Performance-Portable Implicit Scale-Resolving Compressible Flow Using libCEED

SIAM CSE 2023

James Wright, Jed Brown, Kenneth Jansen, Leila Ghaffari

February 27, 2023

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. Viscous Outflow Boundary Conditions
4. Efficient Implicit Timestepping

libCEED Overview

What is libCEED?

- C library for element-based discretizations
  - Bindings available for Fortran, Rust, Python, and Julia

What is libCEED?

- C library for element-based discretizations
  - Bindings available for Fortran, Rust, Python, and Julia
- Designed for matrix-free operator evaluation

What is libCEED?

- C library for element-based discretizations
    - Bindings available for Fortran, Rust, Python, and Julia
- Designed for matrix-free operator evaluation
- 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

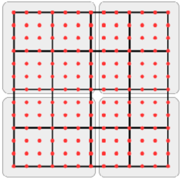
What is libCEED?

- C library for element-based discretizations
  - Bindings available for Fortran, Rust, Python, and Julia
- Designed for matrix-free operator evaluation
- 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

Finite Element Operator Decomposition

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

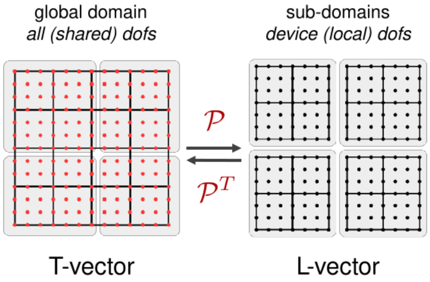
global domain
all (shared) dofs



T-vector

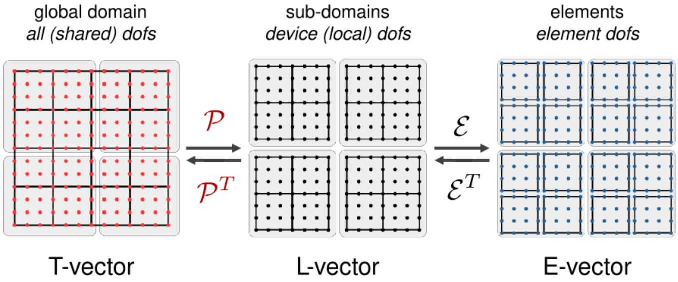
Finite Element Operator Decomposition

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



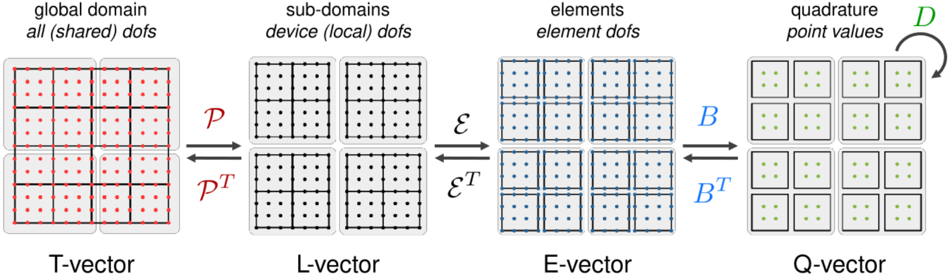
Finite Element Operator Decomposition

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



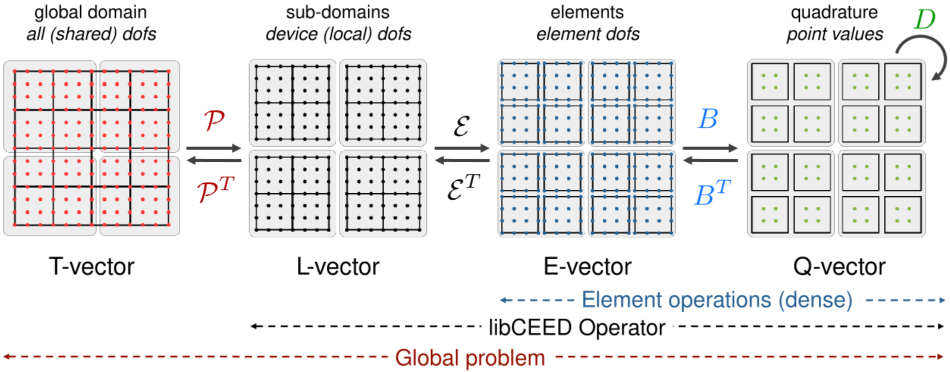
Finite Element Operator Decomposition

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



Finite Element Operator Decomposition

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



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

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

Compressible Navier-Stokes for Continuous-Galerkin FEM

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

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

Compressible Navier-Stokes for Continuous-Galerkin FEM

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

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

Simplify into residual form:

