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. Viscous Outflow Boundary Conditions
4. Efficient Implicit Timestepping

libCEED Overview

What is libCEED?

- C library for element-based discretizations
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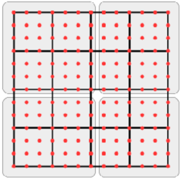
- Geared toward high-order finite element discretizations

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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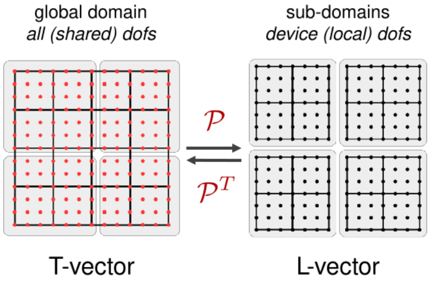

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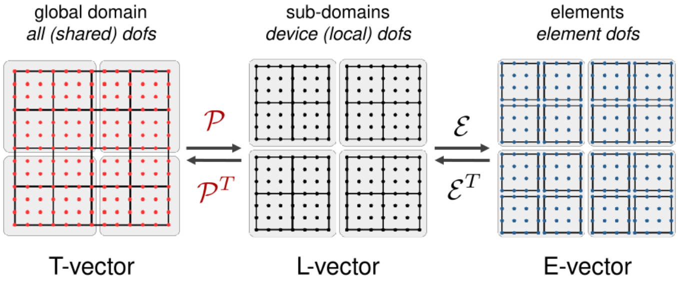

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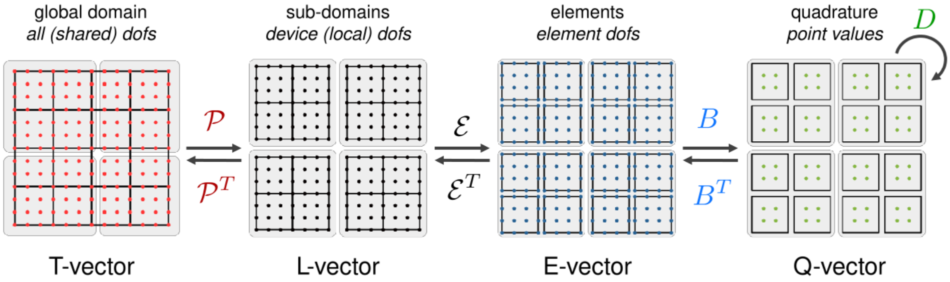

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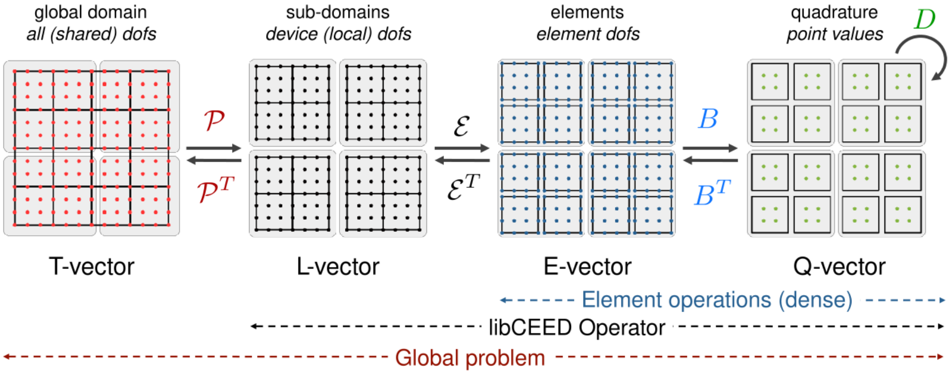

Compressible Fluid Equations in libCEED

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

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Simplify into residual form:

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

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

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

Viscous Outflow Boundary Conditions

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- Riemann Flux BCs everywhere is ideal

$$\boldsymbol{F}_i = \boldsymbol{F}_i^{\text{adv}}$$

p^{int}	p^{ext}
u_i^{int}	u_i^{ext}
T^{int}	T^{ext}

Riemann Flux

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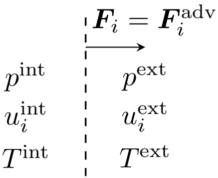
Solution

- Calculate $\boldsymbol{F}_i^{\text{adv}}$ via Riemann solver, setting $u_i^{\text{ext}} = u_i^{\text{int}}$



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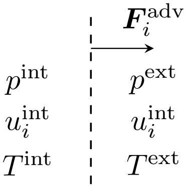

Riemann Outflow Boundary Condition Flux

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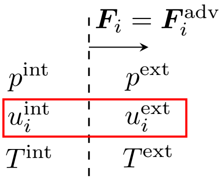

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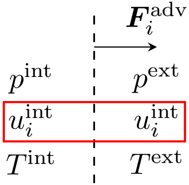

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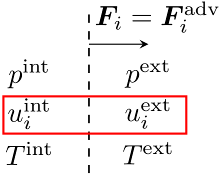
- Calculate $\boldsymbol{F}_i^{\text{adv}}$ via Riemann solver, setting $u_i^{\text{ext}} = u_i^{\text{int}}$
- Calculate $\boldsymbol{F}_i^{\text{diff}}$ from solution, then $\boldsymbol{F}_i = \boldsymbol{F}_i^{\text{adv}} + \boldsymbol{F}_i^{\text{diff}}$



