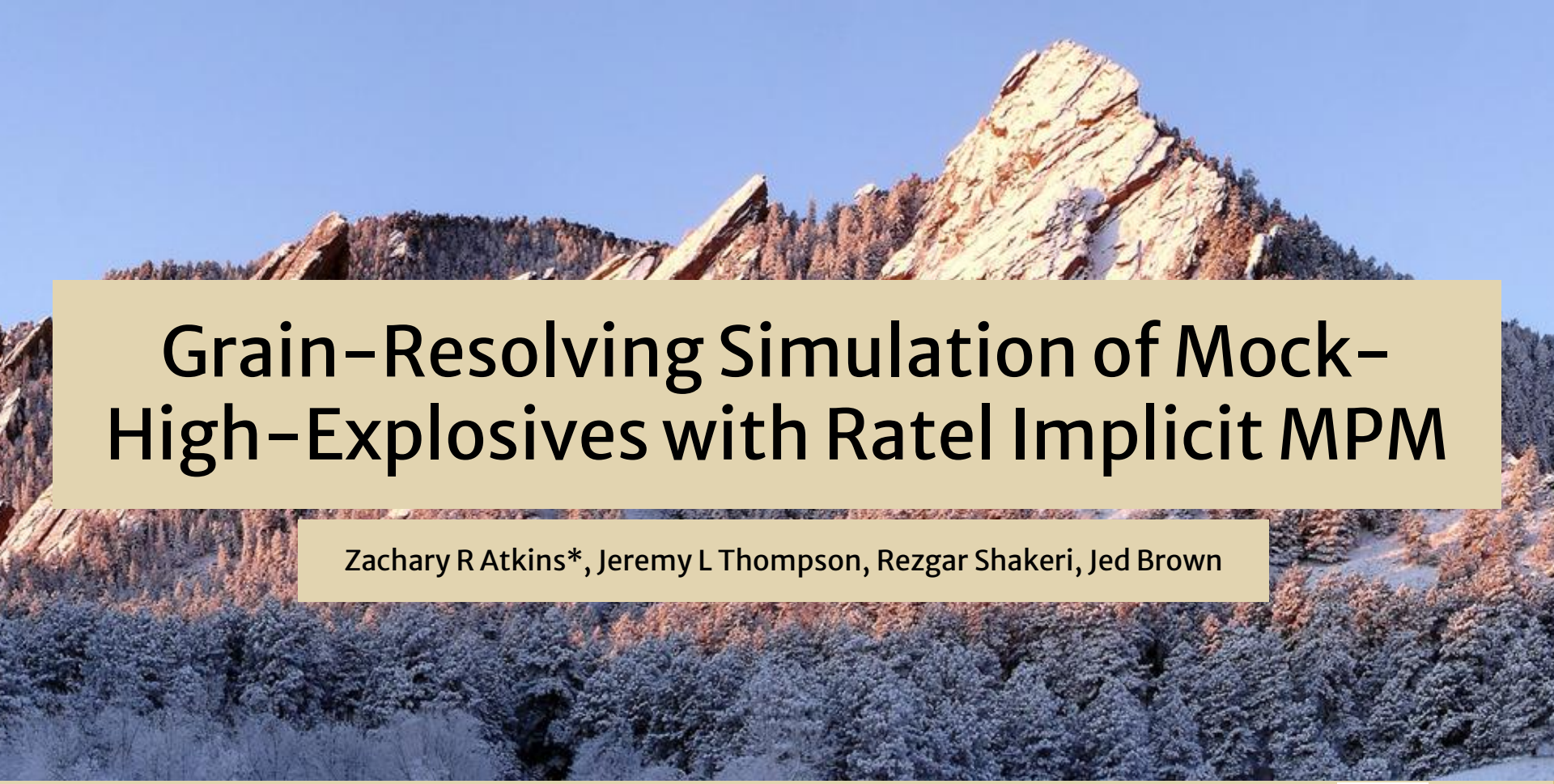

Grain-Resolving Simulation of Mock-High-Explosives with Ratel Implicit MPM

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Outline

- Mock-HE Manufacturing Problem
- Implicit Material Point Method Formulation
- Challenges with Grain-Resolving Scale

Mock-High Explosive (HE) Manufacturing

- **Grains** of mock-HE crystals (IDOX) are coated with a nitro-plasticized polymer **binder** (Estane) to form **prills**
- By volume, each prill is 95% grain, 5% binder
  - This will be an issue in a few slides!

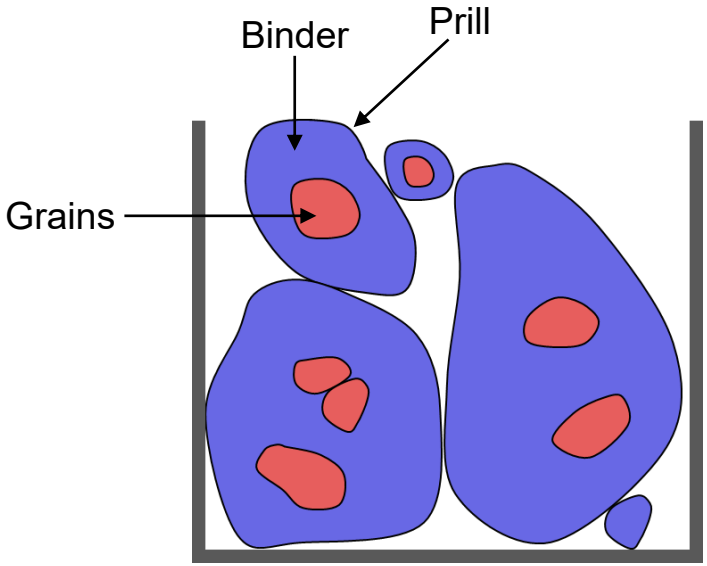

Image credits: Zachary White, CU Boulder

Mock-High Explosive (HE) Manufacturing

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- By volume, each prill is 95% grain, 5% binder
  - This will be an issue in a few slides!
- Prills are poured into a 5mm diameter cylindrical die, 8.5mm high unpressed
  - At this point, prills are *very* loosely packed – about 30% void
- Compressed to 3kPa loading force, ~5mm height pressed

