Toward efficient, high-order solvers for Computational Fluid Dynamics applications

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Global System Laboratory Seminar, NOAA

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CEED
EXASCALE DISCRETIZATIONS

ECP
EXASCALE COMPUTING PROJECT

Where do I come from?

Siena, Tuscany, Italy

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Ok, where do I come from, mathematically speaking?

Master's thesis:
Catmull-Clark *Subdivision Surfaces* (Computer-Aided Design, '78)

The limit-surface obtained is a bicubic uniform B-spline surface of class C^2, except at *extraordinary* points

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PhD dissertation: Viscoelastic fluids

PhD in Applied Math from NJIT on numerical simulations of thin films (long-waves) of viscoelastic fluids

Viscoelastic materials:

- hysteresis: loop in stress-strain rate curve
- stress relaxation: constant $\epsilon \Rightarrow$ decreasing σ
- creep: constant $\sigma \Rightarrow$ increasing ϵ

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Mechanical system analogs

- Hookean: elastic solids

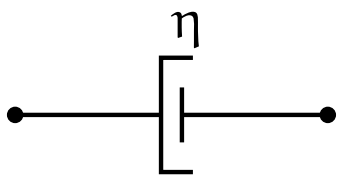
$\sigma_{ij} = 2G\epsilon_{ij}$

G shear elastic modulus

- Newtonian: viscous fluids

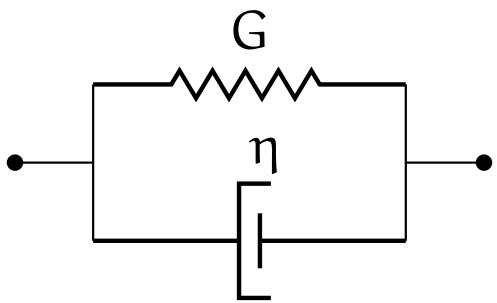
$\sigma_{ij} = 2\eta\dot{\epsilon}_{ij}$

η dynamic (shear) viscosity



- Kelvin-Voigt: linear viscoelastic solids

$\sigma_{ij} = 2G\epsilon_{ij} + 2\eta\dot{\epsilon}_{ij}$



- Maxwell: linear viscoelastic fluids

$\sigma_{ij} + \lambda_1 \partial_t \sigma_{ij} = 2\eta\dot{\epsilon}_{ij}$

λ_1 relaxation time, s. t. $\lambda_1 = \eta/G$.

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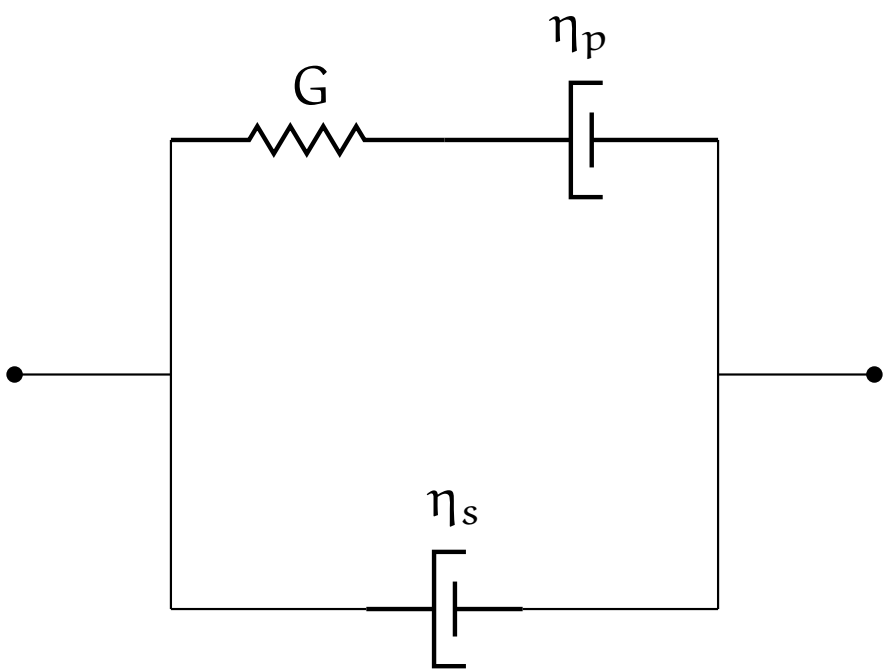
Mechanical system analog for Jeffreys

Jeffreys Model: linear viscoelastic fluids

$$\sigma_{ij} + \lambda_1 \partial_t \sigma_{ij} = 2\eta \left(\dot{\epsilon}_{ij} + \lambda_2 \partial_t \dot{\epsilon}_{ij} \right) \ ,$$

with $\lambda_2 = \lambda_1 \frac{\eta_s}{\eta_s + \eta_p}$, and $\eta = \eta_s + \eta_p \Rightarrow \lambda_1 \geqslant \lambda_2$. With η_s and η_p viscosity of Newtonian solvent and polymeric solute, respectively.

λ_1 relaxation time, λ_2 retardation time.



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Governing equations

Conservation laws:

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla(p+\Pi) + \nabla\cdot\boldsymbol{\sigma} + \mathbf{F_b}\ , \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0\,, \tag{2}$$

where, in 2D, $\mathbf{u} = (u(x,y,t), v(x,y,t))$, is the vector velocity field, $\nabla = (\partial_x, \partial_y)$, p is the pressure, Π is the van-der-Waals attraction/repulsion force, and $\mathbf{F_b} = (\rho g \sin\alpha, -\rho g\cos\alpha)$ body force.

Jeffreys' model:

$$\boldsymbol{\sigma} + \lambda_1 \partial_t \boldsymbol{\sigma} = 2\eta(\dot{\boldsymbol{\epsilon}} + \lambda_2 \partial_t \dot{\boldsymbol{\epsilon}})$$

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Schematic

Setup and boundary conditions:

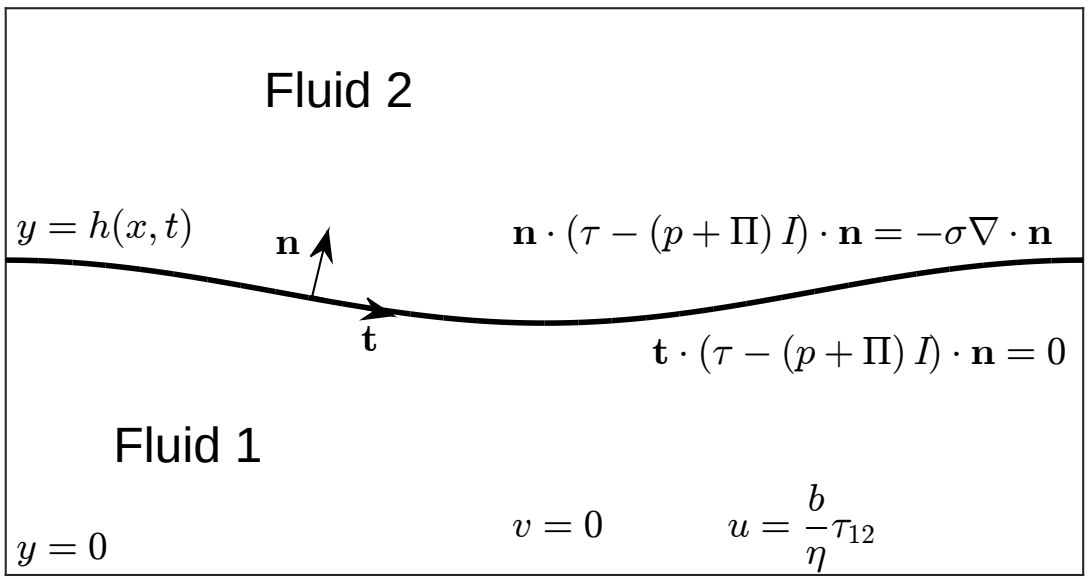

Figure: Schematic of the fluid interface and boundary conditions.

Kinematic BC: $\mathrm{Df/Dt} = \mathrm{f_t} + \mathbf{u} \cdot \nabla \mathrm{f} = 0$, with $\mathrm{f}(\mathrm{x}, \mathrm{y}, \mathrm{t}) = \mathrm{y} - \mathrm{h}(\mathrm{x}, \mathrm{t})$.

