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

Multi-disciplinary Simulation Center (MSC)

Ratel Overview

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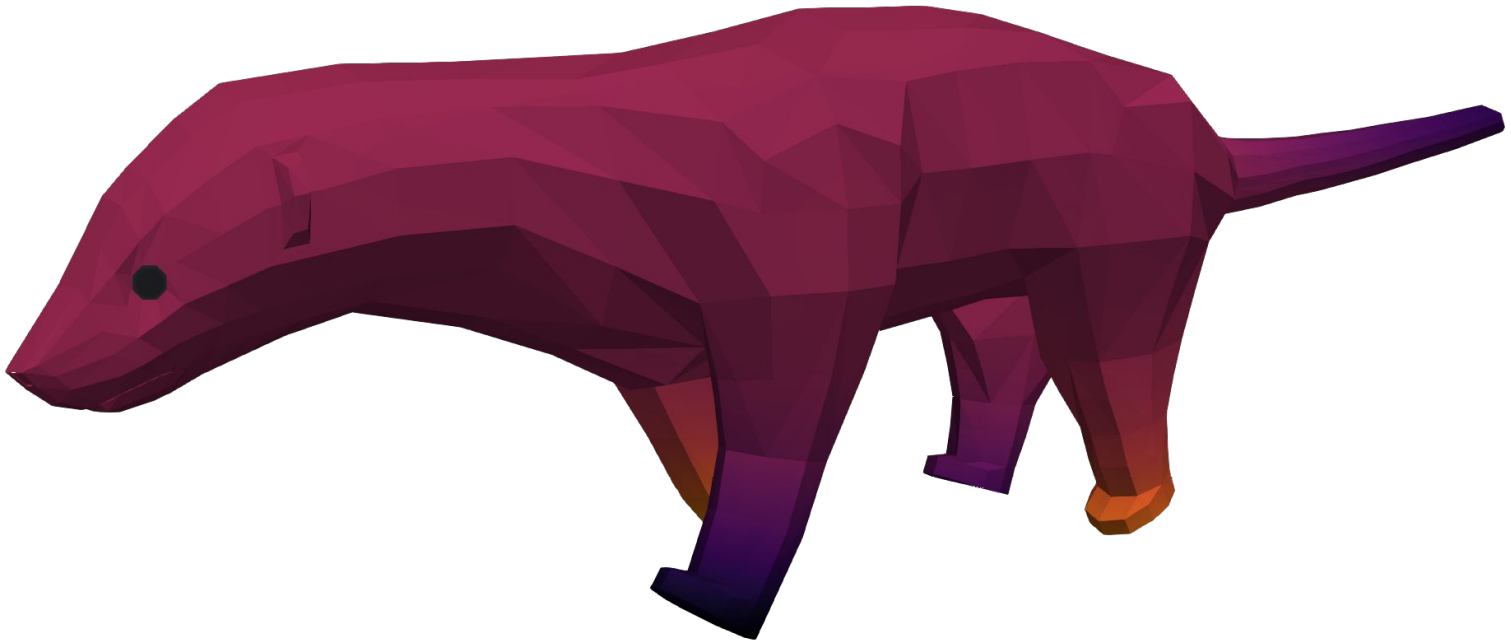
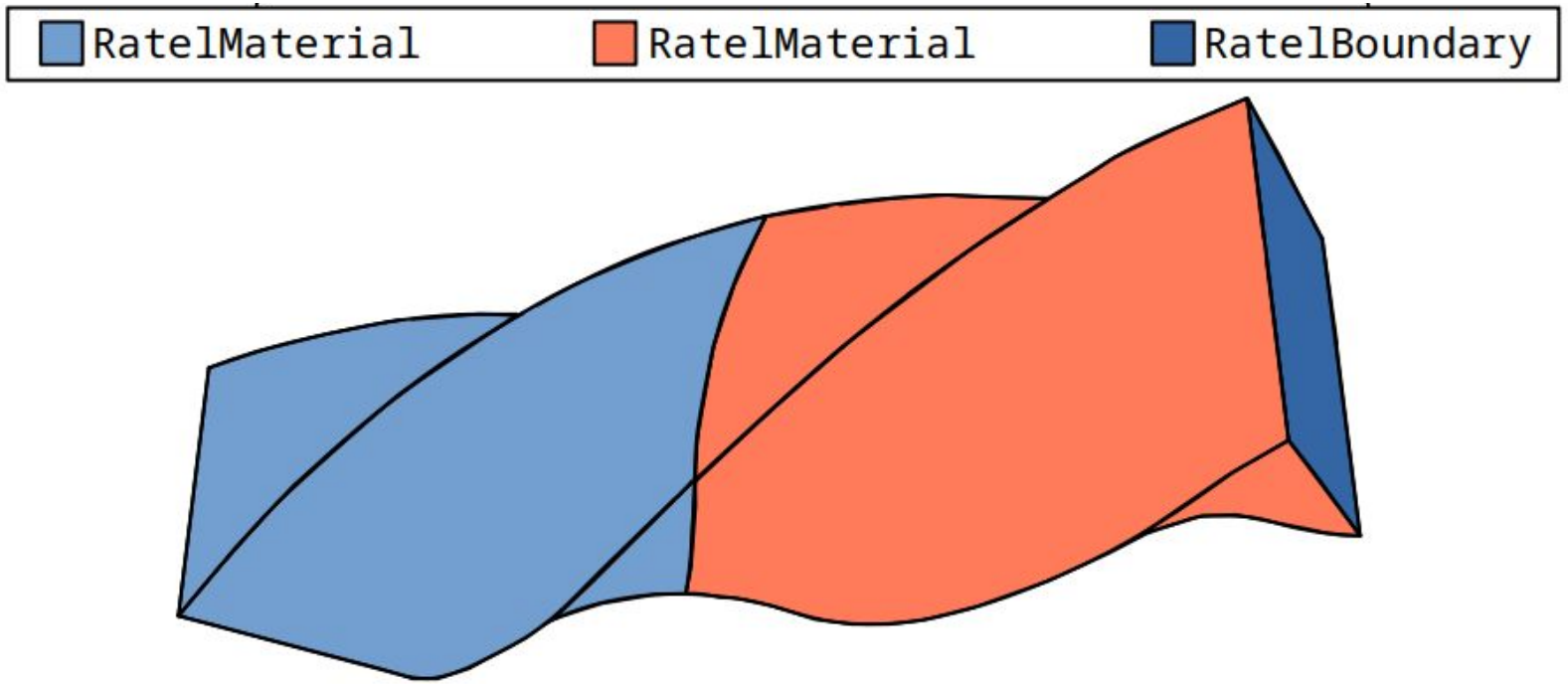
Ratel



