Efficient solver composition with high-order methods

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SIAM CSE19, Spokane, Washington

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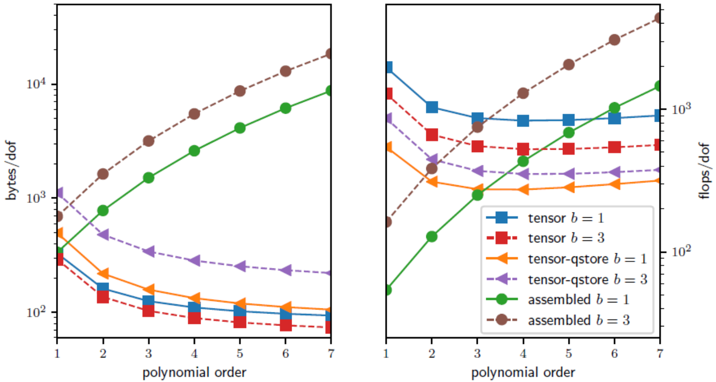
Motivation



Memory bandwidth (left) and flops per dof (right) to apply a Jacobian matrix, obtained from discretizations of a b-variable PDE system. Assembled matrix vs matrix-free (exploits the tensor product structure by either storing at q-points or computing on the fly)

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Overview

- A sparse matrix is no longer a good representation for high-order operators
- libCEED uses a matrix-free operator description, based on a purely algebraic interface, where user only specifies action of weak form operators
- libCEED operator representation is optimal with respect to the FLOPs needed for its evaluation, as well as the memory transfer needed for operator evaluations (matvec)
    - Matrix-free operators that exploit tensor product structures reduce the work load from $\mathrm{O}(\mathrm{p}^6)$ (for sparse matrix) to $\mathrm{O}(\mathrm{p}^4)$, and memory storage from $\mathrm{O}(\mathrm{p}^6)$ to $\mathrm{O}(\mathrm{p}^3)$
- We demonstrate the usage of libCEED with PETSc for a compressible Navier Stokes solver

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libCEED: the library of the CEED (Center for Efficient Extensible Discretizations)

- Primary target: high order finite element methods (FEM) exploiting tensor product structure
- Extensible backends:
  - CPU: reference and vectorized implementations
  - OCCA (just-in-time compilation) for CPUs, GPUs, OpenMP (Open Multi-Processing: API that supports multi-platform shared memory programming), OpenCL (framework for writing programs that execute across several platforms, e.g., CPUs, GPUs, etc.)
  - MAGMA (dense Linear Algebra library for GPUs and Multicore Architectures)
  - CUDA (parallel computing platform and API for general purpose processing on GPUs)
  - AVX (Advanced Vector Extensions instruction set architecture extension) and LIBXSMM (library for small dense and sparse matrix multiplications)
- Same source code can call multiple CEEDs with different backends. On-device operator implementation with unique interface
- Open source (BSD-2 license) C library with Fortran interface

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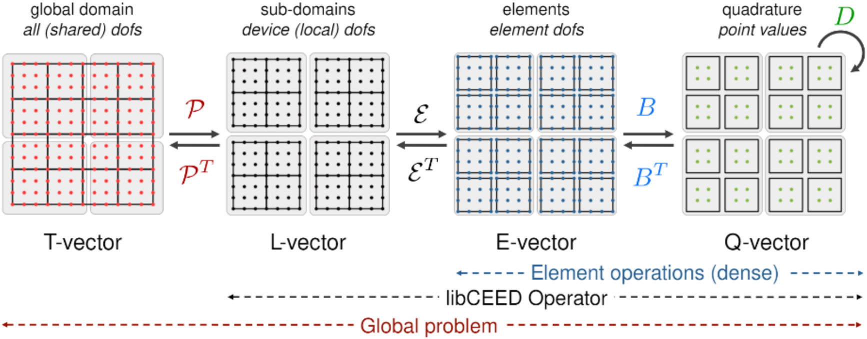
libCEED decomposition

