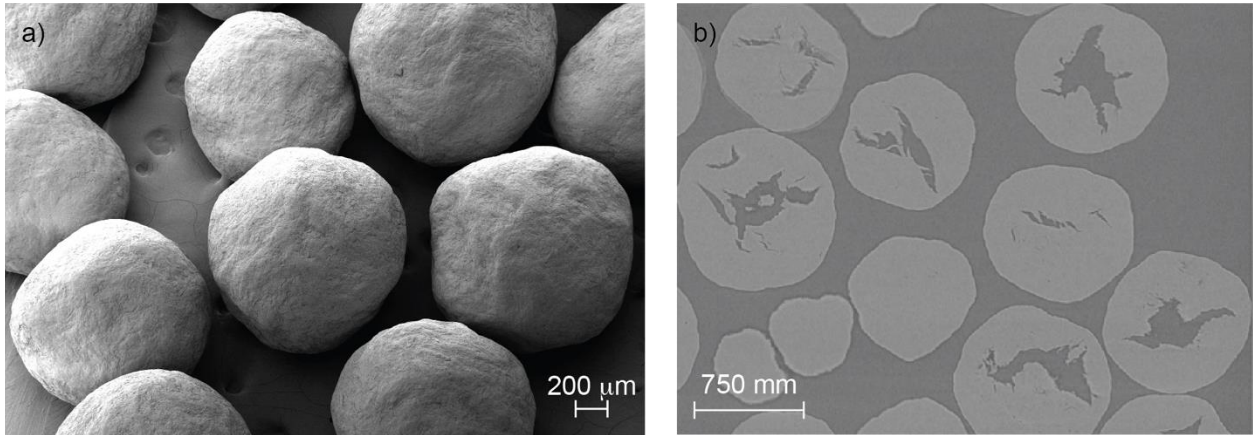


Colors show damage

Detailed modeling of a compaction experiment

- Microcrystalline cellulose (MCC), 1.0mm diameter.

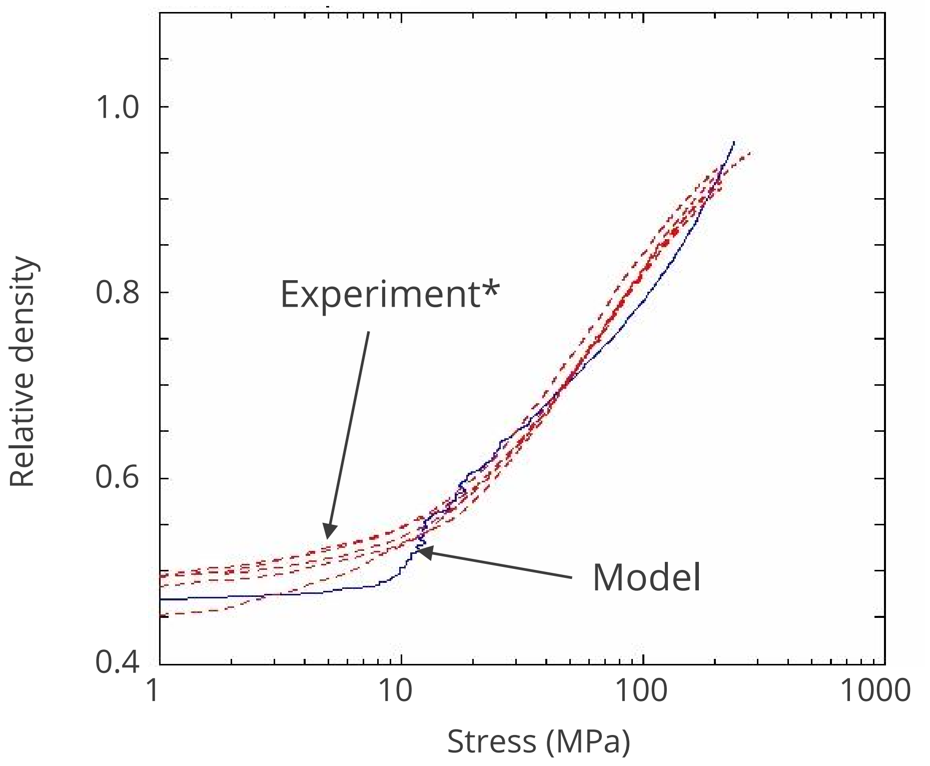




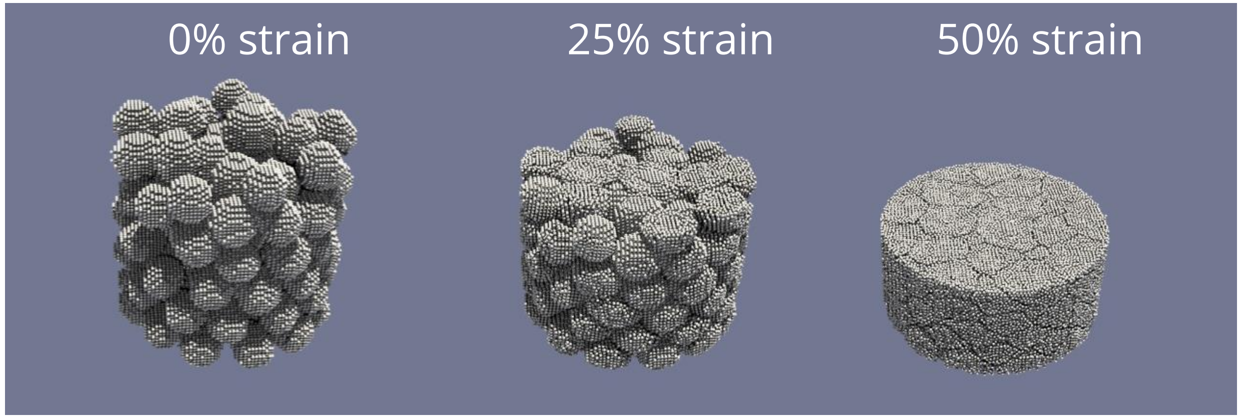
M.A. Cooper et al., 2022, “Mesostructure Evolution During Powder Compression: Micro-CT Experiments and Particle-Based Simulations”, In Thermomechanics & Infrared Imaging, Inverse Problem Methodologies, Mechanics of Additive & Advanced Manufactured Materials, and Advancements in Optical Methods & Digital Image Correlation, Volume 4 2022 (pp. 15-22).