- Ratel - matrix-free solid mechanics with PETSc + libCEED
- Grew out of libCEED mini-app

Mesh support

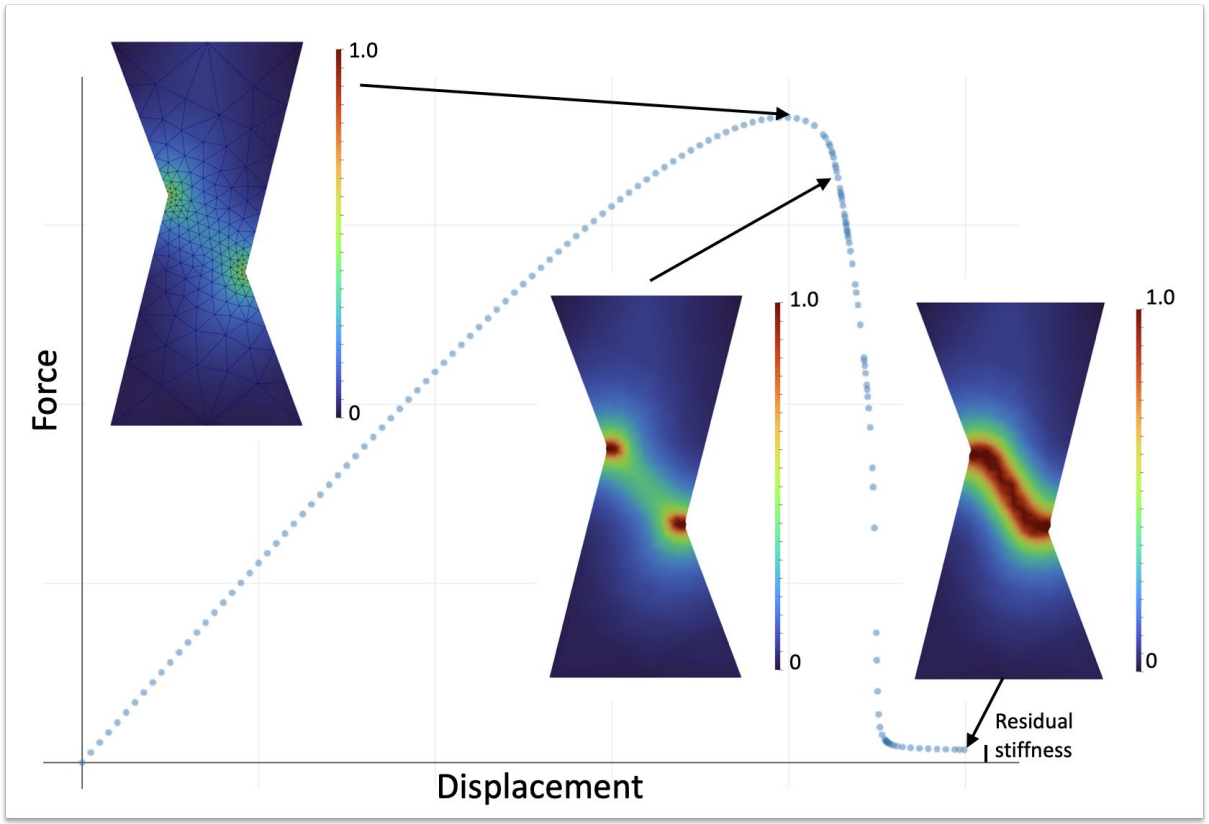
Mini-app	Ratel
● Single material ● Hex only	● Multiple materials ● Hex and tet support ● Mixed FEM support



Material Models

Mini-app

- Linear elasticity
- Neo-Hookean hyperelasticity
  - small strain, finite strain



Ratel

- Hyperelasticity
  - Linear, mixed linear, Neo-Hookean, mixed NH, Mooney Rivlin, Ogden, Hencky (some with AD)
- Plasticity
  - Linear, Hencky
- Damage
  - Neo-Hookean, Henky
- Poromechanics
  - Linear, Neo-Hookean
- Viscoelasticity (Hencky)

