Performance-Portable Implicit Scale-Resolving Compressible Flow Using libCEED

SIAM CSE 2023

James Wright, Jed Brown, Kenneth Jansen, Leila Ghaffari

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

Smead Aerospace
UNIVERSITY OF COLORADO **BOULDER**

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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- Performance demonstrated for solids.......

Finite Element Operator Decomposition

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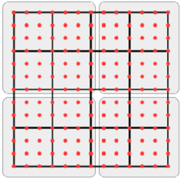
$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$

global domain
all (shared) dofs



T-vector

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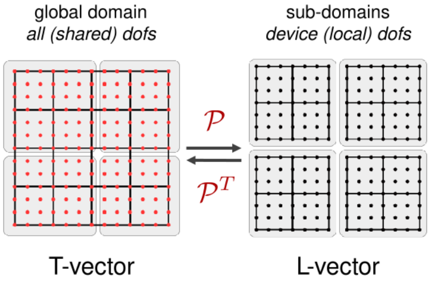

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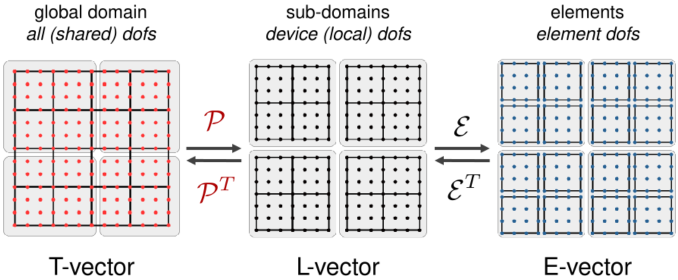

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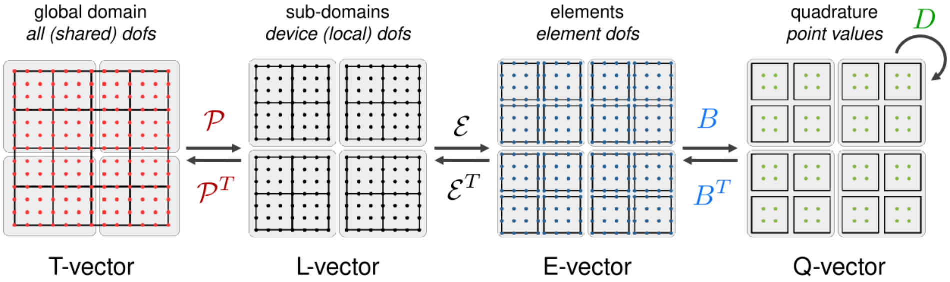

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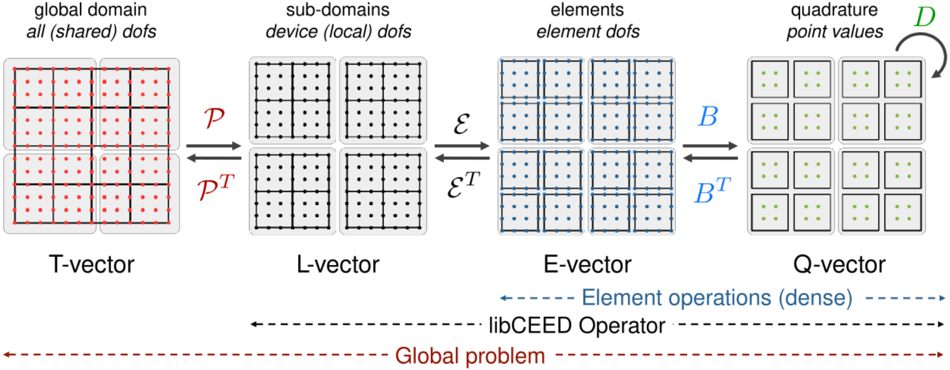

Compressible Fluid Equations in libCEED

Compressible Navier-Stokes

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

for

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

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

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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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

How to compute $\dfrac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \Delta \boldsymbol{Y}$?