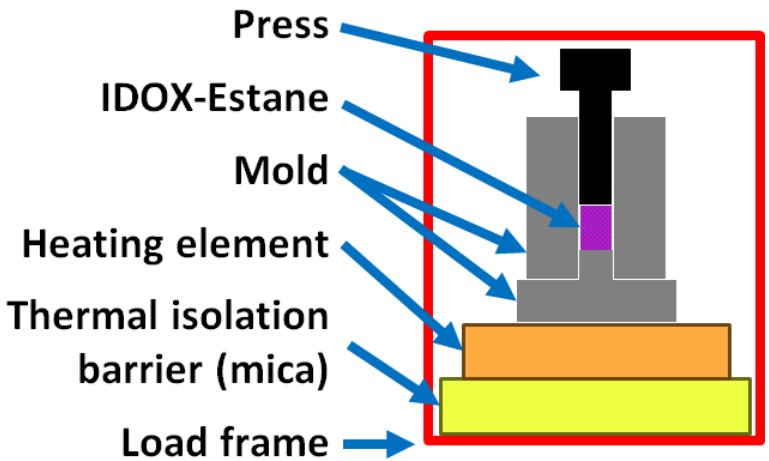
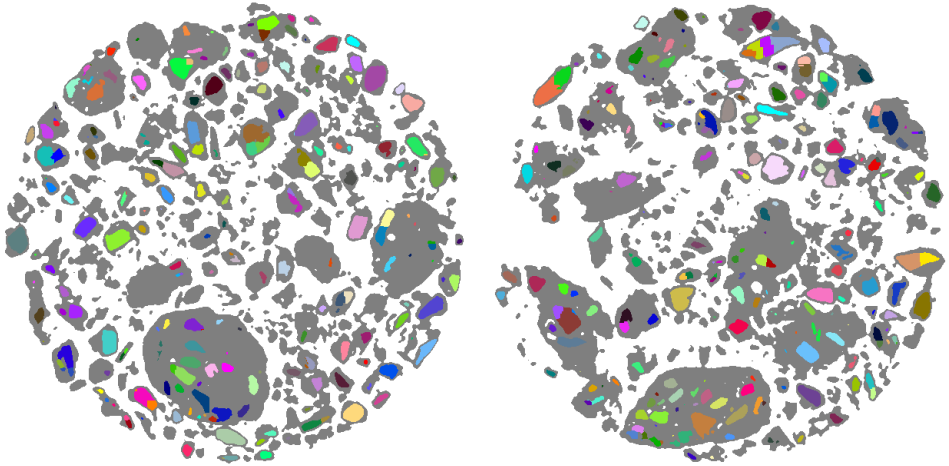


Image credits: Zachary White, CU Boulder; Trevor Lyons, Mines

Resolving Grains – Experimental Data

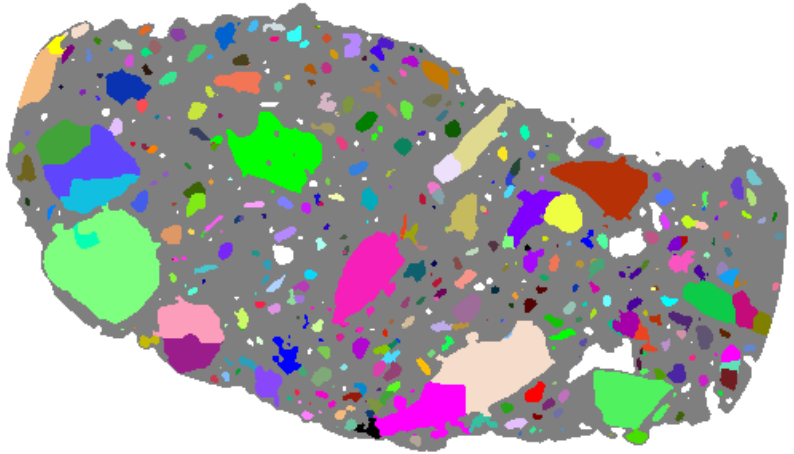
- Before pouring into the die, first pour into a plastic cylinder and perform computed tomography (CT) scan
- After post-processing, have a "stack" of TIFF image files
  - Each pixel is ~8.5um cubed
  - Value of each pixel is
    - 0: Void
    - 1: Binder
    - 2-N: Labeled grain (up to ~14000)
  - Roughly 400 million voxels total
  - We only care about ~290 million voxels



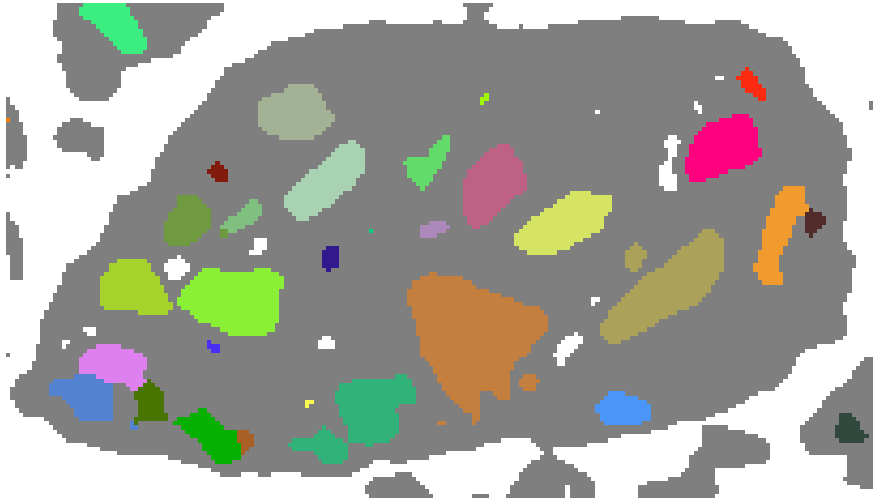
Sample horizontal slices of processed CT data
Gray: Binder, Colors: Grains
Credit: Nate Peterson (Mines), Gus Becker (CU Boulder)

Resolving Grains – Major Issue

- Problem: Where are all the grains?
  - Recall, each prill should be 95% grain, 5% binder



CT data of a real prill (grains still under-resolved)
Gray: Binder, Colors: Grains