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Nondimensionalization

Scalings:

$$x = Lx^*\,,\ (y, h, h_\star, b) = H(y^*, h^*, h_\star^*, b^*)\,,\ (p, \Pi) = P(p^*, \Pi^*)\,,$$

$$u = Vu^*\,,\ v = \varepsilon V v^*\,,\ (t, \lambda_1, \lambda_2) = T(t^*, \lambda_1^*, \lambda_2^*)\,,\ \gamma = \frac{V\eta}{\varepsilon^3}\gamma^*\,,$$

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} = \frac{\eta}{T}\begin{pmatrix} \sigma_{11}^* & \frac{\sigma_{12}^*}{\varepsilon} \\ \frac{\sigma_{21}^*}{\varepsilon} & \sigma_{22}^* \end{pmatrix}\,,$$

where $H/L = \varepsilon \ll 1$ is the small parameter. Pressure is scaled with $P = \eta/(T\varepsilon^2)$, and time with $T = L/V$.

Dimensionless governing equations

Long-wave approximation in two spatial dimensions:

$$(1+\lambda_2\partial_t)h_t + \frac{\partial}{\partial x}\left\{(\lambda_2-\lambda_1)\left(\frac{h^2}{2}Q - hR\right)h_t + \left[(1+\lambda_1\partial_t)\frac{h^3}{3} + (1+\lambda_2\partial_t)bh^2\right]\frac{\partial}{\partial x}\left(\frac{\partial^2 h}{\partial x^2} + \Pi(h)\right)\right\} = 0\,,$$

$$Q + \lambda_2 Q_t = -\frac{\partial}{\partial x}\left(\frac{\partial^2 h}{\partial x^2} + \Pi(h)\right),$$
$$R + \lambda_2 R_t = -h\frac{\partial}{\partial x}\left(\frac{\partial^2 h}{\partial x^2} + \Pi(h)\right).$$

disjoining pressure: $\Pi(h) = \frac{\gamma(1-\cos\theta_e)}{M h_\star}\left[\left(\frac{h_\star}{h}\right)^n - \left(\frac{h_\star}{h}\right)^m\right]$,
θ_e contact angle, $M = 0.5$, $(n = 3, m = 2)$, $h_\star$ precursor film thickness.

Jeffreys' constitutive law:

$$\boldsymbol{\sigma} + \lambda_1\partial_t\boldsymbol{\sigma} = 2\eta(\dot{\boldsymbol{\epsilon}} + \lambda_2\partial_t\dot{\boldsymbol{\epsilon}})$$

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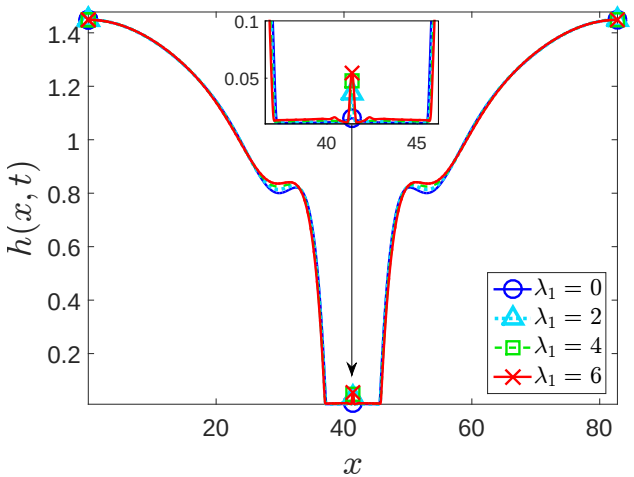
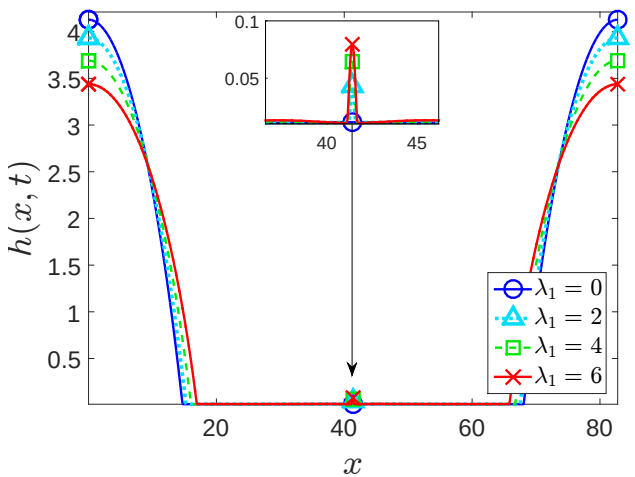
Dewettin films

Viscoelastic films with $\lambda_2 = 0$, and $b = 0$



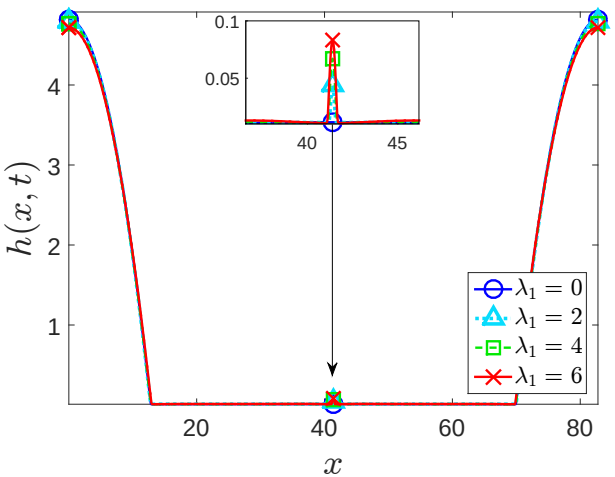
(a)

$t = 3.345 \times 10^5$



(b)

$t = 3.37 \times 10^5$



(c)

$t = 3.38 \times 10^5$

The Newtonian film does not exhibit any secondary droplet.

Dewetting films

A higher slippage with the substrate suppresses formation of satellite droplets

Rayleigh-Taylor instabilities in the case of an inverted plane

Spreading and receding drops

The viscoelastic drop spreads faster and recedes slower compared to the Newtonian one

Membranes

Shear and extensional free-boundary flows of viscoelastic membranes

Linear finite elements with plane stress formulation. Different constitutive models considered: elastic, viscous, viscoelastic (Maxwell)

References

Some references:

V. Barra, S. Afkhami, L. Kondic, *Mathematical and numerical modeling of thin viscoelastic films of Jeffreys type subjected to the van der Waals and gravitational forces*, EPJE, **42**, 1 – 14 (2019)

V. Barra, S. A. Chester, S. Afkhami, *Numerical Simulations of Nearly Incompressible Viscoelastic Membranes*, Computers & Fluids, **175**, 36 – 47 (2018)

V. Barra, S. Afkhami, L. Kondic, *Interfacial dynamics of thin viscoelastic films and drops*, J. Non-Newt. Fluid Mech. **237**, 26 – 38 (2016)

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Internship at Pixar

12-week internship program at PIXAR

Developed 2 proprietary libraries in C++ for viscous fluid simulations on curved surfaces

A vorticity-formulation Navier-Stokes solver with fluid-structure interactions, using Discrete Exterior Calculus (DEC) and time-splitting

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Internship at Pixar

A thin film (long-wave) solver on curved surfaces

Arbitrary topology
and element shapes

Prototyped a plugin
for Side FX Houdini

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Overview

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Overview

- For decades, high-order numerical methods have been considered too expensive
- A sparse matrix is no longer a good representation for high-order operators. In particular, the Jacobian of a nonlinear operator is known to rapidly lose sparsity as the order is increased
- 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, its integration with other packages, and some PETSc application examples

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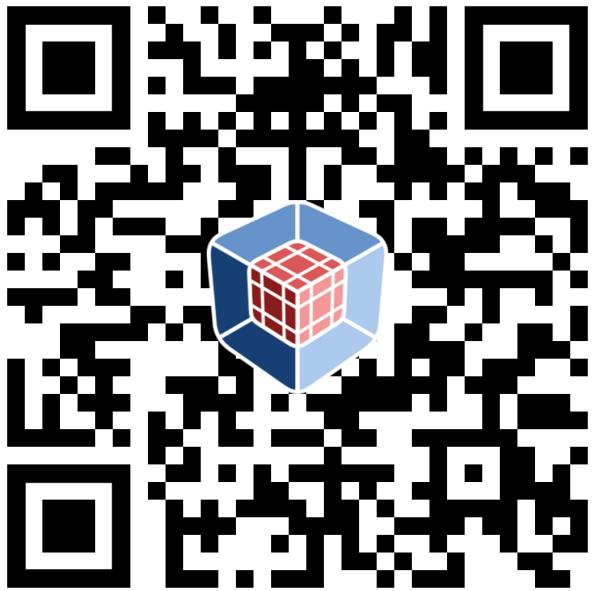
libCEED: the library of CEED (Center for Efficient Exascale Discretizations)

