

Performance-Portable Implicit Scale-Resolving Compressible Flow Using libCEED

SIAM CSE 2023

James Wright, Jed Brown, Kenneth Jansen, Leila Ghaffari

February 27, 2023

Ann and H.J. Smead Department of Aerospace Engineering Sciences



Smead Aerospace
UNIVERSITY OF COLORADO **BOULDER**

1. libCEED Overview
2. Compressible Fluid Equations in libCEED
3. Efficient Implicit Timestepping
4. Performance and Results of Flat Plate Boundary Layer Simulation



libCEED Overview



What is libCEED?

- C library for element-based discretizations
 - Bindings available for Fortran, Rust, Python, and Julia



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 - Code that runs on CPU also runs on GPU without changes
 - Computational backend selectable at runtime, using runtime compilation
- Geared toward high-order finite element discretizations
- Performance demonstrated for solids in Brown *et al.* 2022¹
 - Want to apply those methods and lessons-learned to fluids

¹*Performance Portable Solid Mechanics via Matrix-Free p -Multigrid*, Brown *et al.*, arXiv:2204.01722



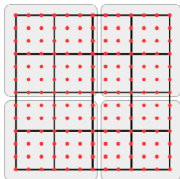
Finite Element Operator Decomposition



Finite Element Operator Decomposition

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

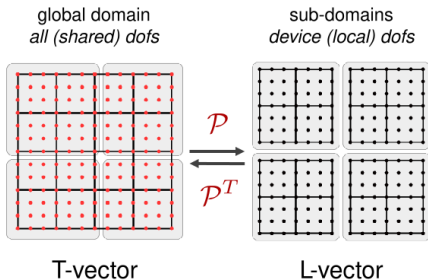
global domain
all (shared) dofs



T-vector

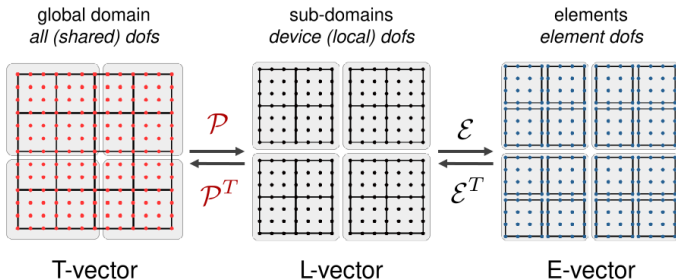
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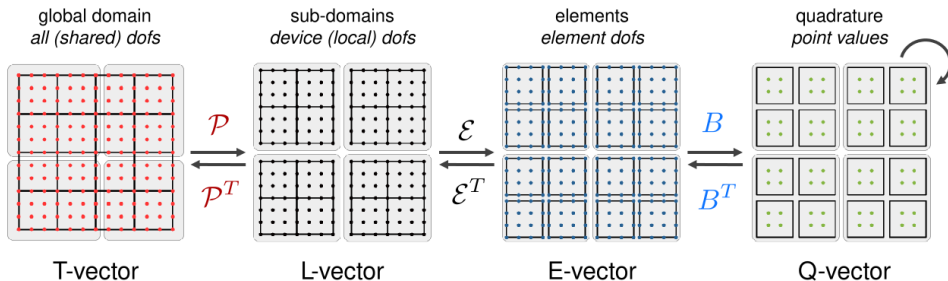
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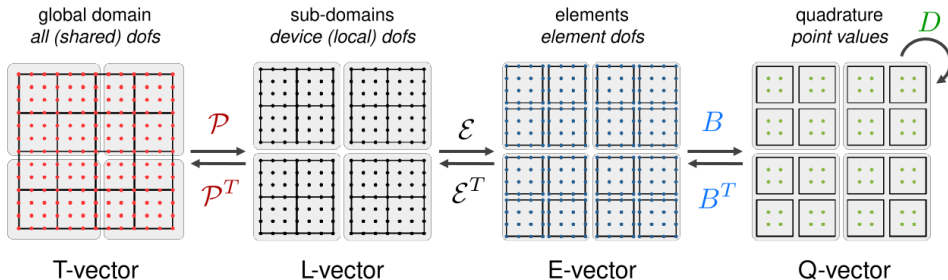
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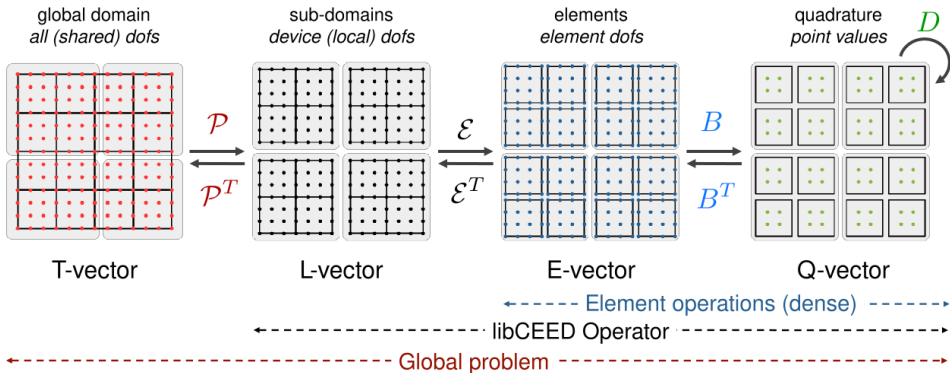
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Compressible Fluid Equations in libCEED