Detailed modeling of compaction

Density vs. stress during compression



Peridynamic simulation



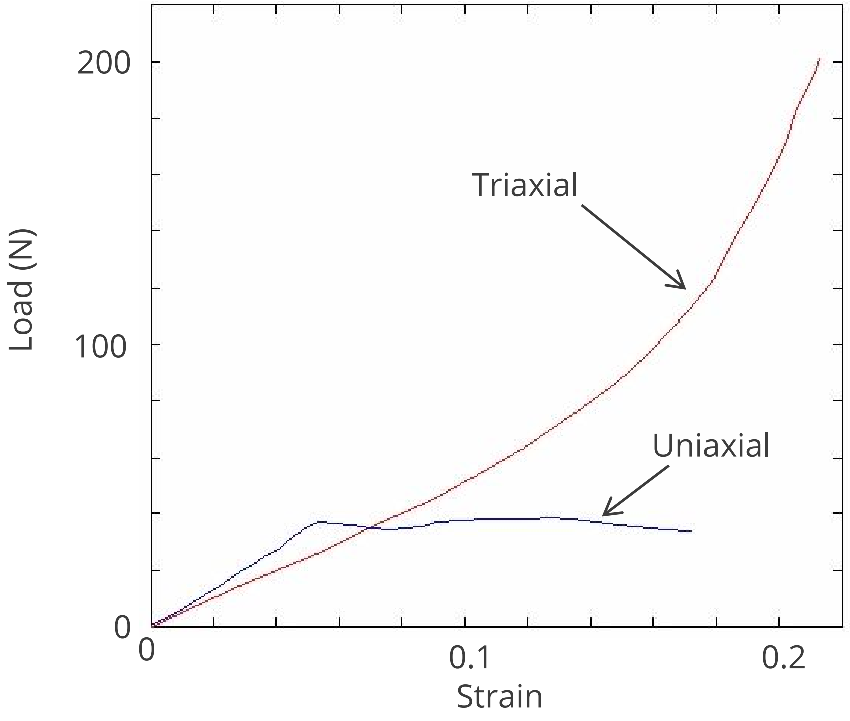
*M.A. Cooper et al., 2022, "Mesostructure Evolution During Powder Compression: Micro-CT Experiments and Particle-Based Simulations", In Thermomechanics & Infrared Imaging, Inverse Problem Methodologies, Mechanics of Additive & Advanced Manufactured Materials, and Advancements in Optical Methods & Digital Image Correlation, Volume 4 2022 (pp. 15-22).

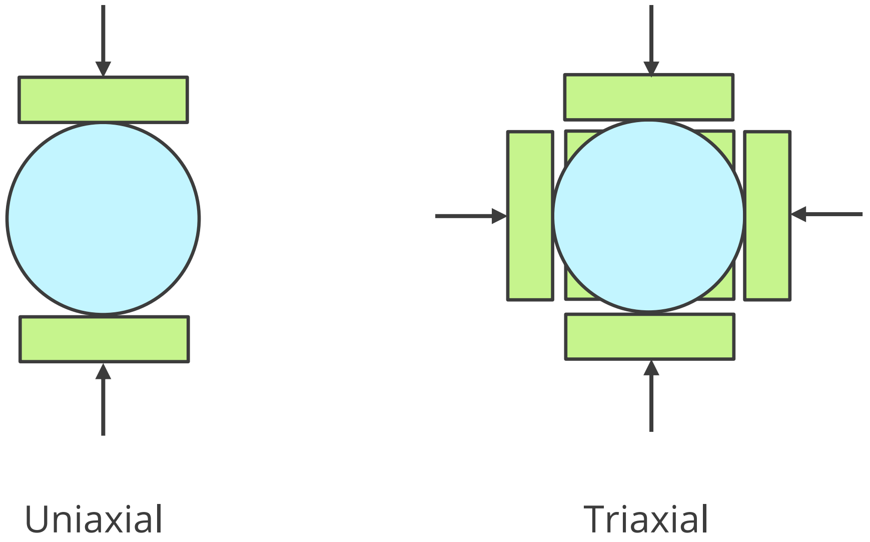
Limits of detailed modeling and another idea

- Too expensive!
- For some applications we want to model many thousands or even millions of grains.
- Instead try to use peridynamics to calibrate a new **high-stress discrete element** (DEM) model.