- Primary target: high-order finite/spectral element methods (FEM/SEM) exploiting tensor-product structure
- Open source (BSD-2 license) C library with Fortran and Python interfaces
- Releases: v0.1 (January 2018), v0.2 (March 2018), v.0.3 (September 2018), v0.4 (March 2019), v0.5 (September 2019)



For latest release:

Tomov S., Abdelfattah A., **Barra V.**, Beams N., Brown J. et al., *CEED ECP Milestone Report: Performance tuning of CEED software and 1st and 2nd wave apps* (2019, Oct 2nd) DOI: `https://doi.org/10.5281/zenodo.3477618`

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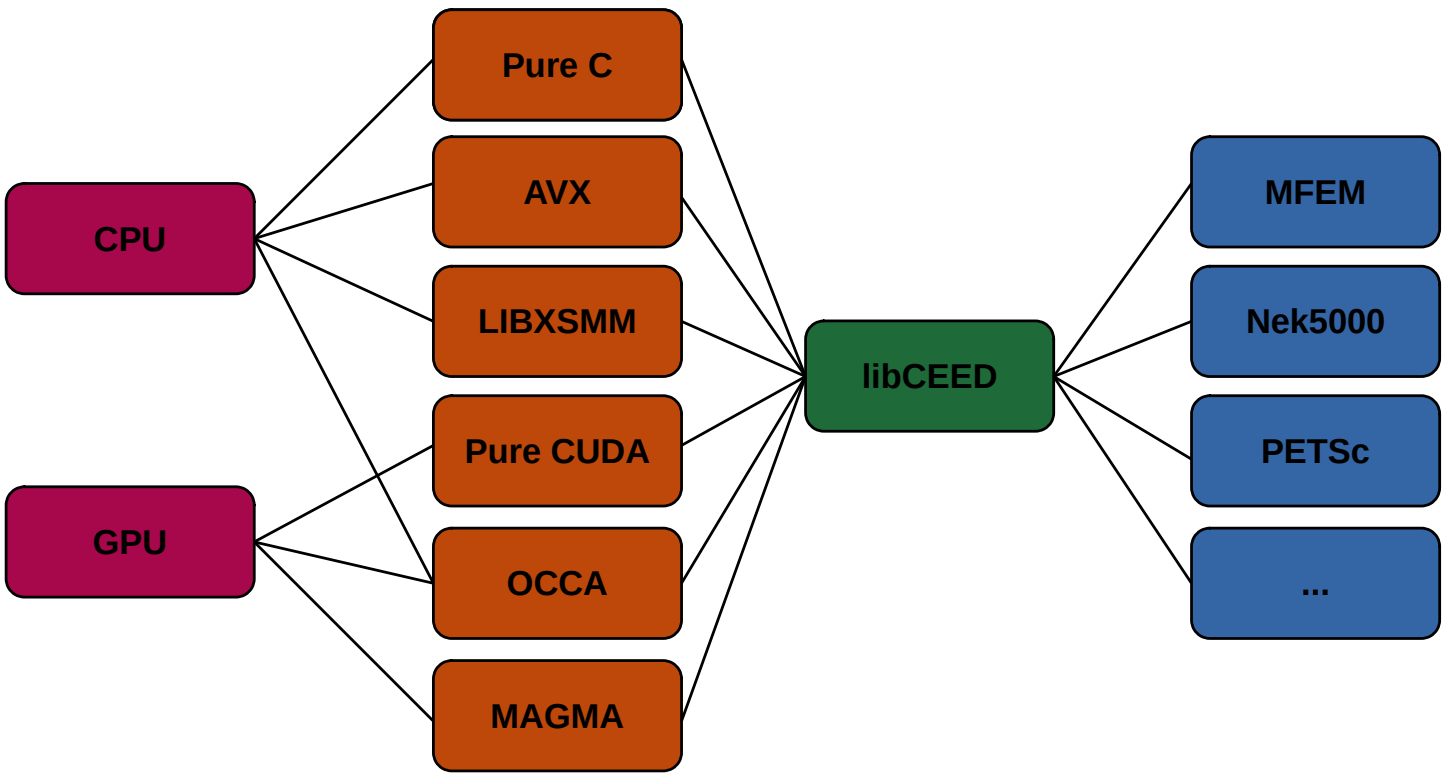
libCEED backends



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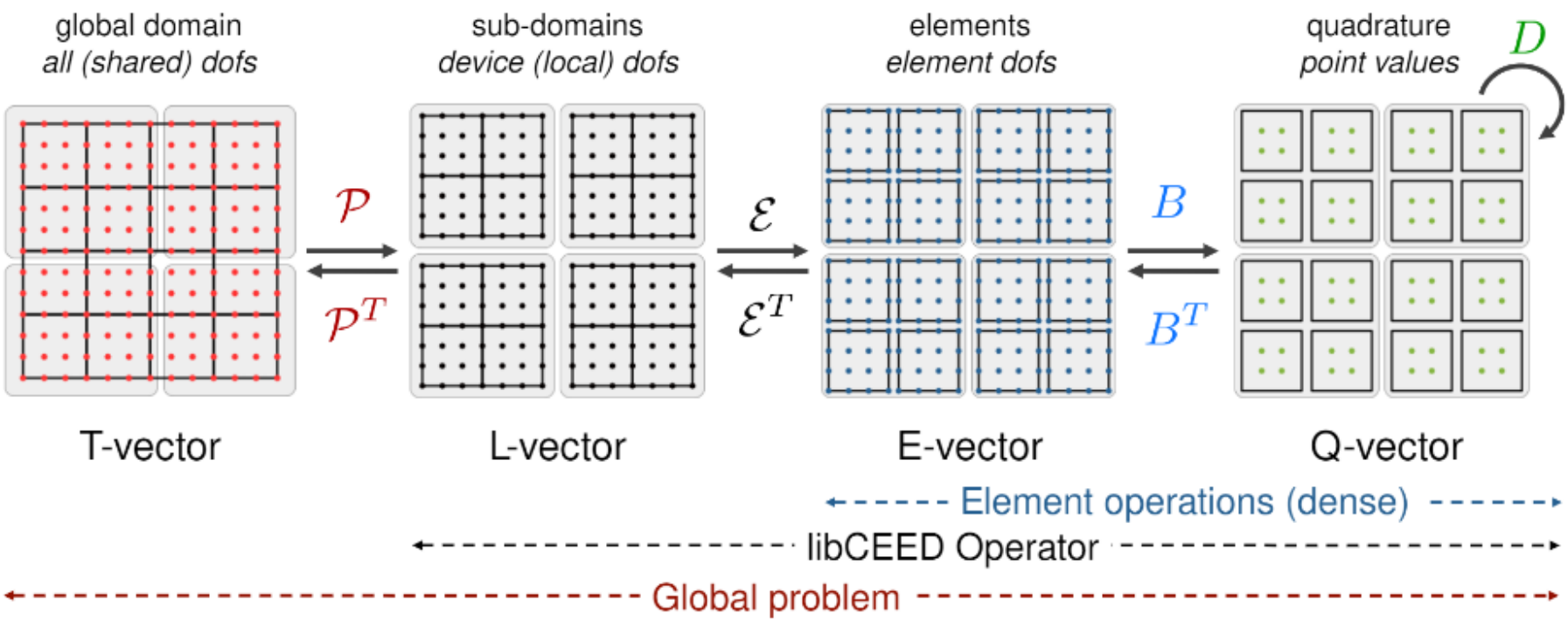
libCEED decomposition

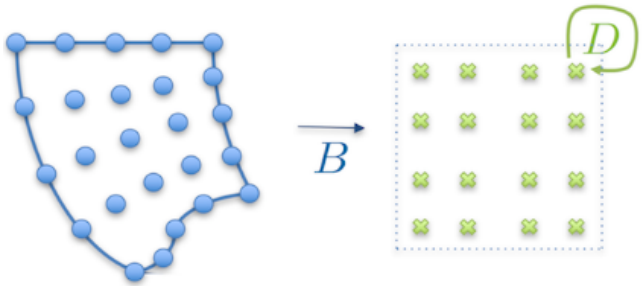
$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$



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

  - $\mathrm{C} = \mathcal{E}^{\mathsf{T}}\mathrm{B}^{\mathsf{T}}\mathrm{D}\mathrm{B}\mathcal{E}$: CeedOperator

    Composition of different operators defined on different element topologies possible

