Performance-Portable Implicit Scale-Resolving Compressible Flow Using libCEED

SIAM CSE 2023

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Outline

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

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- Geared toward high-order finite element discretizations
- Performance demonstrated for solids in Brown *et al.* 2022[1]
  - 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

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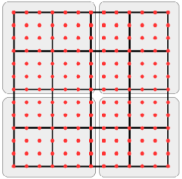
$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$

global domain
all (shared) dofs



T-vector

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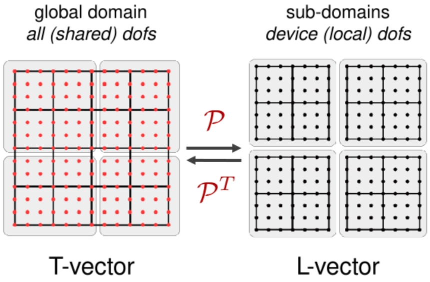

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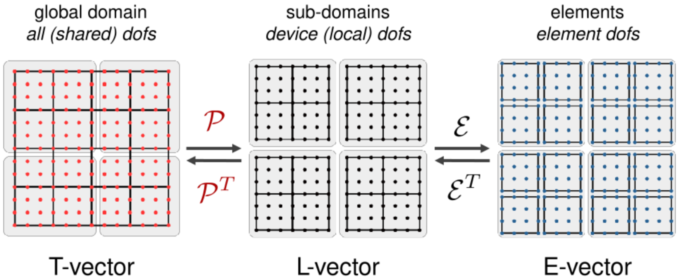

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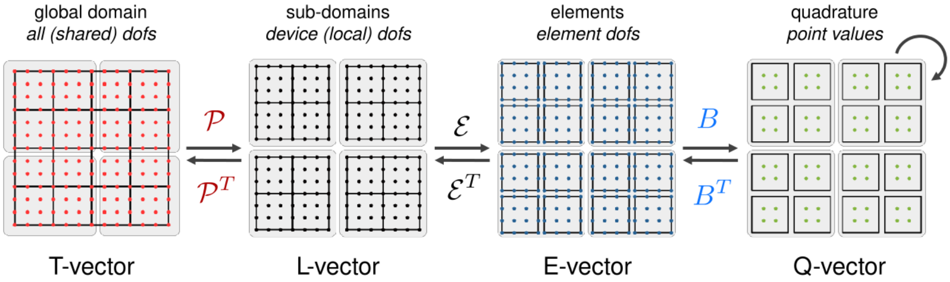

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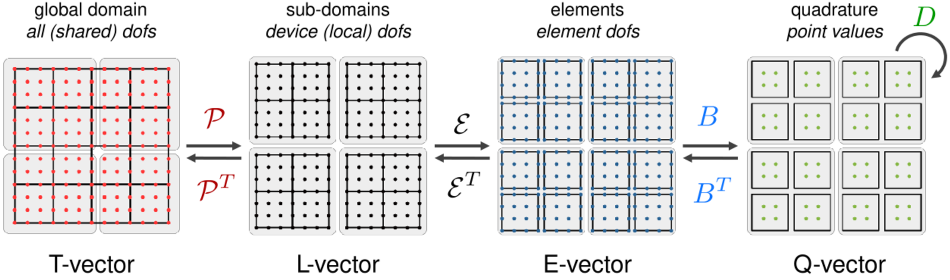

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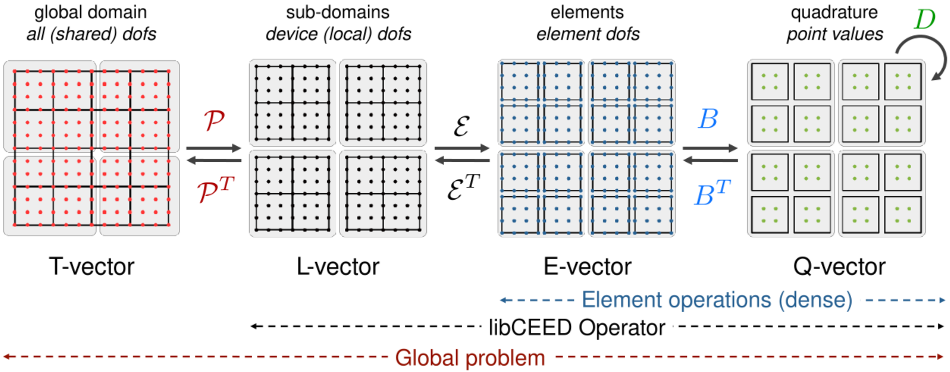