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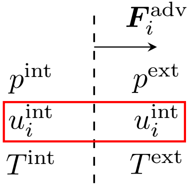
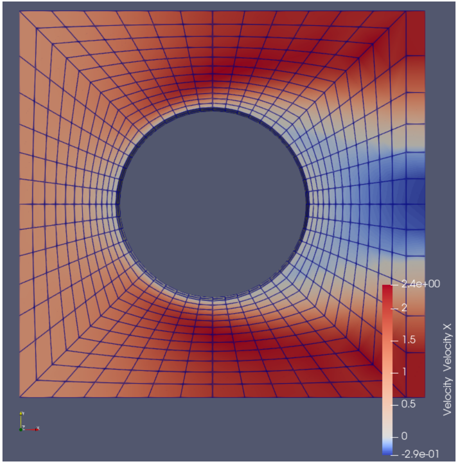


Riemann Outflow Boundary Condition Flux

Viscous Outflow Boundary Conditions Demonstration



- Cylinder in cross flow torture test
- Stable despite recirculation
- Only p and T set at boundary

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 $\mathrm{span}\left\{ \left[\frac{\mathrm{d}\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})}{\mathrm{d}\boldsymbol{Y}} \right]^n \Delta \boldsymbol{Y} \right\}_{n=0}$

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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

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

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- Store $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}$ directly (sparse matrix representation)
  - **Pros:** Opens up preconditioning 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 $\sqrt{\epsilon_{\text{machine}}}$, 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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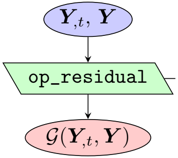

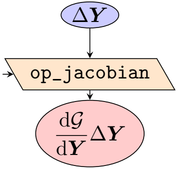

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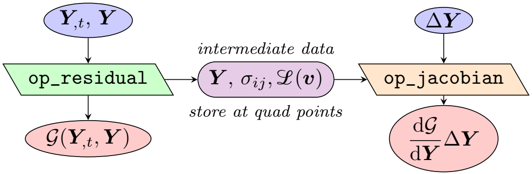

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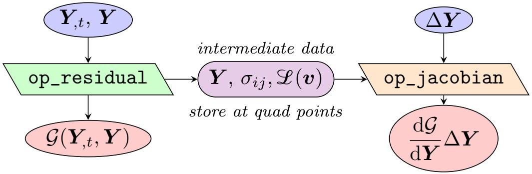
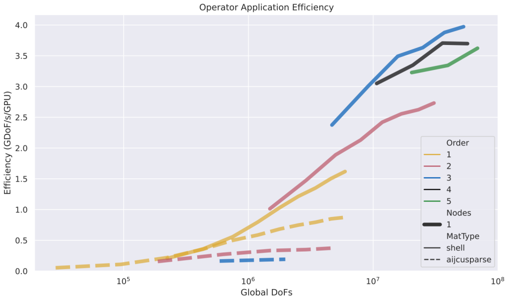


- **Pros:** Exact Jacobian matrix-vector product (potentially faster convergence)
- **Cons:** Preconditioning requires partial assembly

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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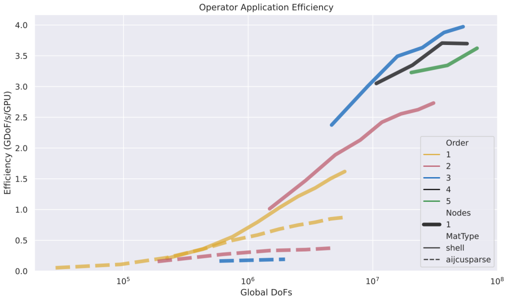

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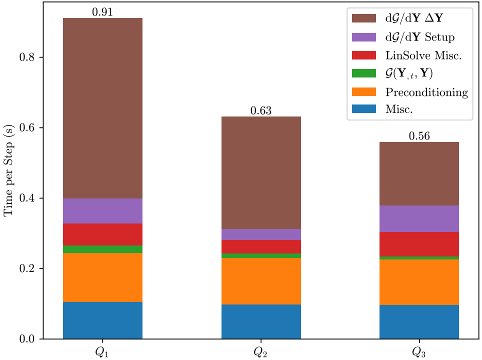

Fluids performance, DoFs fixed.
Run on ALCF's Polaris on two nodes ($8\times$ NVIDIA A100)

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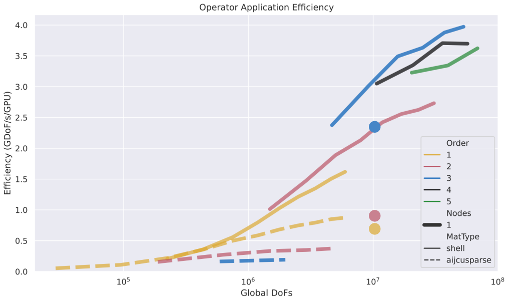

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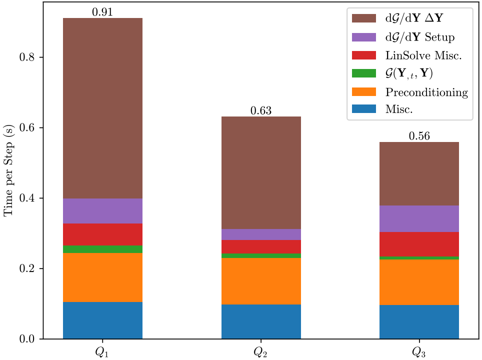

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Support and References

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