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

Compressible Navier-Stokes for Continuous-Galerkin FEM

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

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

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

Simplify into residual form:

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

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

Viscous Outflow Boundary Conditions

Viscous Outflow Boundary Conditions

Viscous Outflow Boundary Conditions

- Riemann Flux BCs everywhere is ideal

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

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

Riemann Flux

Viscous Outflow Boundary Conditions

- Riemann Flux BCs everywhere is ideal
- Velocity not known *a priori* $\longrightarrow$ traditional Riemann BCs not applicable

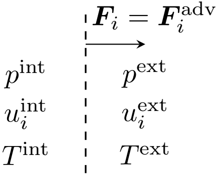
$$\boldsymbol{F}_i = \boldsymbol{F}_i^{\text{adv}}$$

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

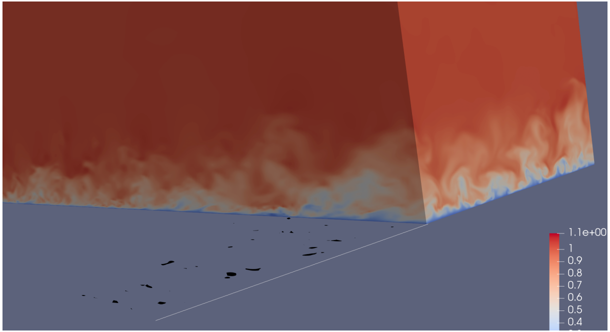
Riemann Flux

Viscous Outflow Boundary Conditions

- Riemann Flux BCs everywhere is ideal
- Velocity not known *a priori* $\longrightarrow$ traditional Riemann BCs not applicable
- Weak-pressure prescription ill-posed for recirculation



Riemann Flux



Viscous Outflow Boundary Conditions

- Riemann Flux BCs everywhere is ideal
- Velocity not known *a priori* $\longrightarrow$ traditional Riemann BCs not applicable
- Weak-pressure prescription ill-posed for recirculation

Solution

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

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

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

Riemann Flux

$$\boldsymbol{F}_i^{\mathrm{adv}}$$

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

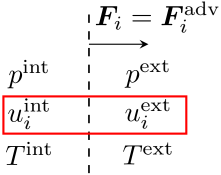
Riemann Outflow Boundary Condition Flux

Viscous Outflow Boundary Conditions

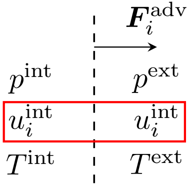
- Riemann Flux BCs everywhere is ideal
- Velocity not known *a priori* $\longrightarrow$ traditional Riemann BCs not applicable
- Weak-pressure prescription ill-posed for recirculation

Solution

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



Riemann Flux



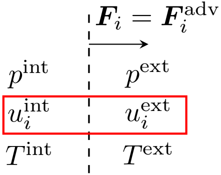
Riemann Outflow Boundary Condition Flux

Viscous Outflow Boundary Conditions

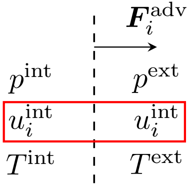
- Riemann Flux BCs everywhere is ideal
- Velocity not known *a priori* $\longrightarrow$ traditional Riemann BCs not applicable
- Weak-pressure prescription ill-posed for recirculation

Solution

- 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 $\boldsymbol{F}_i = \boldsymbol{F}_i^{\text{adv}} + \boldsymbol{F}_i^{\text{diff}}$

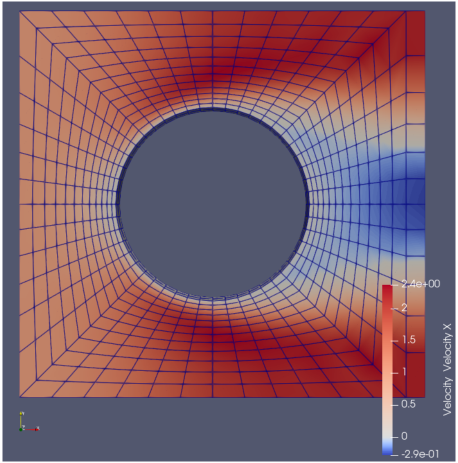


Riemann Flux



Riemann Outflow Boundary Condition Flux

Viscous Outflow Boundary Conditions Demonstration



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

Efficient Implicit Timestepping

Implicit Timestepping

Implicit timestepping requires solving:

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

Implicit Timestepping

Implicit timestepping requires solving:

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

- Store $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}$ directly (sparse matrix representation)
    - **Pros:** Opens up preconditioning options
    - **Cons:** Is large, expensive to store

Implicit Timestepping

Implicit timestepping requires solving:

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

- Store $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}$ directly (sparse matrix representation)
  - **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:** Approximation, accuracy limited to $\sqrt{\epsilon_{\text{machine}}}$