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  - **Pros:** Opens up preconditioning options
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- 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 $\sqrt{\epsilon_{\text{machine}}}$, preconditiong require partial assembly

Exact Matrix-Free Jacobian via CeedOperator

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

$$= \left[\mathcal{P}^T \mathcal{E}^T B^T \frac{\mathrm{d}G}{\mathrm{d}\boldsymbol{Y}} B \mathcal{E} \mathcal{P}\right] \Delta\boldsymbol{Y}$$

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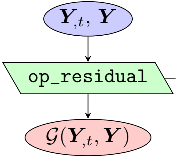

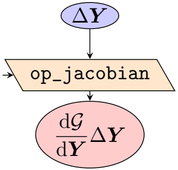

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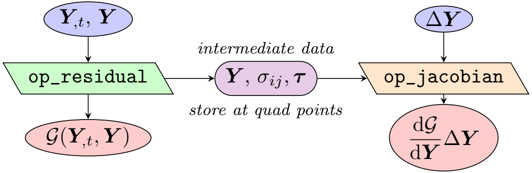

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&= \left[\mathcal{P}^T\mathcal{E}^T B^T \frac{\mathrm{d}G}{\mathrm{d}\boldsymbol{Y}} B\mathcal{E}\mathcal{P}\right]\Delta\boldsymbol{Y}
\end{aligned}
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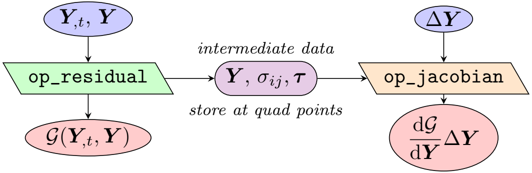

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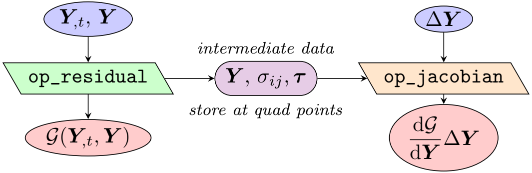

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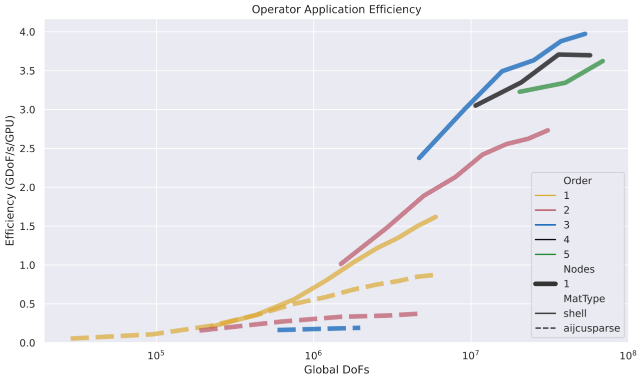
[1] Affect of specific terms may be ignored from the Jacobian. This is done for $\mathrm{d}\boldsymbol{\tau}/\mathrm{d}\boldsymbol{Y}$

Performance Exact Matrix-Free Jacobian via CeedOperator



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

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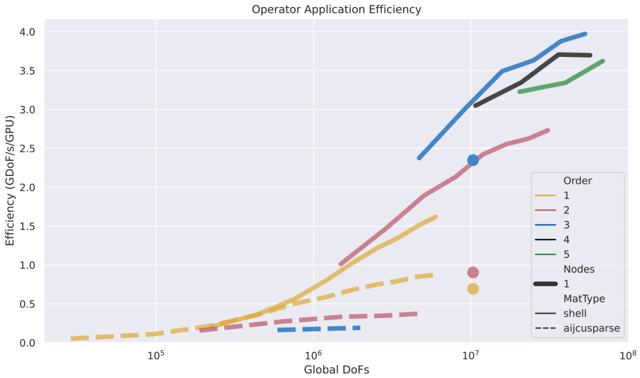

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  - Fluids run over 2 nodes ⟶ network latency present
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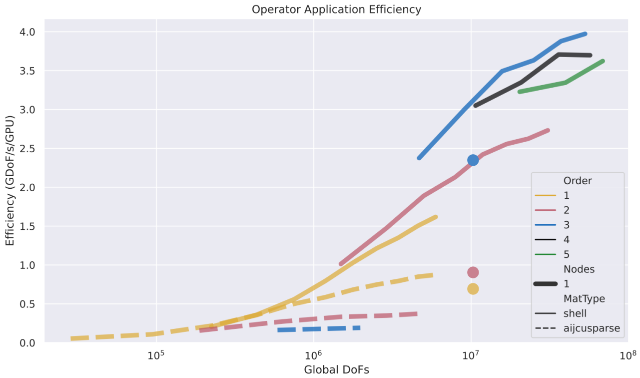