Need for multipoint interactions in DEM

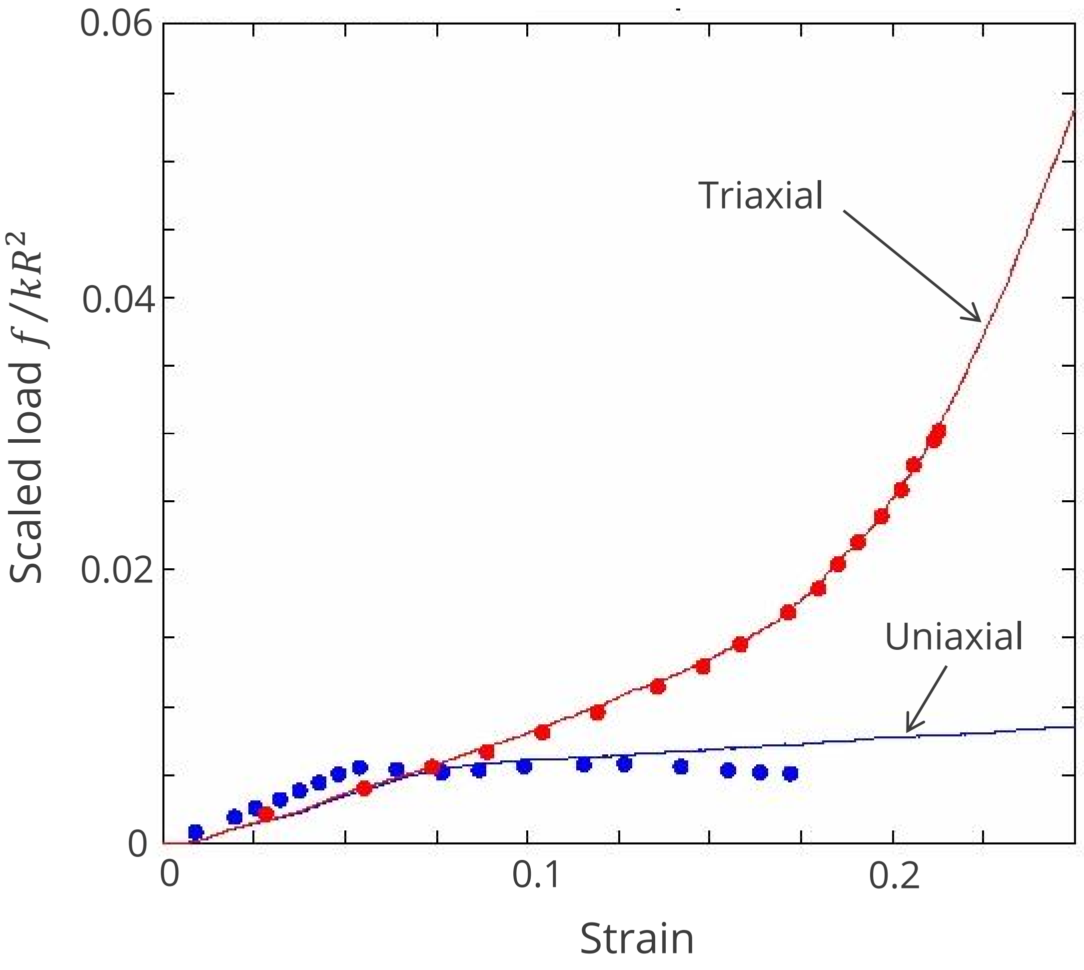
- Traditional DEM assumes each pair of elements has a force independent of all the others.
- Experiments* show this assumption is no good at high stress.
  - Triaxial response of a single MCC grain is much different from uniaxial.

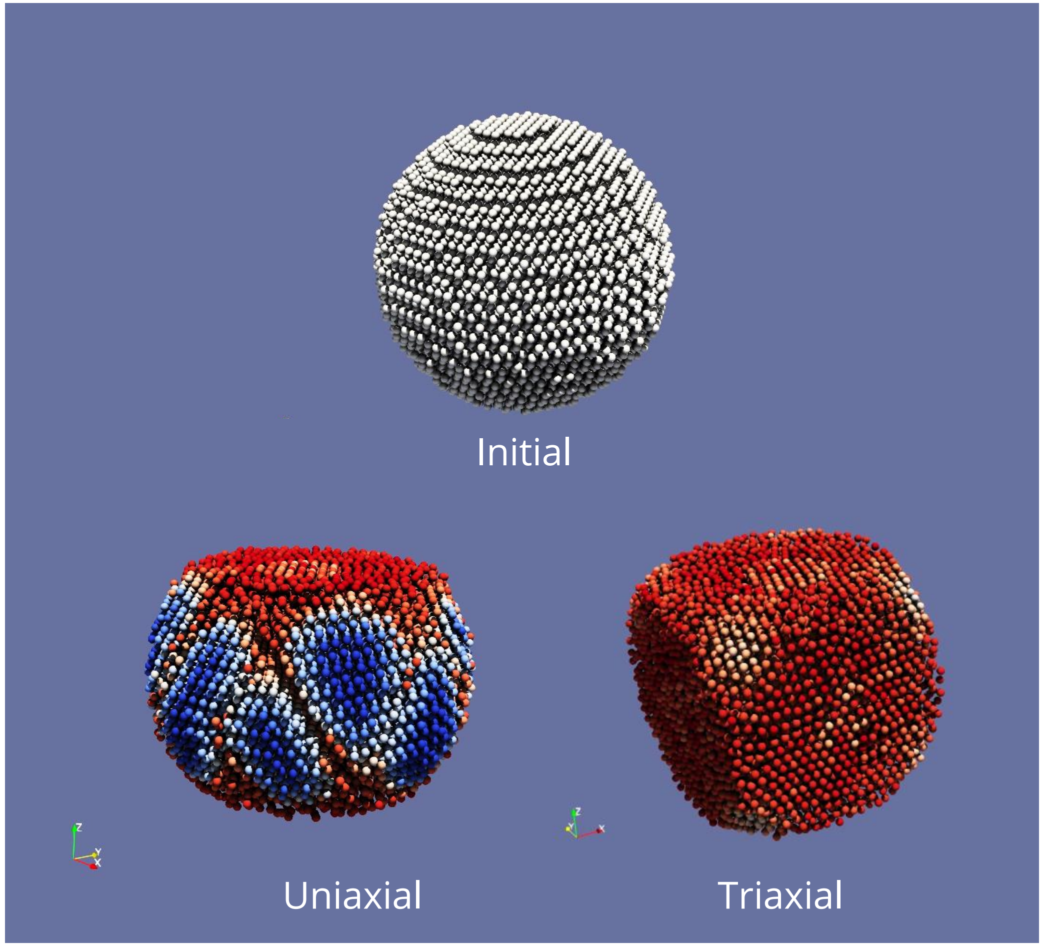




*H. Jonsson and G. Frenning. 2016, “Investigations of single microcrystalline cellulose-based granules subjected to conned triaxial compression.” *Powder Technology*

Single grain simulations capture effect of triaxiality





Proposed multipoint DEM model

- Energy of each grain i with current position $\mathbf{x}_i$:

$$E_i = \hat{E}_i(\mathbf{r}_{1i}, \mathbf{r}_{2i}, \dots, \mathbf{r}_{Ni}), \qquad \mathbf{r}_{ji} = \mathbf{x}_j - \mathbf{x}_i.$$

- Total potential energy under external load $\mathbf{b}_i$:

