Ratel - New Foundations of Computational Mechanics for the Exascale Era

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Interrupt Me!

Please interrupt with questions/comments

(Yes, especially you students!)

Overview

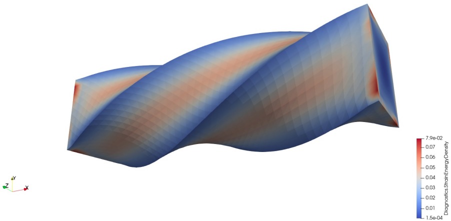
1. libCEED
2. Ratel
3. Mentoring
4. Questions

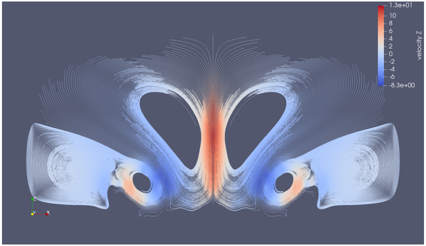
libCEED Team

libCEED Repo: https://github.com/CEED/libCEED

Developers: Ahmad Abdelfattah, Zach R. Atkins, Valeria Barra, Natalie Beams, Jed Brown, Jean-Sylvain Camier, Veselin Dobrev, Yohann Dudouit, Leila Ghaffari, Sebastian Grimberg, Tzanio Kolev, David Medina, Will Paznel, Thilina Ratnayaka, Rezgar Shakeri, Stan Tomov, James Wright III, Jeremy L Thompson

Background





libCEED solid mechanics (left) and fluid dynamics (right) mini-apps

- Physics based simulations important in science/engineering
- Intuition: FEM solves equations with piecewise polynomial solution
- libCEED supports FEM-like simulations on modern hardware

libCEED Projects

Several projects built using libCEED

- Ratel - solid mechanics FEM (H1) and iMPM (PSAAP)
- HONEE - fluid dynamics FEM (H1) & differential filtering (PHASTA)
- MFEM - various applications, libCEED integrators (LLNL)
- Palace - Electromagnetics FEM with MFEM + libCEED (Amazon)
  H(div) and H(curl) elements
- RDycore - FV river dynamical core with PETSc + libCEED (SciDAC)

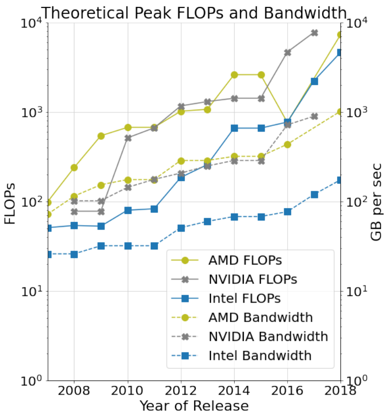
Top 500

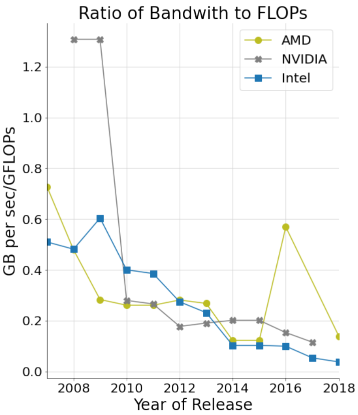
Machine	HPL	HPCG
Fugaku	442.01 PFLOPs	16.01 PFLOPs
Frontier	1,353.00 PFLOPs	14.05 PFLOPs
Aurora	1,012.00 PFLOPs	5.61 PFLOPs
LUMI	379.70 PFLOPs	4.59 PFLOPs
Alps	434.90 PFLOPs	3.57 PFLOPs

