Performance Portability with Matrix-Free Finite Element Operators

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PETSc User Meeting 2019, Georgia Tech, Atlanta, GA, USA

Abstract

One of the challenges with high-order finite element and spectral element methods is that a global sparse matrix is no longer a good representation of a high-order linear operator, both with respect to the FLOPs needed for evaluation and the memory transfer needed for a matrix-vector multiply. Thus, high-order methods require a new operator description that still represents a linear or non-linear operator. libCEED is an extensible library that provides a portable algebraic interface and optimized implementations suitable for high-order operators. libCEED’s operator description is easy to incorporate in a wide variety of applications, without significant refactoring of the discretization infrastructure. We introduce the libCEED API, show performance results for CEED Benchmark Problems, and introduce a Navier-Stokes demo solver using libCEED and PETSc.

Operator Decomposition

Finite element operators are typically defined through weak formulations of PDEs that involve integration over a computational mesh. The required integrals are computed by splitting them as a sum over the mesh elements, mapping each element to a simple reference element, and applying a quadrature rule in the reference space. This is illustrated below for the simple case of symmetric linear operator on third order (Q3) scalar continuous (H1) elements, where we use the notions T-vector, L-vector, E-vector and Q-vector to represent the sets corresponding to the (true) degrees of freedom on the global mesh, the split local degrees of freedom on the subdomains, the split degrees of freedom on the mesh elements, and the values at quadrature points, respectively.

Figure 1: Algebraic Operator Decomposition

- Process decomposition P
- Element restriction G
- Basis (Dofs-to-Qs) evaluator B
- Operator at quadrature points D
- A = GTEBDG
- Not in libCEED (used PETSc)
-CEEDElemRestriction
-CEEDBasis
-CEEDFunction
-CEEDOperator

Backends

The libCEED API takes an algebraic approach, where the user describes in the frontend the operators G, B, D, and D and the library provides backend implementations and coordinates their action to the original operator independently on each device/MPI task. This purely algebraic description includes all the finite element information, so backends can operate on the linear algebra level without explicit finite element code. The separation of the frontend and backends enables applications to easily change backends.

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Performance w.r.t. DOFs

CEED uses Benchmark Problems to test and compare the performance of high order finite element codes. Benchmark Problem 1 (BP1): L² projection problem with homogeneous Neumann BCs,

\[ \nabla u = f, \]

where B is the mass matrix.

We analyze the performance on BP1 over 20 iterations of unpreconditioned Conjugate Gradient on hexahedral 3D elements with 2 more quadrature points than the nodes of the shape function in 1D.

Performance w.r.t. time

Navier-Stokes Demo

This example solves the time-dependent Navier-Stokes equations of compressible gas dynamics in a static Eulerian three-dimensional frame using structured high-order finite element/spectral element spatial discretization and explicit high-order time-stepping. The mathematical formulation is given in what follows. The compressible Navier-Stokes equations in conservative form are

\[ \begin{align*}
\partial_t \rho + \nabla \cdot (\rho U) &= 0, \\
\partial_t (\rho U) + \nabla \cdot (\rho UU + P I) &= -\nabla P + \rho \nabla \mathbf{F}, \\
\partial_t (\rho E) + \nabla \cdot ((\rho E + P) \mathbf{U}) &= \nabla \cdot (\mathbf{F} \times \mathbf{U}) - \nabla \cdot (\mu \nabla \mathbf{U}), \\
\end{align*} \]

where \( \sigma = \mu (\nabla U + (\nabla U)^T) + \lambda (\nabla \cdot \mathbf{U}) I \) is the Cauchy (symmetric) stress tensor, with \( \mu \) the dynamic viscosity coefficient, and \( \lambda = -\frac{2}{3} \text{ the Stokes hypothesis constant.} \) In equations (1), \( \sigma \) represents the volume mass density, \( \rho \) the momentum density (defined as \( \rho U = \rho u \) where \( u \) is the vector velocity field), \( P \) the total energy density (defined as \( E = \rho u \)), \( I \) represents the 3 x 3 identity matrix, \( g \) the gravitational acceleration constant, \( k \) the unit vector in the z direction, \( T \) the thermal conductivity constant. \( T \) represents the temperature, and \( P = (\gamma - 1) \rho \) \( (E - U U^T) / (\gamma - 1) \) is the pressure, where \( \gamma \) is the specific heat at constant pressure and \( \gamma \) is the specific heat at constant volume (that is, \( \gamma = \gamma / \gamma - 1 \)). We solve the density current problem: a cold air bubble rises in a neutrally stratified atmosphere.

Outlook

Status: ready for collaborators and friendly users. Ongoing work on CUDA and HIP optimizations.

- Improved non-conforming and mixed-mesh support
- Algorithmic differentiation of Q-functions

Figure 4: BP1: 2x Intel Xeon Platinum 8180M CPU 2.5GHz (Skylake): In (a)-(c), serial implementation. In (d)-(f) blocked implementation.

Figure 5: Solution of the compressible Navier-Stokes equations. In (a) the initial condition; in (b) the evolution at time \( t = 50 \) s.