Compressible Fluid Equations in libCEED

Compressible Navier-Stokes

$$\boldsymbol{A_0} \boldsymbol{Y}_{,t} + \boldsymbol{F}_{i,i}(\boldsymbol{Y}) - S(\boldsymbol{Y}) = 0$$

for

$$\boldsymbol{A_0} \underbrace{\begin{bmatrix} p \\ u_i \\ T \end{bmatrix}}_{\boldsymbol{Y}} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho e \end{bmatrix}, \quad \boldsymbol{F}_i(\boldsymbol{Y}) = \underbrace{\begin{pmatrix} \rho u_i \\ \rho u_i u_j + p\delta_{ij} \\ (\rho e + p) u_i \end{pmatrix}}_{\boldsymbol{F}_i^{\text{adv}}} + \underbrace{\begin{pmatrix} 0 \\ -\sigma_{ij} \\ -\rho u_j \sigma_{ij} - k T_{,i} \end{pmatrix}}_{\boldsymbol{F}_i^{\text{diff}}}, \quad S(\boldsymbol{Y}) = -\begin{pmatrix} 0 \\ \rho \boldsymbol{g} \\ 0 \end{pmatrix}$$

Compressible Navier-Stokes for Continuous-Galerkin FEM

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

$$\int_\Omega \boldsymbol{v} \cdot \left[\boldsymbol{A_0} \boldsymbol{Y}_{,t} - \boldsymbol{S}(\boldsymbol{Y})\right] \,\mathrm{d}\Omega + \int_\Omega \boldsymbol{v} \cdot \boldsymbol{F}_{i,i}(\boldsymbol{Y}) \,\mathrm{d}\Omega$$

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$$\underbrace{+ \int_\Omega \mathscr{L}^{\mathrm{adv}}(\boldsymbol{v}) \boldsymbol{\tau} \left[\boldsymbol{A_0} \boldsymbol{Y}_{,t} + \boldsymbol{F}_{i,i}(\boldsymbol{Y}) - S(\boldsymbol{Y})\right] \,\mathrm{d}\Omega}_{\text{SUPG}} = 0$$

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$$\Rightarrow \quad {\color{red}\mathcal{P}^T}\mathcal{E}^T{\color{blue}B^T}{\color{green}G}{\color{blue}B}\mathcal{E}{\color{red}\mathcal{P}} \begin{bmatrix} \boldsymbol{Y}_{,t} \\ \boldsymbol{Y} \end{bmatrix} = 0$$

Efficient Implicit Timestepping

Implicit Timestepping

Implicit timestepping requires solving:

$$\frac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \Delta \boldsymbol{Y} = -\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})$$

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- Krylov solvers form solution basis from $\operatorname{span}\left\{ \left[\frac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \right]^n \Delta \boldsymbol{Y} \right\}_{n=0}$

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Bottom Line

Cost of $\frac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \Delta \boldsymbol{Y}$ dominates implicit timestepping cost

Jacobian Matrix-Vector Multiply Options

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  - **Pros:** Opens up preconditioning options
  - **Cons:** Is large, expensive to store
- Finite difference matrix-free approximation:

$$\frac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \Delta \boldsymbol{Y} \approx \frac{\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y} + \epsilon \Delta \boldsymbol{Y}) - \mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\epsilon}$$

  - **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{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}\Delta\boldsymbol{Y} &= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{Y}} \overbrace{\left[\mathcal{P}^T \mathcal{E}^T B^T G B \mathcal{E} \mathcal{P}\right]}^{\mathcal{G}(\boldsymbol{Y}_{,t},\boldsymbol{Y})} \Delta\boldsymbol{Y} \\
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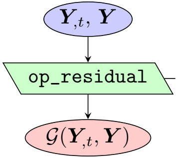

