Performance-Portable Implicit Scale-Resolving Compressible Flow Using libCEED

SIAM CSE 2023

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Outline

1. What is libCEED?
2. libCEED Overview
3. Fluid Simulations with libCEED
4. Accuracy and Performance of High-Order Scale-Resolving Simulations

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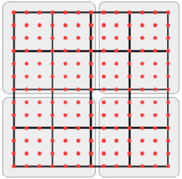
- Portable to different hardware via computational backends
  - Code that runs on CPU also runs on GPU without changes
  - Computational backend selectable at runtime, using runtime compilation
- Geared toward high-order finite element discretizations

libCEED Overview

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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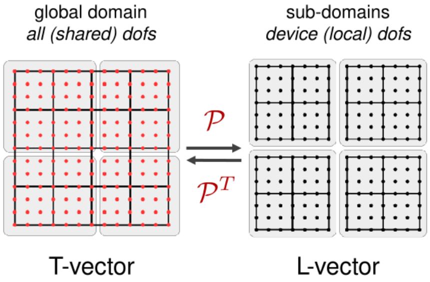

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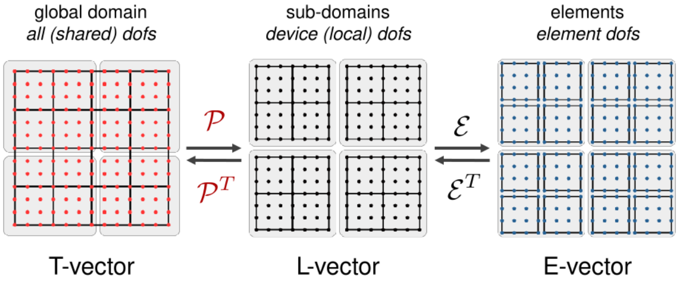

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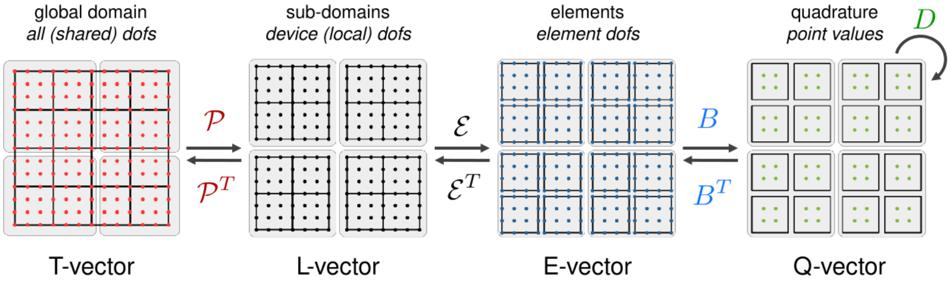

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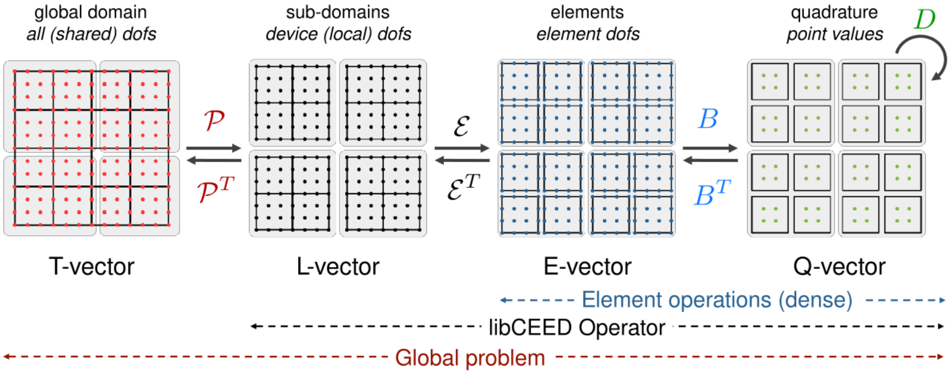

Fluid Simulations with libCEED

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

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

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

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Simplify into residual form:

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Simplify into residual form:

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

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

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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  - **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:** Approximation, accuracy limited to $\sqrt{\epsilon_{\text{machine}}}$

Exact Matrix-Free Jacobian via CeedOperator

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

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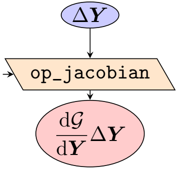

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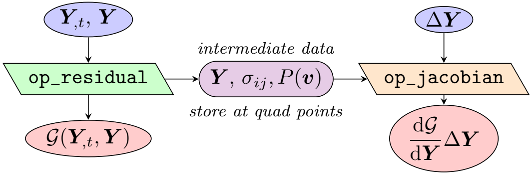

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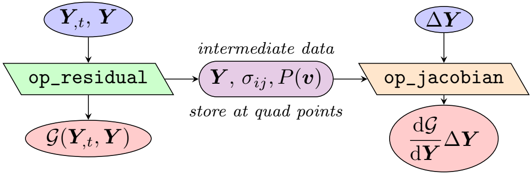

- **Pros:** Exact Jacobian matrix-vector product (potentially faster convergence)
- **Cons:** More expensive than residual evaluation (but not by too much)
  - Still faster than just *applying* sparse $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}$

Accuracy and Performance of High-Order Scale-Resolving Simulations

Flat Plate Boundary Layer, Zero Pressure Gradient

Problem Description:

- $Re_\theta \approx 970$ boundary layer at inflow, $M \approx 0.1$
- Synthetic turbulence generation (STG) used for inflow structures
- Internal damping layer (IDL) used in STG development region to prevent pressure wave growth
- asdf
- Domain size of $\{27 \times 24 \times 4\}\delta_0$

High-Order Approach

- Test 3 different order elements, Q_1, Q_2, Q_3 tensor-product hexes
- Maintain *DOF resolution* (DOFs per physical length)
- DOF resolution for streamwise and spanwise was $\Delta x^+ = 30$ and $\Delta z^+ = 12$
    - For Q_1, this is about half the resolution required for DNS resolution

Support and References

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