Zoomed-in CT data of full press, single prill
Gray: Binder, Colors: Grains

Resolving Grains – Solutions

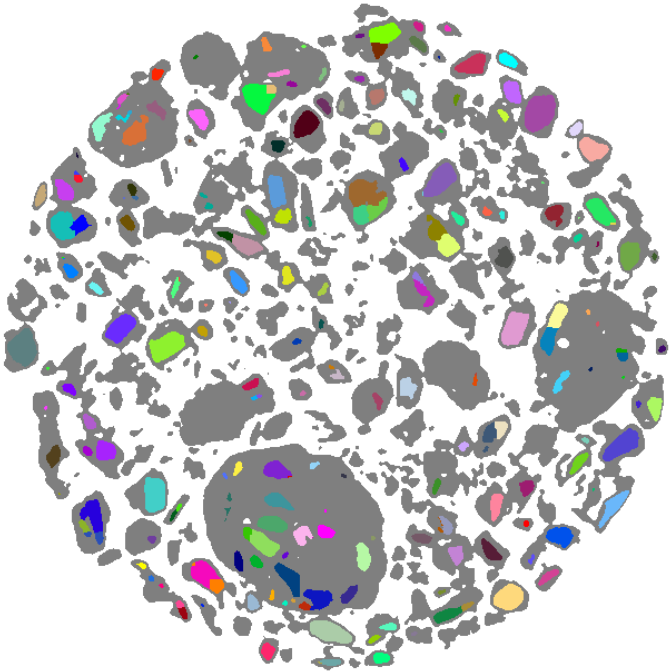
- Current solution: represent Estane binder + fine grains as homogenized material
  - Expect the material properties to be more like the grains
  - Limits our ability to accurately model the binder

- Ongoing work with collaborators:
  - CT scans of individual prills (Trevor Lyons, Mines)
  - Generate artificial prills (Jarett Poliner, Columbia)
  - Simulate a pour of the artificial prills (LAMMPS – Zachary White, CU Boulder)
  - Load simulated pour data into Ratel (Jeremy Thompson & me, CU Boulder)

Why MPM?

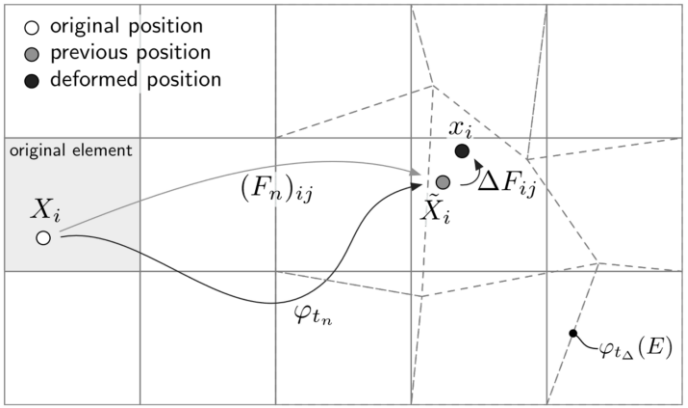
FEM just won't work!

- Highly heterogeneous material
  - Smaller grains cannot be meshed easily
  - Resulting mesh is poorly conditioned and must be smoothed
- Large void regions
  - Likely to cause overlap/inversion of cells
  - Modeling internal contact would be very difficult and expensive
- Very large deformations
  - Need to compress >40% of volume
  - High likelihood of extreme mesh distortion



Implicit MPM Formulation

- Previously-converged Lagrangian (Coombs et al. 2020)
- Currently, quasi-static time discretization



Reframe equilibrium equations to be with respect to $\widetilde{\Omega}$ at time t_n using stored deformation gradient $\boldsymbol{F}_n$

$$\boldsymbol{F} = \tilde{\boldsymbol{F}}\boldsymbol{F}_n, \quad J = \tilde{J}J_n, \quad \Delta\boldsymbol{F} = \tilde{\boldsymbol{F}},$$

$$J = \frac{d\mathrm{v}}{dV}, \quad \tilde{J} = \frac{d\mathrm{v}}{d\tilde{V}}, \quad J_n = \frac{d\tilde{V}}{dV},$$

$$\nabla\boldsymbol{u} = \nabla\boldsymbol{u}_n + \nabla\tilde{\boldsymbol{u}} + \nabla\tilde{\boldsymbol{u}} \cdot \nabla\boldsymbol{u}_n$$

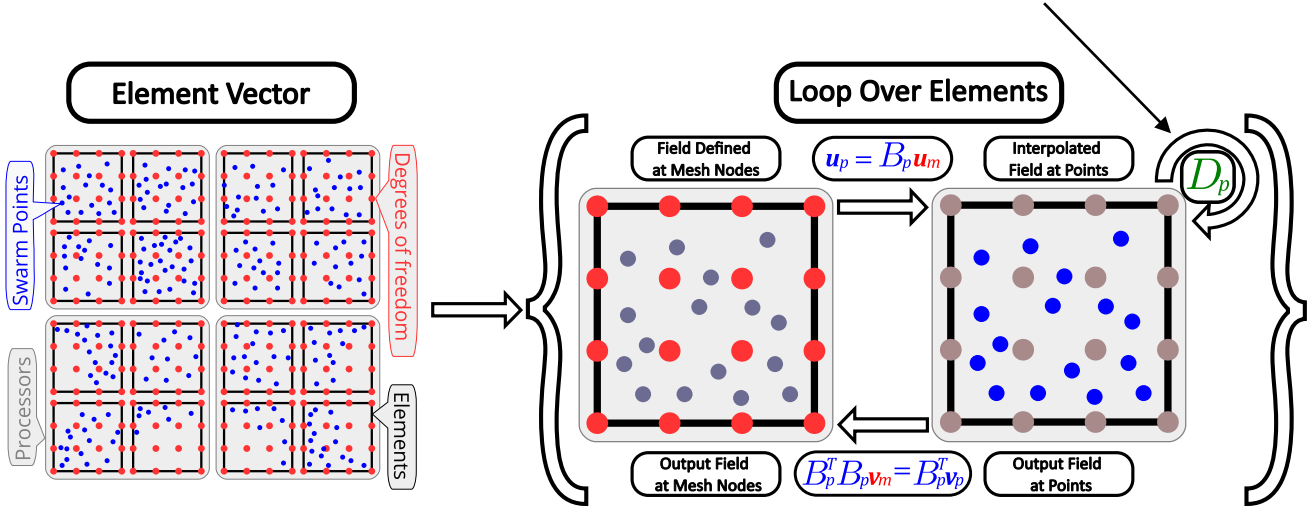
Solve for $\Delta\boldsymbol{u}$ such that

$$r(\Delta\boldsymbol{u}; \boldsymbol{u}_n) \coloneqq \int_{\widetilde{\Omega}} \nabla_{\tilde{X}}\boldsymbol{v} : \underbrace{\frac{1}{J_n}\boldsymbol{\tau}(\nabla\boldsymbol{u}^{\mathrm{p}})\tilde{\boldsymbol{F}}^{-T}}_{\tilde{\boldsymbol{P}}} \, \mathrm{d}\tilde{V} - \int_{\widetilde{\Omega}} \boldsymbol{v} \cdot \frac{1}{J_n}\rho_0\boldsymbol{g} \, \mathrm{d}\tilde{V} = \boldsymbol{0}$$