$$\mathbf{A}_0 \mathbf{Y}_{,t} + \mathbf{F}_{i,i}(\mathbf{Y}) - S(\mathbf{Y}) = 0$$

for

$$\underbrace{\mathbf{A}_0 \begin{bmatrix} p \\ u_i \\ T \end{bmatrix}}_{\mathbf{Y}} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho e \end{bmatrix}, \quad \mathbf{F}_i(\mathbf{Y}) = \underbrace{\begin{pmatrix} \rho u_i \\ \rho u_i u_j + p \delta_{ij} \\ (\rho e + p) u_i \end{pmatrix}}_{\mathbf{F}_i^{\text{adv}}} + \underbrace{\begin{pmatrix} 0 \\ -\sigma_{ij} \\ -\rho u_j \sigma_{ij} - k T_{,i} \end{pmatrix}}_{\mathbf{F}_i^{\text{diff}}}, \quad S(\mathbf{Y}) = - \begin{pmatrix} 0 \\ \rho \mathbf{g} \\ 0 \end{pmatrix}$$



Compressible Navier-Stokes for Continuous-Galerkin FEM

Find $\mathbf{Y} \in \mathcal{S}^h$, $\forall \mathbf{v} \in \mathcal{V}^h$

$$\int_{\Omega} \mathbf{v} \cdot [\mathbf{A}_0 \mathbf{Y}_{,t} - \mathbf{S}(\mathbf{Y})] \, d\Omega + \int_{\Omega} \mathbf{v} \cdot \mathbf{F}_{i,i}(\mathbf{Y}) \, d\Omega$$



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$$\mathcal{G}(\mathbf{Y}_{,t}, \mathbf{Y}) = 0$$



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Efficient Implicit Timestepping



Implicit Timestepping

Implicit timestepping requires solving:

$$\frac{d\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{d\mathbf{Y}} \Delta \mathbf{Y} = -\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})$$



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Bottom Line

Cost of $\frac{d\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{d\mathbf{Y}} \Delta \mathbf{Y}$ dominates implicit timestepping cost



Jacobian Matrix-Vector Multiply Options

How to compute $\frac{d\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{d\mathbf{Y}} \Delta \mathbf{Y}$?



Jacobian Matrix-Vector Multiply Options

How to compute $\frac{d\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{d\mathbf{Y}} \Delta \mathbf{Y}$?

- Store $\frac{d\mathcal{G}}{d\mathbf{Y}}$ directly (sparse matrix representation)
 - **Pros:** Opens up preconditioning options
 - **Cons:** Is large, expensive to store



Jacobian Matrix-Vector Multiply Options

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- Store $\frac{d\mathcal{G}}{d\mathbf{Y}}$ directly (sparse matrix representation)
 - **Pros:** Opens up preconditioning options
 - **Cons:** Is large, expensive to store
- Finite difference matrix-free approximation:

$$\frac{d\mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{d\mathbf{Y}} \Delta \mathbf{Y} \approx \frac{\mathcal{G}(\mathbf{Y}_t, \mathbf{Y} + \epsilon \Delta \mathbf{Y}) - \mathcal{G}(\mathbf{Y}_t, \mathbf{Y})}{\epsilon}$$

- **Pros:** Just need a residual evaluation, cheap (in programming and computation)
- **Cons:** Accuracy limited to $\sqrt{\epsilon_{\text{machine}}}$, preconditioning require partial assembly