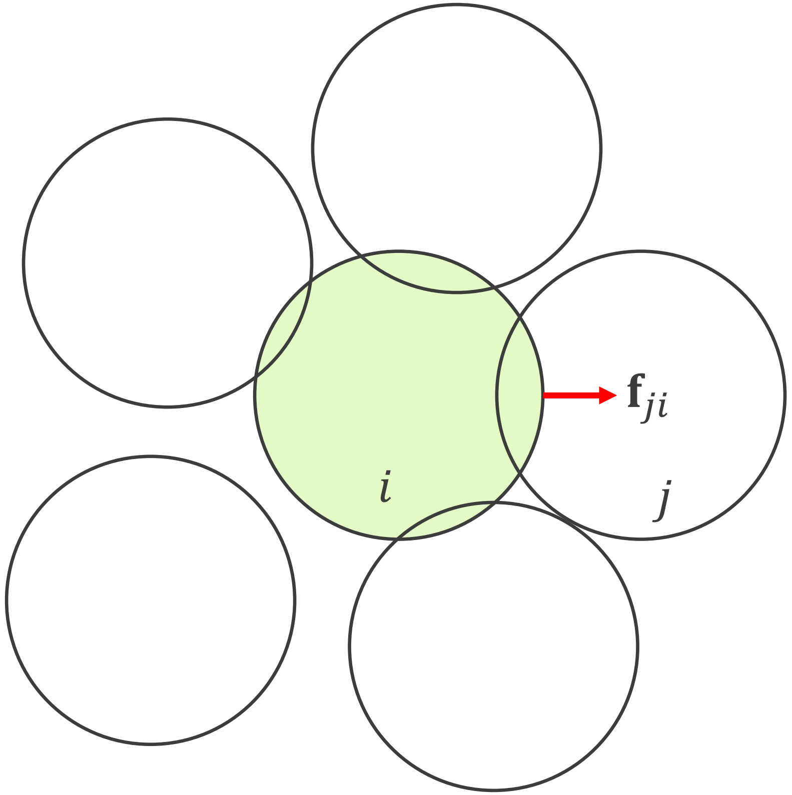
$$\Phi = \sum_i (E_i - \mathbf{b}_i \cdot \mathbf{x}_i)$$

- Stationary Φ in equilibrium. Euler-Lagrange equation is

$$\sum_j (\mathbf{f}_{ji} - \mathbf{f}_{ij}) + \mathbf{b}_i = \mathbf{0}, \qquad i = 1, 2, \dots, N$$

where

$$\mathbf{f}_{ji} = \frac{\partial \hat{E}_i}{\partial \mathbf{r}_{ji}}, \qquad \mathbf{f}_{ij} = \frac{\partial \hat{E}_j}{\partial \mathbf{r}_{ij}}.$$

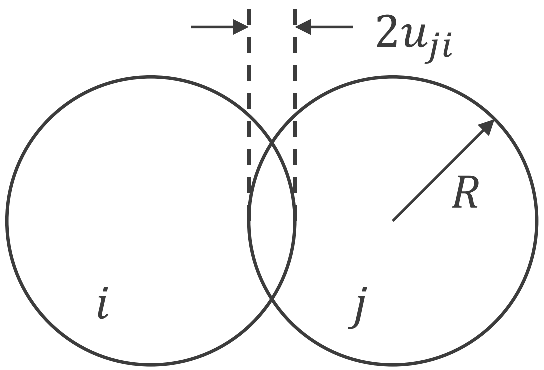


Each $\mathbf{f}_{ji}$ can depend on all the contact displacements.
Very similar to molecular dynamics.

Proposed multipoint DEM model, ctd.

- Define the overlap displacement and strains:

$$
\begin{aligned}
u_{ji} &= R - \frac{r_{ji}}{2} && \ldots \text{displacement of the contact point,} \\
\epsilon_{ji} &= \frac{u_{ji}}{R} && \ldots \text{strain,} \\
\xi_{ji} &= \max\{0, \epsilon_{ji}\} && \ldots \text{compressive strain.}
\end{aligned}
$$



- Dilatation-like variable:

$$\theta_i = \sum_j \xi_{ji}$$

- Effective dilatation that accounds for bulging:

$$\eta_{ji} = \max\{0, \epsilon_{ji} + \beta\theta_i\}$$

where β is a constant that is conceptually similar to a Poisson ratio.

Proposed multipoint DEM model, ctd.

- Force from j on i due to multipoint contact:

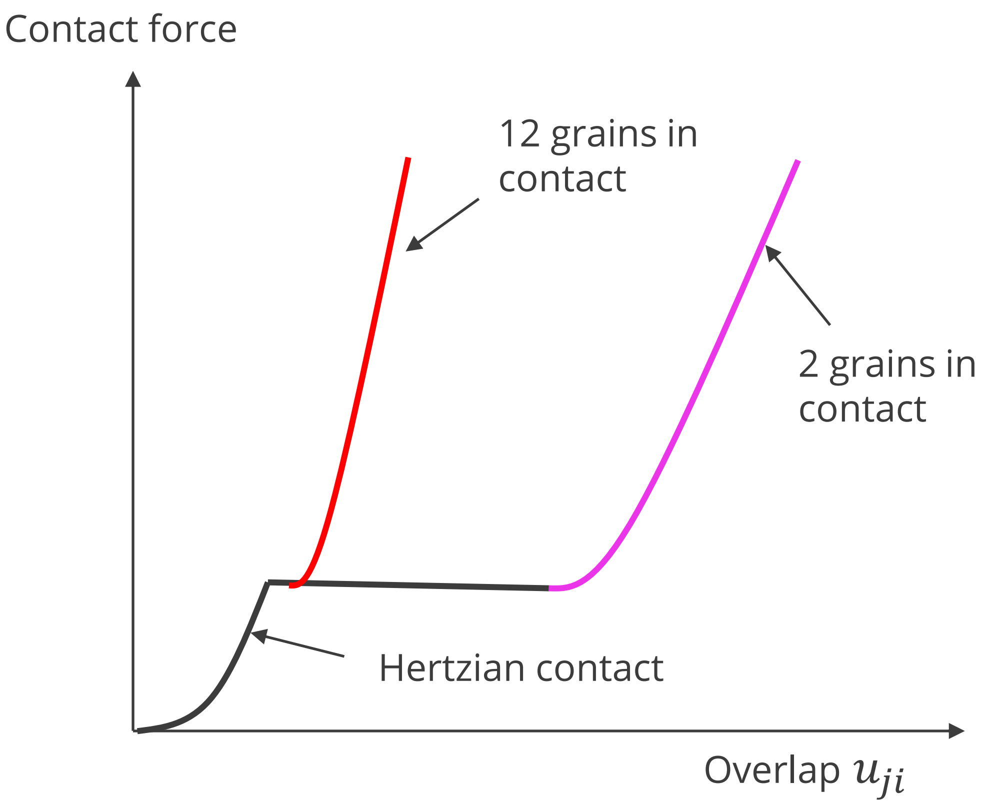
$$f_{ji} = AkR^2\tau^m\eta_{ji}^p$$

  where

$$\tau = \sum_j \eta_{ji}^{p+1}$$

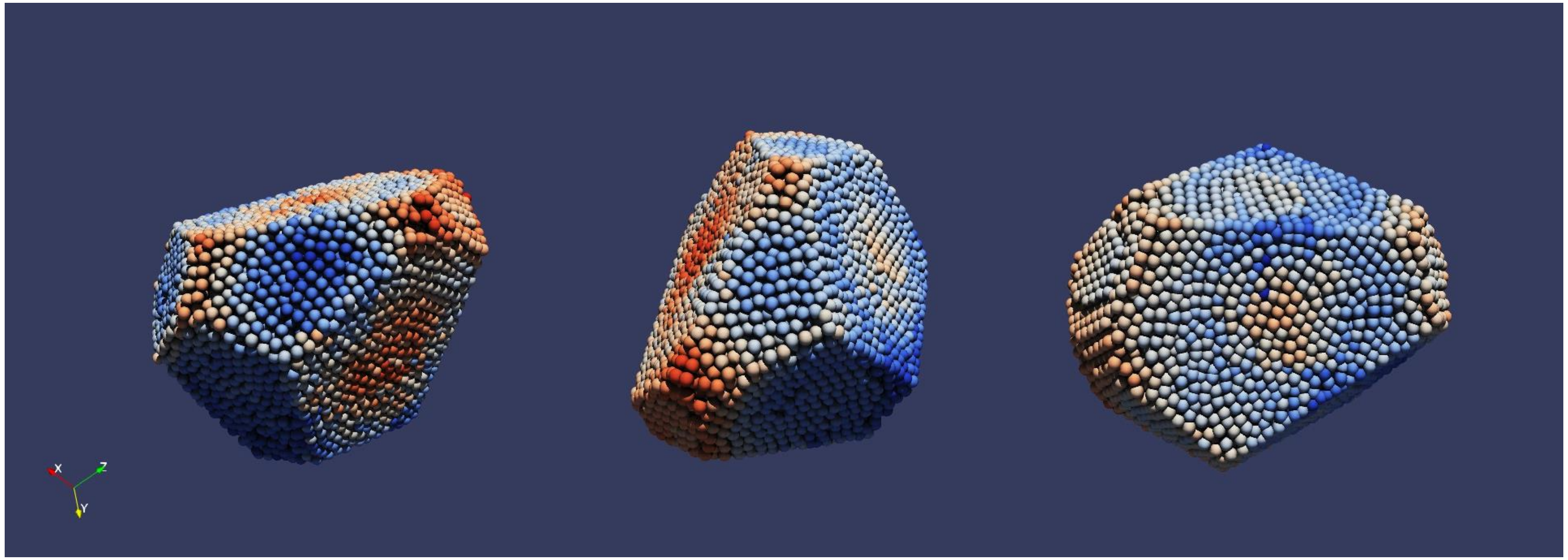
  and A, m, and p are constants. k is the bulk modulus.

- $AkR^2\tau^m$ is like a hydrostatic pressure.
- η_{ji}^p distributes this pressure among the grains in contact with i.
- There is also a conventional pair (Hertzian) interaction term.



Calibration

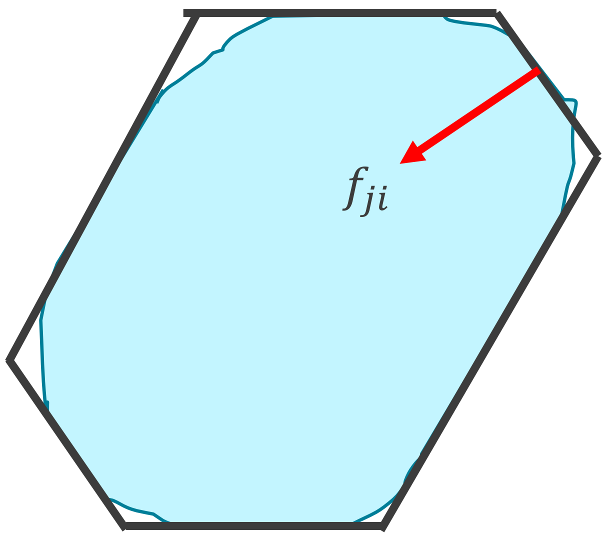
- Use peridynamic detailed grain simulations of a sphere confined by 12 plates moving radially at different rates.
- There is a direct procedure to find A, p, m from the results.



