Matrix-Free MPM on High-Order Meshes with Ratel and libCEED

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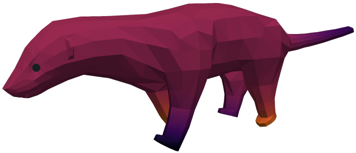
Ratel Team



Repository: https://gitlab.com/micromorph/ratel

Developers: Zach R. Atkins, Jed Brown, Fabio Di Gioacchino,
Leila Ghaffari, Zach Irwin, Rezgar Shakeri,
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Overview

Ratel - high order, performance portable solid mechanics

Built on libCEED and PETSc

GPU and CPU performance

Overview

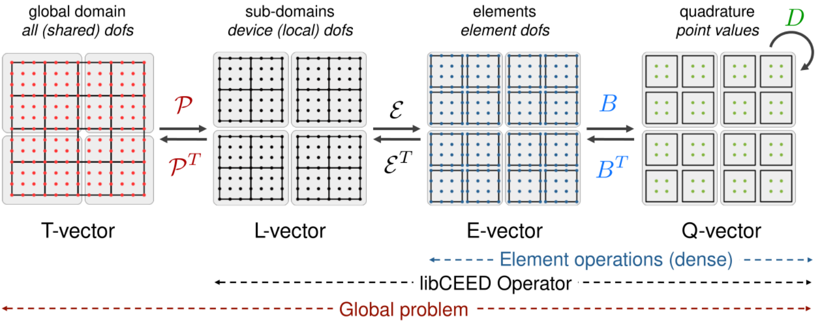
1. Ratel Background
2. AtPoints Evaluation
3. Performance
4. Multigrid
5. Future Work

ECP Roots

- Ratel built directly on results from ECP CEED project
- libCEED provides high-performance operator evaluation
- PETSc provides linear/non-linear solvers and time steppers
- Ratel built from libCEED + PETSc solid mechanics demo app

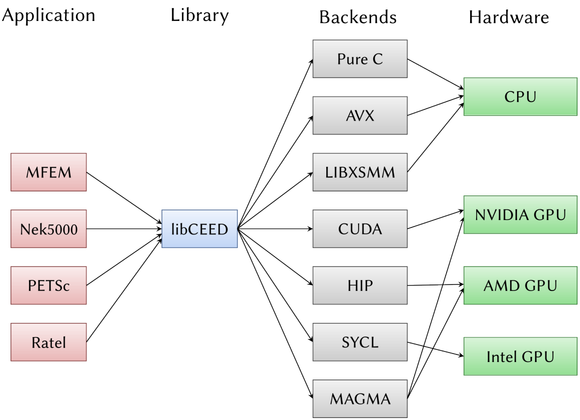
Matrix-Free Operators from libCEED

$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$



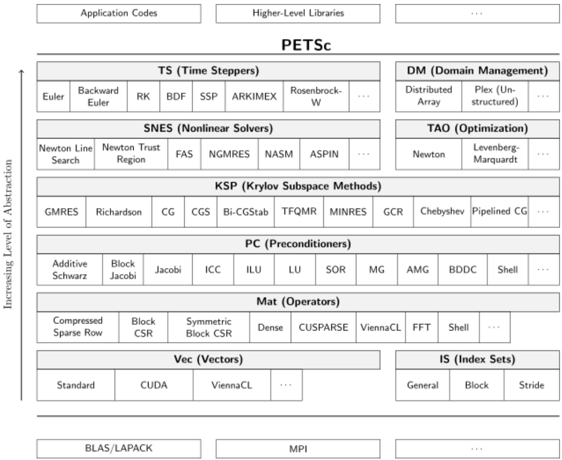
libCEED provides arbitrary order matrix-free operator evaluation

Performance Portability from libCEED



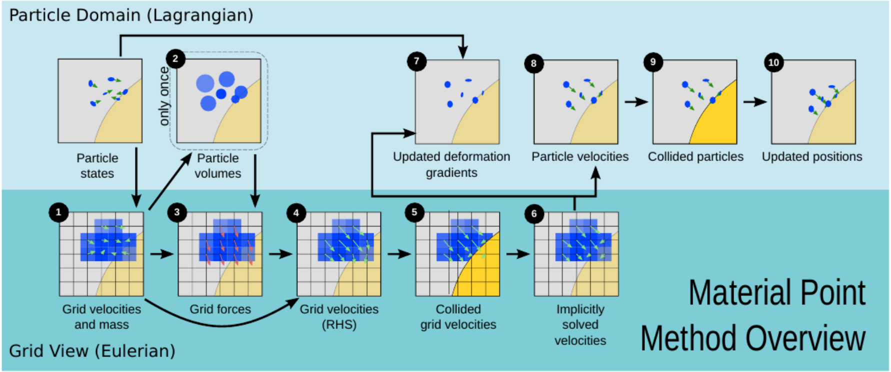
Performance portability with libCEED's matrix-free operators

Extensible Solvers from PETSc



PETSc provides extensible, scalable solvers

What is MPM?