  - $\mathrm{A} = \mathrm{P}^{\mathsf{T}}\mathrm{C}\mathrm{P}$: User code responsible for parallelization on different compute devices. We use PETSc

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Point-wise QFunctions

User-defined QFunctions:

$$-\nabla \cdot (\kappa(\mathbf{x}) \nabla u) - f$$

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$$-\nabla \cdot (\kappa(\mathbf{x}) \nabla u) - f$$

or from libCEED's Gallery:

$$\nabla \cdot (\nabla u) - f$$

are point-wise functions that do not depend on element resolution, topology, or basis order

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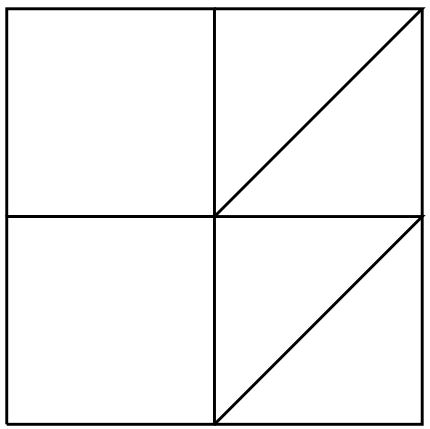

are point-wise functions that do not depend on element resolution, topology, or basis order

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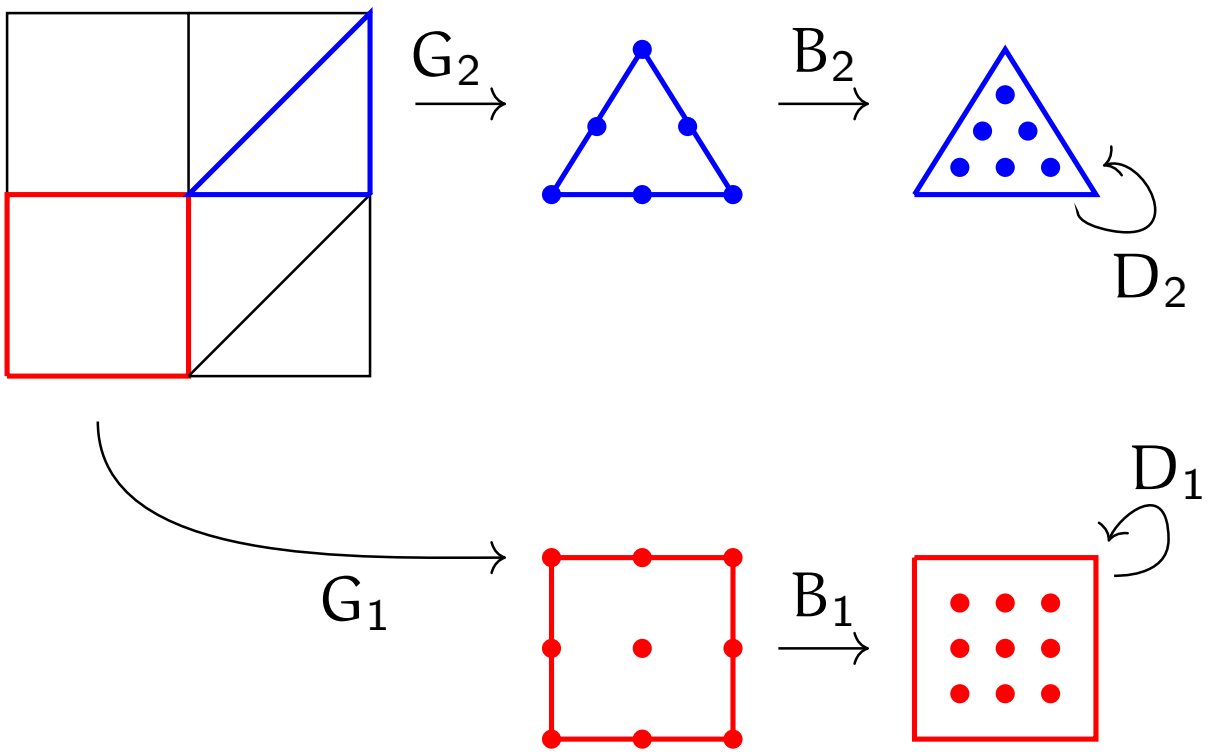
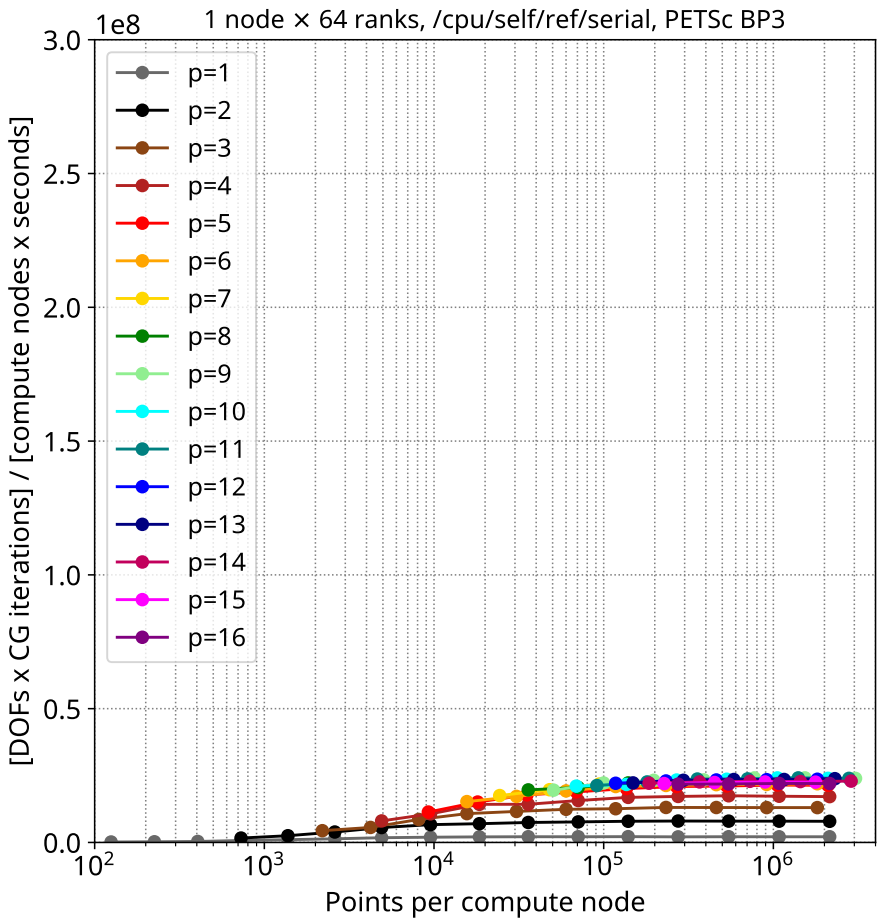
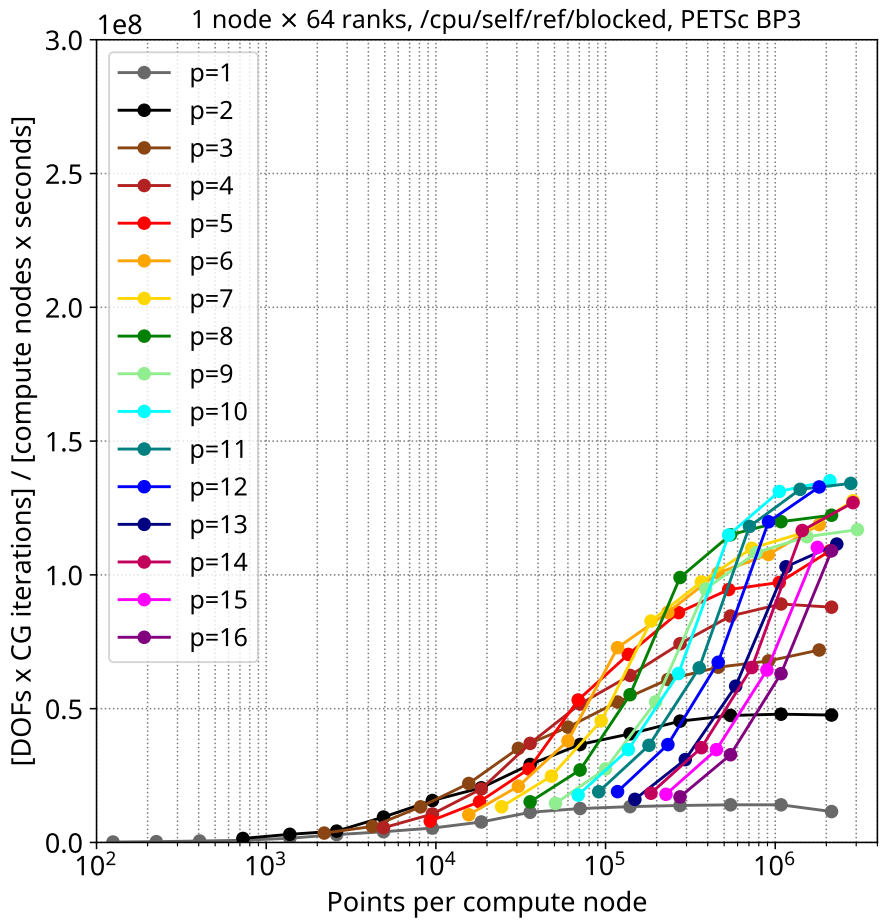