Material Models - Automatic Differentiation

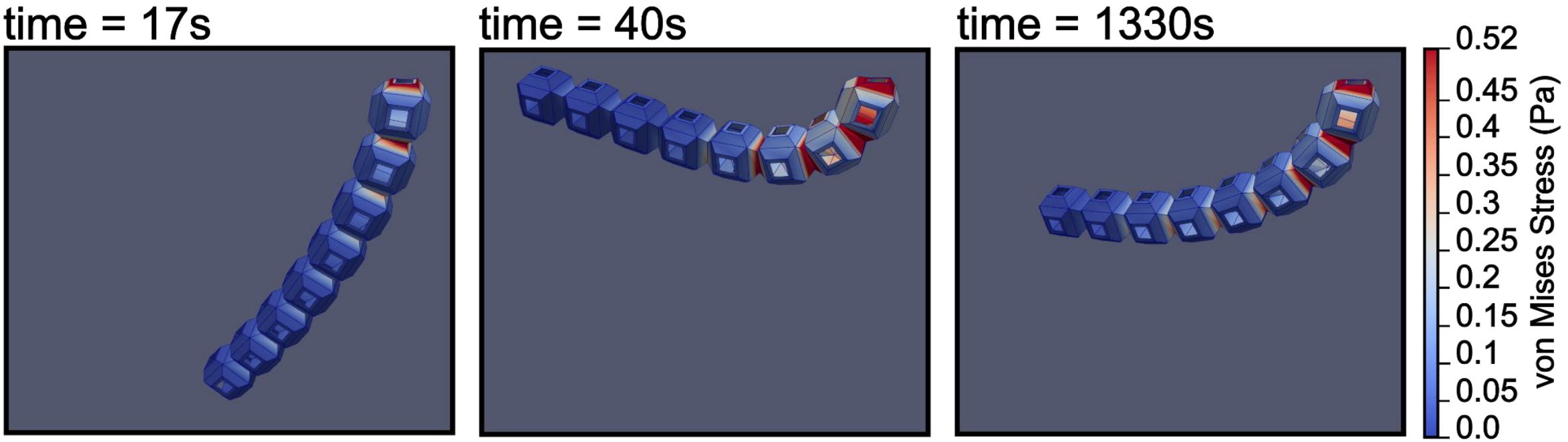
- ❑ Material model development is time intensive
- ❑ Jacobians are easy bug opportunity
- ❑ AD speeds up development, can reduce bugs

Ratel

- Hyperelasticity
  - Neo-Hookean, Ogden
- Plasticity
  - In progress
- Enzyme AD, ADOL-C
- Long term - Rust + Enzyme

Solver Modes

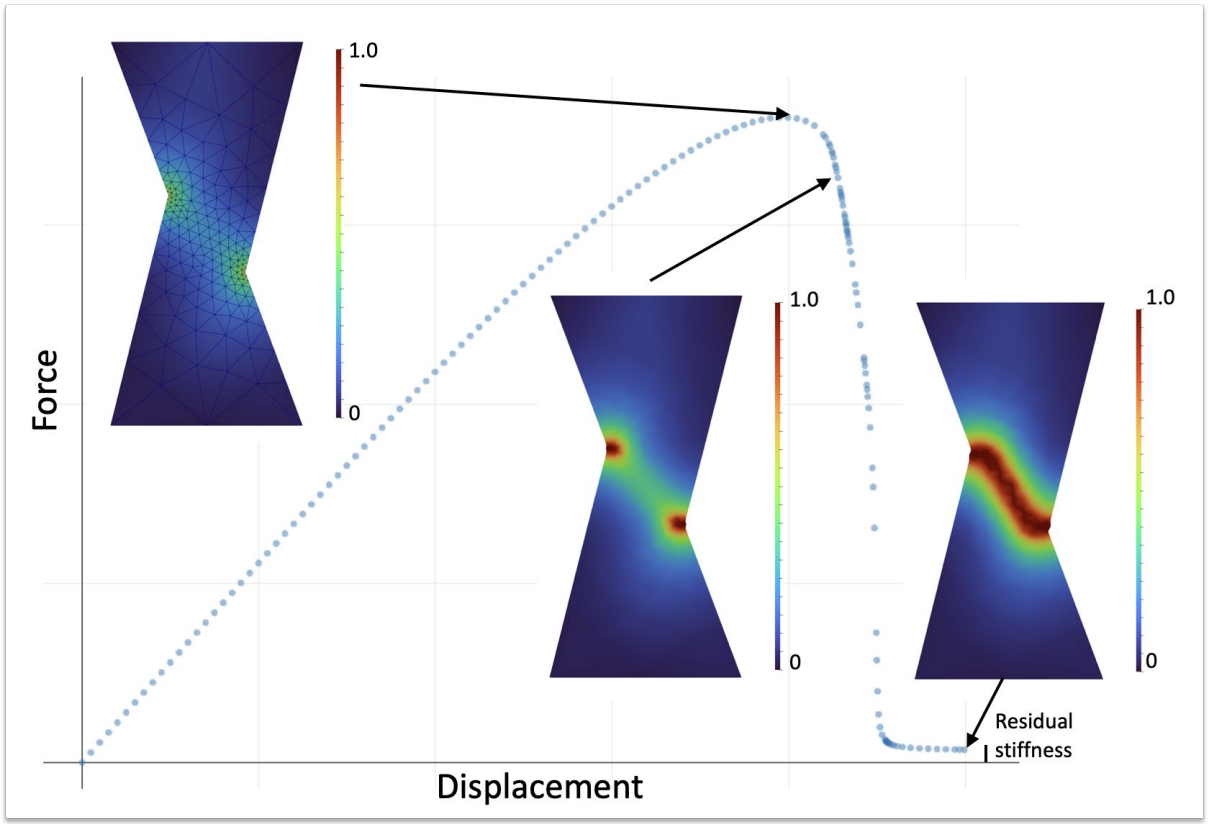
Mini-app	Ratel
• Static	• Static • Quasistatic • Dynamic