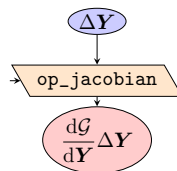
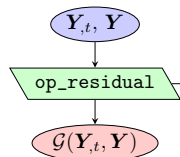
Exact Matrix-Free Jacobian via CeedOperator

$$\begin{aligned}\frac{d\mathcal{G}}{d\mathbf{Y}}\Delta\mathbf{Y} &= \frac{d}{d\mathbf{Y}} \overbrace{\left[\mathcal{P}^T \mathcal{E}^T \mathbf{B}^T \mathbf{G} \mathbf{B} \mathcal{E} \mathcal{P} \right]}^{\mathcal{G}(\mathbf{Y},t,\mathbf{Y})} \Delta\mathbf{Y} \\ &= \left[\mathcal{P}^T \mathcal{E}^T \mathbf{B}^T \frac{d\mathbf{G}}{d\mathbf{Y}} \mathbf{B} \mathcal{E} \mathcal{P} \right] \Delta\mathbf{Y}\end{aligned}$$



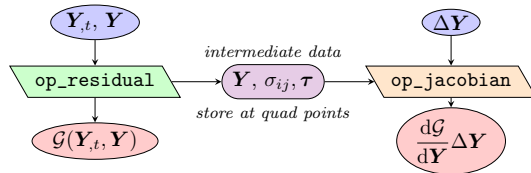
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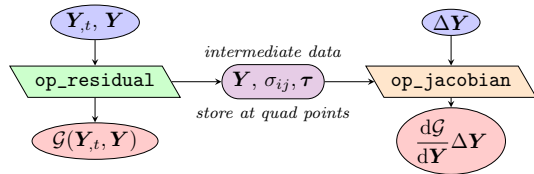
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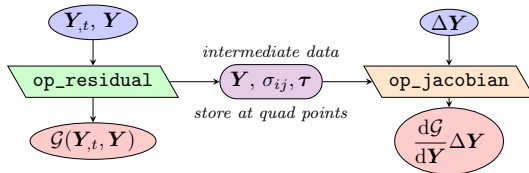
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- **Cons:** Preconditioning requires partial assembly, requires coding Jacobian

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²Affect of specific terms may be ignored from the Jacobian. This is done for $d\tau/d\mathbf{Y}$

Performance and Results of Flat Plate Boundary Layer Simulation

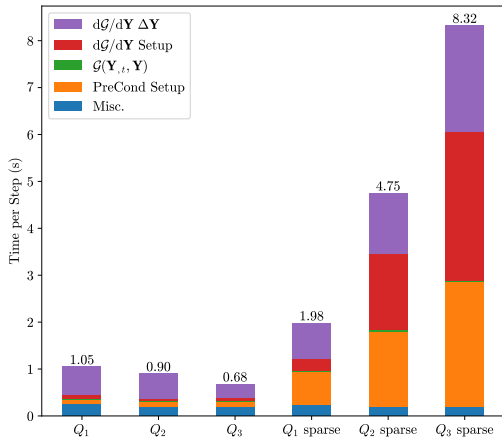


Problem Description

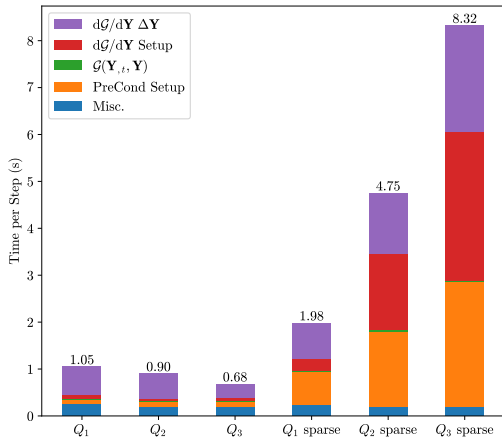
- Flat plate boundary layer with zero pressure gradient
 - $Re_\theta \approx 970$ boundary layer at inflow, $M \approx 0.1$
 - Synthetic turbulence generation (STG) used for inflow structures
 - Run at implicit large eddy simulation (ILES) resolution for linears (higher orders may be DNS level, tbd)
- Test 3 different order elements, Q_1, Q_2, Q_3 tensor-product hexes
- Maintain *DOF resolution* (DoFs per physical length/ global DoF count)
- Performance results shown for two nodes of ALCF's Polaris (4× NVIDIA A100 per node)