Performance w. r. t. problem size on KNL: ref



(a)



(b)

Figure: Knight Landing (Intel Xeon Phi 7230 SKU 1.3 GHz) with Intel-18 compiler. In (a) serial implementation; in (b) blocked implementation ($q = P + 2$, $P = p + 1$)

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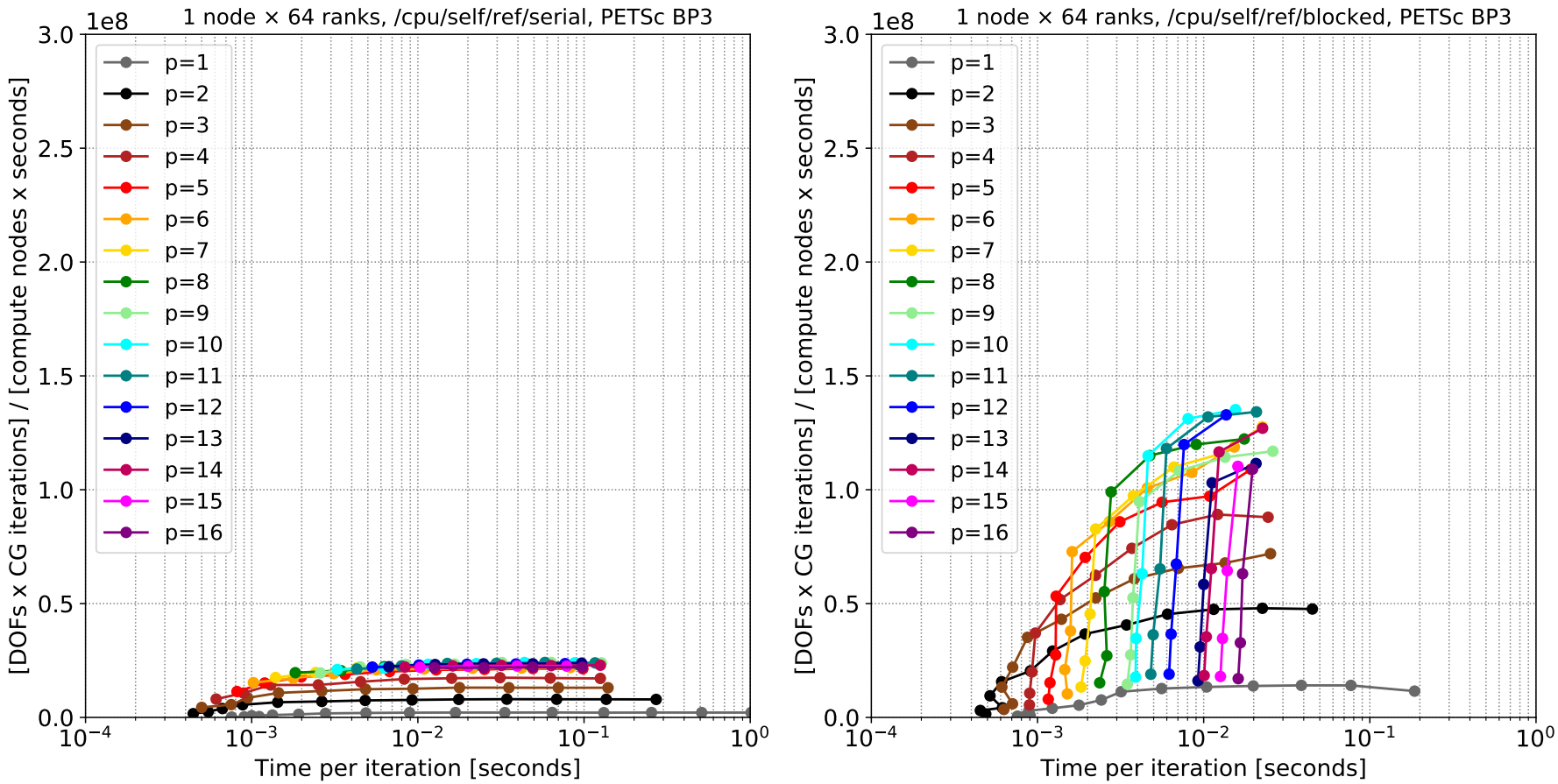
Performance w. r. t. time on KNL: ref



(a) (b)

Figure: Knight Landing (Intel Xeon Phi 7230 SKU 1.3 GHz) with Intel-18 compiler. In (a) serial implementation; in (b) blocked implementation ($q = P + 2$, $P = p + 1$)

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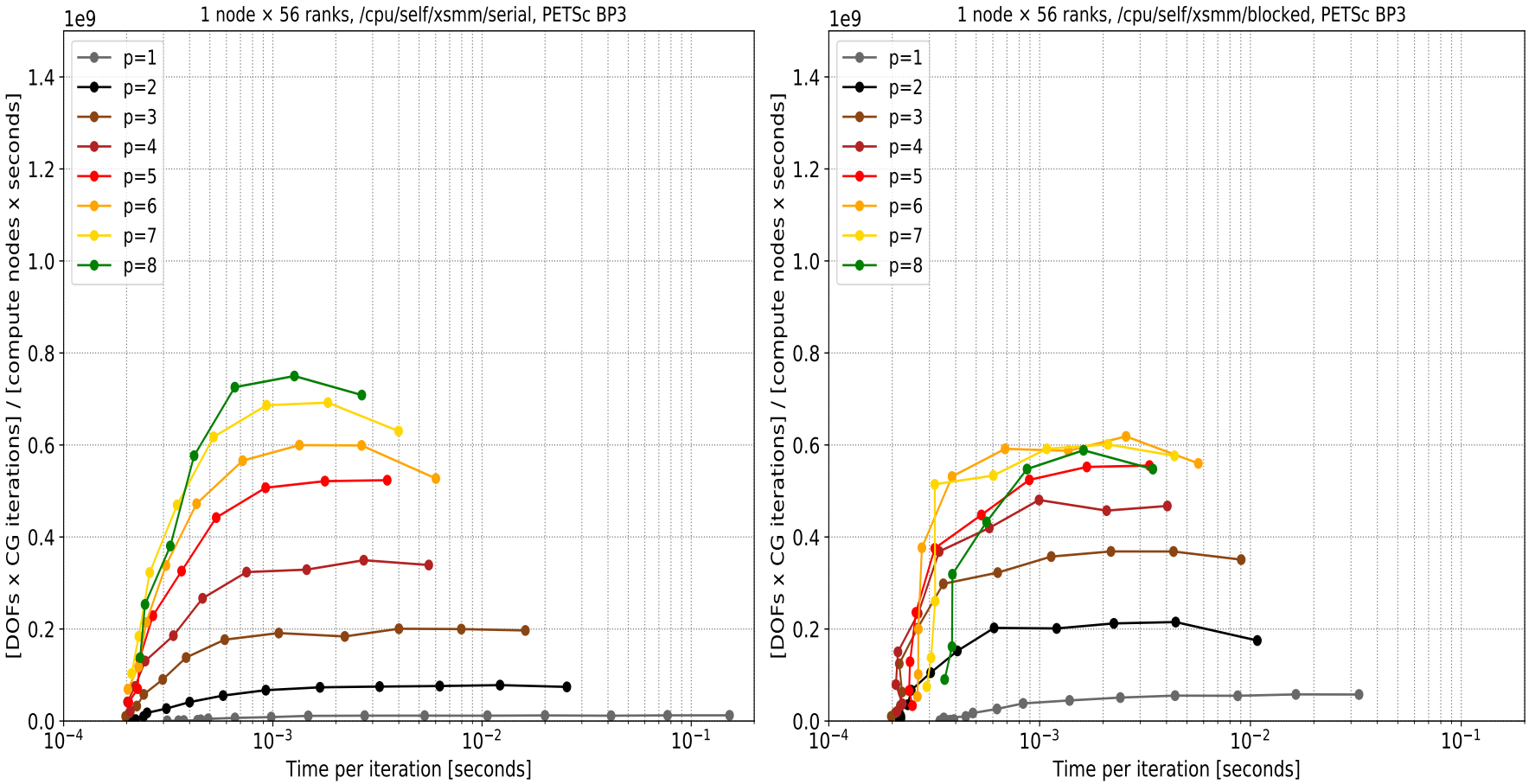
Performance w. r. t. time on Skylake: libXSMM