Boundary Conditions

Mini-app

- Dirichlet
  - clamp
- Neumann (traction)



Ratel

- Dirichlet
  - Clamp, slip
- Neumann (traction)
- Pressure
- Contact
  - Nitsche, penalty
  - Platen, cylinder
- All BCs incremental time varying

Diagnostic Quantities

Mini-app	Ratel
• Displacement • Pressure • Strain energy	• Displacement • Cauchy stress tensor • Pressure • Strain tensor invariants • Strain energy • von-Mises stress • Mass density

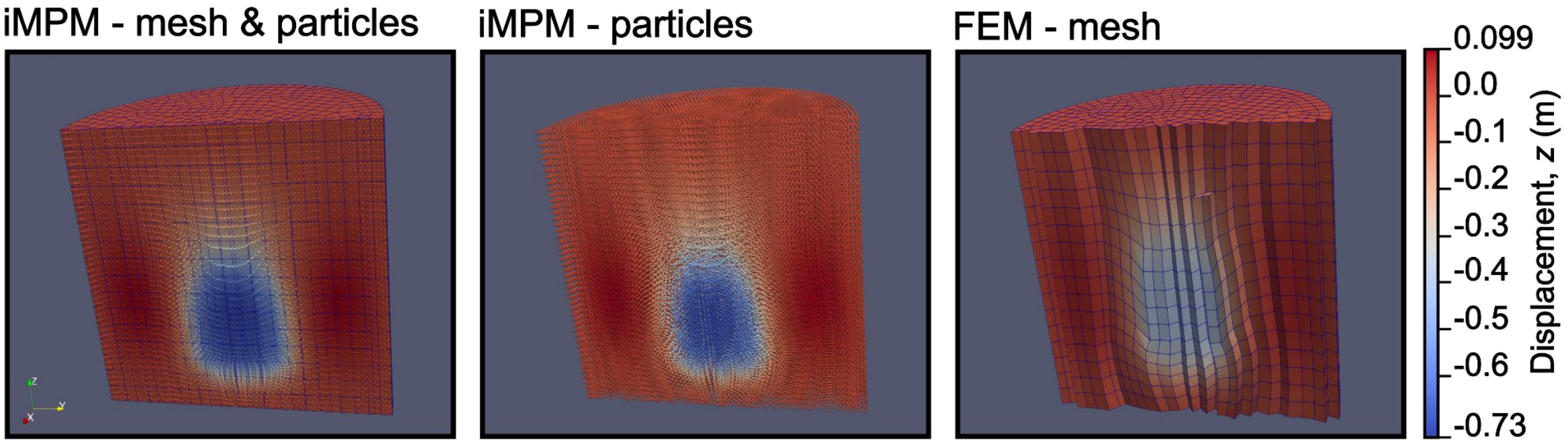
Numerical Methods

Mini-app

- FEM

Ratel

- FEM
- Mixed FEM
- iMPM



Preconditioning

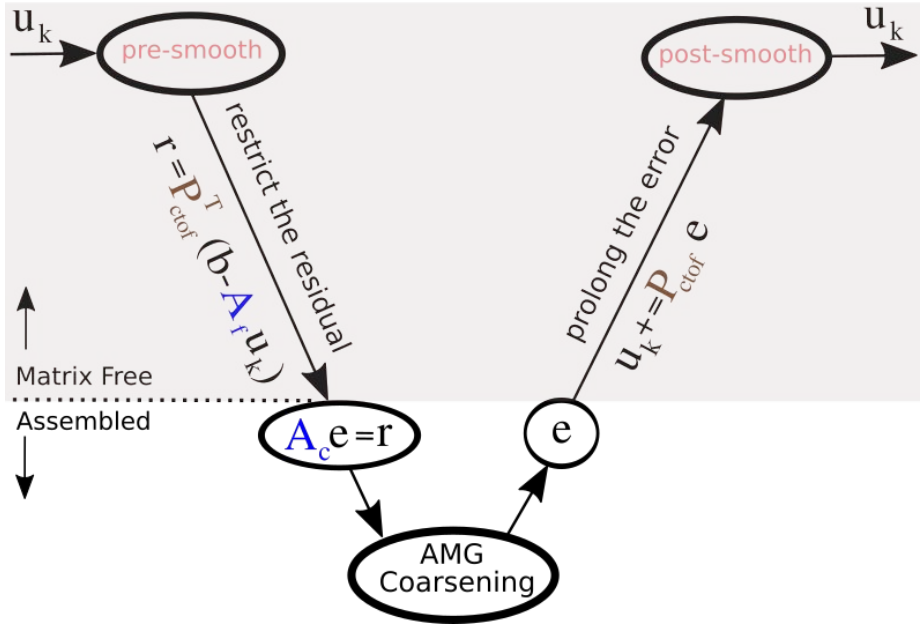
Mini-app

- Jacobi
- P-multigrid

Ratel

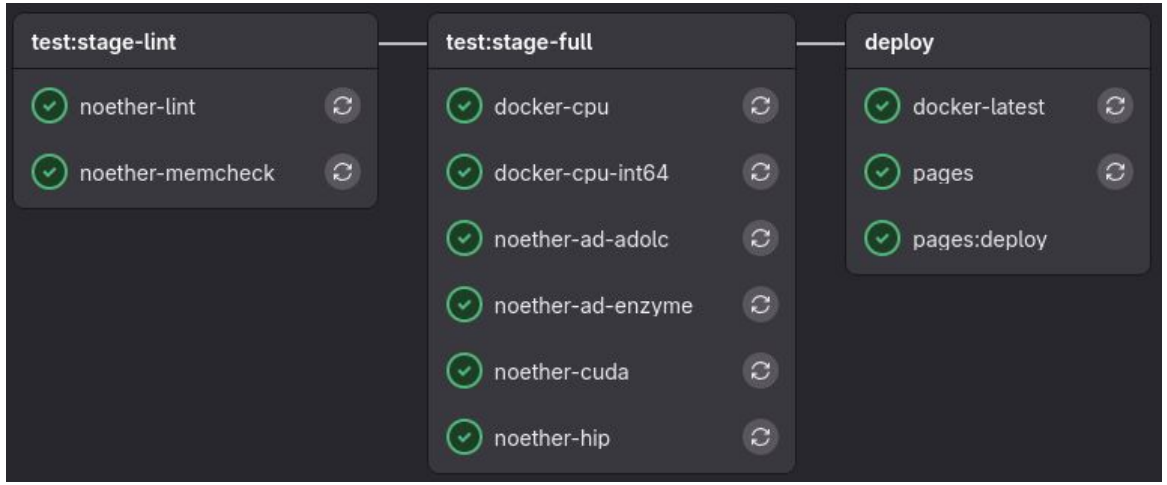
- Jacobi (diagonal, block)
- P-multigrid (including iMPM)
- Fieldsplit
- Any PETSc preconditioner