3D simulations of an initially spherical grain
Colors show displacement magnitude

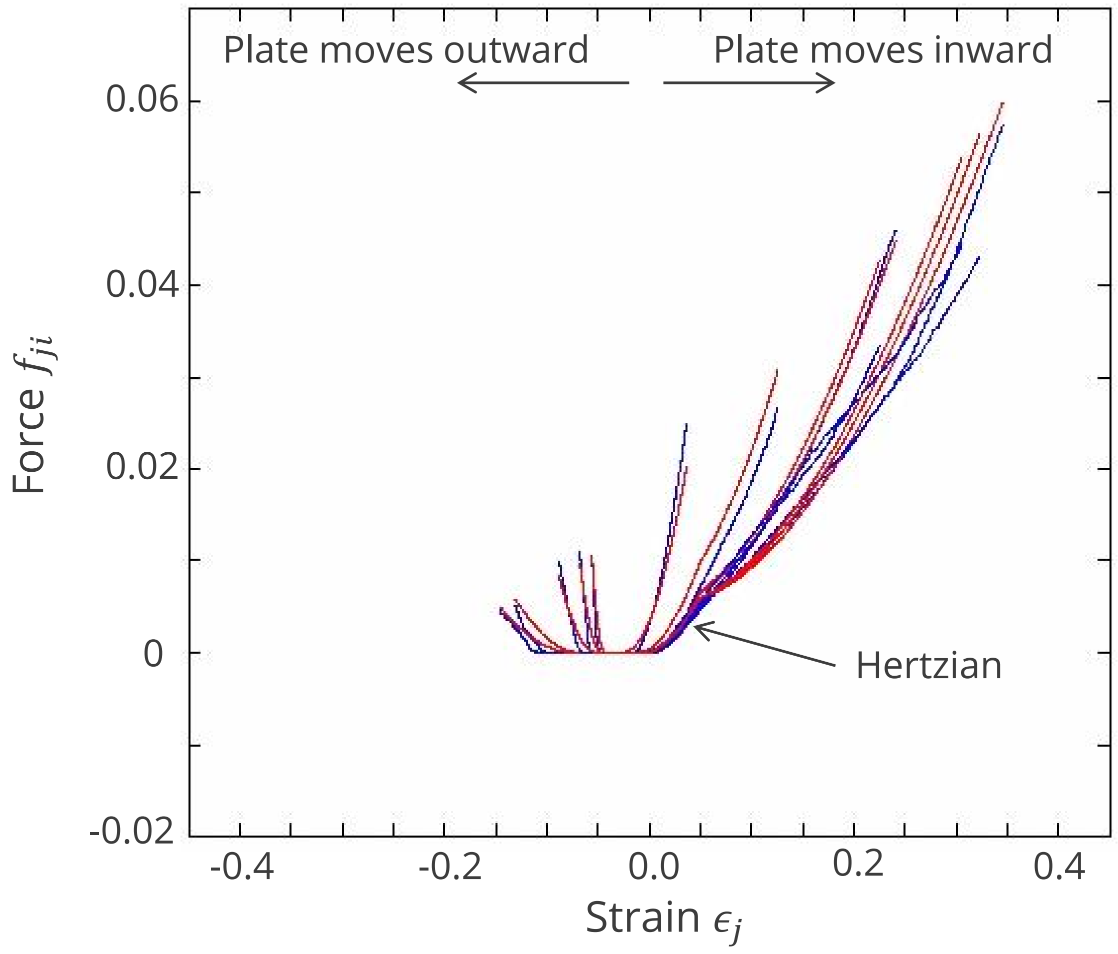
Comparison of new DEM model with detailed 3D

- The two main nonlinear effects are captured:
  - Pressure vs. compression within a grain.
  - Competition among the plates for surface area.