(a) (b)

Figure: Skylake (2x Intel Xeon Platinum 8180M CPU 2.50GHz) with gcc-8 compiler. Backends: in (a) libXSMM serial; in (b) libXSMM blocked ($q = P + 2$, $P = p + 1$)

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Performance w. r. t. time on Summit: ref (non optimized)

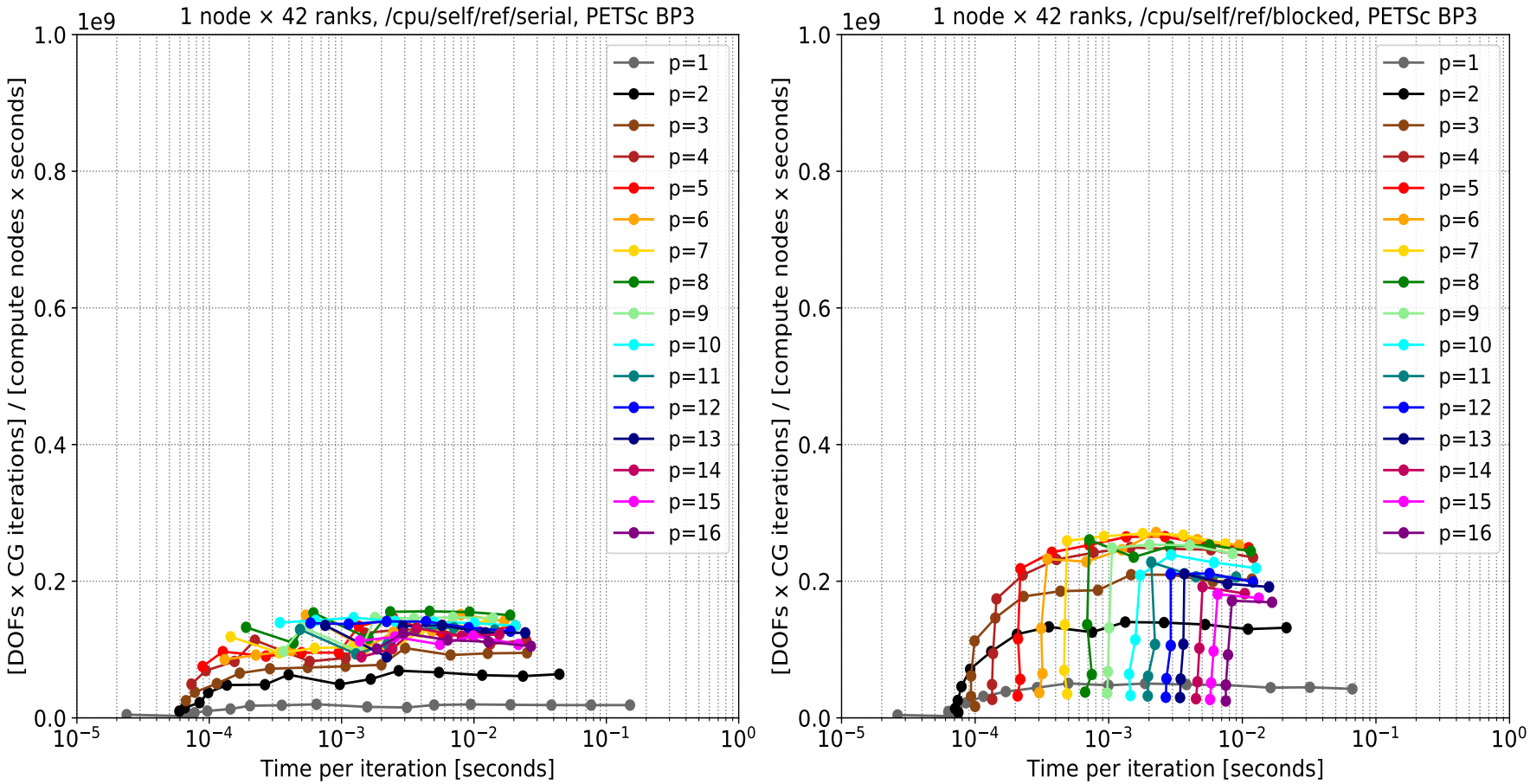

Figure: OLCF Summit (2x IBM POWER9) with gcc-9 compiler. Backends: in (a) ref serial; in (b) ref blocked ($q = P + 2$, $P = p + 1$)

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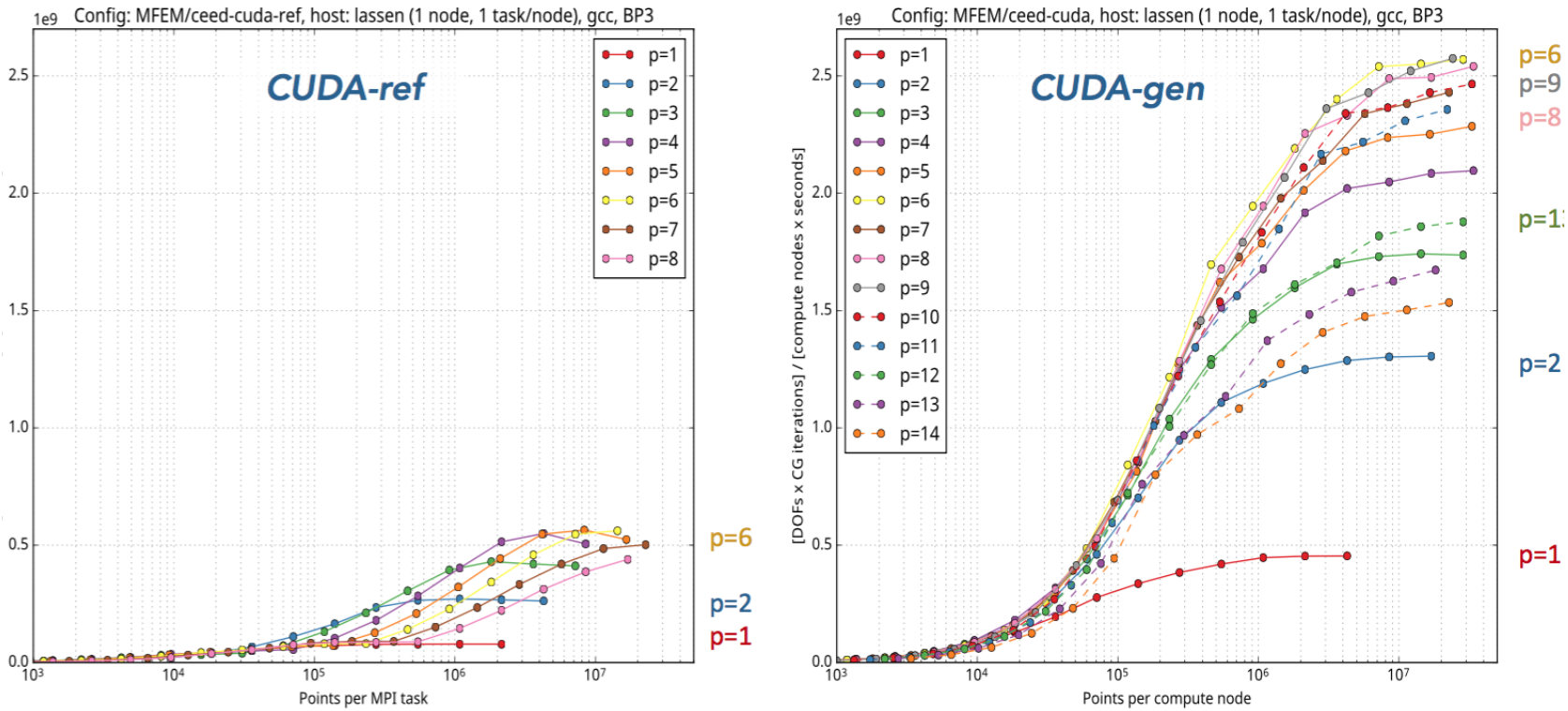
GPU results: MFEM + libCEED



Results by Yohann Dudouit on Lassen (LLNL): CUDA-ref (left) and CUDA-gen (right) backends performance for 3D BP3 on a NVIDIA V100 GPU.