Top 500 Machines for HPCG with HPL peak FLOPs

Difficult to realize peak FLOPs with CG on modern machines

Modern Hardware



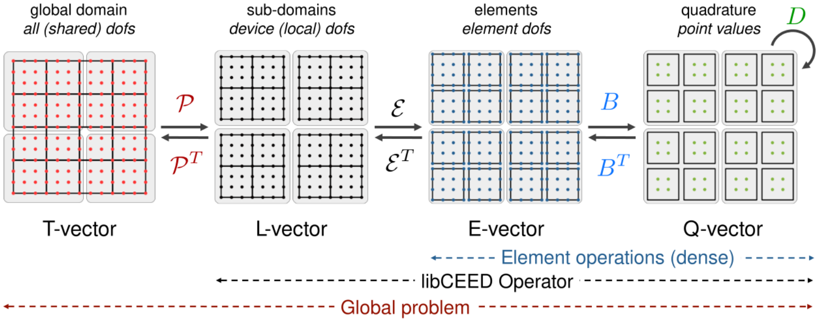


Memory bandwidth is improving slower than FLOPs [2]

Mirrors difference between Top 500 HPL vs HPCG benchmarks [1]

Matrix-Free Operators from libCEED

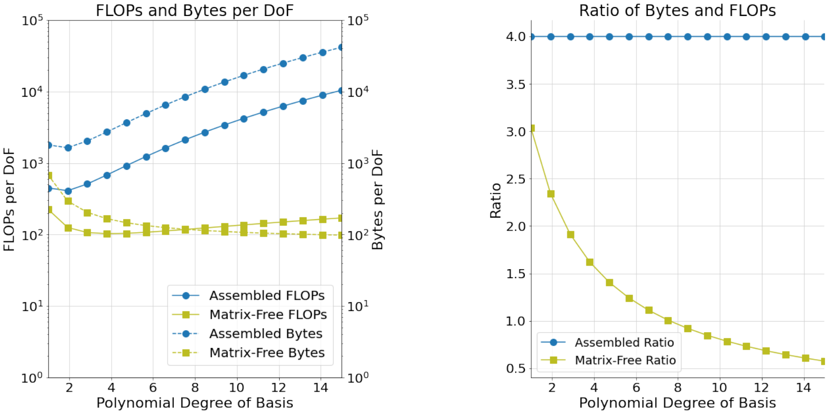
$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$



libCEED provides matrix-free operator evaluation on various hardware

Matrix-free operators apply these steps instead of populating a matrix

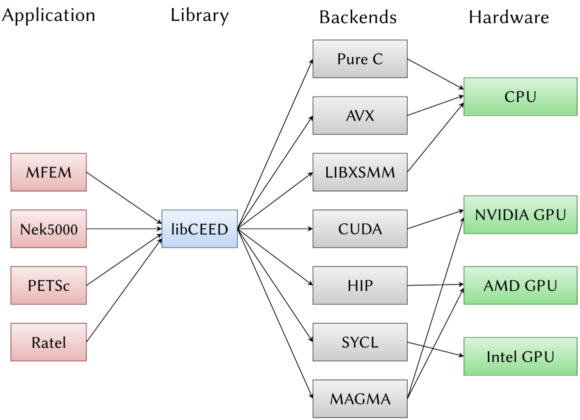
Benefits of Matrix-Free



Requirements for matrix-vector product with sparse matrix vs matrix-free for screened Poisson $\nabla^2 u - \alpha^2 u = f$ in 3D

Matrix-free representations using tensor product bases better match modern hardware

Performance Portability



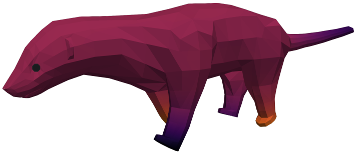
libCEED's design naturally allows multiple hardware implementations

Design Implications

Using matrix-free operators drives design decisions

- Direct solvers are out (require assembled matrix)
- Iterative solvers are in (Krylov methods, etc)
- High order $=$ high accuracy & bad condition numbers
- Preconditioning is needed for fast convergence

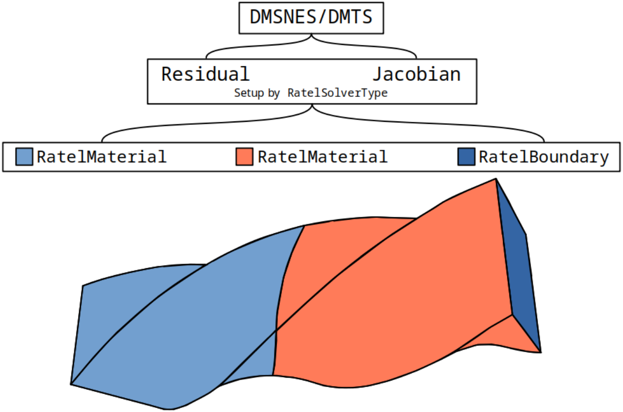
Ratel Team



Ratel Repo: https://gitlab.com/micromorph/ratel

Developers: Zach R. Atkins, Jed Brown, Fabio Di Gioacchino,
Leila Ghaffari, Zach Irwin, Rezgar Shakeri,
Ren Stengel, Jeremy L Thompson