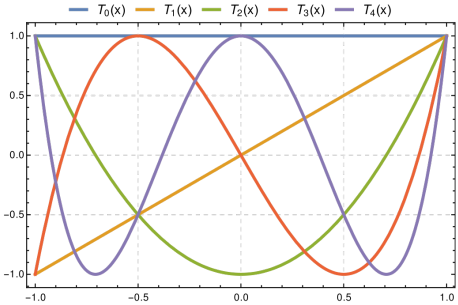
- Continuum based particle method with background mesh for gradients
- Extension of FLIP (which is an extension of PIC)
- Enables large deformation simulations with complex features

MPM vs FEM

MPM can be formulated as very similar to FEM

- Problem on background mesh changes when material points move
- Can be viewed as FEM with arbitrary quadrature point locations
- Natural fit for libCEED matrix-free representation
- Ratel FEM infrastructure provides fast background mesh solves

libCEED Basis Evaluation to Points



- Interpolate from primal to dual (quadrature) space
- Fit Chebyshev polynomials to values at quadrature points
- Evaluate Chebyshev polynomials at arbitrary points

libCEED Basis Evaluation to Points

Interpolation to Chebyshev has same FLOPs as FEM $\mathcal{O}\left(q^4\right)$

- Invert map C^{-1} from quadrature points to Chebyshev coeffs
- Create 1D interpolation matrix $B = CN$
- Tensor product:
  $B = \left(C \otimes C \otimes C\right)\left(N \otimes N \otimes N\right) = \left(CN\right) \otimes \left(CN\right) \otimes \left(CN\right)$
- Additional cost from evaluation to arbitrary points

libCEED Basis Evaluation to Points

Per point evaluation has higher FLOPs $\mathcal{O}\left(q^6\right)$

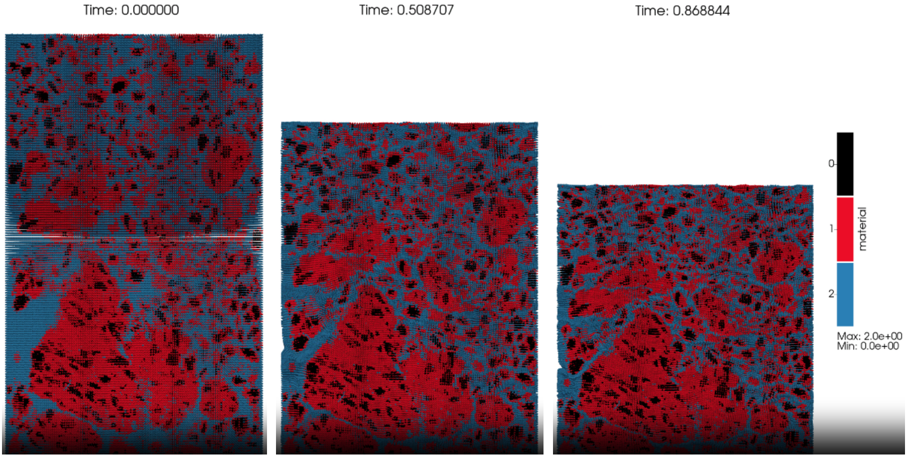
- Recurrence for Chebyshev values at point
  $f_0 = 1,\ f_1 = 2x,\ f_n = 2xf_{n-1} - f_{n-2}$
  $f_0' = 0,\ f_1' = 2,\quad f_n' = 2xf_{n-1}' + 2f_{n-1} - f_{n-2}'$
- Contract pencil of values with element coefficients
- Operation is independent per quadrature point
- $\mathcal{O}\left(q^3\right)$ FLOPs at $\mathcal{O}\left(q^3\right)$ points