- We only use traditional material points, due largely to the parallelization strategy

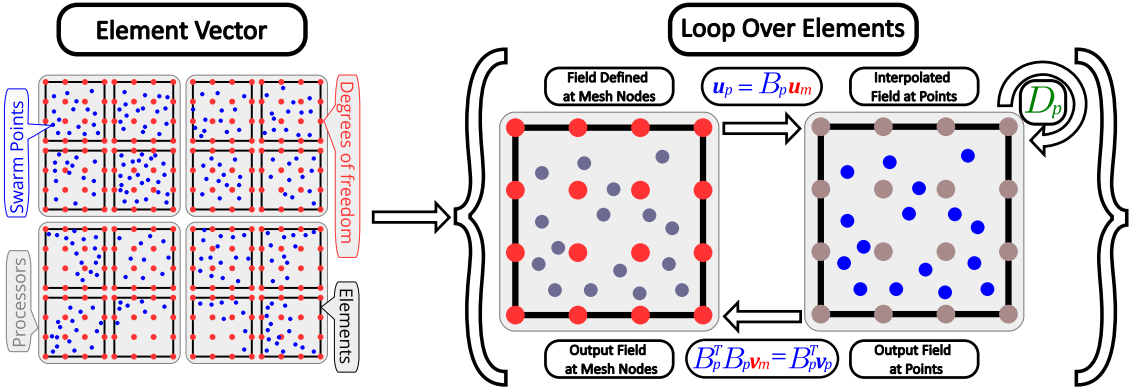
Implicit MPM Formulation

- Each material point must store $\nabla \boldsymbol{u}_n$ (9 components) as well as any state variables
- Constitutive properties, e.g., etc., are also stored per-point
  - E.g., density, bulk and shear moduli, fracture toughness
- Constitutive models are defined by action at a single material point (QFunction)



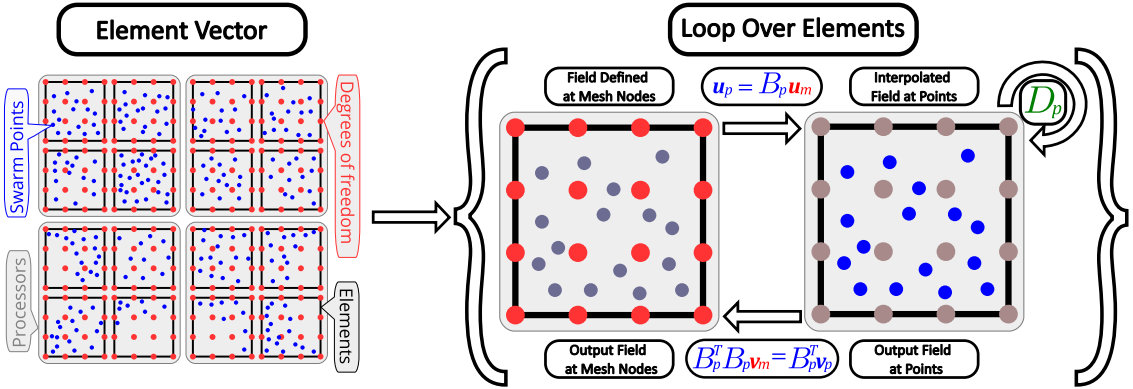
Matrix-Free Operators

- Strategy:
  - Group material points by cell
  - Use FEM basis functions to compute interpolation/gradient at nodes
  - Interpolate to points using Chebyshev interpolating polynomials
  - Apply constitutive model point-wise
  - Apply transpose interpolation operators to recover FEM output fields



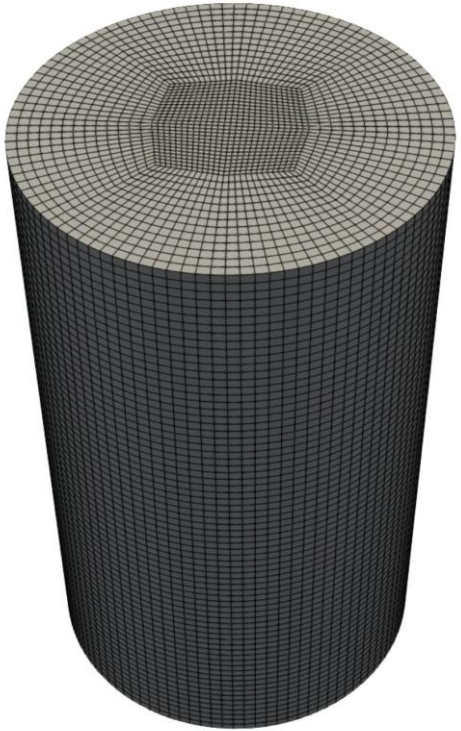
Matrix-Free Operators

- Advantages:
  - Utilizes the same matrix-free infrastructure used for FEM
  - Assembly for preconditioners is nearly identical as FEM
  - Take advantage of memory-limited, high-compute accelerators (i.e. GPUs)
  - Existing FEM constitutive models can be used with minor adjustments for extra stored state and material parameters



Simulation Setup – Meshing and Point Initialization

- Our MPM only supports hex meshes
  - Non-affine hexes are fine, though
- Externally generate a cylinder mesh, GMSH
  - Target an average characteristic length (here, 120 um)
- Place material points uniformly within each cell



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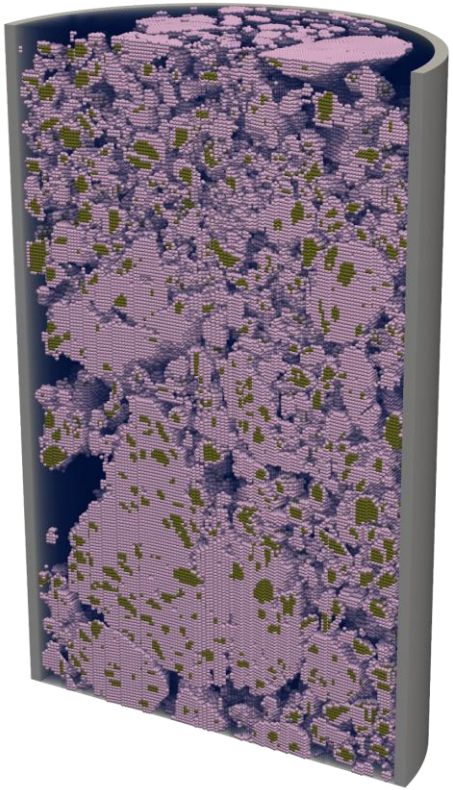
  - Non-affine hexes are fine, though
- Externally generate a cylinder mesh, GMSH
  - Target an average characteristic length (here, 120 um)
- Place material points uniformly within each cell
- Load voxel data into 3D array, one entry per pixel
- Locate each material point's enclosing voxel
  - The voxel size is used to rescale the mesh coordinates
- Set material properties based on the voxel value