Basic Design



Each material region sets up part of the non-linear and linear equations

Preconditioning Support

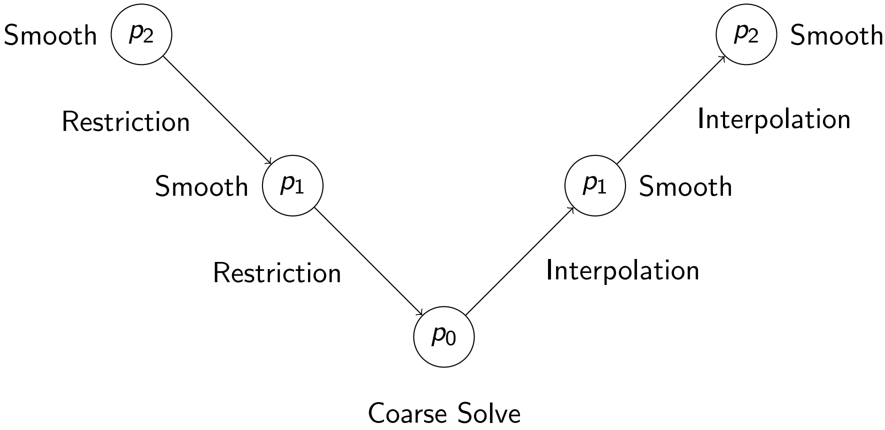
Iterative solvers need preconditioning, especially with high-order operators

- Jacobi - diagonal assembly
- Point Block Jacobi - block diagonal assembly
- Variable Point Block Jacobi - variable block diagonal assembly
- Algebraic Multigrid - full assembly (best for linear elements)

Preconditioning support for matrix-free is an interesting research area

Need to balance setup costs and preconditioner effectiveness

p-multigrid

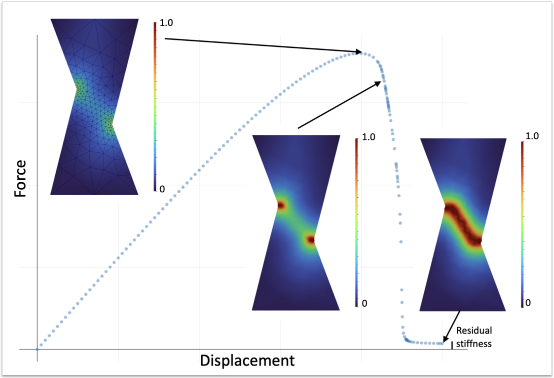


libCEED provides grid transfer operators and smoothers from operators

Too General, Need Specifics

Ok, lets look at some specific simulations

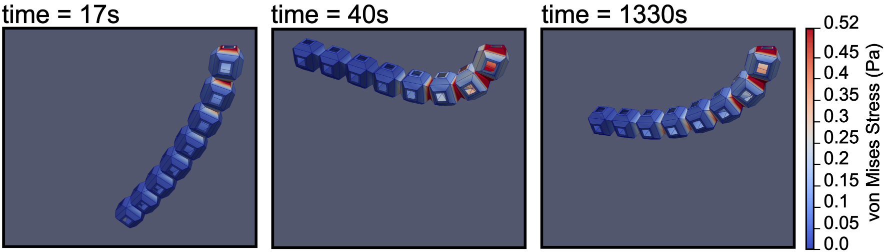
Example - Linear Damage




```
$ bin/ratel-quasistatic -options_file examples/ymls/ex02-
    quasistatic-elasticity-linear-damage-compressiveshear-
    AT2-face-forces.yml
```