ECP EXASCALE COMPUTING PROJECT

CEED EXASCALE DISCRETIZATIONS

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



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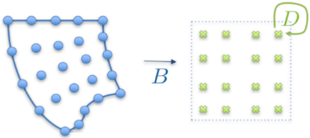
libCEED API objects



- $\mathcal{E}$: Ceed Element Restriction

  Restrict to single element

  User choice in ordering

- B: Ceed Basis Applicator

  Describes the actions on basis such as interpolation, gradient, div, curl

  Independent of geometry and element topology
- D: Ceed QFunction

  Operator that defines the action of the physics at quadrature points

  Choice of interlaced (by fields) or blocked (by element) for multi-component vectors
- $\mathrm{C} = \mathcal{E}^{\mathcal{T}}\mathrm{B}^{\mathsf{T}}\mathrm{D}\mathrm{B}\mathcal{E}$: CeedOperator

  Composition of different operators defined on different element topologies possible
- $A = \mathrm{P}^{\mathsf{T}}\mathrm{C}\mathrm{P}$: User code responsible for parallelization on different compute devices. We use PETSc

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Composition of solvers for multiphysics problems

The algebraic system obtained by the discretization of an m-variable nonlinear PDE is $\mathbf{F}(\mathbf{u}) = \mathbf{0}$:

$$\begin{pmatrix} F_1(u_1, u_2, \dots, u_m) \\ F_2(u_1, u_2, \dots, u_m) \\ \vdots \\ F_m(u_1, u_2, \dots, u_m) \end{pmatrix} = \mathbf{0} \quad \xrightarrow{\text{Jacobian}} \quad \begin{pmatrix} J_{11} & J_{12} & \cdots & J_{1m} \\ J_{21} & J_{22} & \cdots & J_{2m} \\ \vdots & & \ddots & \\ J_{m1} & J_{m2} & \cdots & J_{mm} \end{pmatrix}$$

solved via Newton's method: $\mathbf{u}^{n+1} = \mathbf{u}^n - \lambda \hat{J}^{-1}(\mathbf{u}^n)\mathbf{F}(\mathbf{u}^n)$.

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Ex: For a Dirichlet Stokes flow

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma} &= \mathbf{F}_b \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \Rightarrow \begin{pmatrix} J_{uu} & J_{pu}^T \\ J_{pu} & 0 \end{pmatrix}$$

where $\boldsymbol{\sigma} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - p\mathbf{I}_3$, and where the Schur's complement is $S = -J_{pu}J_{uu}^{-1}J_{pu}^T$ (needs preconditioning). If we use the simple block Jacobi preconditioner $\rightarrow$ block Gauss-Seidel, that can be solved by only partial assembly of the Jacobian, where each block can be computed independently and we can reuse the same QFunction for the blocks corresponding to different physical variables.

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libCEED API for operator composition

Creation of QFunctions and CEED operators:

```
CeedQFunctionCreateInterior(ceed, 1, Mass, __FILE__":Mass", &qf_mass);
CeedQFunctionAddInput(qf_mass, "u", 5, CEED_EVAL_INTERP);
CeedQFunctionAddInput(qf_mass, "weights", 1, CEED_EVAL_NONE);
CeedQFunctionAddOutput(qf_mass, "v", 5, CEED_EVAL_INTERP);

CeedOperatorCreate(ceed, qf_mass, NULL, NULL, &op_mass);
CeedOperatorSetField(op_mass, "u", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
CeedOperatorSetField(op_mass, "weights", Erestrictudi, CEED_NOTRANSPOSE, basisx, weights);
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$$f(\mathbf{u}, \mathbf{p}; \Theta) \rightleftharpoons f(u, p; \boldsymbol{\Theta})$$

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Composition of operators for multiphysics or mixed element meshes:

```
CeedCompositeOperatorCreate(ceed, &op_comp);
CeedCompositeOperatorAddSub(op_comp, op_1);
CeedCompositeOperatorAddSub(op_comp, op_2);
```

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Towards a libCEED miniapp: a Navier-Stokes solver

Compressible Navier-Stokes equations in conservation form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{U} = 0\,, \tag{1a}$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \left(\frac{\mathbf{U} \otimes \mathbf{U}}{\rho} + P \mathbf{I}_3 \right) + \rho g \mathbf{k} = \nabla \cdot \boldsymbol{\sigma}\,, \tag{1b}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left(\frac{(E + P)\mathbf{U}}{\rho} \right) = \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma} + k \nabla T)\ , \tag{1c}$$

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where $\boldsymbol{\sigma} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T + \lambda(\nabla \cdot \mathbf{u})\mathbf{I}_3)$, and

$$\begin{aligned}
(c_p/c_v - 1)\left(E - \mathbf{U}\cdot\mathbf{U}/(2\rho) - \rho g z\right) = P \quad &\leftarrow \quad \text{pressure} \\
\mu \quad &\leftarrow \quad \text{dynamic viscosity} \\
g \quad &\leftarrow \quad \text{gravitational acceleration} \\
k \quad &\leftarrow \quad \text{thermal conductivity} \\
\lambda \quad &\leftarrow \quad \text{Stokes hypothesis constant} \\
c_p \quad &\leftarrow \quad \text{specific heat, constant pressure} \\
c_v \quad &\leftarrow \quad \text{specific heat, constant volume}
\end{aligned}$$

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Vector form

The system (1) can be rewritten in vector form

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = S(\mathbf{q})\,, \tag{2}$$

for the state variables

$$\mathbf{q} = \begin{pmatrix} \rho \\ \mathbf{U} \equiv \rho \mathbf{u} \\ E \equiv \rho e \end{pmatrix} \begin{array}{l} \leftarrow \text{ volume mass density} \\ \leftarrow \text{ momentum density} \\ \leftarrow \text{ energy density} \end{array} \tag{3}$$

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where

$$\mathbf{F}(\mathbf{q}) = \begin{pmatrix} \mathbf{U} \\ (\mathbf{U} \otimes \mathbf{U})/\rho + P\mathbf{I}_3 - \boldsymbol{\sigma} \\ (E + P)\mathbf{U}/\rho - (\mathbf{u} \cdot \boldsymbol{\sigma} + k\nabla T) \end{pmatrix},$$

$$S(\mathbf{q}) = -\begin{pmatrix} 0 \\ \rho g \hat{k} \\ 0 \end{pmatrix}$$

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Space discretization

We use high-order finite elements/spectral elements: high-order Lagrange polynomials over non-uniformly spaced nodes, the Legendre-Gauss-Lobatto (LGL) points (roots of the p^{th}-order Legendre polynomial P_p). We let $\mathbb{R}^3 \supset \Omega = \bigcup_{e=1}^{N_e} \Omega_e$, with N_e disjoint hexaedral elements.

The physical coordinates are $\mathbf{x} = (x, y, z) \in \Omega_e$, while the reference coords are $\boldsymbol{\xi} = (\xi, \eta, \zeta) \in \mathbf{I} = [-1, 1]^3$.

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Define the discrete solution

$$\mathbf{q}_N(\mathbf{x}, t)^{(e)} = \sum_{k=1}^{P} \psi_k(\mathbf{x}) \mathbf{q}_k^{(e)} \tag{4}$$

with P the number of nodes in the element (e).

We use tensor-product bases $\psi_{kji} = h_i(\xi) h_j(\eta) h_k(\zeta)$.

Strong and weak formulations

The strong form of (3):

$$\int_{\Omega} v \left(\frac{\partial \mathbf{q}_N}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}_N) \right) d\Omega = \int_{\Omega} v \mathbf{S}(\mathbf{q}_N)\, d\Omega \,, \ \forall v \in \mathcal{V}_p \tag{5}$$