Contact force vs. plate position

Red=DEM model Blue=Full 3D model

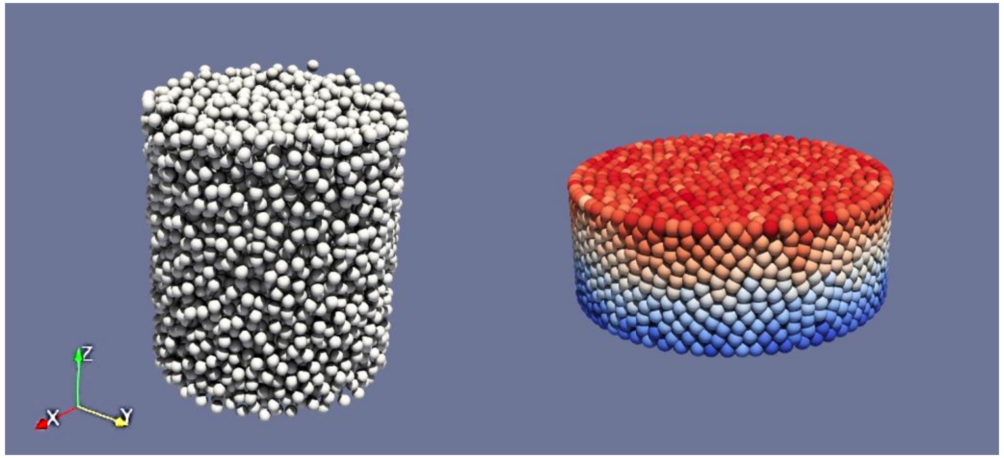


Validation: Bulk powder compaction with DEM

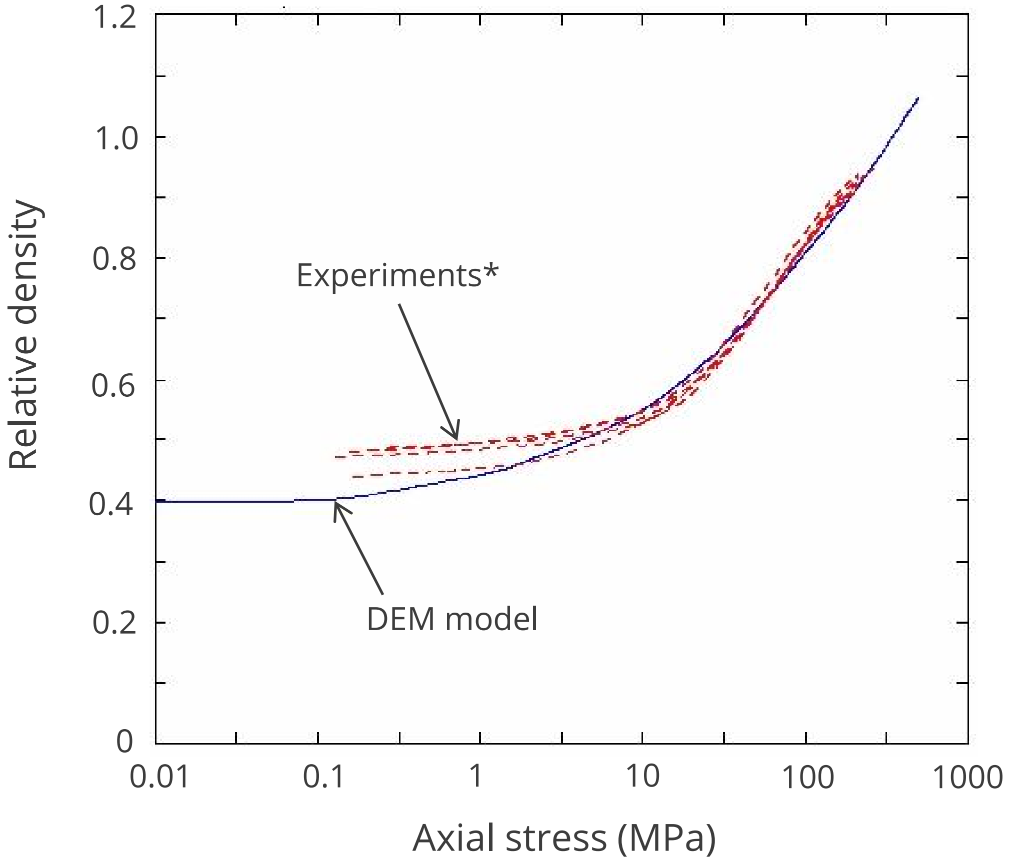
- MCC powder
- Random initial grain positions
- Friction is included as a drag term