Exact Matrix-Free Jacobian vs Sparse



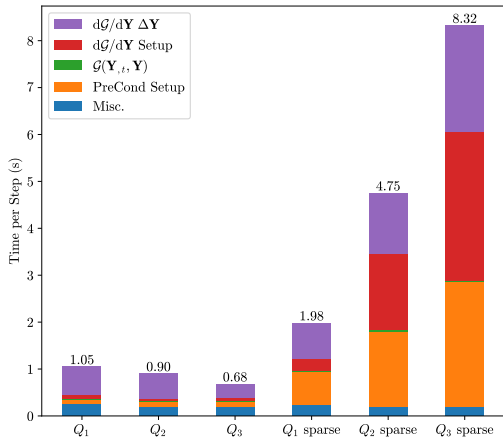
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- Sparse $d\mathcal{G}/d\mathbf{Y} \Delta\mathbf{Y}$ significantly slower than matrix-free



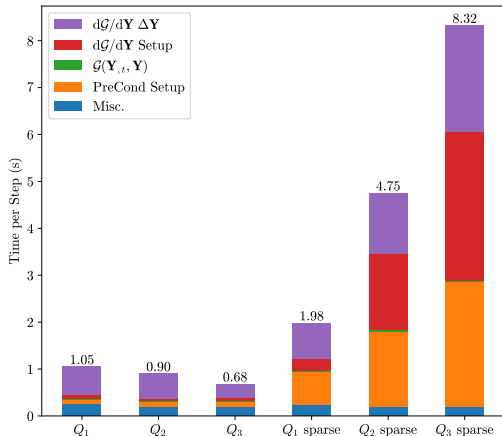
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- Time to assemble $d\mathcal{G}/d\mathbf{Y}$ quite large



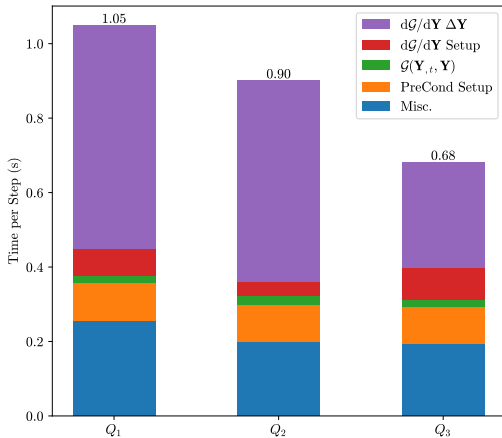
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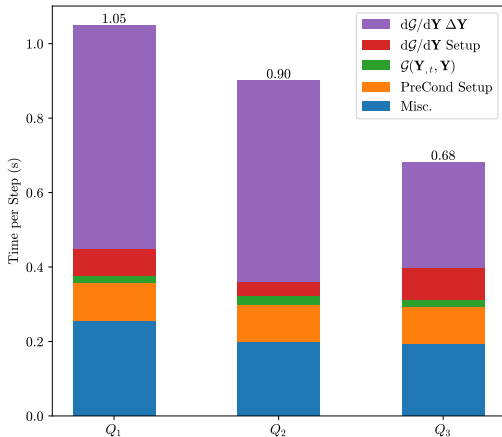
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- Associated costs rise with element order



Fluids Performance Analysis



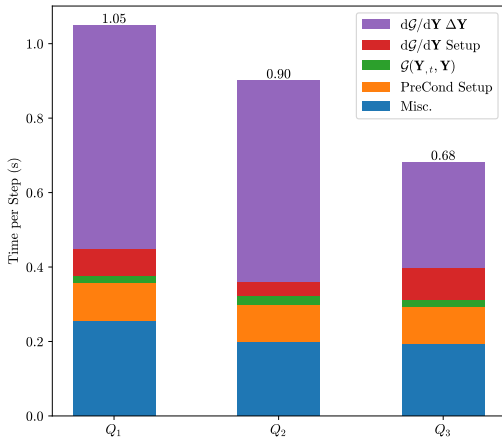
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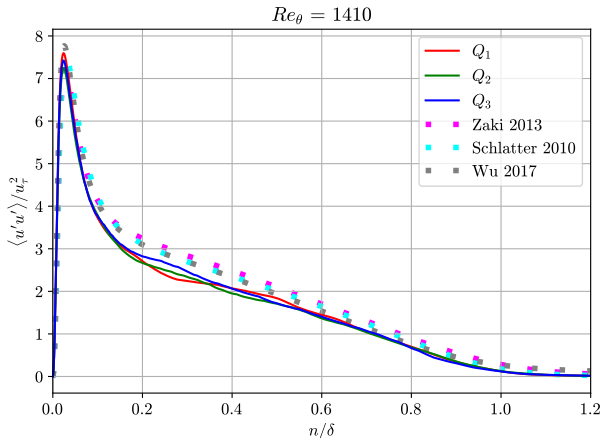
Fluids Performance Analysis



