Center for micromorphic multiphysics porous and particulate materials simulations within exascale computing workflows

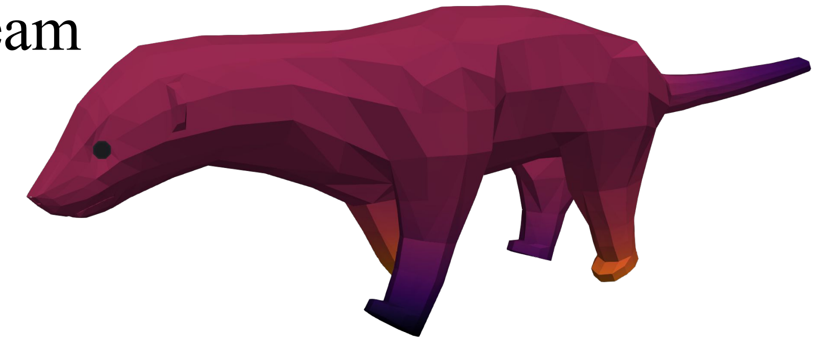
Multi-disciplinary Simulation Center (MSC)

Ratel Implicit MPM Update

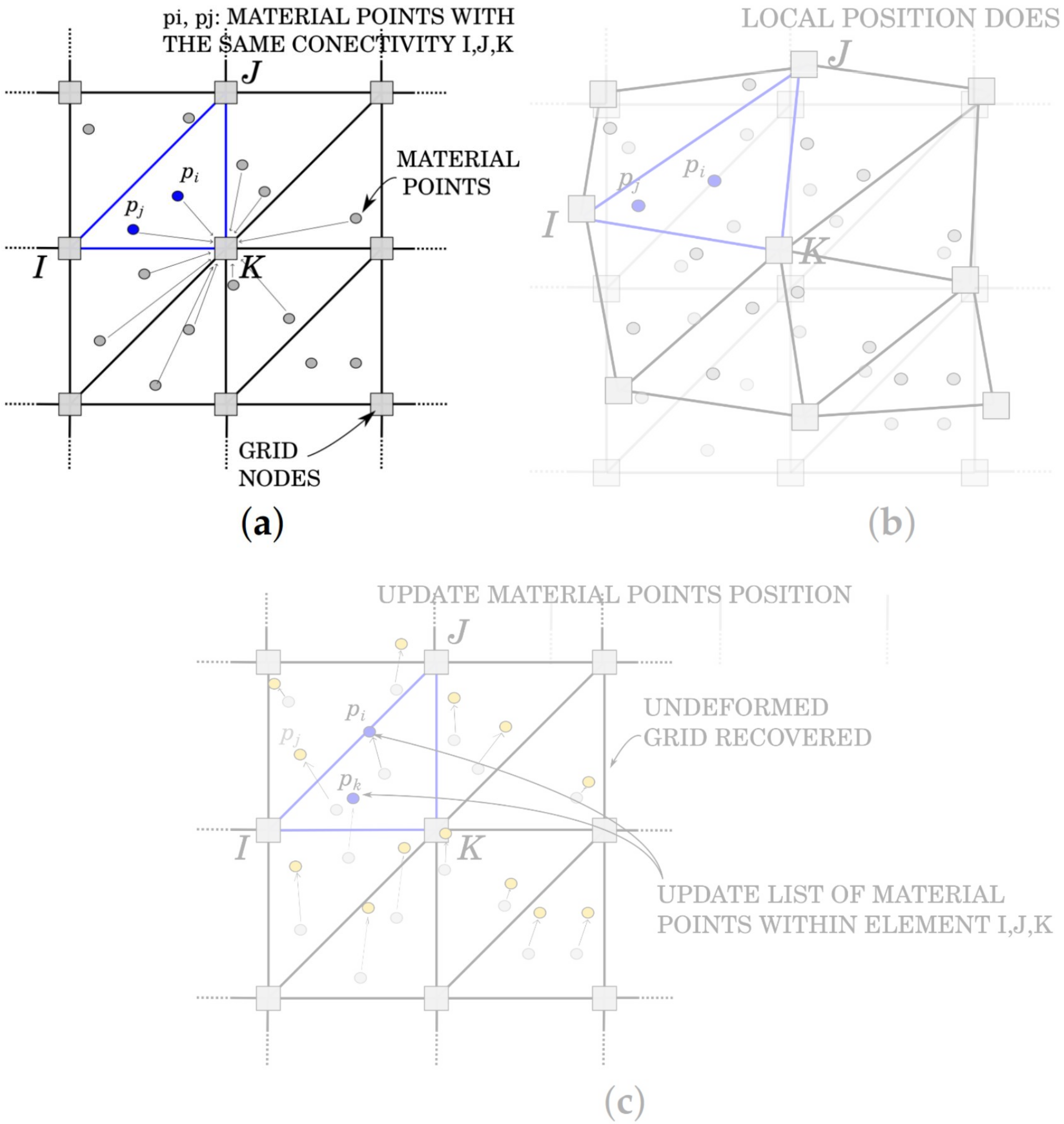
Jeremy L Thompson, Ratel Team

4 Oct 2024

Boulder, CO



Material Point Method - Basics



Start of Timestep $t_n + \Delta t$

Material Point Data:

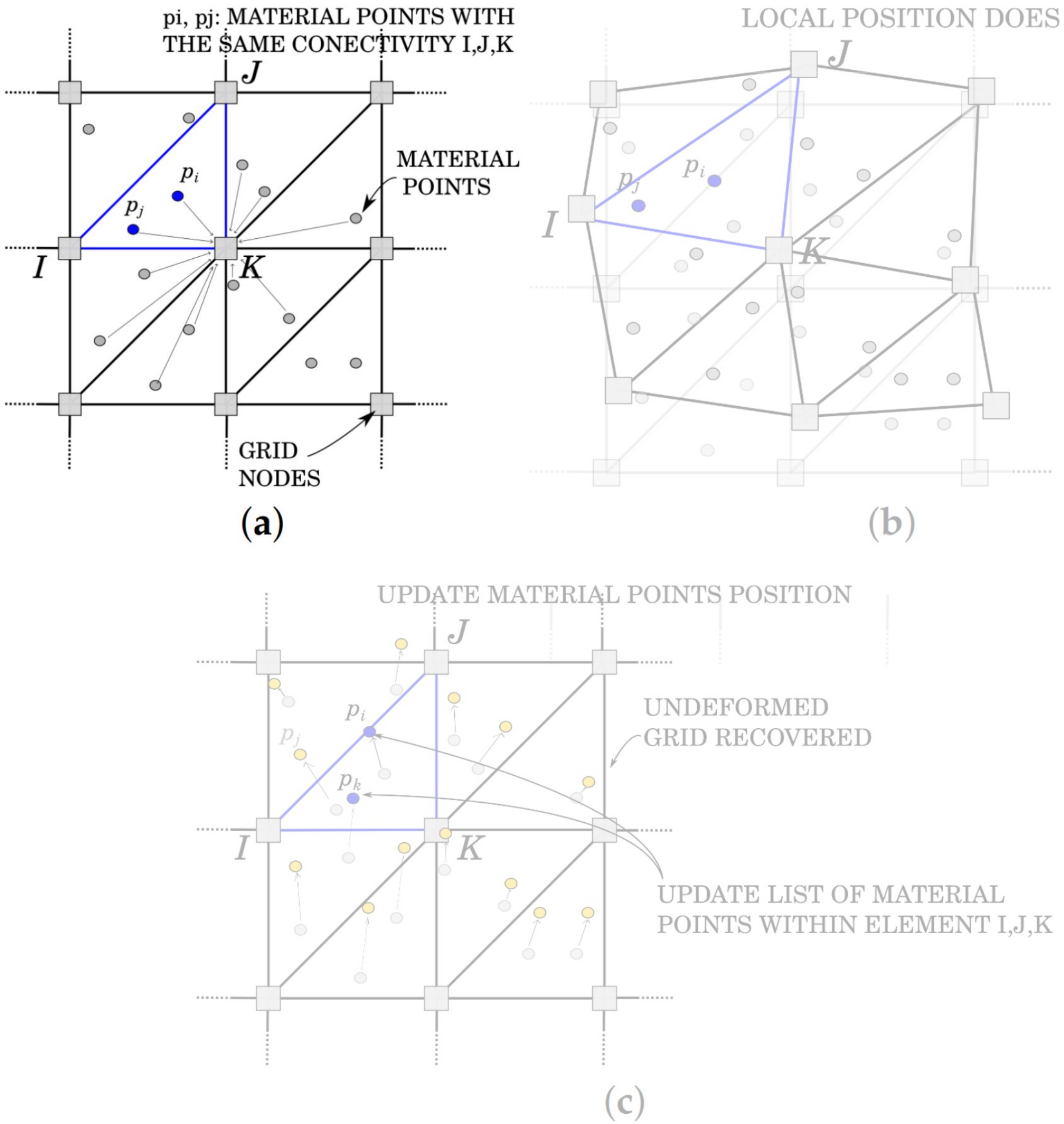
- Previous converged deformation gradient $\boldsymbol{F}_p^n$
- Previous converged position $\boldsymbol{x}_p^n$
- Previous converged displacement $\boldsymbol{u}_p^n$
- Material properties, e.g., bulk and shear moduli K, μ
- Initial density ρ_0

Mesh Data:

- Nothing, in initial configuration

Diagram from I. Iaconeta, A. Larese, R. Rossi, and Z. Guo, "Comparison of a Material Point Method and a Galerkin Meshfree Method for the Simulation of Cohesive-Frictional Materials," *Materials*, vol. 10, no. 10, Art. no. 10, Oct. 2017, doi: 10.3390/ma10101150.

Material Point Method - Basics



Goal: Compute $\boldsymbol{u}$ such that

(Not currently considered)

$$\int_{\Omega_0} \nabla_{\boldsymbol{X}} \boldsymbol{v} : \boldsymbol{P}(\boldsymbol{u})\, \mathrm{d}V - \int_{\Omega_0} \boldsymbol{v} \cdot \rho_0 \boldsymbol{g}\, \mathrm{d}V - \cancel{\int_{\partial\Omega_0} \boldsymbol{v} \cdot \boldsymbol{t}\, \mathrm{d}S} = 0$$

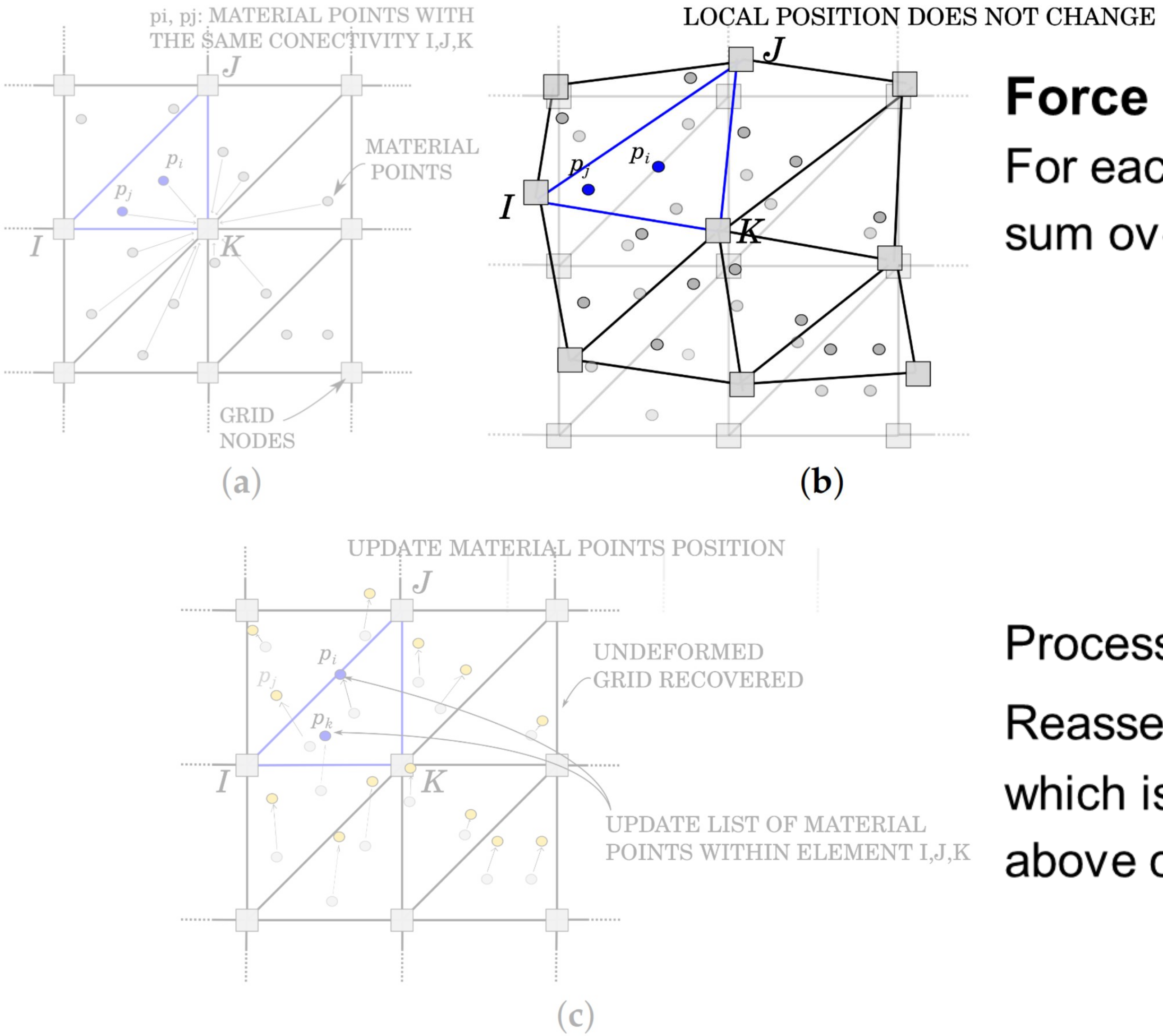
Note: $\boldsymbol{X}$ is the initial configuration coordinates – these are lost at material points as they move through the domain.

