

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

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15 July 2025

Ratel Team



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

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The authors acknowledge support by the Department of Energy, National Nuclear Security Administration, Predictive Science Academic Alliance Program (PSAAP) under Award Number DE-NA0003962.



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Ratel - high order, performance portable solid mechanics

Built on libCEED and PETSc

GPU and CPU performance

Overview

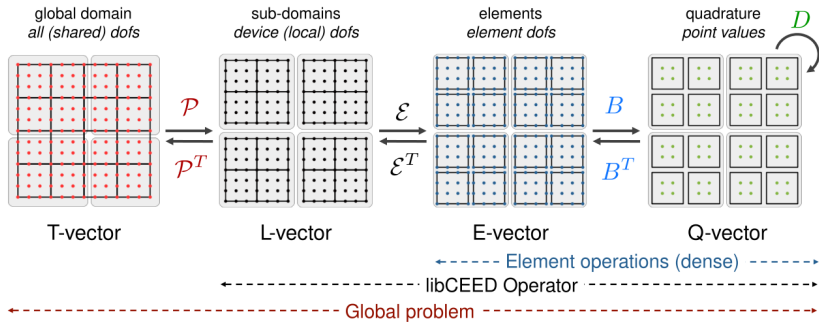
- 1 Ratel Background
- 2 AtPoints Evaluation
- 3 Performance
- 4 Multigrid
- 5 Future Work

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

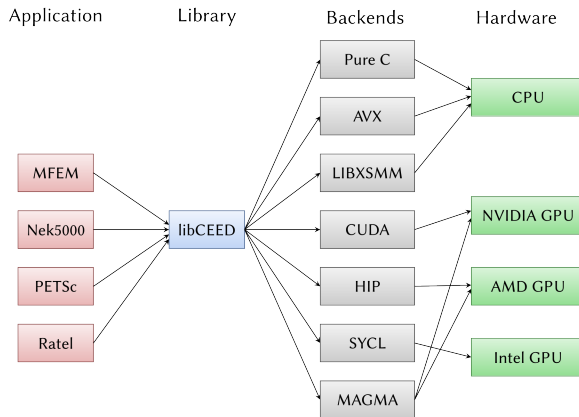
Matrix-Free Operators from libCEED

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



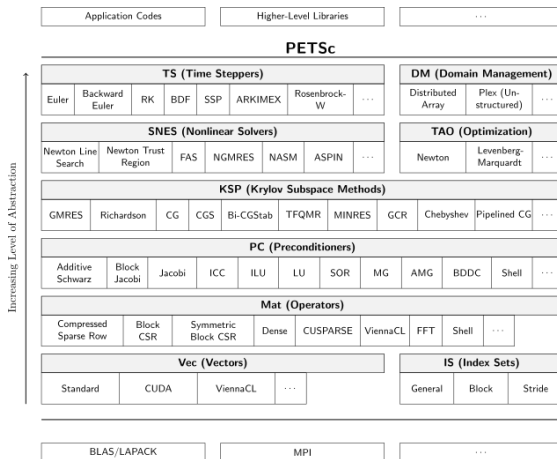
libCEED provides arbitrary order matrix-free operator evaluation

Performance Portability from libCEED



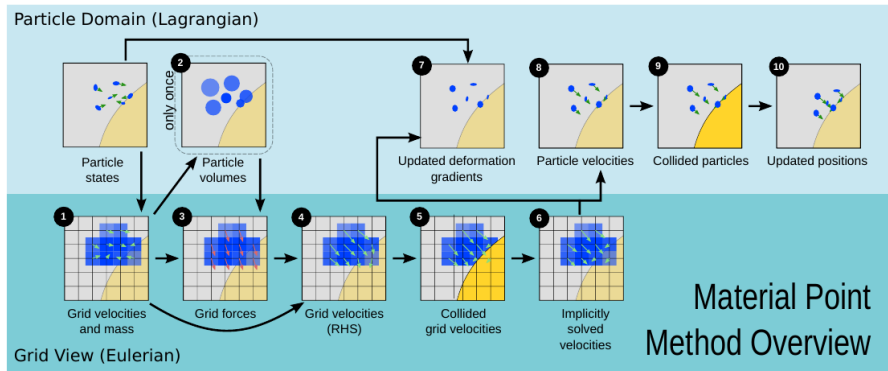
Performance portability with libCEED's matrix-free operators

Extensible Solvers from PETSc



PETSc provides extensible, scalable solvers

What is MPM?