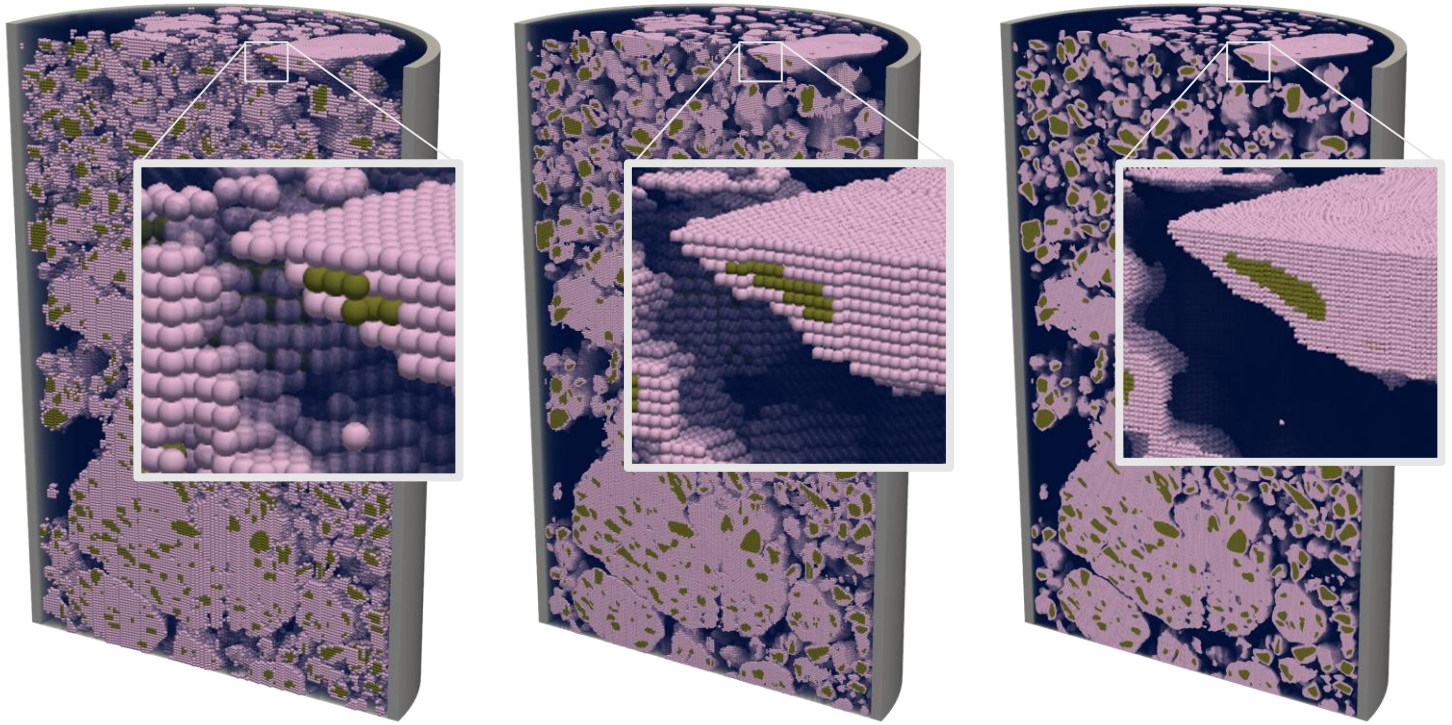


Simulation Setup – Meshing and Point Initialization

3.04 MPoints

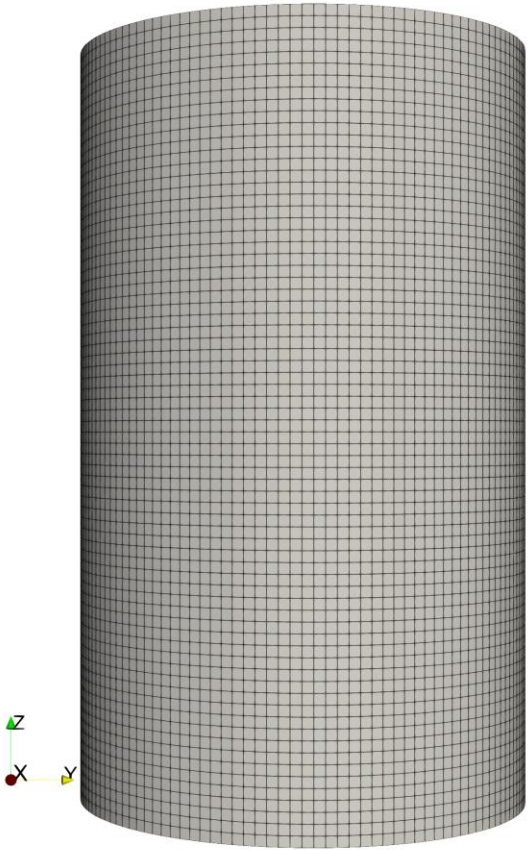
22.7 MPoints

316 MPoints



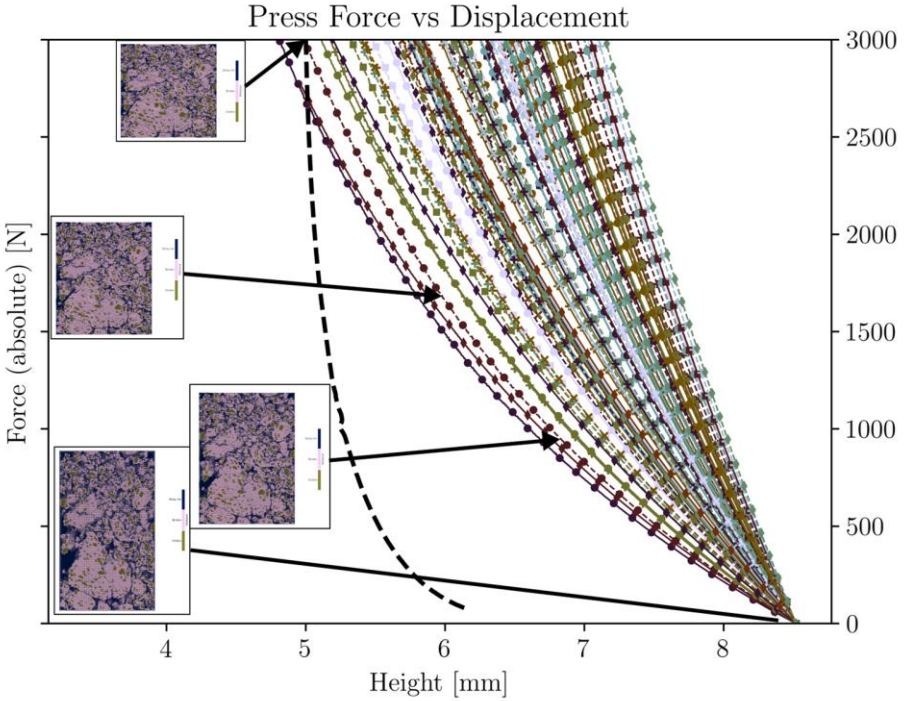
Boundary Conditions

- Ideally, we would use traction boundaries
  - This would ensure that we reach (and stop at) 3kPa
- But…traction boundaries are difficult to apply once points leave the boundary cells
  - Future work
- Instead, we use incrementally applied Dirichlet boundaries – outside and bottom are fixed
- Top is fixed in x-y directions and displaced by fixed increment in z
  - At the end of timestep, the mesh is transformed by the same increment



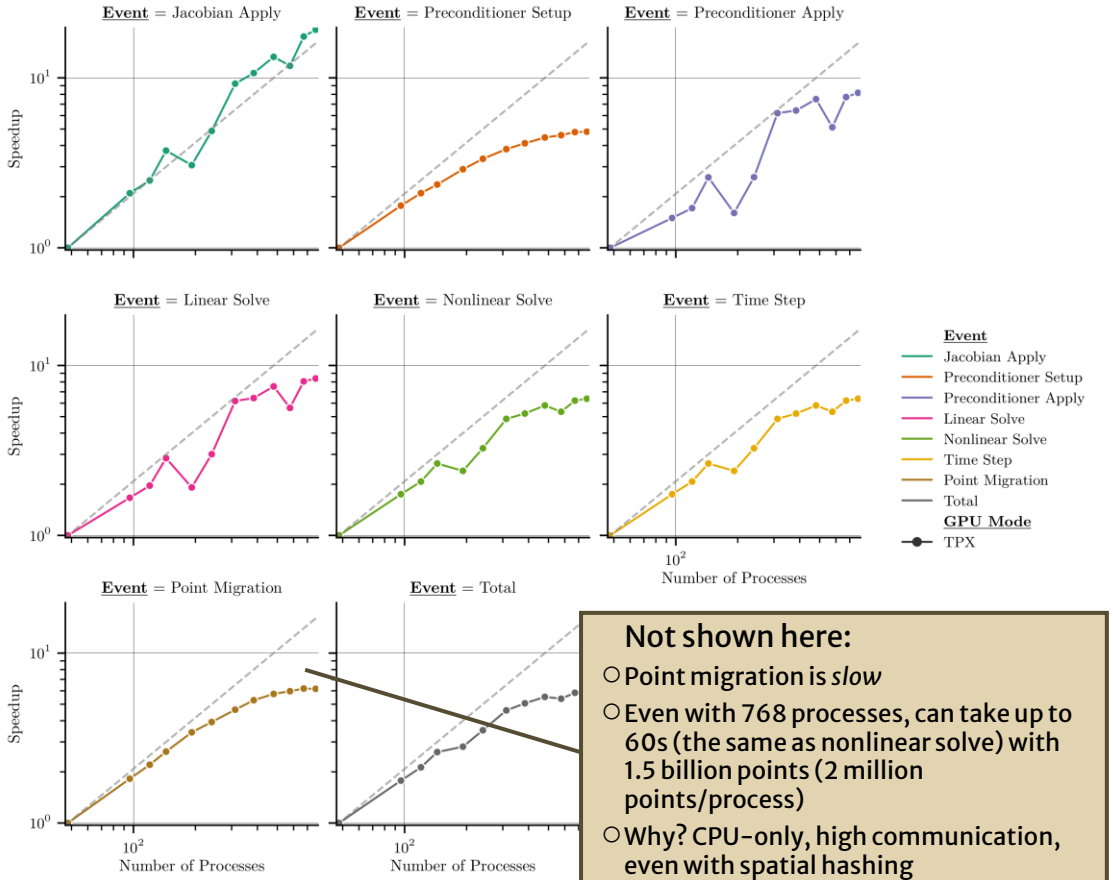
Quantities of Interest

- Force-Displacement, expect:
  - Compress ~40% to 5mm height
  - Peak loading force of 3kPa
- Determine:
  - Young's Modulus E for grains
  - Young's Modulus E for binder
- Want to add:
  - Viscoelastic parameters
  - Fracture toughness for phase-field damage
  - Plasticity (yield strength, etc.)



Performance

- Strong scaling
  - 400 million points
  - AMD MI300A APUs, 3 LGPUs/GPU, XNACK=1
  - 4–64 Tuolumne Nodes
- Solver configuration
  - PETSc GAMG multigrid preconditioner
  - PETSc BCGS(2) linear solver
  - PETSc Newton nonlinear solver, bisection line search
- Results
  - Matrix-free operators scale great
  - Preconditioner and point migration, not so much