Instead, find $\Delta \boldsymbol{u}$ such that

$$\int_{\Omega_n} \nabla_{\tilde{\boldsymbol{X}}} \boldsymbol{v} : \underbrace{\left(\frac{1}{J_n} \boldsymbol{\tau}(\Delta \boldsymbol{u}) \cdot \Delta \boldsymbol{F}^{-T} \right)}_{\tilde{\boldsymbol{P}}(\Delta \boldsymbol{u})} dV - \int_{\Omega_n} \boldsymbol{v} \cdot \underbrace{\left(\frac{\rho_0}{J_n} \Delta \boldsymbol{g} \right)}_{\rho(\boldsymbol{x}_n, t) \Delta \boldsymbol{g}} = 0$$

Diagram from I. Iaconeta, A. Larese, R. Rossi, and Z. Guo, “Comparison of a Material Point Method and a Galerkin Meshfree Method for the Simulation of Cohesive-Frictional Materials,” *Materials*, vol. 10, no. 10, Art. no. 10, Oct. 2017, doi: 10.3390/ma10101150.

Material Point Method - Basics



Force and Stiffness at Material Points

For each node i, compute force contributions via the sum over each material point p in its support:

$$\boldsymbol{f}_i^{int} = \sum_p V_p^n \nabla \boldsymbol{N}_i(\boldsymbol{x}_p^n) : \widetilde{\boldsymbol{P}}(\Delta \boldsymbol{u}_p)$$

$$\boldsymbol{f}_i^{ext} = \sum_p V_p^n \boldsymbol{N}_i(\boldsymbol{x}_p^n) \frac{\rho_p^0}{J_p^n} \cdot \Delta \boldsymbol{g}$$

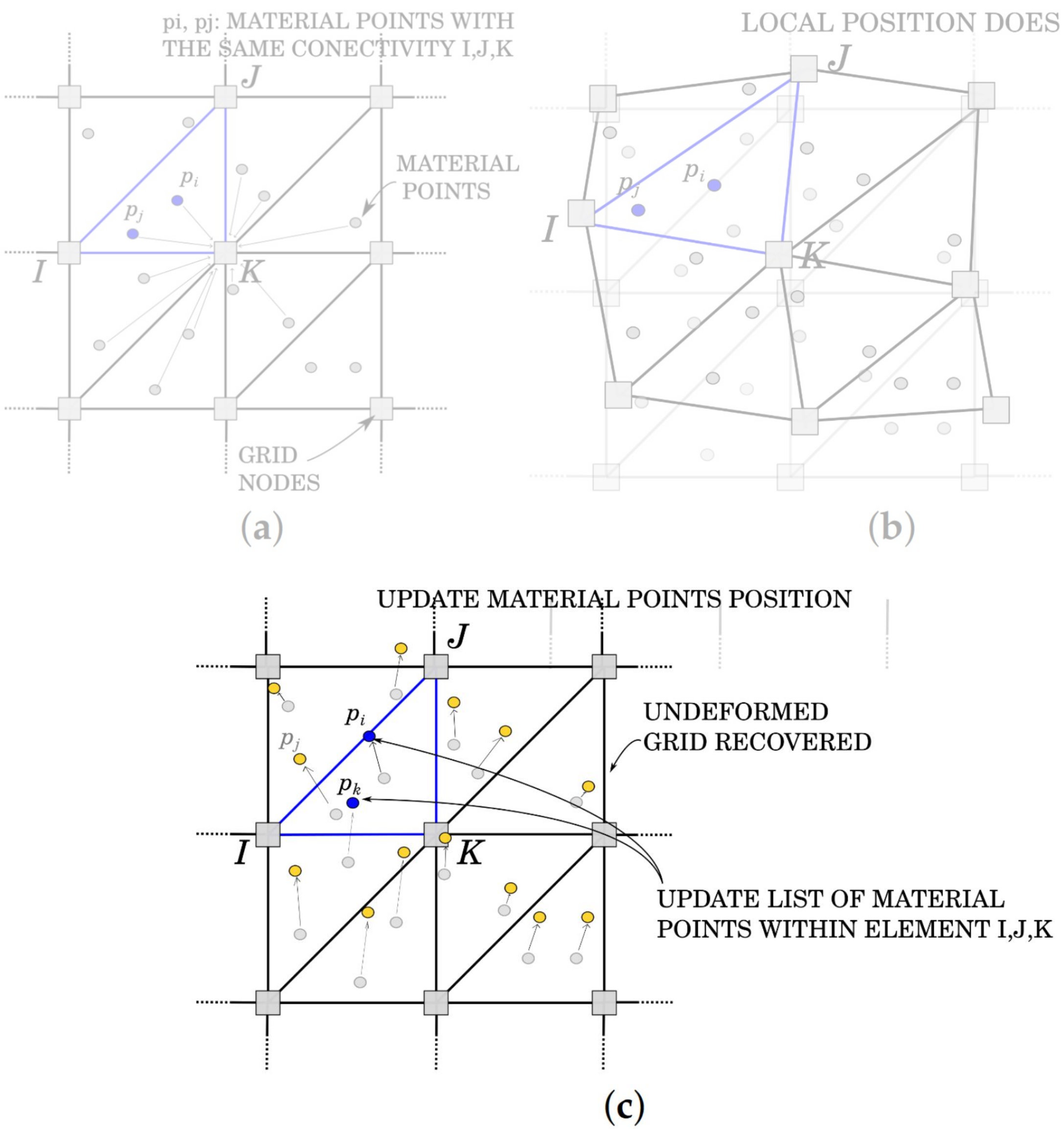
Process is similar for stiffness matrix.