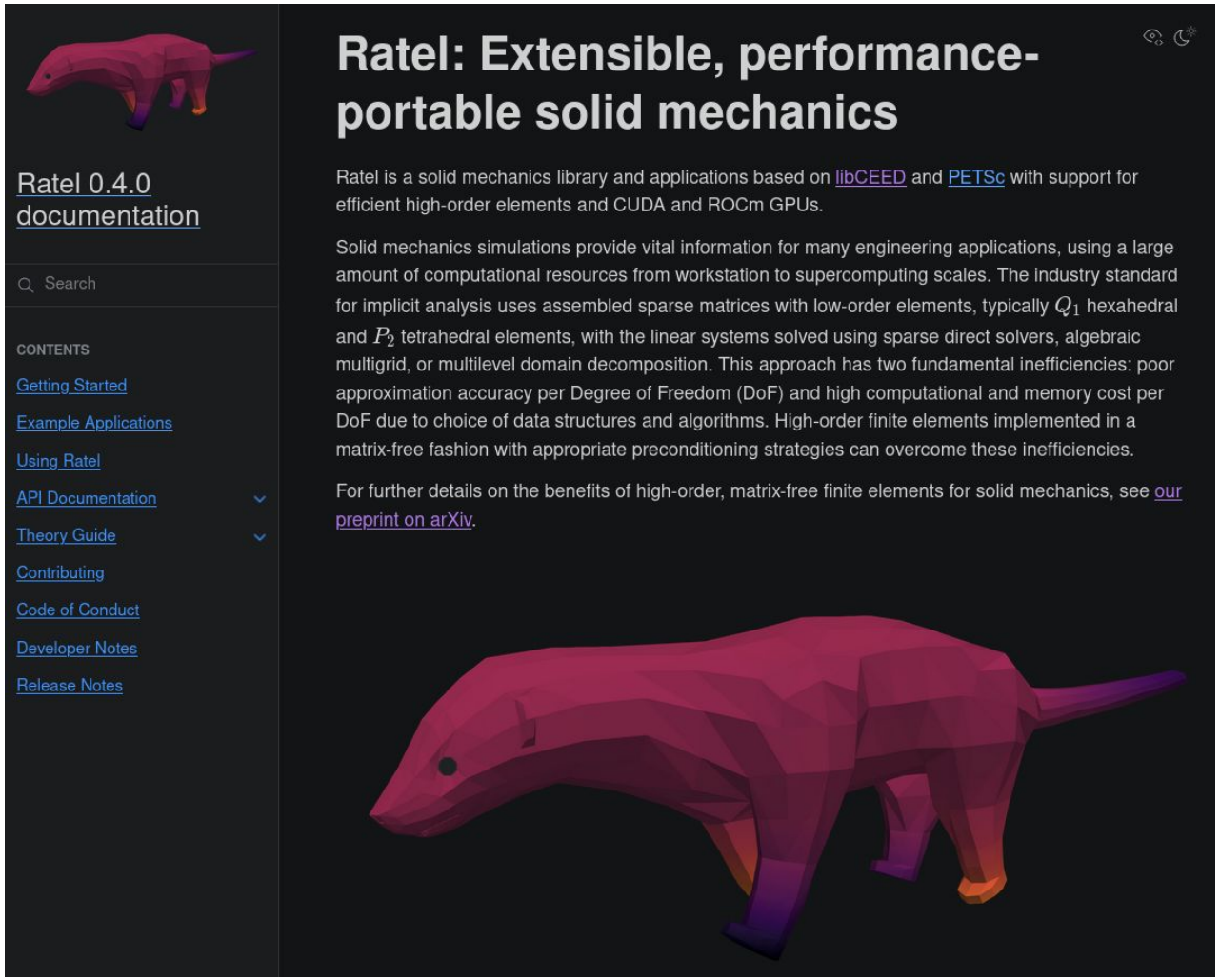
smoother: $u_k \mathrel{+}= \text{cheby}(u_k; A_f, b, \lambda_{max})$