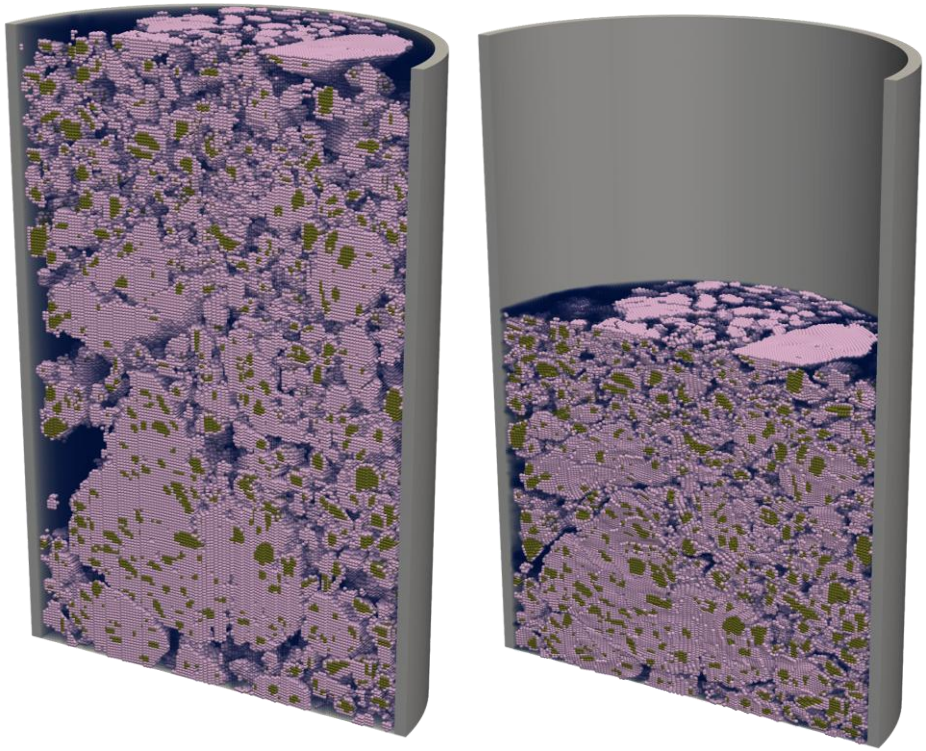


Not shown here:

- Point migration is *slow*
- Even with 768 processes, can take up to 60s (the same as nonlinear solve) with 1.5 billion points (2 million points/process)
- Why? CPU-only, high communication, even with spatial hashing

Challenges in Modeling

- Large voids
  - We don't currently support disabling cells – instead, use "sticky air": perfectly compressible, low stiffness material which does not retain state
- Heterogeneous materials on boundaries with fine details
  - Surface force decreases significantly under refinement
  - Only converges near grain-resolving scale*



What does “grain-resolving” mean?

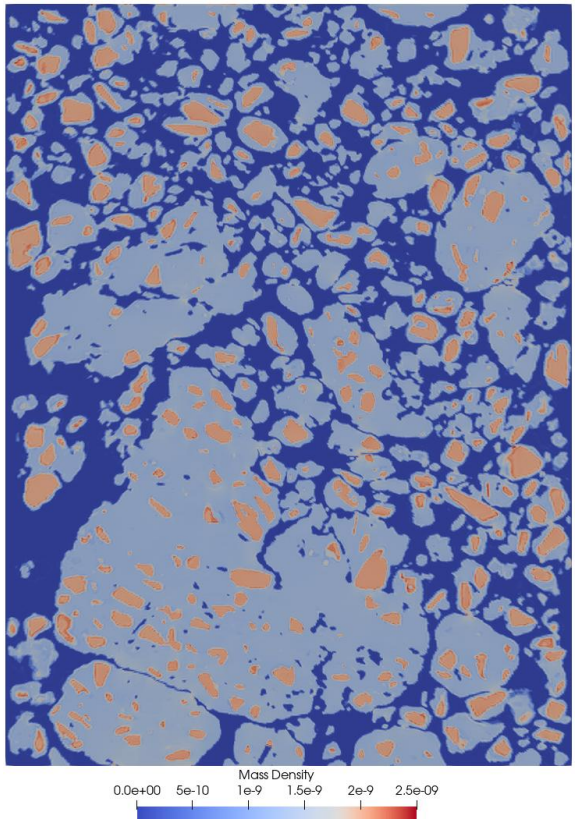
316 MPoints

- At least N points per grain
  - Relatively easy due to number/size of grains
  - Requires ~25 million points
- At least N points per voxel
  - Much harder, ~290 million voxels in domain
  - For approximately 1 cell/voxel, need ~8 billion material points
    - Checkpoint files at this resolution are about 1.5 TB each
    - Even projected mesh outputs are ~60GB
  - Even ~1 point per voxel is ~300 million points

- Unfortunately, it seems like we need the latter for surface forces to converge and to avoid numerical fracture

Challenges at Scale

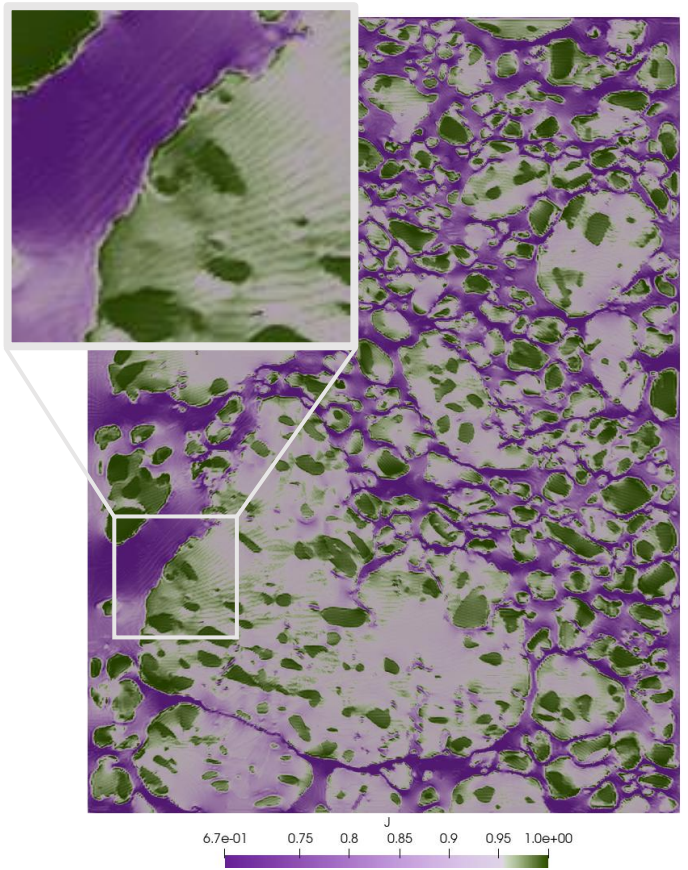
- Preconditioning/Linear Solver
  - More refined mesh ⇒ more linear iterations with Jacobi preconditioning
  - Solution: Use Algebraic Multigrid (AMG) preconditioner
- AMG Memory Requirements
  - Requires explicit assembly of libCEED matrix-free operators
  - Requires computing matrix triple products ($P^T AP$)
  - Just for memory, 1.5 billion points requires ~256 MI300A (128 GB)
- Point Migration/Location
  - Implemented in PETSc DMSwarm using spatial hashing
  - 1 spatial hash lookup + N cell/hash box pointwise nonlinear solves *per point* on process *and* for any points that left another process
  - Future work: Move this to GPU kernel and reduce communication