Reassemble at each Newton iteration to compute $\Delta \boldsymbol{u}_i^{(k)}$, which is temporarily interpolated back to points for the above computation as

$$\Delta \boldsymbol{u}_p^{(k)} = \sum_i \boldsymbol{N}_i(\boldsymbol{x}_p^n) \Delta \boldsymbol{u}_i^{(k)}$$

Diagram from I. Iaconeta, A. Larese, R. Rossi, and Z. Guo, "Comparison of a Material Point Method and a Galerkin Meshfree Method for the Simulation of Cohesive-Frictional Materials," *Materials*, vol. 10, no. 10, Art. no. 10, Oct. 2017, doi: 10.3390/ma10101150.

Material Point Method - Basics



Moving the Material points

Interpolate the final nodal displacement increment to material points:

$$\Delta \boldsymbol{u}_p^* = \sum_i \boldsymbol{N}_i(\boldsymbol{x}_p^n)\Delta \boldsymbol{u}_i^*$$

Update position and state data at material points as

$$\boldsymbol{x}_p^{n+1} = \boldsymbol{x}_p^n + \Delta \boldsymbol{u}_p^*$$
$$\boldsymbol{u}_p^{n+1} = \boldsymbol{u}_p^n + \Delta \boldsymbol{u}_p^*$$
$$V_p^{n+1} = \det(\Delta F_p^*)\, V_p^n$$
$$\boldsymbol{F}_p^{n+1} = \Delta \boldsymbol{F}_p^* \cdot \boldsymbol{F}_p^n,$$

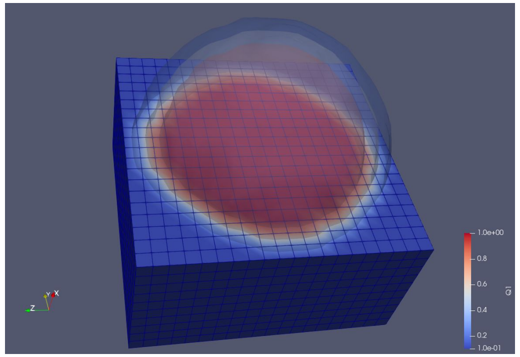
where $\Delta \boldsymbol{F}_p^* = \boldsymbol{I} + \nabla_{\tilde{X}}(\Delta \boldsymbol{u}_p^*)$.

Background grid is reset, and operators are rebuilt for the next timestep.

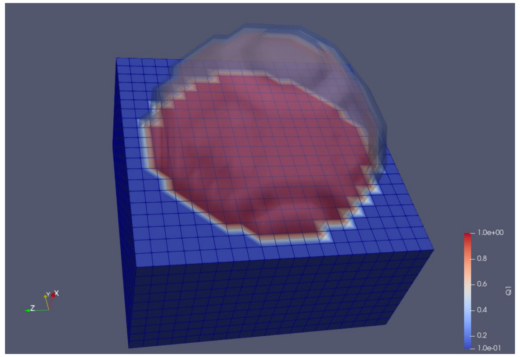
Diagram from I. Iaconeta, A. Larese, R. Rossi, and Z. Guo, “Comparison of a Material Point Method and a Galerkin Meshfree Method for the Simulation of Cohesive-Frictional Materials,” *Materials*, vol. 10, no. 10, Art. no. 10, Oct. 2017, doi: 10.3390/ma10101150.

Where we were: Spring 2024 TST

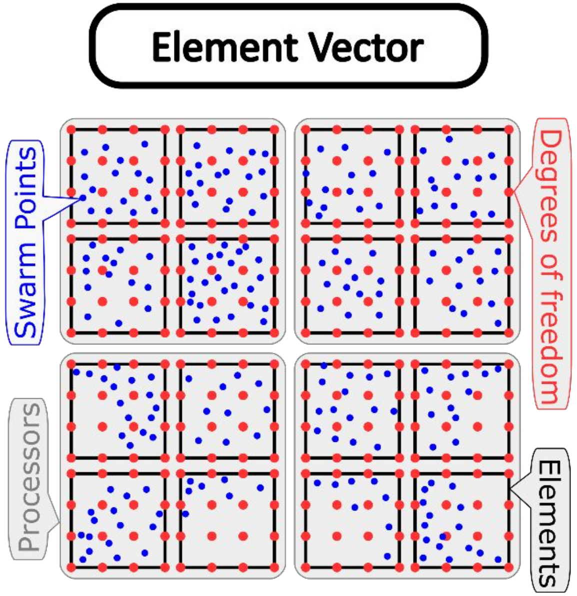
- libCEED infrastructure
  - Operator evaluation at arbitrary points
  - Projection (lumped and consistent) from point to FEM fields
  - CPU diagonal assembly
- PETSc: DMSwarm for material point management
- Ratel: Initial MPM implementation

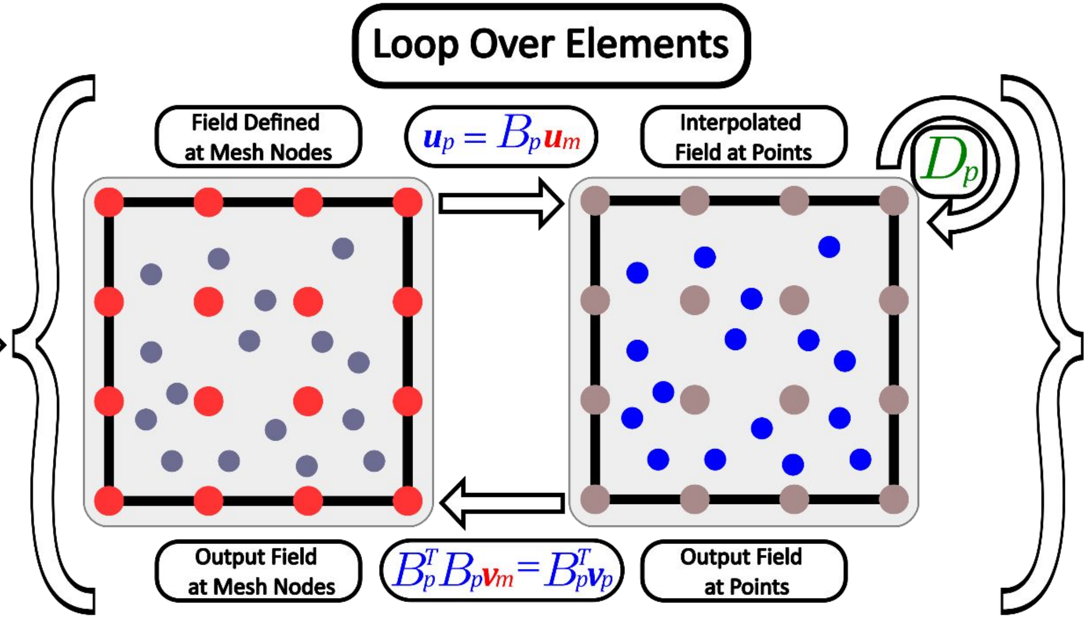


Consistent



Lumped





Where we are: Fall 2024 Retreat

libCEED + Ratel

- Operators defined at points, with mixed FEM/point input/output
- Diagonal assembly of points operators for preconditioning
- Porting to GPU complete
- Bake-off Problems (BPs) implemented and verified for points operators:
  - Scalar and vector projection, Laplace, and collocated Laplace problems
- Linear and mixed linear elasticity implemented and verified
- Neo-Hookean elasticity implemented