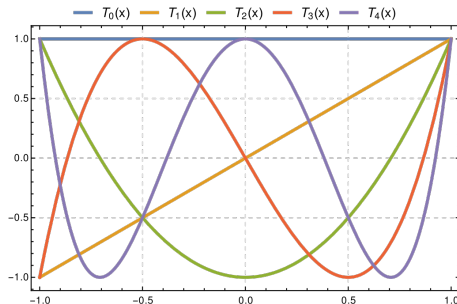
- Continuum based particle method with background mesh for gradients
- Extension of FLIP (which is an extension of PIC)
- Enables large deformation simulations with complex features

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 $\mathcal{O}(q^4)$

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

libCEED Basis Evaluation to Points

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

- Recurrence for Chebyshev values at point

$$f_0 = 1, f_1 = 2x, f_n = 2xf_{n-1} - f_{n-2}$$

$$f'_0 = 0, f'_1 = 2, f'_n = 2xf'_{n-1} + 2f_{n-1} - f'_{n-2}$$

- Contract pencil of values with element coefficients
- Operation is independent per quadrature point
- $\mathcal{O}(q^3)$ FLOPs at $\mathcal{O}(q^3)$ points

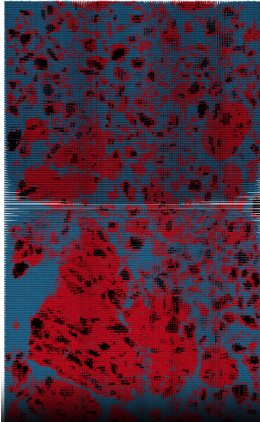
AtPoints Operator

Final operator very similar to FEM

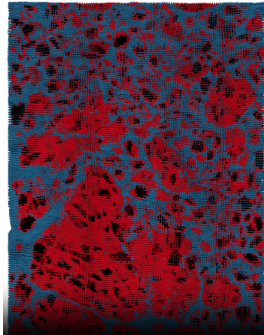
- $L = \mathcal{E}^T B^T B^e{}^T D B^e B \mathcal{E}$ - CeedOperator
- All other operations identical to FEM
- libCEED gives action of local MPM operator
- PETSc responsible for communication between devices
 $A = P^T L P$

Sample Run

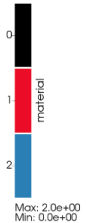
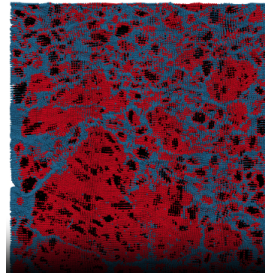
Time: 0.000000



Time: 0.508707



Time: 0.868844



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

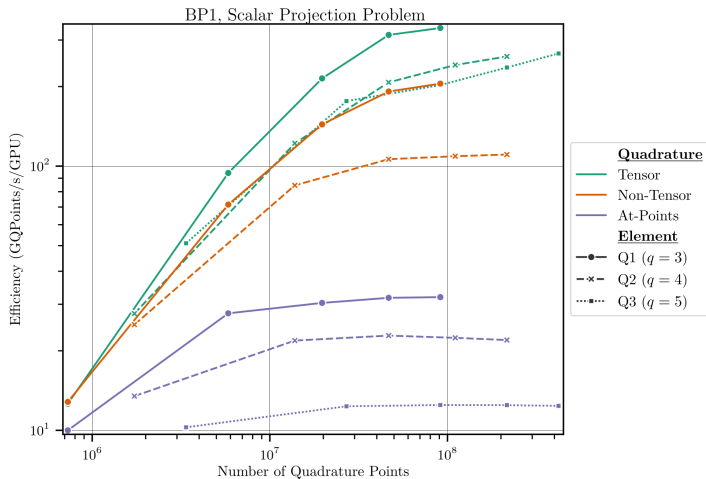
CEED Benchmark Problems

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, $a = 0.5$, $b = 1.5$, $N = 2$

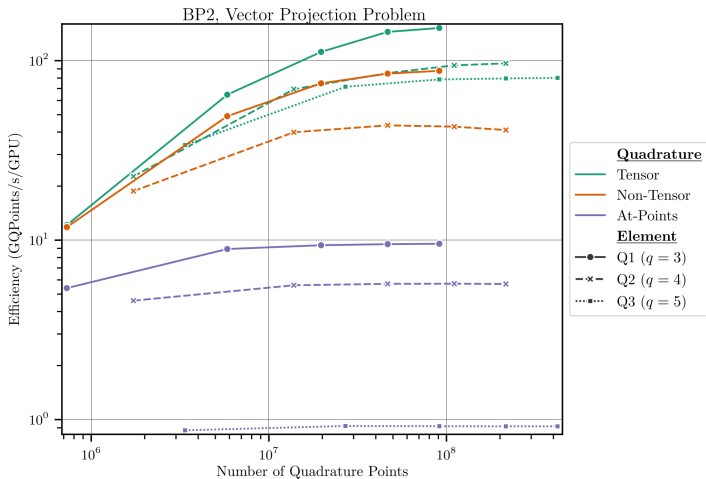
Using 4x AMD Instinct™ MI300A Accelerated Processing Units (APUs)