Simulation with new DEM model

Colors show axial displacement



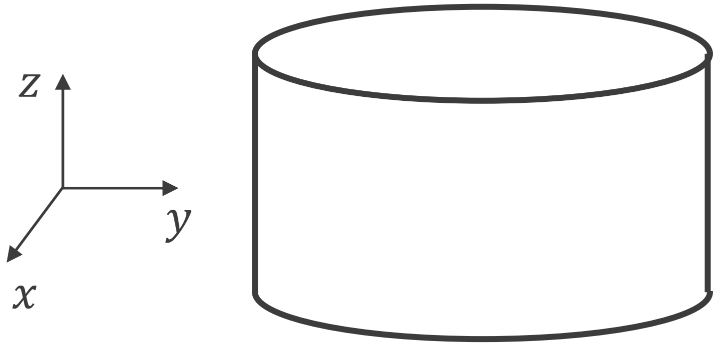
Density vs. stress during compaction

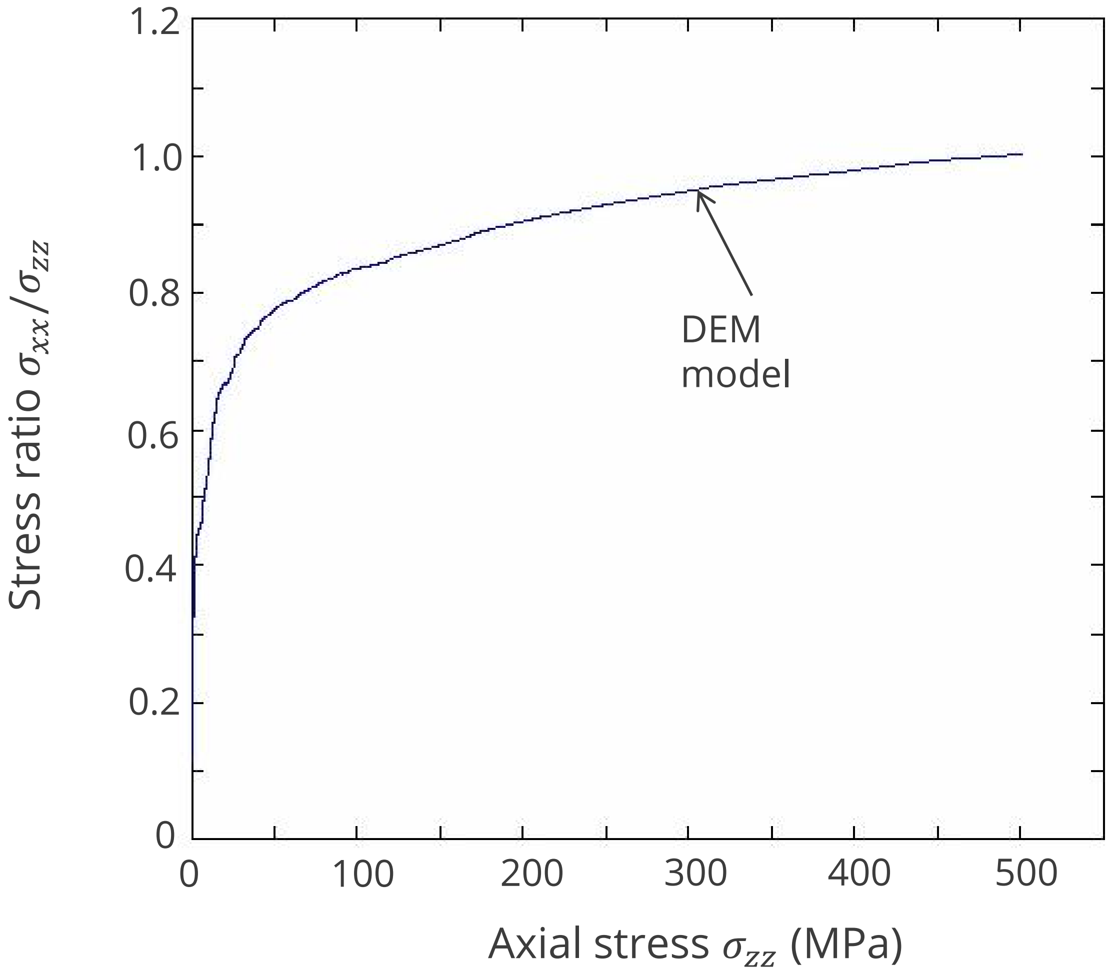


*M.A. Cooper et al., 2022

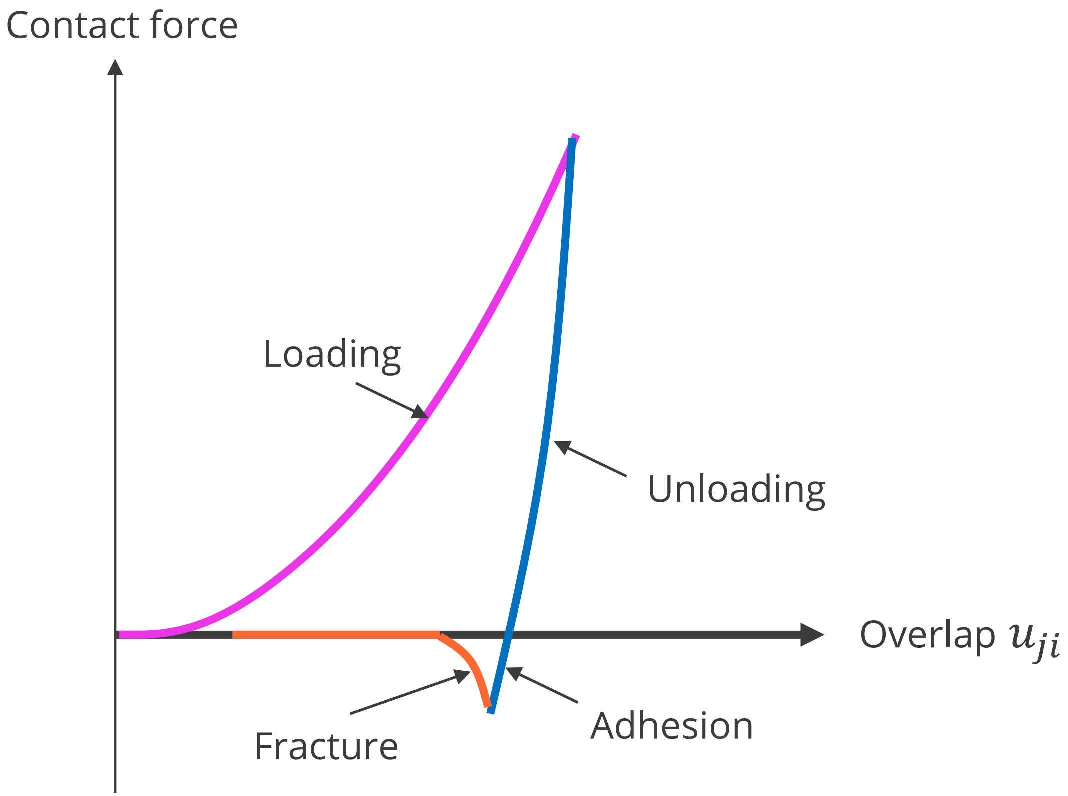
Poisson effect during compaction

- MCC powder
- Ratio of lateral to axial stress changes
- Fluid-like stress state at high compression

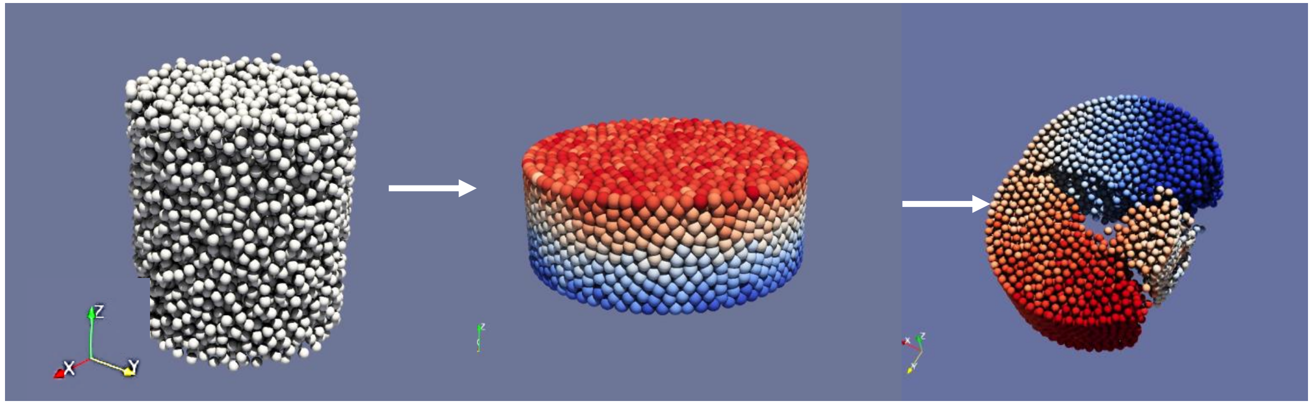


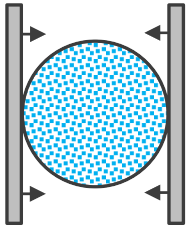


Can add unloading effects to the DEM interactions



Compaction followed by Brazilian test on compact





New model is (almost) a special case of state-based PD

- Compare the above DEM momentum balance

$$\sum_j (\mathbf{f}_{ji} - \mathbf{f}_{ij}) + \mathbf{b}_i = \mathbf{0}, \qquad i = 1, 2, \ldots, N$$

with the momentum balance for state-based peridynamics:

$$\int_{\mathcal{H}} \Big(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{q} - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{q}]\langle \mathbf{x} - \mathbf{q} \rangle \Big)\, \mathrm{d}\mathbf{q} + \mathbf{b}(\mathbf{x}) = \mathbf{0}.$$

- Similar structure: vector difference of gradients of potential energy at material points.

- Main difference: DEM uses Eulerian coordinates, PD Lagrangian.

Summary

- We used peridynamics 3 ways:
  - Full 3D model of powder compaction
  - State-based PD model (in effect) of multipoint DEM interaction forces
  - Calibration of the DEM model with 3D grain-scale simulations