Big Picture

MPM material modeling is being abstracted to the same interfaces as FEM operations in Ratel

Where we are: Fall 2024 Retreat

Ratel iMPM

- Support for iMPM in Ratel improving
  - Drop-in replacement for standard FEM operators
  - **Verified** with BPs and static elasticity (linear and mixed linear) MMS
    - BPs include scalar and vector projection and Laplace problems
  - Quasistatic examples for linear and Neo-Hookean elasticity
  - Existing materials relatively easy to translate to iMPM now
  - Linear and Neo-Hookean damage in iMPM on the horizon
  - Performance optimization ongoing

Where we are: Fall 2024 Retreat

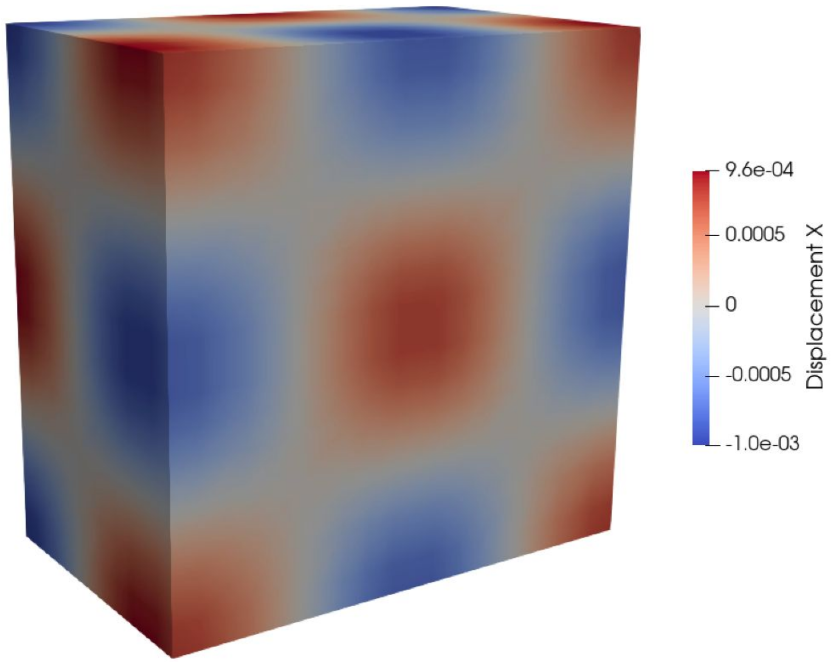
Verification via Method of Manufactured Solutions: Linear Elasticity

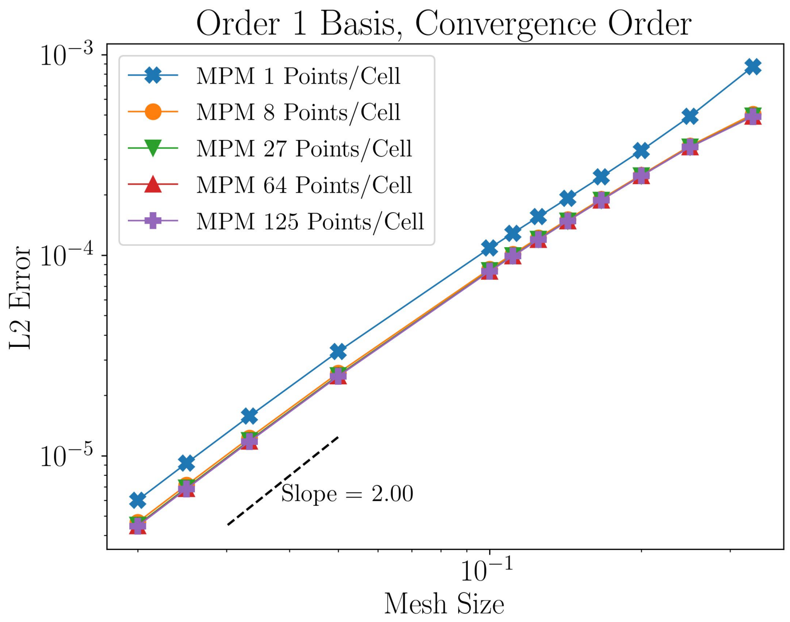
- Consider the prescribed displacement field

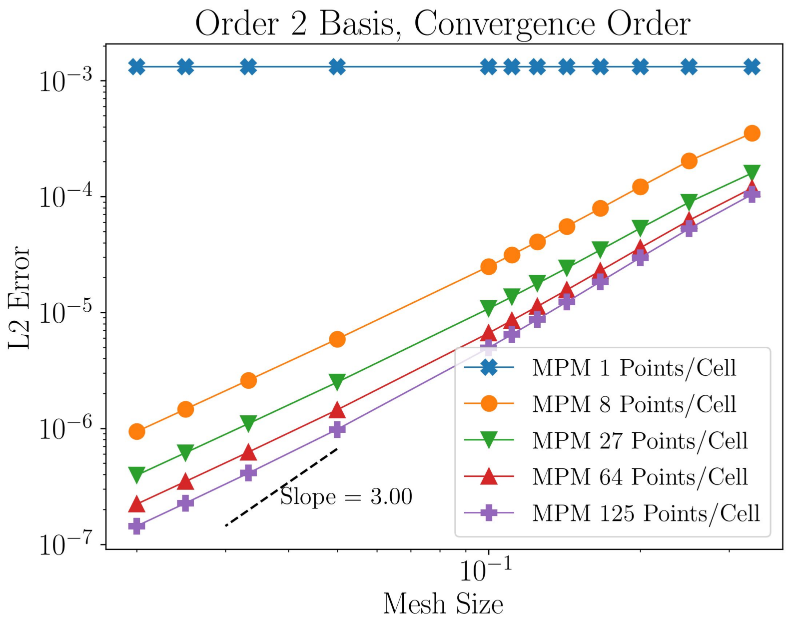
$$u_i = (i+1)A_0 \sin\left(2\pi x_0 - {}^{\pi}/_{2}\right) \sin\left(2\pi x_1 - {}^{\pi}/_{2}\right) \sin\left(2\pi x_2 - {}^{\pi}/_{2}\right), \qquad i = 0,1,2$$