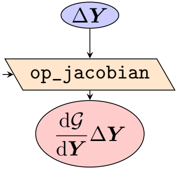

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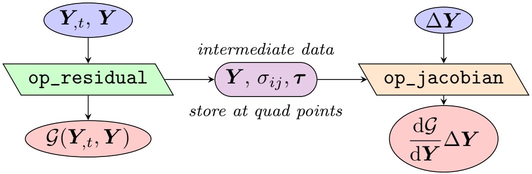

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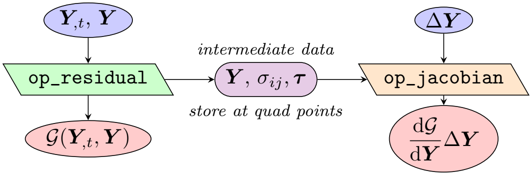

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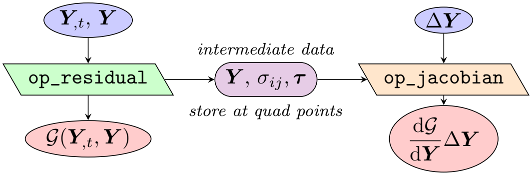

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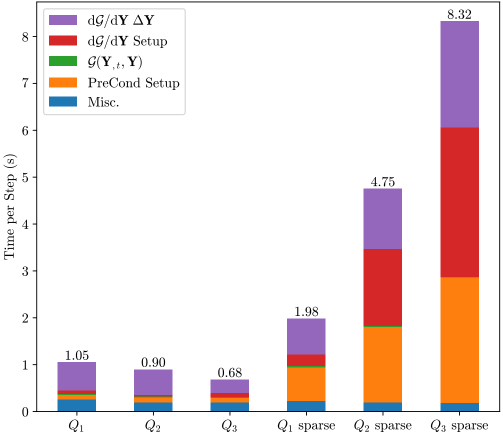
[2]Affect of specific terms may be ignored from the Jacobian. This is done for $\mathrm{d}\boldsymbol{\tau}/\mathrm{d}\boldsymbol{Y}$

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 ($4\times$ NVIDIA A100 per node)

Exact Matrix-Free Jacobian vs Sparse



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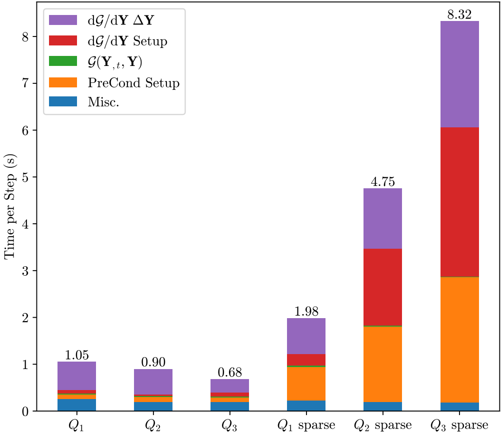

- Sparse $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}\Delta\boldsymbol{Y}$ significantly slower than matrix-free

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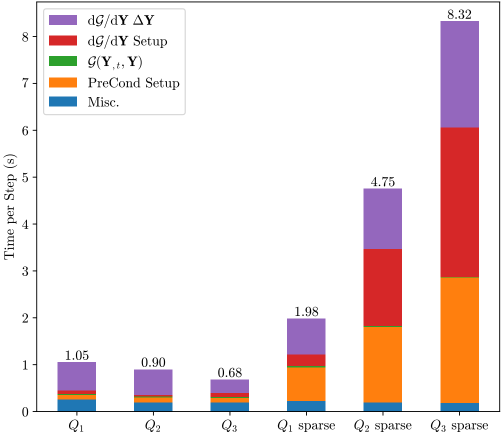

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- Time to assemble $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}$ quite large