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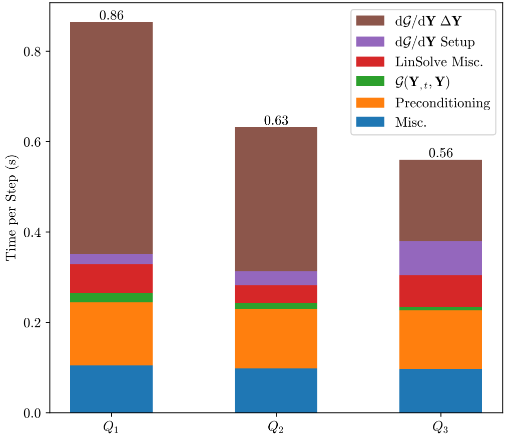
- Significant increase in efficiency for $Q_1, Q_2 \rightarrow Q_3$

Performance and Results of Flat Plate Boundary Layer Simulation

Fluids Performance Analysis



Run on ALCF's Polaris on two nodes (8× NVIDIA A100, global DoF count fixed

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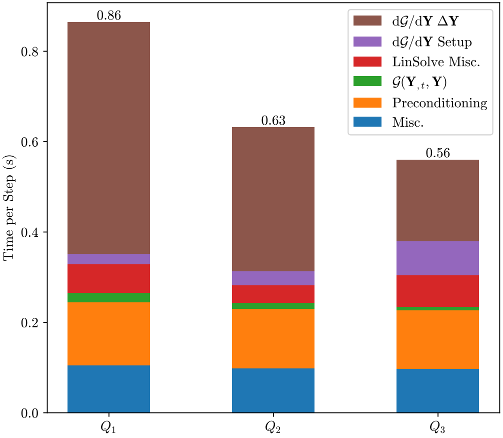

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- Time of $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}\,\Delta\boldsymbol{Y}$ decreases as order increases
  - Despite increase in $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}\,\Delta\boldsymbol{Y}$ calculations per timestep:

Q_1	Q_2	Q_3
250	221	360

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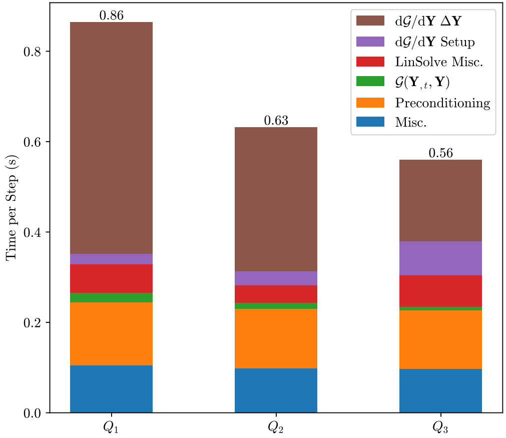

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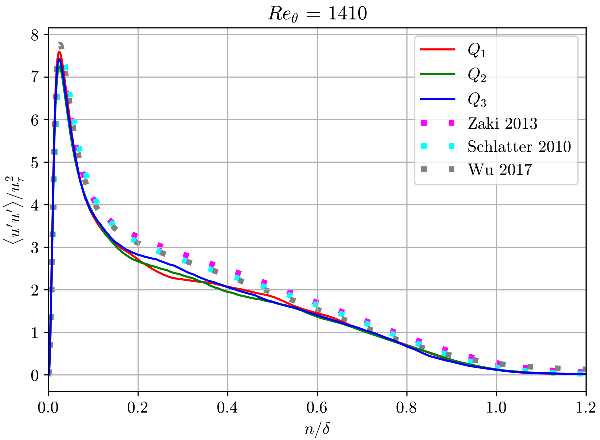
- $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}$ setup time increases with order
  - Dominant cost is partial matrix assembly for preconditioning
  - For Q_3, eats up gains from faster $\mathrm{d}\mathcal{G}/\mathrm{d}\boldsymbol{Y}\Delta\boldsymbol{Y}$ calculations

Results of Flat Plate Boundary Layer



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

Support and References

This work was supported by.... Add in sponsor support (ALCF, FastMATH DOE, ECP, etc)