- Generate a body forcing term which yields this displacement field as

$$\boldsymbol{\phi} = -\nabla_X \cdot \boldsymbol{\sigma}(\boldsymbol{u}) = -\nabla_X \cdot [2\mu\boldsymbol{\epsilon} + \lambda \mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I}], \qquad \boldsymbol{\epsilon} = \frac{1}{2}\left(\boldsymbol{F} + \boldsymbol{F}^T\right) - \mathbf{I}$$







Where we are: Fall 2024 Retreat

Ratel iMPM

- Quasistatic Implicit complete
  - Point migration and projections all working
  - Newton linearization implemented
  - Jacobi preconditioner working
- Non-homogeneous material support
  - Support for material properties defined at points (e.g. λ, μ for Neo-Hookean)
  - Potentially, projecting material properties to the mesh will work better

<u>Big Picture</u>

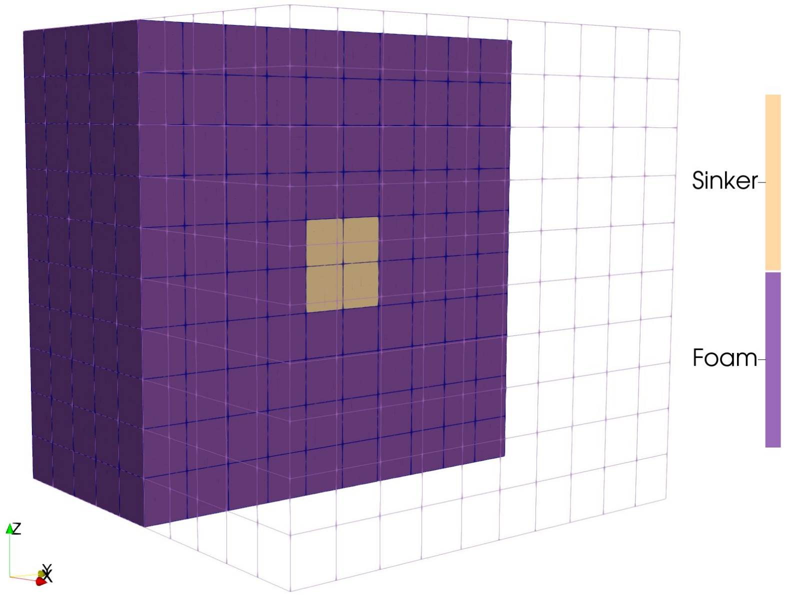
Ratel can do finite-deformation, implicit MPM with improving material support

Code-to-code Sinker Verification problem

- Dense, stiff cube inside less dense, soft cube; both nearly incompressible
  - "Sinker": $E = 190\ GPa,\ \nu = 0.49,\ \rho = 8050\ {}^{kg}/_{m^3}$, side length $0.2\ m$
  - "Foam": $E = 5\ GPa,\ \nu = 0.49,\ \rho = 15\ {}^{kg}/_{m^3}$, side length $1\ m$
- Gravity-like body force with acceleration vector $\boldsymbol{g} = -60\widehat{\boldsymbol{k}}\ {}^{m}/_{s^2}$ over 20 timesteps
- Homogenous zero Dirichlet BCs on all sides
- Refinement study over 5^3, 10^3, and 15^3 element regular hex mesh, order 2

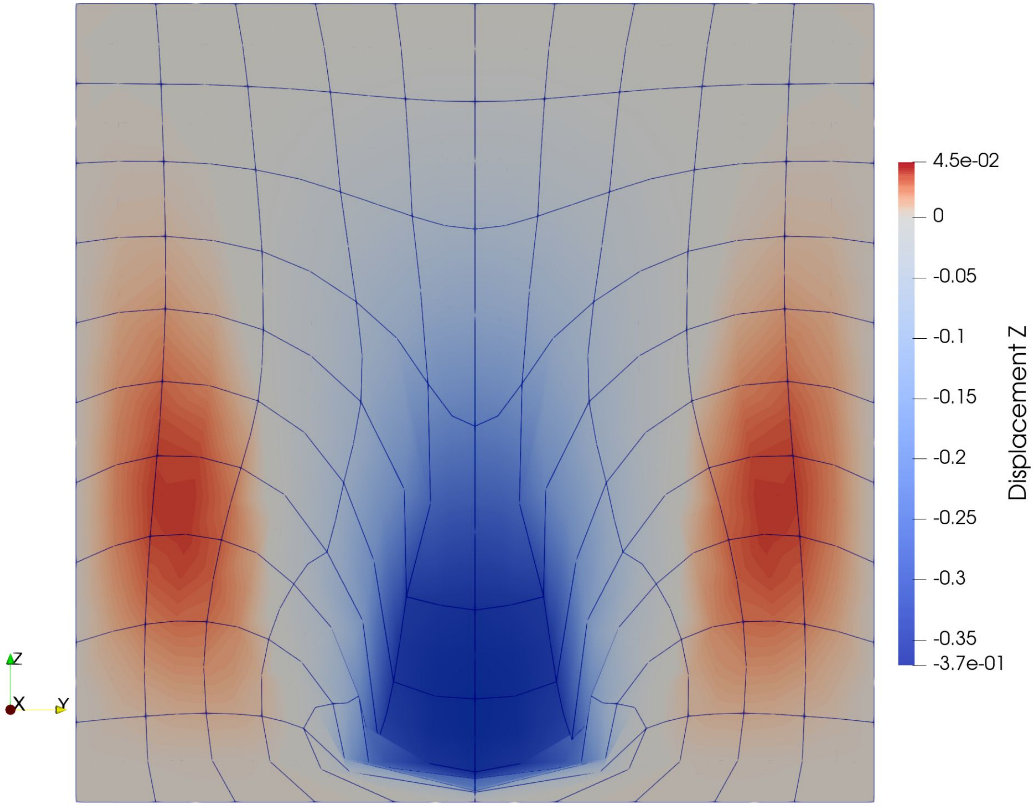
$$\boxed{\begin{aligned} \boldsymbol{f}_p^{ext} &= V_p^n \rho_p \cdot \boldsymbol{g}, && \text{(MPM)} \\ \boldsymbol{f}_i^{ext} &= \int_{e_i} \boldsymbol{v} \cdot (\rho_i \boldsymbol{g})\, \mathrm{d}V\,, && \text{(FEM)} \end{aligned}}$$