Mass Density – 1.5 billion points, lumped projection onto background mesh at ~20% deformation

Challenges due to MPM

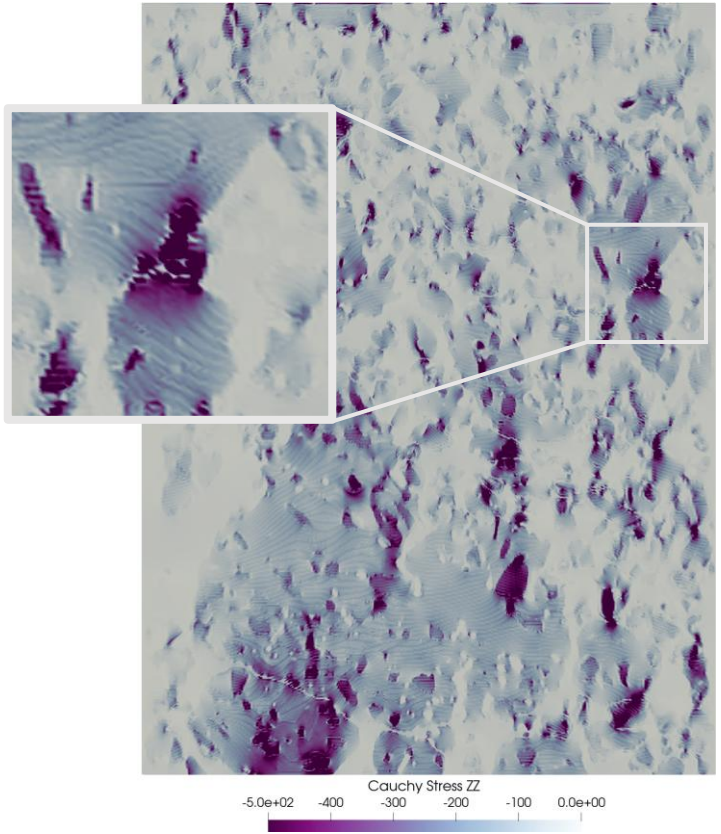
- Ringing/Cell-Crossing instability in projected output fields



$J = \det(\boldsymbol{F})$*: 1.5 billion points, lumped projection onto background mesh at ~20% deformation*

Challenges due to MPM

- Ringing/Cell-Crossing instability in projected output fields
- Stress singularities on prill boundaries
  - Prills effectively merge when they touch
  - Want prills to slide and rotate
  - Future work: inter-prill contact modeling



σ_{zz}: 1.5 billion points, lumped projection onto background mesh at ~20% deformation

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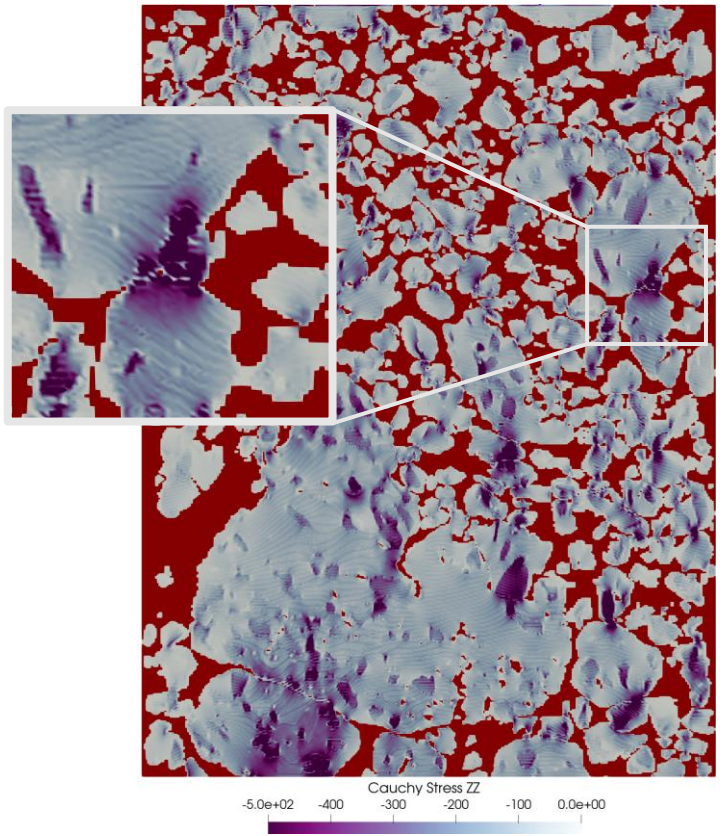
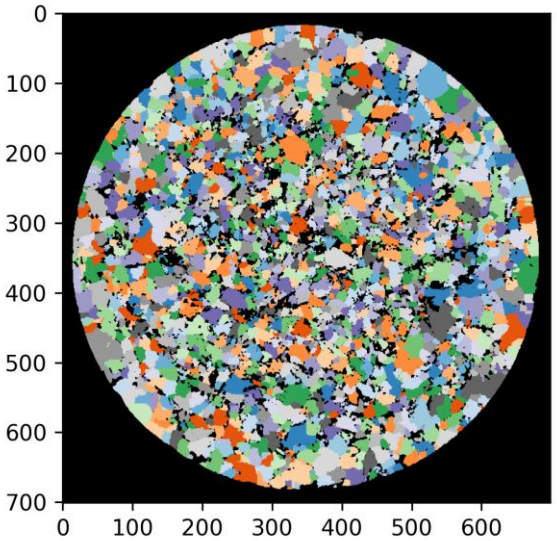


σ_{zz}: 1.5 billion points, lumped projection onto background mesh at ~20% deformation, air masked

Future Work

- Better input data
- Performance
  - GPU kernels for point location
- Material Modeling
  - Anisotropy
  - Viscoelasticity
  - Plasticity
- Simulation Capabilities
  - Traction boundaries
  - Inter-grain contact & friction



Hand-pressed sample (50N), credit: Trevor Lyons, Mines

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