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Towards a libCEED miniapp: a Navier-Stokes solver

Compressible Navier-Stokes equations in conservation form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{U} = 0\,, \tag{3a}$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \left(\frac{\mathbf{U} \otimes \mathbf{U}}{\rho} + P\mathbf{I}_3 \right) + \rho g \mathbf{k} = \nabla \cdot \boldsymbol{\sigma}\,, \tag{3b}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left(\frac{(E + P)\mathbf{U}}{\rho} \right) = \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma} + k \nabla T)\,, \tag{3c}$$

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

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Towards a libCEED miniapp: a Navier-Stokes solver

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

$$(c_p/c_v - 1)\,(E - \mathbf{U} \cdot \mathbf{U}/(2\rho) - \rho g z) = P \quad \leftarrow \text{ pressure}$$

$\mu \leftarrow$ dynamic viscosity

$g \leftarrow$ gravitational acceleration

$k \leftarrow$ thermal conductivity

$\lambda \leftarrow$ Stokes hypothesis constant

$c_p \leftarrow$ specific heat, constant pressure

$c_v \leftarrow$ specific heat, constant volume

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Vector form

The system (3) can be rewritten in vector form

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = S(\mathbf{q}), \tag{4}$$

for the state variables

$$\mathbf{q} = \begin{pmatrix} \rho \\ \mathbf{U} \equiv \rho \mathbf{u} \\ E \equiv \rho e \end{pmatrix} \begin{matrix} \leftarrow \text{ volume mass density} \\ \leftarrow \text{ momentum density} \\ \leftarrow \text{ energy density} \end{matrix} \tag{5}$$

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where

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

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

Space discretization

We use high-order finite/spectral elements: high-order Lagrange polynomials over non-uniformly spaced nodes, $\{x_i\}_{i=0}^{p}$, 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 $\mathbf{X} = (X, Y, Z) \in \mathbf{I} = [-1, 1]^3$.

Space discretization

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Define the discrete solution

$$\mathbf{q}_N(\mathbf{x}, t)^{(e)} = \sum_{k=1}^{P} \psi_k(\mathbf{x}) \mathbf{q}_k^{(e)} \tag{6}$$

with P the number of nodes in the element e.

We use tensor-product bases $\psi_{kji} = h_i(X) h_j(Y) h_k(Z)$.

Strong and weak formulations

The strong form of (5):

$$\int_\Omega v \left(\frac{\partial \mathbf{q}_N}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}_N) \right) \, d\Omega = \int_\Omega v \mathbf{S}(\mathbf{q}_N) \, d\Omega \,, \ \forall v \in \mathcal{V}_p \tag{7}$$

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

$$\int_\Omega v \frac{\partial \mathbf{q}_N}{\partial t} \, d\Omega + \int_\Gamma v \hat{\mathbf{n}} \cdot \mathbf{F}(\mathbf{q}_N) \, d\Omega - \int_\Omega \nabla v \cdot \mathbf{F}(\mathbf{q}_N) \, d\Omega = \int_\Omega v \mathbf{S}(\mathbf{q}_N) \, d\Omega \,, \ \forall v \in \mathcal{V}_p \tag{8}$$

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Strong and weak formulations

The strong form of (5):

$$\int_\Omega v \left(\frac{\partial \mathbf{q}_N}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}_N) \right) \, d\Omega = \int_\Omega v \mathbf{S}(\mathbf{q}_N) \, d\Omega \, , \; \forall v \in \mathcal{V}_p \tag{7}$$

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

$$\int_\Omega v \frac{\partial \mathbf{q}_N}{\partial t} \, d\Omega + \int_\Gamma v \hat{\mathbf{n}} \cdot \mathbf{F}(\mathbf{q}_N) \, d\Omega - \int_\Omega \nabla v \cdot \mathbf{F}(\mathbf{q}_N) \, d\Omega = \int_\Omega v \mathbf{S}(\mathbf{q}_N) \, d\Omega \, , \; \forall v \in \mathcal{V}_p \tag{8}$$

For the Time Discretization we use an explicit formulation

$$\mathbf{q}_N^{n+1} = \mathbf{q}_N^n + \Delta t \sum_{i=1}^{s} b_i k_i \, , \tag{9}$$

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

A very simple example: The advection equation

We analyze the transport of total energy

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u} E) = 0\,, \tag{10}$$

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

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, $\pi(\mathbf{x}, t)$, and potential temperature, $\theta(\mathbf{x}, t)$, that relate to the state variables via

$$\rho = \frac{P_0}{(c_p - c_v)\theta(\mathbf{x}, t)} \pi(\mathbf{x}, t)^{\frac{c_v}{c_p - c_v}}, \tag{11a}$$

$$e = c_v \theta(\mathbf{x}, t)\pi(\mathbf{x}, t) + \mathbf{u} \cdot \mathbf{u}/2 + gz, \tag{11b}$$

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

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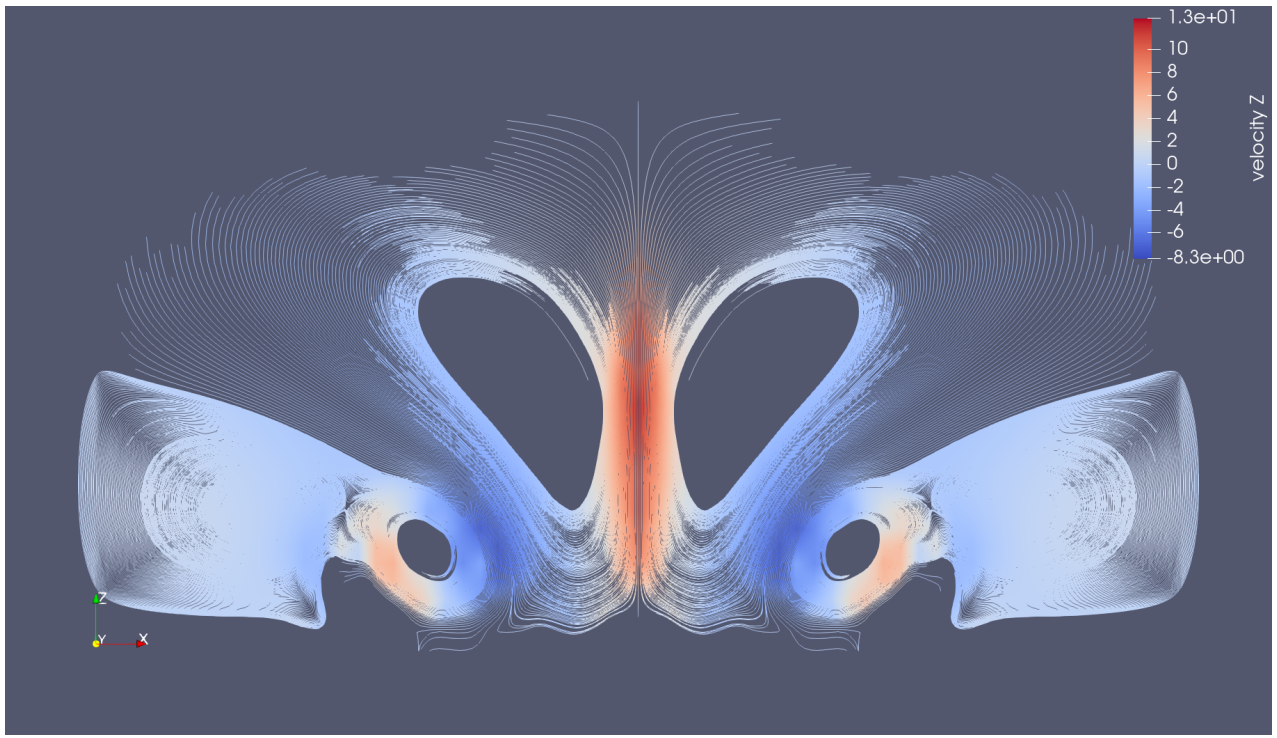
Recent Developments: Implicit time-stepping