$\boldsymbol{f}_p^{ext}$ or $\boldsymbol{f}_i^{ext}$

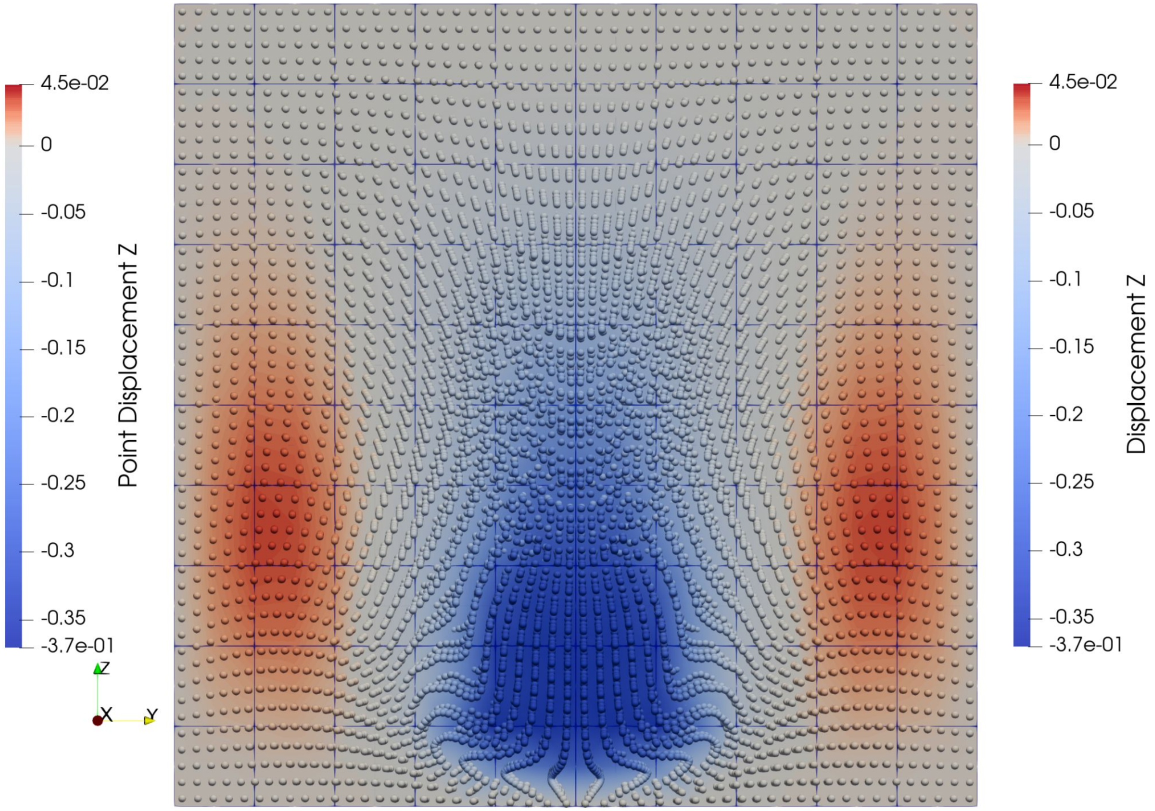


Where we are: Fall 2024 Retreat

Code-to-code Sinker Verification problem



FEM

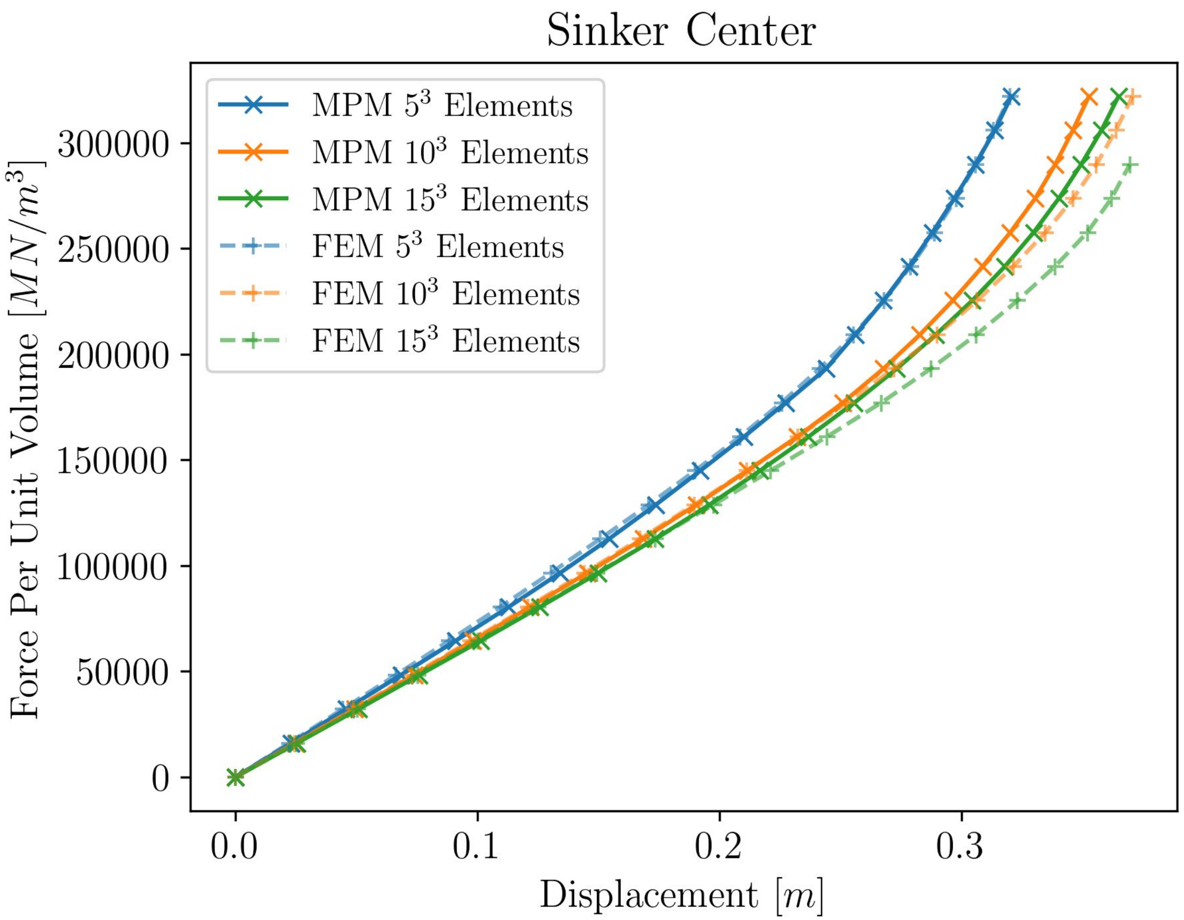


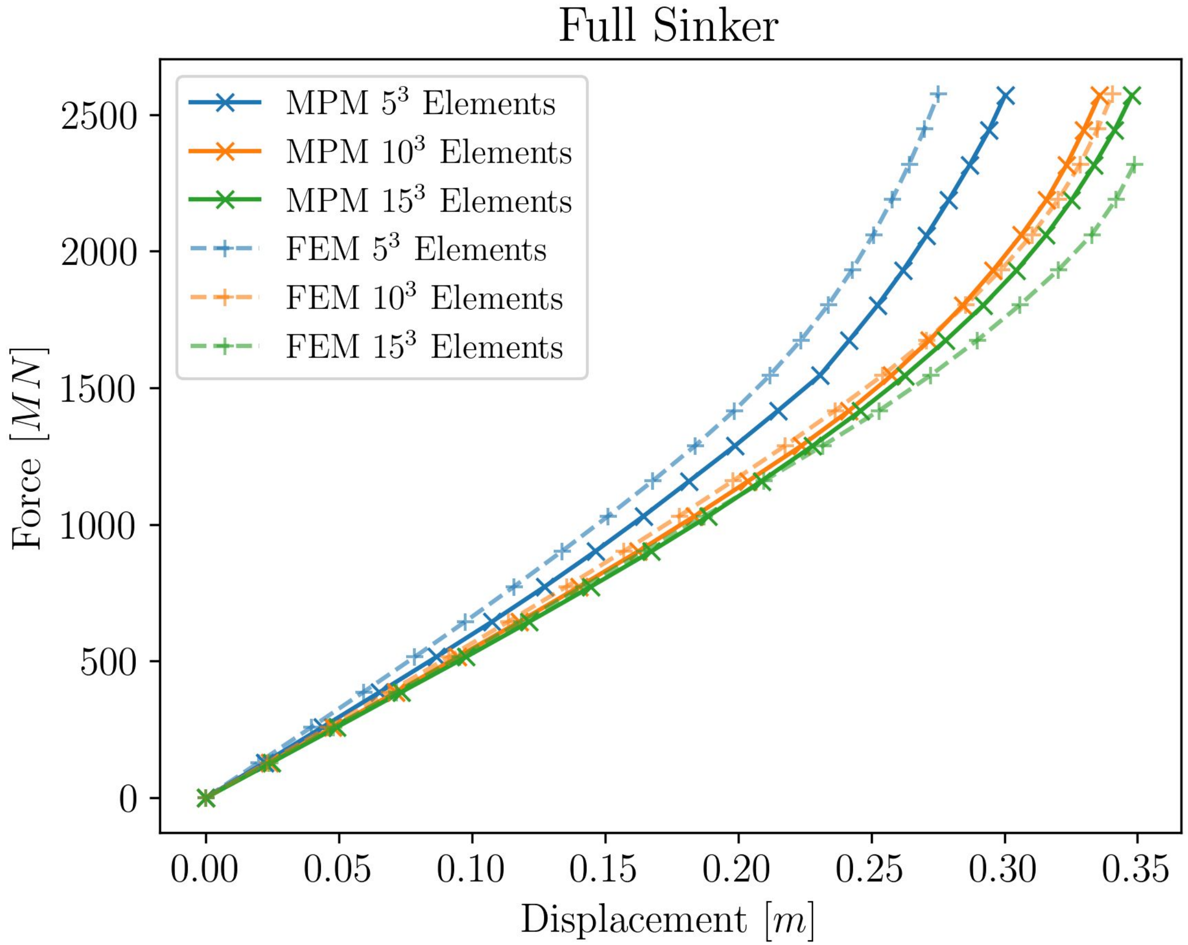
MPM

Where we are: Fall 2024 Retreat

Code-to-code Sinker Verification QOIs: Force-Displacement

- Refinement over 5^3, 10^3, and 15^3 element regular hex mesh, order 2
- Consistent projection shown, no substantial difference from lumped

