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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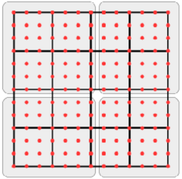
  - Computational backend selectable at runtime via JIT compilation
- Geared toward high-order element discretizations

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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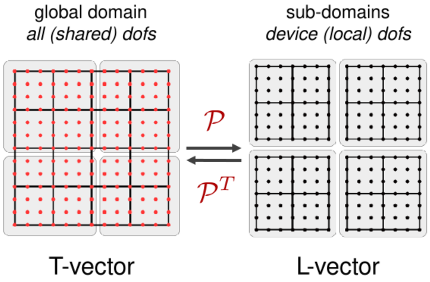

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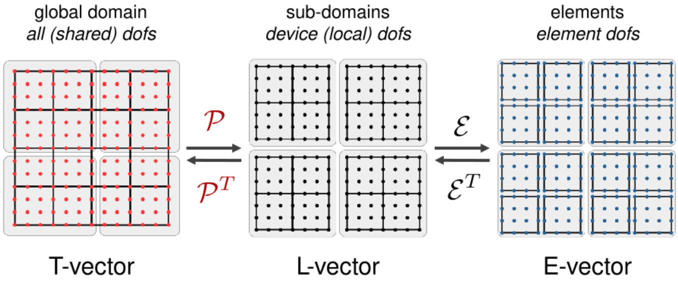

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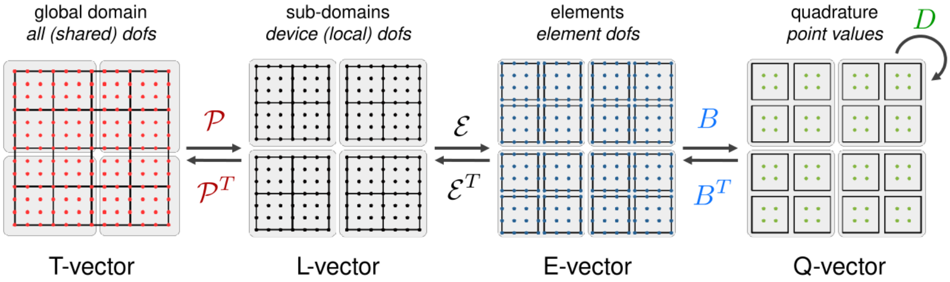

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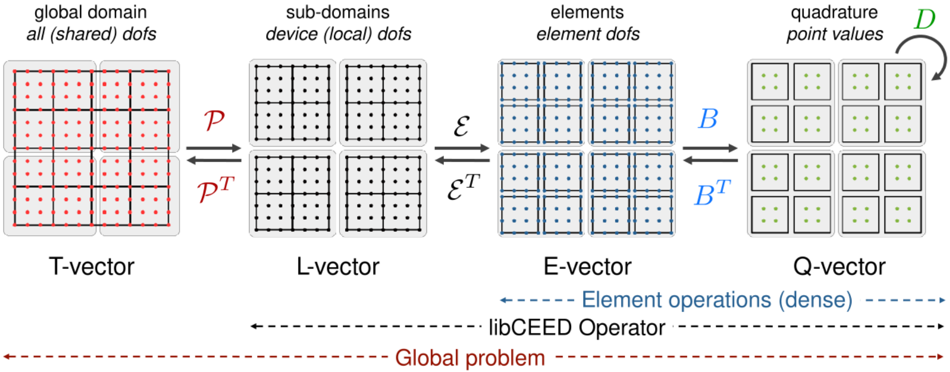

Fluid Simulations with libCEED

Compressible Navier-Stokes

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

for

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

convert to primitive variable formulation

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Compressible Navier-Stokes for FEM

Find $\boldsymbol{U} \in \mathcal{S}^h$

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

Compressible Navier-Stokes for FEM

Find $\boldsymbol{U} \in \mathcal{S}^h$

$$
\begin{aligned}
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+ \int_{\partial\Omega} \boldsymbol{v} \cdot \boldsymbol{F}_i(\boldsymbol{U}) \cdot \widehat{\boldsymbol{n}} \, \mathrm{d}\partial\Omega \\
\underbrace{+ \int_\Omega \mathcal{P}(\boldsymbol{v})^T \, \left(\boldsymbol{U}_{,t} + \boldsymbol{F}_{i,i}(\boldsymbol{U}) - S(\boldsymbol{U})\right) \, \mathrm{d}\Omega}_{\text{SUPG}} &= 0 \,, \; \forall \boldsymbol{v} \in \mathcal{V}^h
\end{aligned}
$$

Compressible Navier-Stokes for FEM

Find $\boldsymbol{U} \in \mathcal{S}^h$

$$\begin{aligned}\int_\Omega \boldsymbol{v} \cdot \big(\boldsymbol{U}_{,t} - \boldsymbol{S}(\boldsymbol{U})\big) \,\mathrm{d}\Omega - \int_\Omega \boldsymbol{v}_{,i} \cdot \boldsymbol{F}_i(\boldsymbol{U}) \,\mathrm{d}\Omega \\ + \int_{\partial\Omega} \boldsymbol{v} \cdot \boldsymbol{F}_i(\boldsymbol{U}) \cdot \widehat{\boldsymbol{n}} \,\mathrm{d}\partial\Omega \\ \underbrace{+ \int_\Omega \mathcal{P}(\boldsymbol{v})^T \,\big(\boldsymbol{U}_{,t} + \boldsymbol{F}_{i,i}(\boldsymbol{U}) - S(\boldsymbol{U})\big) \,\mathrm{d}\Omega}_{\text{SUPG}} = 0\,,\ \forall \boldsymbol{v} \in \mathcal{V}^h\end{aligned}$$

Further simplified into residual form:

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

Code Architecture

- PETSc used for handling everything libCEED doesn't
  - $\mathcal{P}, \mathcal{P}^T$ (Partition global-to-local operations)
  - Time integration, linear, non-linear equation solving
  - Strong boundary conditions

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- PETSc used for handling everything libCEED doesn't
  - $\mathcal{P}, \mathcal{P}^T$ (Partition global-to-local operations)
  - Time integration, linear, non-linear equation solving
  - Strong boundary conditions
- PETSc calls a libCEED operator when it needs the residual evaluation
- libCEED Operator based on user-implemented `CeedQFunctions` (D)
  - Use different `CeedQFunction`s for volume vs boundary integrals
  - Combined into a single `CeedOperator` to represent $\mathcal{G}(\boldsymbol{U}_{,t}, \boldsymbol{U})$

Something Implicit Timestepping

Should mention implicit timestepping since it's in the title

- Big point is the matrix-free exact Jacobian evaluation

Time Step Loop

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3. PETSc gets $\boldsymbol{G}^G = \mathcal{P}^T \boldsymbol{G}^L$
4. PETSc uses $\boldsymbol{G}^G$ to compute new solution value ...or whatever else it wants

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 waves
- Domain size of $\{27 \times 24 \times 4\}\delta_0$

Questions?