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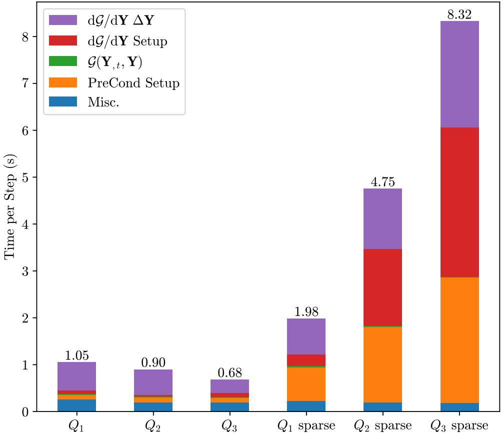

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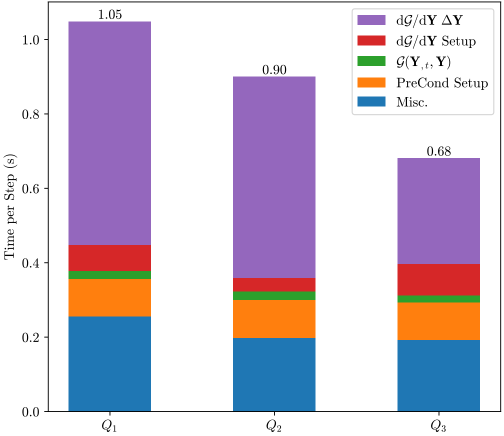
- Time to assemble $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}$ quite large
- Associated costs rise with element order

Fluids Performance Analysis



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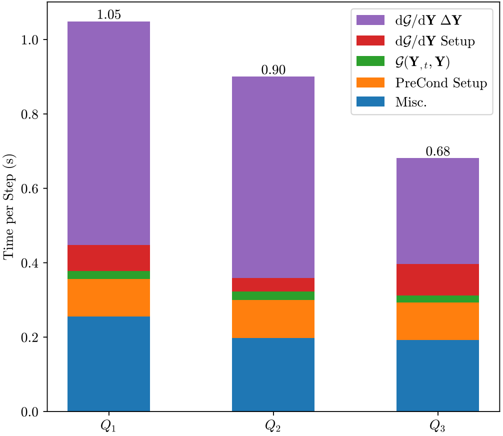

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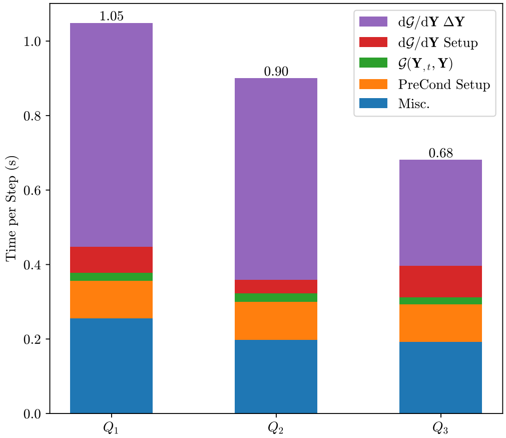
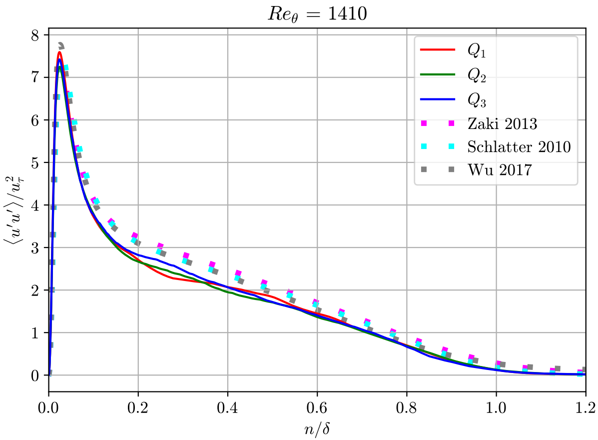


- Time of $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}\,\Delta\boldsymbol{Y}$ decreases as order increases
- $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}$ setup time increases with order
  - Dominant cost is partial matrix assembly for preconditioning

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

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- We thank PETSc and libCEED developers, especially Jeremy Thompson and Junchao Zhang among many others