

Matrix Free P-Multigrid with libCEED and PETSc

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libCEED Team

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Grant: Exascale Computing Project (17-SC-20-SC)

- 1: University of Colorado, Boulder
- 2: Lawrence Livermore National Laboratory
- 3: Virginia Polytechnic Institute and State University
- 4: OCCA
- 5: University of Illinois, Urbana-Champaign

libCEED is an extensible library that provides a portable algebraic interface and optimized implementations of high-order operators

We have optimized implementations targeting CPU and GPU

We investigate a p-multigrid example with PETSc PCMG

Overview

- 1 Introduction
- 2 Multigrid Example
- 3 Future Work
- 4 Questions

Center for Efficient Exascale Discretizations

DoE exascale co-design center

- Design discretization algorithms for exascale hardware that deliver significant performance gain over low order methods
- Collaborate with hardware vendors and software projects for exascale hardware and software stack
- Provide efficient and user-friendly unstructured PDE discretization component for exascale software ecosystem

Matrix Free

libCEED design approach:

- Avoid global matrix assembly
- Map each element to reference element
- Geometry data computed on the fly or precomputed
- Easy to parallelize across heterogeneous nodes

libCEED

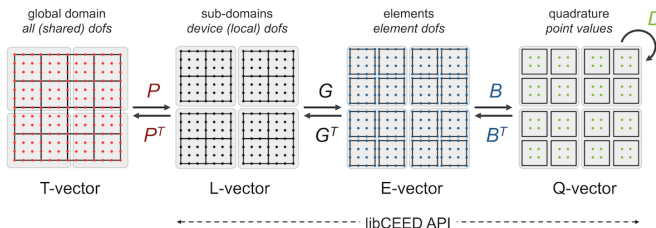
libCEED provides multiple backend implementations

- CPU
 - Pure C
 - Advanced Vector Instructions
 - LIBXSMM
- GPU
 - Pure CUDA
 - OCCA
 - MAGMA

libCEED



$$A = P^T G^T B^T D B G P$$



$$A_L = G^T B^T D B G$$

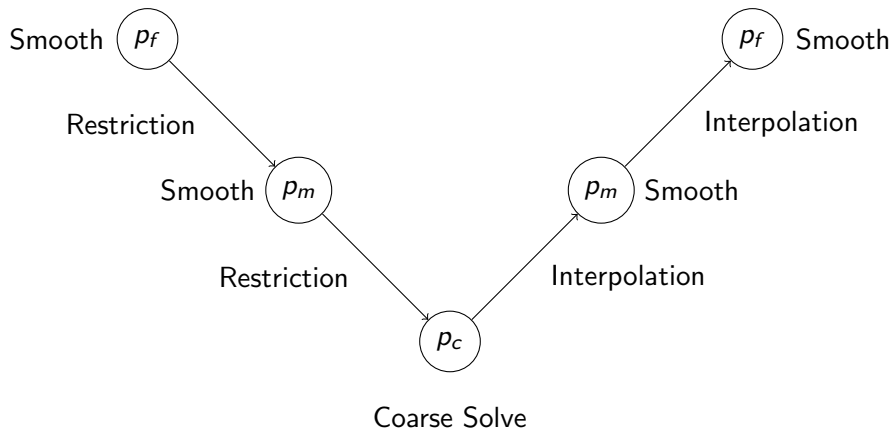
- G - CeedElemRestriction, local gather/scatter
- B - CeedBasis, provides basis operations such as interp and grad
- D - CeedQFunction, representation of PDE at quadrature points
- A_L - CeedOperator, aggregation of Ceed objects for local action of operator

PETSc PCMG

- PCMG - PETSc geometric multigrid preconditioner
- Requires several operators from the user
 - Restriction operator
 - Interpolation operator
 - Smoother
 - Coarse grid solver

PETSc PCMG

3 level multigrid with PCMG



libCEED Operators - Diffusion

Solving the 2D Poisson problem: $-\Delta u = f$

Weak Form: $\int \nabla v \nabla u = \int v f$

- General libCEED Operator

$$A_L = G^T B^T D B G$$

- Diffusion Operator

$$A_L = G^T \hat{D}_{2d}^T D \hat{D}_{2d} G$$

where D is block diagonal by quadrature point:

$$D_i = (w_i \det J_{geo}) J_{geo}^{-T} J_{geo}^{-1} \text{ and } J_{geo} = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial s} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial s} \end{bmatrix}$$

libCEED Operators - Diffusion

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- Diffusion Operator

$$A_L = G^T \hat{D}_{2d}^T D \hat{D}_{2d} G$$

- Computationally Efficient Form

$$A_L = G^T \begin{bmatrix} \hat{D}^T \otimes \hat{J}^T & \hat{J}^T \otimes \hat{D}^T \end{bmatrix} D \begin{bmatrix} \hat{D} \otimes \hat{J} \\ \hat{J} \otimes \hat{D} \end{bmatrix} G$$

