On Performance and Portability for Generic Finite Element Interfaces

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Overview

A global sparse matrix is no longer a good representation of a high-order linear operator

libCEED is an extensible library that provides a portable algebraic interface and optimized implementations

We have preliminary results comparing performance to native implementations in production software

Overview

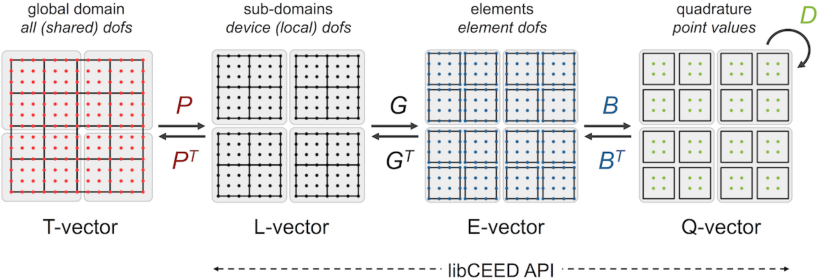
1. Introduction
2. libCEED
3. Production Software
4. Performance Comparison
5. Questions

Weak Form and Finite Elements

- Strong Form of PDE: $A_s u = f$
- Weak Form of PDE: $\int_\Omega Auv = \int_\Omega fv$
- v are test functions defined on each element,
  yields system of equations
- Operator can be decomposed algebraically

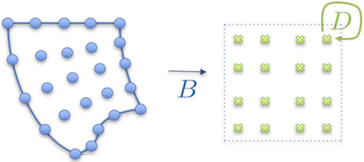
Operator Decomposition

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



Matrix Free Implementation

$$\boxed{A = P^T G^T B^T D B G P}$$



- Avoid global matrix assembly
- Map each element to reference element
- Only store map to reference, action on reference
- Easy to parallelize across nodes

libCEED API

- Provides on-device operator implementation
- Easy to incorporate into existing code
- Supports multiple types of computational devices
  GPUs, CPUs, etc
- Multiple extensible implementations
  Reference on CPUs, OCCA on GPUs

API Objects

- G - CeedRestriction
  Restrict to single element
- B - CeedBasis
  Actions on basis such as interpolation, gradient, divergence, curl
- D - CeedQFunction
  Operator action at quadrature points to include coefficient functions

Device Level Operator

- $L = G^T B^T D B G$ - CeedOperator
- libCEED objects are combined to create a CeedOperator
- CeedOperator gives operator action for elements on device
- User code responsible for communication between devices
  $A = P^T L P$

Benefits

- Extensible library
- Lower memory transfer, no sparse matrix
- Implementations for multiple devices and backends
- libCEED optimization can benefit all operators
  Tensor contraction, basis application, etc

Standalone Implementation

```
// Solve system
if (mpi_rank == 0) {
        globalCGSolve(global_vector, f_vector,
        boundary_vector);
}
else if (mpi_rank > 3) {
        localOperatorApply(&ceed,
       &processor_operator);
}
```

MFEM

```
/// Wrapper for a mass CeedOperator as an
/// mfem::Operator
class CeedMassOperator : public mfem::Operator
 protected:
  const mfem::FiniteElementSpace *fes;
  CeedOperator build_oper, oper;
  CeedBasis basis, mesh_basis;
  CeedElemRestriction restr, mesh_restr;
  CeedQFunction apply_qfunc, build_qfunc;
  CeedVector node_coords, qdata;
```

Nek5000

```
subroutine ceed_axhm1(pap,ap1,p1,h1,h2,ceed,op_mass,
$ vec_ap1,vec_p1,vec_qdata)

include 'ceedf.h'

c Vector conjugate gradient matvec for solution of
c uncoupled Helmholtz equations

include 'SIZE'
include 'TOTAL'
...
call ceedvectorsetarray(vec_p1,ceed_mem_host,
$ ceed_use_pointer, p1,err)
call ceedoperatorapply(op_mass,vec_qdata,vec_p1,vec_ap1,
$ ceed_request_immediate,err)
call ceedvectorgetarray(vec_ap1,ceed_mem_host,ap1,err)
```

PETSc

```
user->op = op_mass;
user->qdata = qdata;

ierr = MatCreateShell(comm, mdof[0]*mdof[1]*mdof[2],
       mdof[0]*mdof[1]*mdof[2],
       PETSC_DECIDE, PETSC_DECIDE, user, &mat);
CHKERRQ(ierr);
ierr = MatShellSetOperation(mat, MATOP_MULT
       (void(*)(void))MatMult_Mass); CHKERRQ(ierr);

...

ierr = KSPSetFromOptions(ksp); CHKERRQ(ierr);
ierr = KSPSetOperators(ksp, mat, mat); CHKERRQ(ierr);
ierr = KSPSolve(ksp, rhs, X); CHKERRQ(ierr);
```

Nek5000

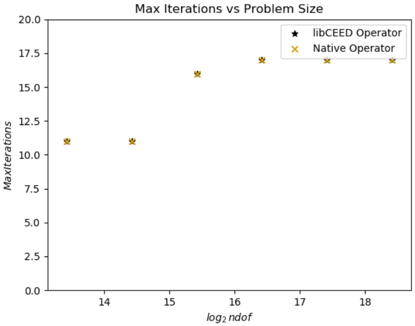
Problem: $\nabla u = f$
CEED Benchmark Problem 1

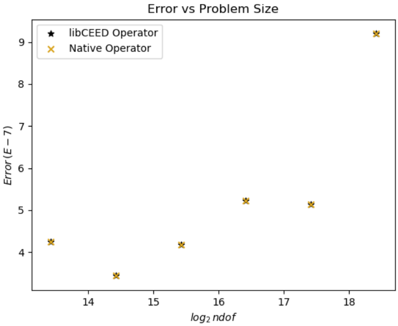
Domain: 3D Cube
Elements: Hexagonal
Number of Elements: 2^n
Shape Function Order: 7
Quadrature Order: 8

Computer: CU Boulder Summit

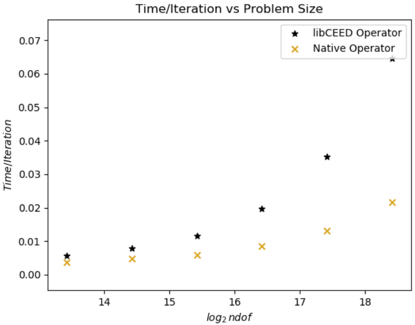
Nodes: 1
CPUs: Intel Xeon Haswell
Processors: 32
Compiler: Intel/17.0.0
MPI: Intel/2017.0.098

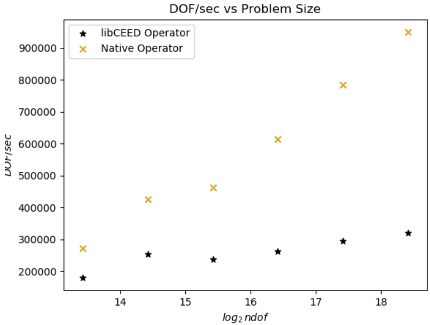
Nek5000 - The Good News





Nek5000 - The Bad News





Future Work

- Optimize reference implementation, tensor contraction
- Create library of user quadrature functions
- Create additional backends
- Compare libCEED operators to native implementation in a wider range of production software

Questions?

Advisor: Jed Brown[1]

Collaborators: Jean-Sylvain Camier[2], Tzanio Kolev[2],
Veselin Dobrev[2], & Thilina Rathnayake[3]

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1: University of Colorado, Boulder
2: Lawrence Livermore National Laboratory
3: University of Illinois, Urbana-Champaign

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