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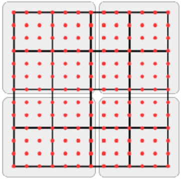
- Portable to different hardware via computational backends
  - Code that runs on CPU also runs on GPU without changes
  - Computational backend selectable at runtime, using runtime compilation
- Geared toward high-order element discretizations

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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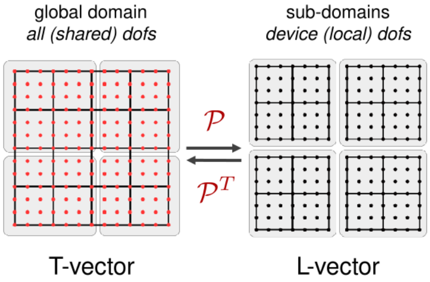

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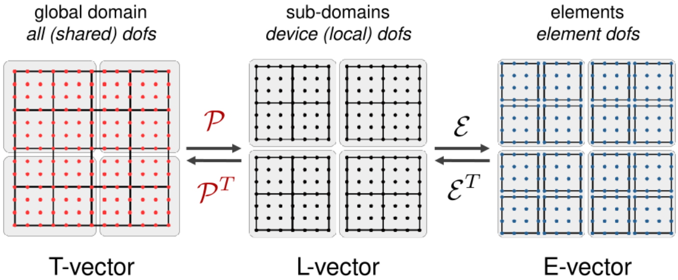

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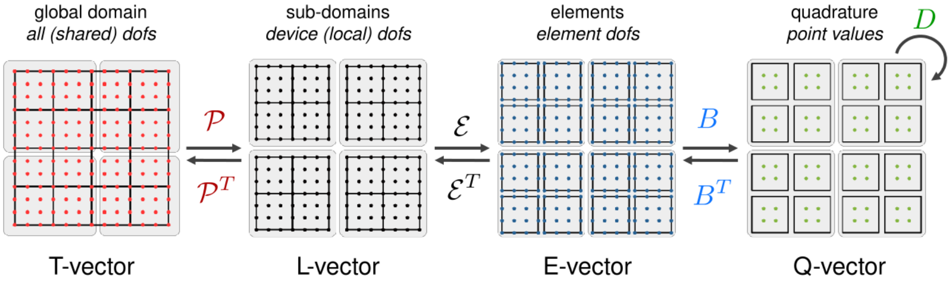

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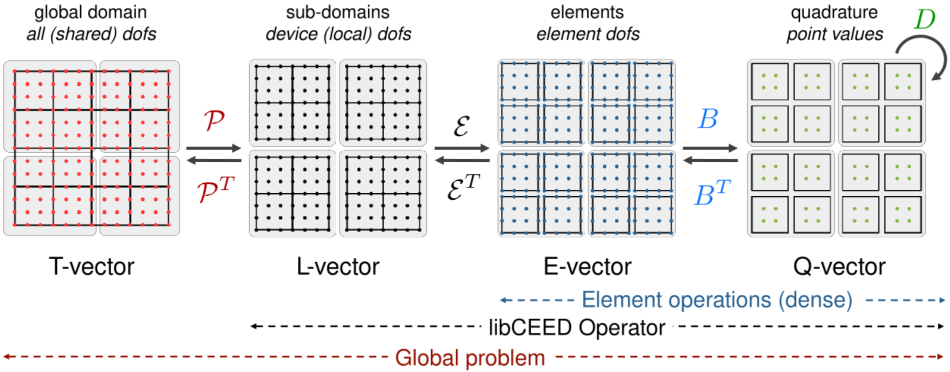

Fluid Simulations with libCEED

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

Compressible Navier-Stokes for FEM

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

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

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\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
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Further simplified into residual form:

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

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$$\Rightarrow \quad \mathcal{P}^T \mathcal{E}^T B^T G B \mathcal{E} \mathcal{P} = 0$$

Implicit Timestepping

Implicit timestepping requires solving:

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

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- Store $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{U}}$ directly
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- Finite difference matrix-free approximation:

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

    - Pros: Just need a residual evaluation, cheap (in programming and computation)
    - Cons: Approximation, accuracy limited to $\sqrt{\epsilon_{\text{machine}}}$

Exact Matrix-Free Jacobian

$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{U}}\Delta\boldsymbol{U} = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{U}}\left[\mathcal{G}(\boldsymbol{U}_{,t}, \boldsymbol{U})\right]\Delta\boldsymbol{U}$$

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\end{aligned}$$

- Store intermediary data at quadrature points to improve efficiency (“taping”)
  - We store $\boldsymbol{U}$, viscous stress, and stabilization perturbation ($\mathcal{P}(\boldsymbol{v})$)
- Pros: Exact Jacobian matrix-vector product (potentially faster convergence)
- Cons: More expensive than residual evaluation (but not by too much)

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

Time Step Loop

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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 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)