libCEED Operators - Diffusion

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- General libCEED Operator

$$A_L = G^T B^T D B G$$

- Diffusion Operator

$$A_L = G^T \hat{D}_{2d}^T D \hat{D}_{2d} G$$

- Computationally Efficient Form

$$A_L = G^T \left(\hat{J}^T \otimes \hat{J}^T \right) \begin{bmatrix} \tilde{D}^T \otimes I & I \otimes \tilde{D}^T \end{bmatrix} D \begin{bmatrix} \tilde{D} \otimes I \\ I \otimes \tilde{D} \end{bmatrix} \left(\hat{J} \otimes \hat{J} \right) G$$

where $\hat{D} = \tilde{D} \hat{J}$

libCEED Operators - Restriction

Restriction / Interpolation is largely a basis operation

- General libCEED Operator

$$A_L = G^T B^T D B G$$

- Restriction / Interpolation Operator

$$A_L = G_c^T I I B_{ftoc} G_f$$

- Computationally Efficient Form

$$A_L = G_c^T \left(\hat{J}_{ftoc} \otimes \hat{J}_{ftoc} \right) G_f$$

libCEED Operators - Smoothing

For smoothing, we use a libCEED diffusion operator with KSPCHEBYCHEV

- General libCEED Operator

$$A_L = G^T B^T D B G$$

- Diffusion Operator

$$A_L = G^T \hat{D}_{2d}^T D \hat{D}_{2d} G$$

- Computationally Efficient Form

$$A_L = G^T \left(\hat{J}^T \otimes \hat{J}^T \right) \begin{bmatrix} \tilde{D}^T \otimes I & I \otimes \tilde{D}^T \end{bmatrix} D \begin{bmatrix} \tilde{D} \otimes I \\ I \otimes \tilde{D} \end{bmatrix} \left(\hat{J} \otimes \hat{J} \right) G$$

QFunction Definition

General libCEED QFunction:

$$v_q = D u_q$$

2D Diffusion QFunction:

$$\begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} D_{00} & D_{01} \\ D_{01} & D_{11} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

Code:

```
CeedQFunctionCreateInterior(ceed, 1, Diff,
                           __FILE__multigrid.c:Diff, &qf_apply);
CeedQFunctionAddInput(qf_apply, "u", 1, CEED_EVAL_GRAD);
CeedQFunctionAddInput(qf_apply, "geo", 3, CEED_EVAL_NONE);
CeedQFunctionAddOutput(qf_apply, "v", 1, CEED_EVAL_GRAD);
```


Operator Definition

General libCEED Operator:

$$\mathbf{v}_L = \mathbf{A}_L \mathbf{u}_L$$

2D Diffusion Operator:

$$\mathbf{A}_L = \mathbf{G}^T \mathbf{B}^T \mathbf{D} \mathbf{B} \mathbf{G}$$

Code:

```
CeedOperatorCreate(ceed, qf_apply, NULL, NULL, &op_apply);
CeedOperatorSetField(op_apply, "u", Erestrictu, CEED_TRANSPOSE,
                    basisu, CEED_VECTOR_ACTIVE);
CeedOperatorSetField(op_apply, "geo", Erestrictqdi, CEED_NOTRANSPOSE,
                    CEED_BASIS_COLLOCATED, geo);
CeedOperatorSetField(op_apply, "v", Erestrictu, CEED_TRANSPOSE,
                    basisu, CEED_VECTOR_ACTIVE);
...
CeedOperatorApply(op_apply, xloc, yloc, CEED_REQUEST_IMMEDIATE);
```

Performance

- 3D Poisson Problem
- Test run on personal computer
- Mesh
 - 8^3 GLL points per element
 - Quadrature on 9^3 GL points per element
 - Cube with 30 elements, 11,880 DoFs

- Unpreconditioned

- $5.0057\text{e-}07$ $\|\cdot\|_\infty$ Error
- 119 CG iterations
- 0.2148 million CG DoFs/sec
- 13.5436 sec CG solve time

- P-Multigrid

- $5.0059\text{e-}07$ $\|\cdot\|_\infty$ Error
- 18 CG iterations
- 0.0795 million CG DoFs/sec
- 4.1058 sec CG solve time

Performance - Highlights

- Significantly decreased number of iterations
- Iterations slower than expected
- Want to decrease iteration time with lighter preconditioner
- Caveats:
 - Small mesh run on laptop for demo purposes
 - Need minor PETSc code adjustments to run well on GPU

Future Work

- Further performance tuning (GPU and CPU)
- Unstructured mesh examples (with AMG coarse solve)
- Expanded set of non-linear examples
- Preconditioning based on libCEED operator decomposition
- Efficient diagonal computation for preconditioning
- Algorithmic differentiation of user quadrature functions
- We invite contributors and friendly users

Questions?

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