Quasistatic simulation of compressive shear for generic brittle material

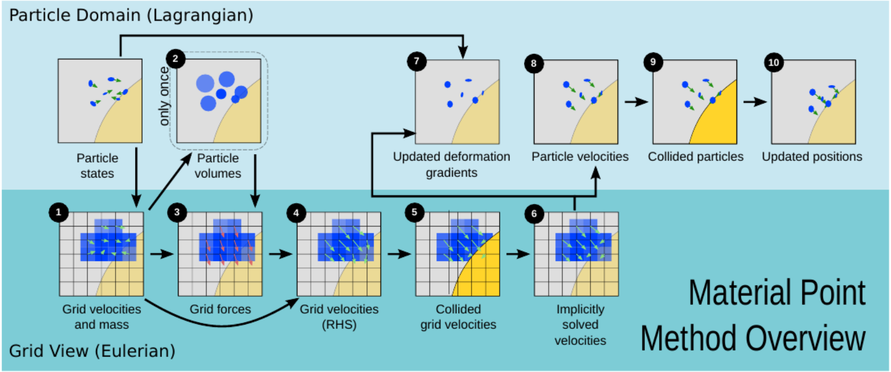
Example - Dynamic Pendulum




```
$ bin/ratel-dynamic -options_file examples/ymls/ex03-dynamic
    -elasticity-schwarz-pendulum-enzyme.yml
```

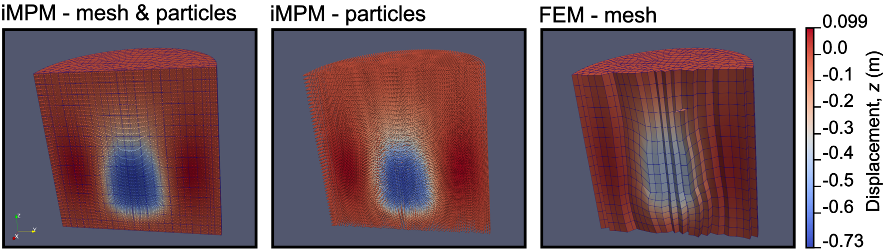
Dynamic simulation of Neo-Hookean Schwarz-P "pendulum" with Enzyme

What is MPM?



- Continuum based particle method with background mesh for gradients
- Extension of FLIP (which is an extension of PIC)
- Used in rendering for the movie *Frozen*

Example - MPM Sinker




```
$ bin/ratel-quasistatic -options_file examples/ymls/ex02-
    quasistatic-elasticity-mpm-neo-hookean-damage-current-
    sinker-cylinder.yml
```

FEM and iMPM simulations of dense sinker in near-incompressible "foam"

Dev Best Practices

Open Source development best practices provide mentoring framework

- Issues/planning act as literature review/research plan
- PR/MRs provide feedback about the work
- Testing verifies correctness, to a degree
- Documentation gives an opportunity to show understanding

Planning

Planning establishes common understanding and goals

- Codebases can easily overwhelm new students/contributors
- Issues help focus the effort and coalesce conversations
- Planning publicly (Issues ideally, or Slack/Zulip) records decisions
- Good example: https://gitlab.com/micromorph/ratel/issues/270

Review

Code review provides feedback and discussions

- All code can be strengthened with review and feedback
- PR/MRs provide tangible assets to guide any discussion
- Public review lets multiple people comment; prevents surprises
- Easy to be more/less explicit as appropriate for the student

Testing

Testing is as essential part of MR acceptance

- Tests communicate intended usage and verify correctness
- New logic must have tests, code coverage is a **guide**
- Minimal reproducers for bugs also make good tests
- Untested code is broken code; tested code is less broken code

Documentation

Documentation ensures understanding and maintainability

- Code needs documentation
- Another avenue to communicate/verify understanding
- Documentation can also be used to start papers/dissertations
- Good documentation facilitates planning for new features

Questions?

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Ratel Repo: https://gitlab.com/micromorph/ratel

Grant: Predictive Science Academic Alliance Program (DE-NA0003962)

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Hans Meuer, Erich Strohmaier, Jack Dongarra, Horst Simon, and Martin Meuer.
Top 500 list, 2020.

Karl Rupp.
CPU-GPU-MIC comparision charts, 2020.

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