with $\mathcal{V}_p = \{v \in H^1(\Omega_e) \,|\, v \in P_p(\mathbf{I}), e = 1, \dots, N_e\}$.
Weak form:

$$\int_{\Omega} v \frac{\partial \mathbf{q}_N}{\partial t}\, d\Omega + \int_{\Gamma} v \widehat{\mathbf{n}} \cdot \mathbf{F}(\mathbf{q}_N)\, d\Omega - \int_{\Omega} \nabla v \cdot \mathbf{F}(\mathbf{q}_N)\, d\Omega = \int_{\Omega} v \mathbf{S}(\mathbf{q}_N)\, d\Omega \,, \ \forall v \in \mathcal{V}_p \tag{6}$$

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For the Time Discretization we use an explicit formulation

$$\frac{\mathbf{q}_N^{n+1} - \mathbf{q}_N^{n}}{\Delta t} = -[\nabla \cdot \mathbf{F}(\mathbf{q}_N)]^n + [S(\mathbf{q}_N)]^n\,, \tag{7}$$

solved with the adaptive Runge-Kutta-Fehlberg (RKF4-5) method

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A very simple example: The advection equation

We analyze the transport of total energy

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u} E) = 0 \,, \tag{8}$$

with $\mathbf{u}$ a uniform circular motion. BCs: no-slip and non-penetration for $\mathbf{u}$, no-flux for E.

order: $p = 6$
$\Omega = [0, 2000]^3$ m
elem. resolution: 250 m
Nodes: 117649

Top view: Advection

Application example: Density current

A cold air bubble drops by convection in a neutrally stratified atmosphere.

Its initial condition is defined in terms of the Exner pressure, $\pi(\boldsymbol{x}, t)$, and potential temperature, $\theta(\boldsymbol{x}, t)$, that relate to the state variables via

$$\rho = \frac{P_0}{(c_p - c_v)\theta(\boldsymbol{x}, t)} \pi(\boldsymbol{x}, t)^{\frac{c_v}{c_p - c_v}} \,, \tag{9a}$$

$$e = c_v \theta(\boldsymbol{x}, t) \pi(\boldsymbol{x}, t) + \mathbf{u} \cdot \mathbf{u}/2 + gz \,, \tag{9b}$$

where P_0 is the atmospheric pressure.

BCs: no-slip and non-penetration for $\mathbf{u}$, no-flux for mass and energy densities.

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Density current

order: $p = 10$, $\Omega = [0, 6000]^2$ m $\times$ $[0, 3000]$ m, elem. resolution: 500 m,
Nodes: 893101

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Side view: Density current

Application example: Wind turbine

We simulate the aerodynamics of a wind turbine through an Actuator Disc Model (ADM). ADM models the turbine as a disc, with a uniform thrust force

$$F_T = \frac{1}{2}\rho u_{1,\infty}^2 A_D C_T \,,$$

$$\begin{aligned} \rho &\leftarrow \text{density of air} \\ u_{1,\infty} &\leftarrow \text{unperturbed (far field) axial velocity} \\ A_D &\leftarrow \text{area swept by rotor} \\ C_T &\leftarrow \text{thrust coefficient} \end{aligned}$$

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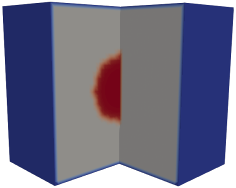

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This adds a source/sink for momentum in the conservation equation $\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = S(\mathbf{q})$, with $S(\mathbf{q}) = \left(0, F_{turbine}\hat{\mathbf{i}} - \rho g \hat{\mathbf{k}}, 0\right)$.

Conclusions and outlook

- We have demonstrated the use of libCEED with PETSc for the numerical high-order solutions of
  - Advection equation
  - Full compressible Navier-Stokes equations
  - Actuator Disc Model for wind turbines
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- Consider deformable meshes
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