- Time of $d\mathcal{G}/d\mathbf{Y} \Delta\mathbf{Y}$ decreases as order increases
- $d\mathcal{G}/d\mathbf{Y}$ setup time increases with order
 - Dominant cost is partial matrix assembly for preconditioning



Results of Flat Plate Boundary Layer



- Spanwise statistics implemented to verify scale-resolving results
- Results *not* converged, but show realistic stress profiles

Zaki et al., 2013, *From Streaks to Spots and on to Turbulence: Exploring the Dynamics of Boundary Layer Transition*
Schlatter et al., 2010, *Assessment of direct numerical simulation data of turbulent boundary layers*
Wu et al., 2017, *Transitional-turbulent spots and turbulent-turbulent spots in boundary layers*



Support and References

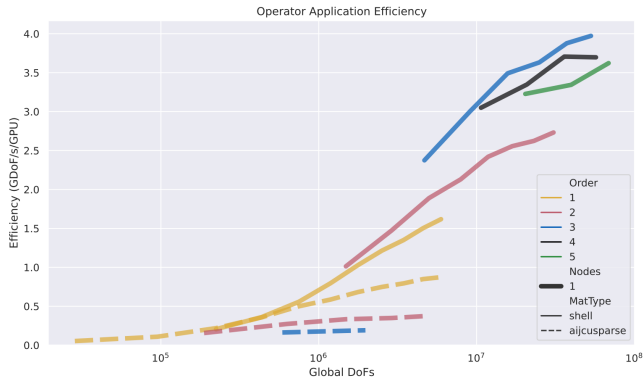
- Research supported by US Department of Energy through DE-SC0021411 FASTMath SciDAC Institute
- Argonne Leadership Computing Facility resources used for this research
- We thank PETSc and libCEED developers, especially Jeremy Thompson and Junchao Zhang among many others



Appendix Slides



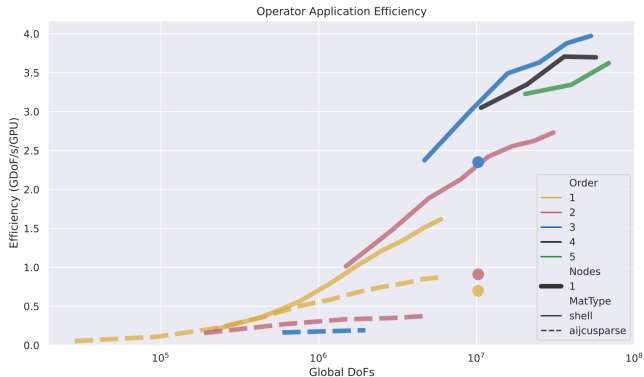
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Matrix-Free Application Comparison (Reproduced from Brown *et al.* 2022). Not from fluids code, but representative of libCEED matrix-free



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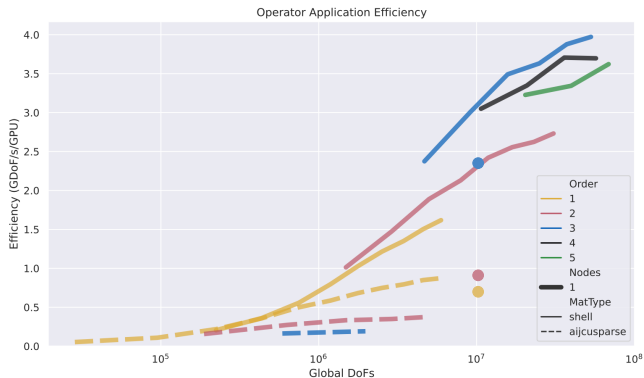


- Significant differences with performance implications
 - Fluids run over 2 nodes → network latency present
 - Solids code lower in FLOPs and storage per DoF

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 - Solids code lower in FLOPs and storage per DoF
- Significant increase in efficiency for $Q_1, Q_2 \rightarrow Q_3$

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