AtPoints Operator

Final operator very similar to FEM

- $L = \mathcal{E}^T B^T B^{eT} D B^e B \mathcal{E}$ - CeedOperator
- All other operations identical to FEM
- libCEED gives action of local MPM operator
- PETSc responsible for communication between devices
  $A = P^T L P$

Sample Run



Confined compression of mock HE material

CEED Benchmark Problems

Performance on CEED BPs

- BP1 - Scalar projection problem
- BP2 - 3 component projection problem
- BP3 - Scalar Poisson problem
- BP4 - 3 component Poisson problem

Bulk of FLOPs are in basis evaluation

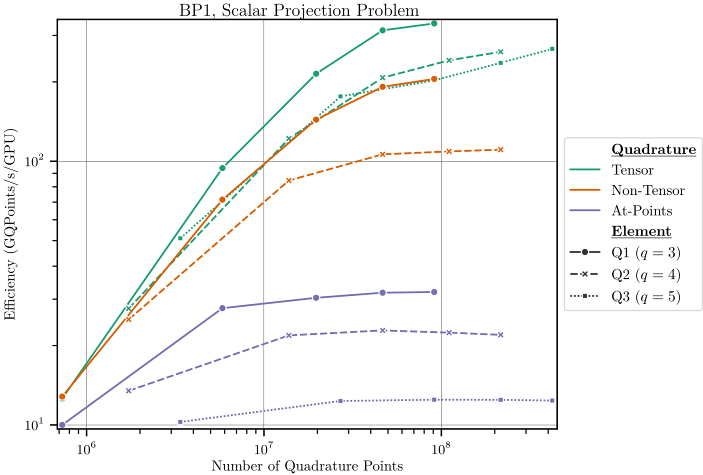
CEED Benchmark Problems

Performance on CEED BPs

- $p = 2, 3, 4$ and $q = p + 1$
- Units cube with 30^3, 60^3, 90^3, 120^3, and 150^3 elements
- Compare tensor, non-tensor, and at-points basis evaluation
- MMS w/ partial sum of Weierstrass function, $a = 0.5$, $b = 1.5$, $N = 2$

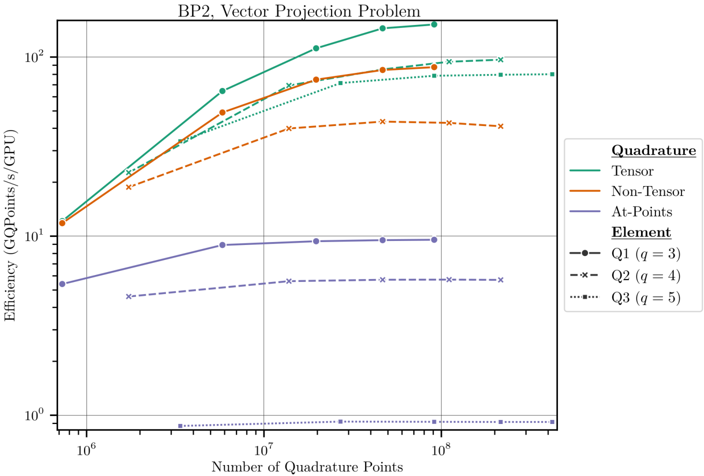
Using 4x AMD Instinct™MI300A Accelerated Processing Units (APUs)