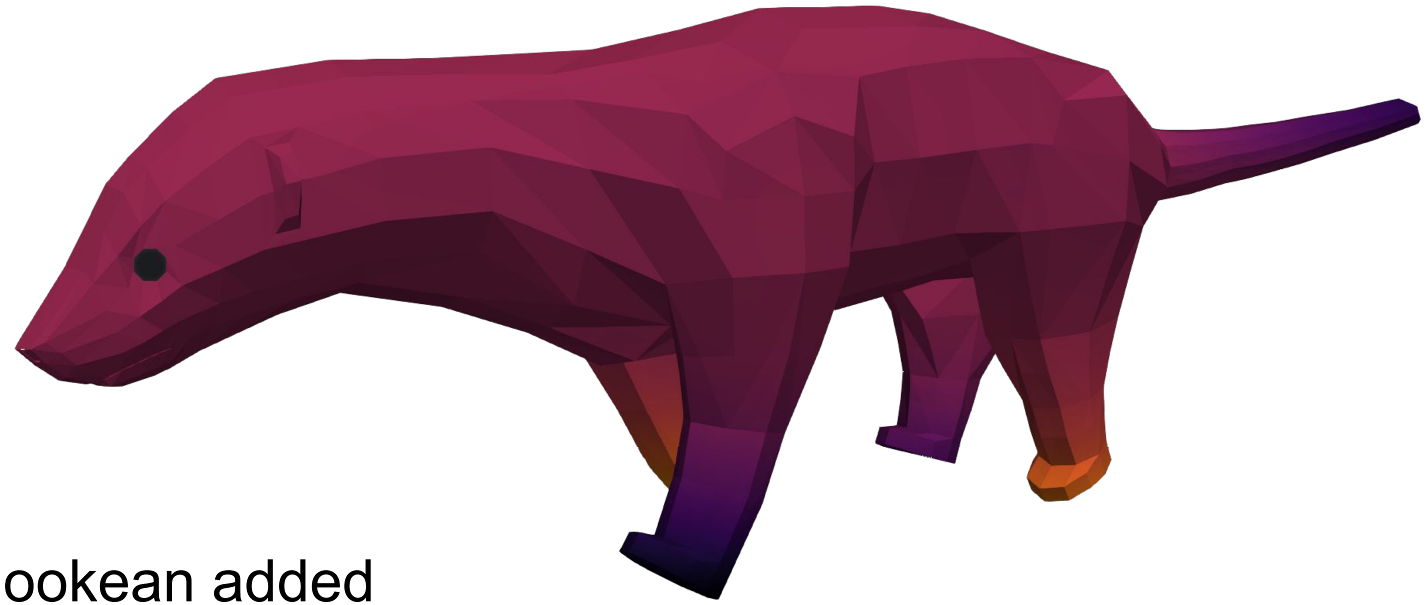




Development Progress

libCEED

- GPU support
  - Operator at points
  - Diagonal assembly at points
  - Fused operator kernels (ToDo)



Ratel

- Materials
  - Linear, mixed linear, and Neo-Hookean added
  - Finite strain damage model added and iMPM version is in progress
  - Linear poroelasticity added and finite strain case is in progress
- Optimizations
  - Project material coefficients to FEM nodes, then use Gauss quadrature
  - Total memory usage improvements ongoing