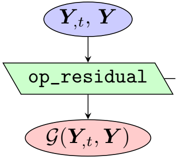
Exact Matrix-Free Jacobian via CeedOperator

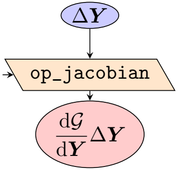
$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}\Delta\boldsymbol{Y} = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{Y}} \overbrace{\left[\mathcal{P}^T \mathcal{E}^T B^T G B \mathcal{E} \mathcal{P}\right]}^{\mathcal{G}(\boldsymbol{Y}_{,t}, \boldsymbol{Y})} \Delta\boldsymbol{Y}$$

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

Exact Matrix-Free Jacobian via CeedOperator

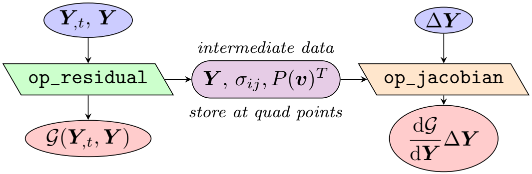
$$\begin{aligned}\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}\Delta\boldsymbol{Y} &= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{Y}}\overbrace{\left[\mathcal{P}^T\mathcal{E}^T B^T G B \mathcal{E}\mathcal{P}\right]}^{\mathcal{G}(\boldsymbol{Y}_{,t},\boldsymbol{Y})}\Delta\boldsymbol{Y} \\ &= \left[\mathcal{P}^T\mathcal{E}^T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





Exact Matrix-Free Jacobian via CeedOperator

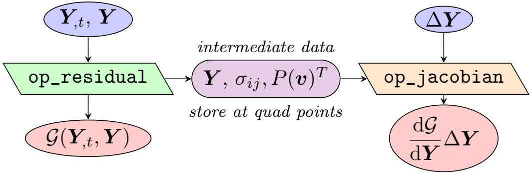
$$
\begin{aligned}
\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}\Delta\boldsymbol{Y} &= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{Y}} \overbrace{\left[\mathcal{P}^T\mathcal{E}^T B^T G B \mathcal{E}\mathcal{P}\right]}^{\mathcal{G}(\boldsymbol{Y}_{,t},\boldsymbol{Y})} \Delta\boldsymbol{Y} \\
&=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



Exact Matrix-Free Jacobian via CeedOperator

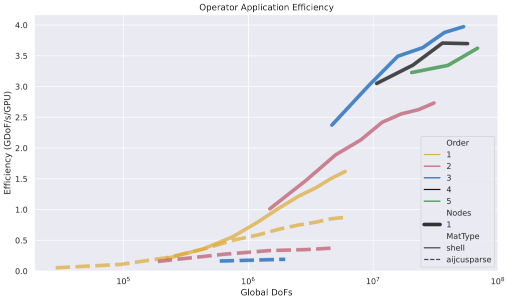
$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}\Delta\boldsymbol{Y} = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{Y}}\overbrace{\left[\mathcal{P}^T\mathcal{E}^T B^T G B \mathcal{E}\mathcal{P}\right]}^{\mathcal{G}(\boldsymbol{Y}_{,t},\boldsymbol{Y})}\Delta\boldsymbol{Y}$$

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



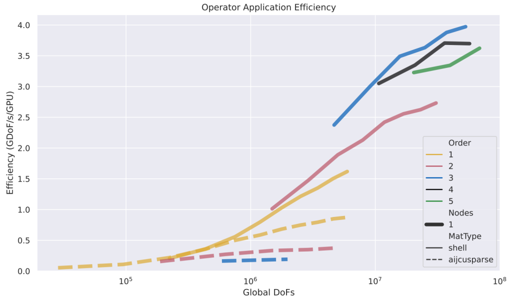
- **Pros:** Exact Jacobian matrix-vector product (potentially faster convergence)
- **Cons:** More expensive than residual evaluation (but not by too much)
  - Still faster than just *applying* sparse $\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}\boldsymbol{Y}}$

Performance Exact Matrix-Free Jacobian via CeedOperator

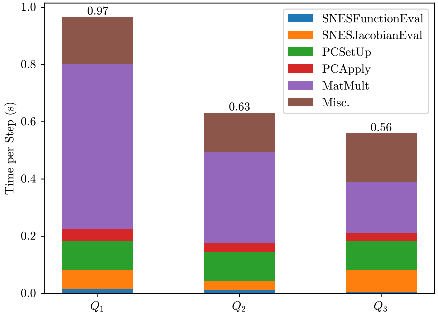


Matrix-Free Application Comparison (Reproduced from Brown *et al.* 2022).
Not from fluids code, but representative of libCEED matrix-free

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



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

Support and References

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