BP1



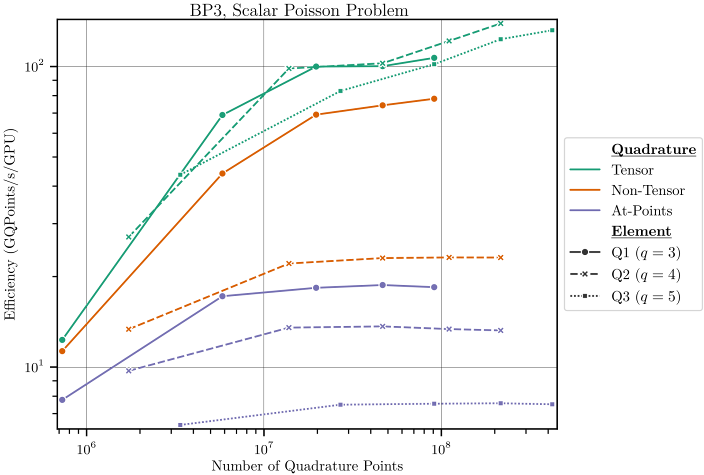
More FLOPs leads to lower efficiency

BP2



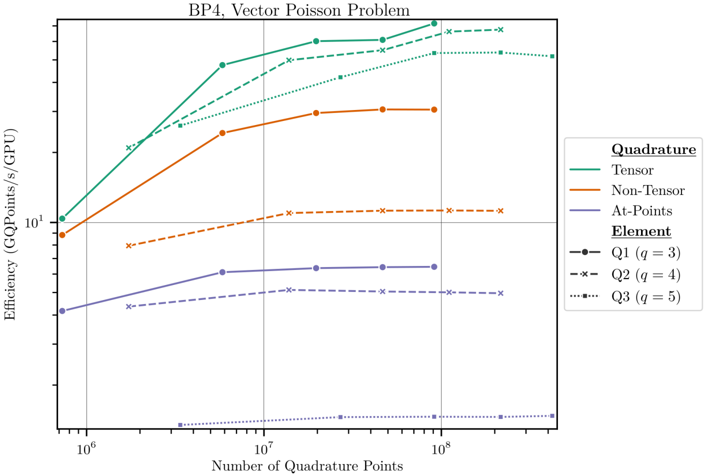
With more components, reach peak efficiency faster

BP3



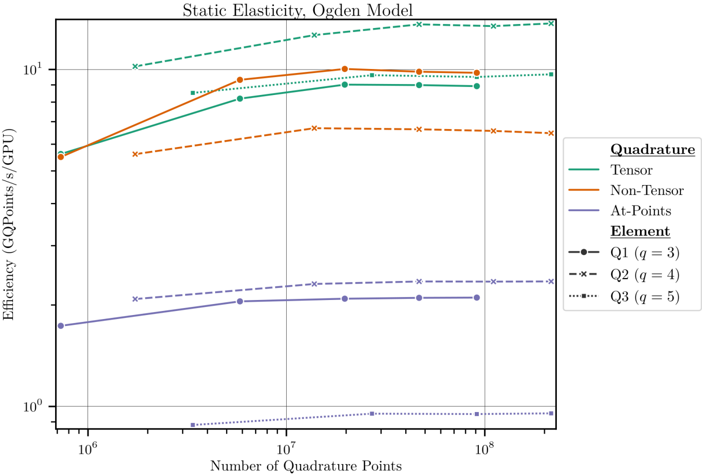
With derivatives, at-points closer to non-tensor

BP3



Derivatives and more components worst for at-points

Ogden



Still see cost with heavier QFunctions

Preconditioning

Practical problems require preconditioning

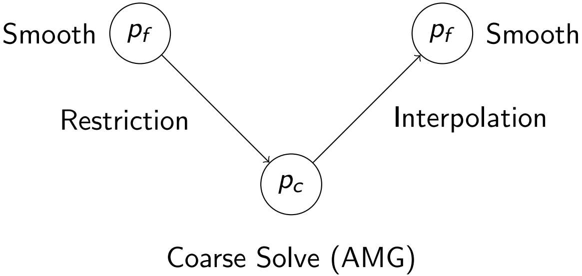
- Problems for MPM tend to be poorly conditioned
- Poor conditioning + expensive Mat-Vec = need preconditioning
- Varying structure between elements makes assembly more difficult

PETSc PCMG

- PCMG - PETSc geometric multigrid preconditioner
- Requires several operators from the user
    - Restriction operator
    - Interpolation operator
    - Smoother
    - Coarse grid solver

Ratel PCpMG

2 level multigrid with PCpMG



Ratel PCpMG

pMG giving promising initial results with GPU impl

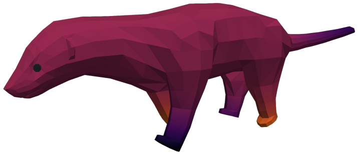
- Finite strain elasticity with damage
- Confined press of grain/binder with "sticky air" voids
- Jacobi iterations tend to double with 2x refinement
- pMG iteration counts robust with refinement

	# MPM Points	Jacobi its	pMG its
Coarse	388,800	900-1000	35-45
Fine	7,372,800	-	25-40

Future Work

- Continued iMPM development
- AtPoints basis and assembly perf tuning
- More models using Automatic Differentiation
- Further contact models development
- Rust QFunctions
- UHyper, UMat integration
- Addition of fluid dynamics models
- Upstream PETSc + libCEED integration
- We invite contributors and friendly users

Questions?



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