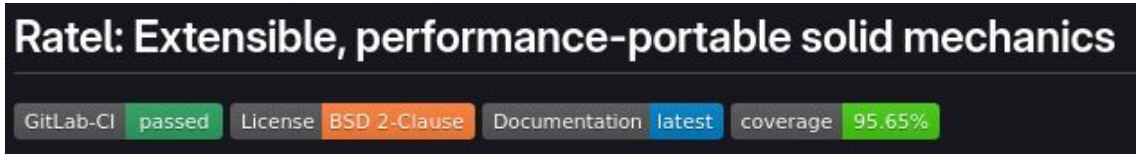


Software Engineering

- Theory and API docs
- GPU and CPU CI
- Auto deployed Dockerfiles

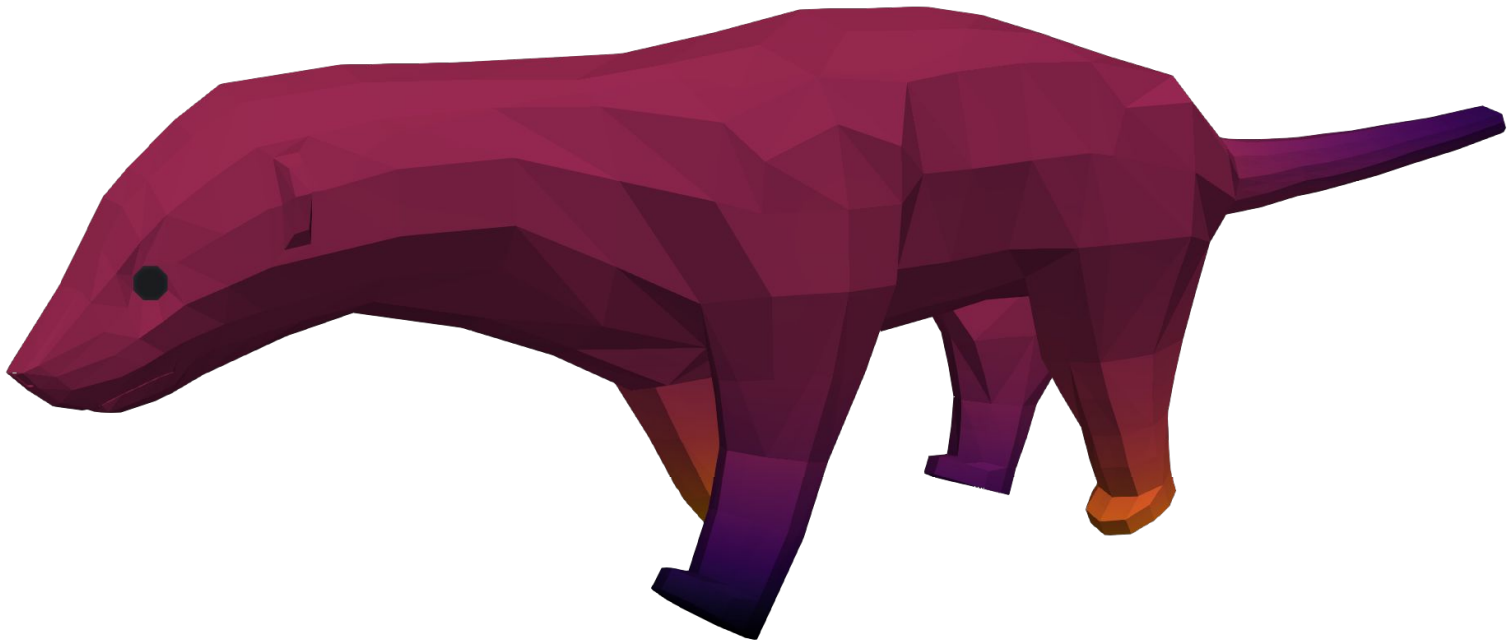






Summary

- Huge expansion of material models and BCs
- iMPM and more preconditioners now supported
- Well positioned for further work



Thank you