BP1



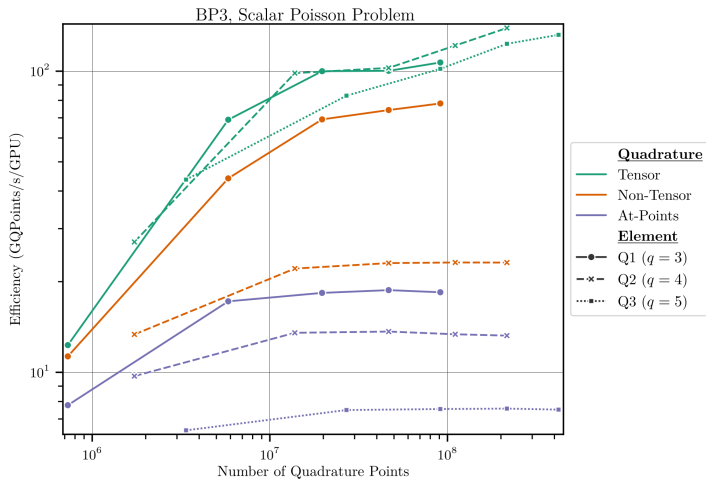
More FLOPs leads to lower efficiency

BP2



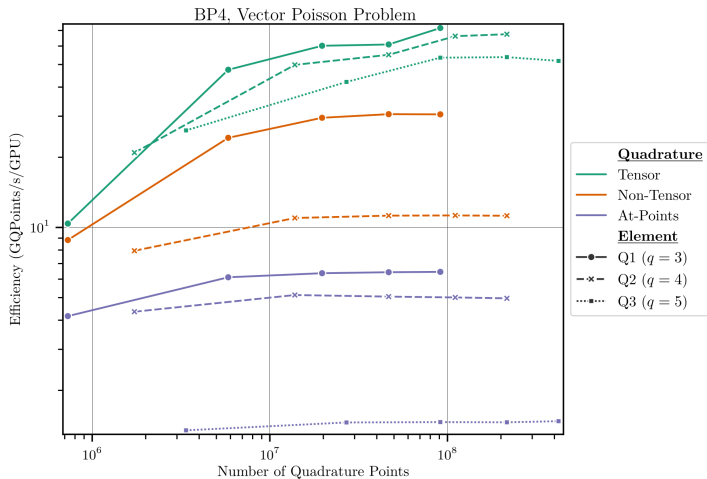
With more components, reach peak efficiency faster

BP3



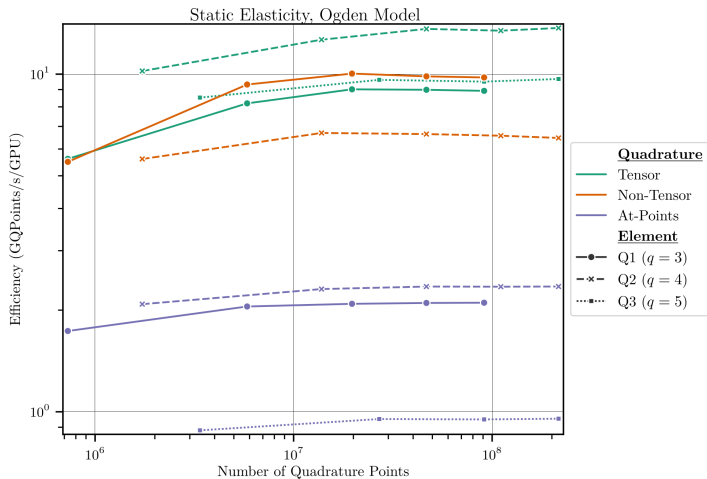
With derivatives, at-points closer to non-tensor

BP4



Derivatives and more components worst for at-points

Ogden



Still see cost with heavier QFunctions

Preconditioning

Practical problems require preconditioning

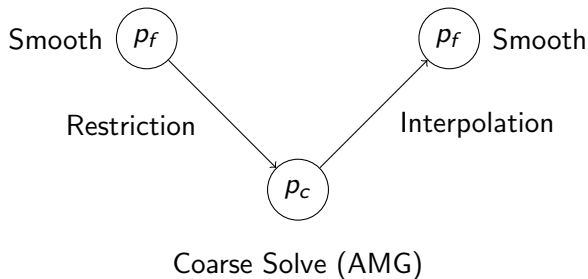
- Problems for MPM tend to be poorly conditioned
- Poor conditioning + expensive Mat-Vec = need preconditioning
- Varying structure between elements makes assembly more difficult

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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