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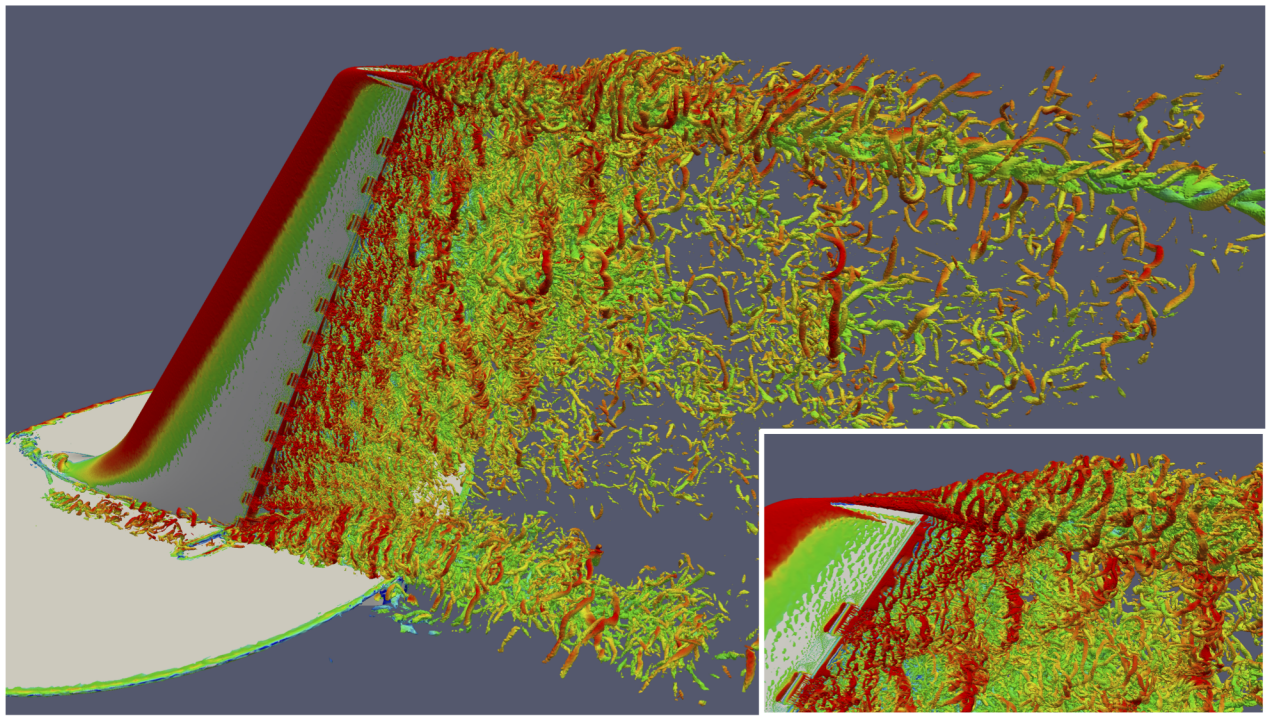
Recent Developments: PHASTA

In collaboration with PHASTA (FastMath) we have worked on libCEED's integration.



[Ref: `phasta.scigap.org`]

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Stabilization methods

We have ported Streamline Upwind (SU) and Streamline Upwind/Petrov-Galerkin (SUPG) stabilization methods to our CFD examples.

For the advection case:

Not stabilized version.

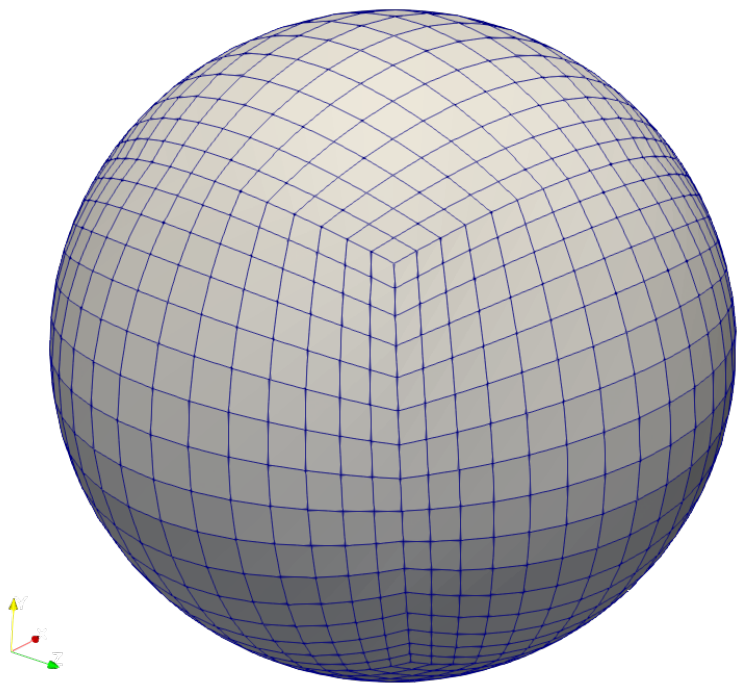
Stabilized version.

Some work in progress

Converted BP1 (Mass operator) & BP3 (Poisson's equation) on the cubed-sphere as a prototype for shallow-water equations solver

$$\frac{\partial \mathbf{u}}{\partial t} = -(\omega + f)\hat{k} \times \mathbf{u} - \nabla\left(\frac{1}{2}|\mathbf{u}|^2 + g(h + h_s)\right) \tag{12a}$$

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h_0 + h)\mathbf{u} \tag{12b}$$



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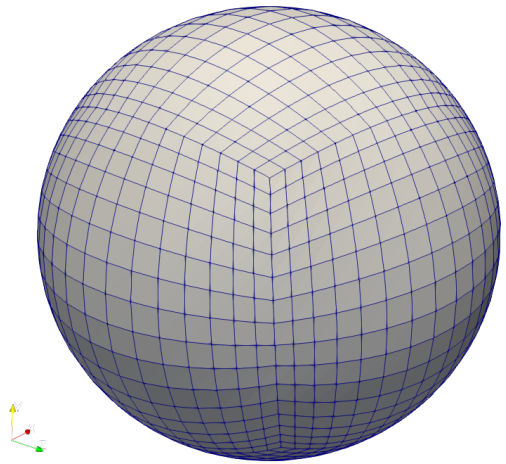
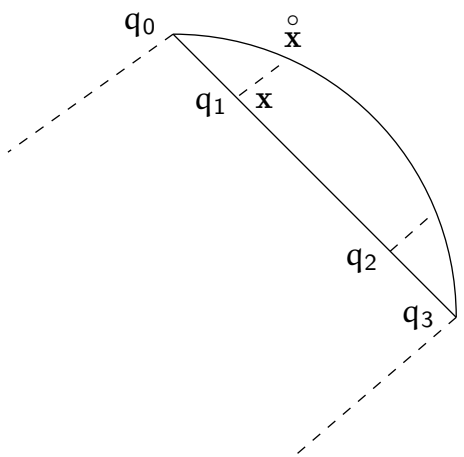
Problems on the sphere





Transform $\mathring{\mathbf{x}} = (\mathring{x}, \mathring{y}, \mathring{z})$ on the sphere $\hookrightarrow$
$\mathbf{x} = (x, y, z)$ on the discrete surface $\hookrightarrow$
$\mathbf{X} = (X, Y) \in \mathbf{I} = [-1, 1]^2$

$$\underset{(3\times 2)}{\frac{\partial \mathring{\mathbf{x}}}{\partial \mathbf{X}}} = \underset{(3\times 3)}{\frac{\partial \mathring{\mathbf{x}}}{\partial \mathbf{x}}} \underset{(3\times 2)}{\frac{\partial \mathbf{x}}{\partial \mathbf{X}}}$$

$$|J| = \left| \mathrm{col}_1 \left(\frac{\partial \mathring{\mathbf{x}}}{\partial \mathbf{X}} \right) \times \mathrm{col}_2 \left(\frac{\partial \mathring{\mathbf{x}}}{\partial \mathbf{X}} \right) \right|$$

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Conclusions

- We have showed libCEED's performance portability on several architectures, when integrated with PETSc and MFEM
- We have demonstrated the use of libCEED with PETSc for the numerical high-order solutions of
  - Advection equation
  - Full compressible Navier-Stokes equations
- We have included implicit time-stepping and stabilization methods

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Outlook

Ongoing and future work:

- BDDC and FDM preconditioners
- Algorithmic differentiation of Q-functions
- Ongoing work on CUDA and HIP optimizations
- Our (first!) user manual and educational Jupyter-notebook tutorials
- We always welcome contributors and users
  `https://github.com/CEED/libCEED`

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- We always welcome contributors and users
  `https://github.com/CEED/libCEED`

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

Thank you!

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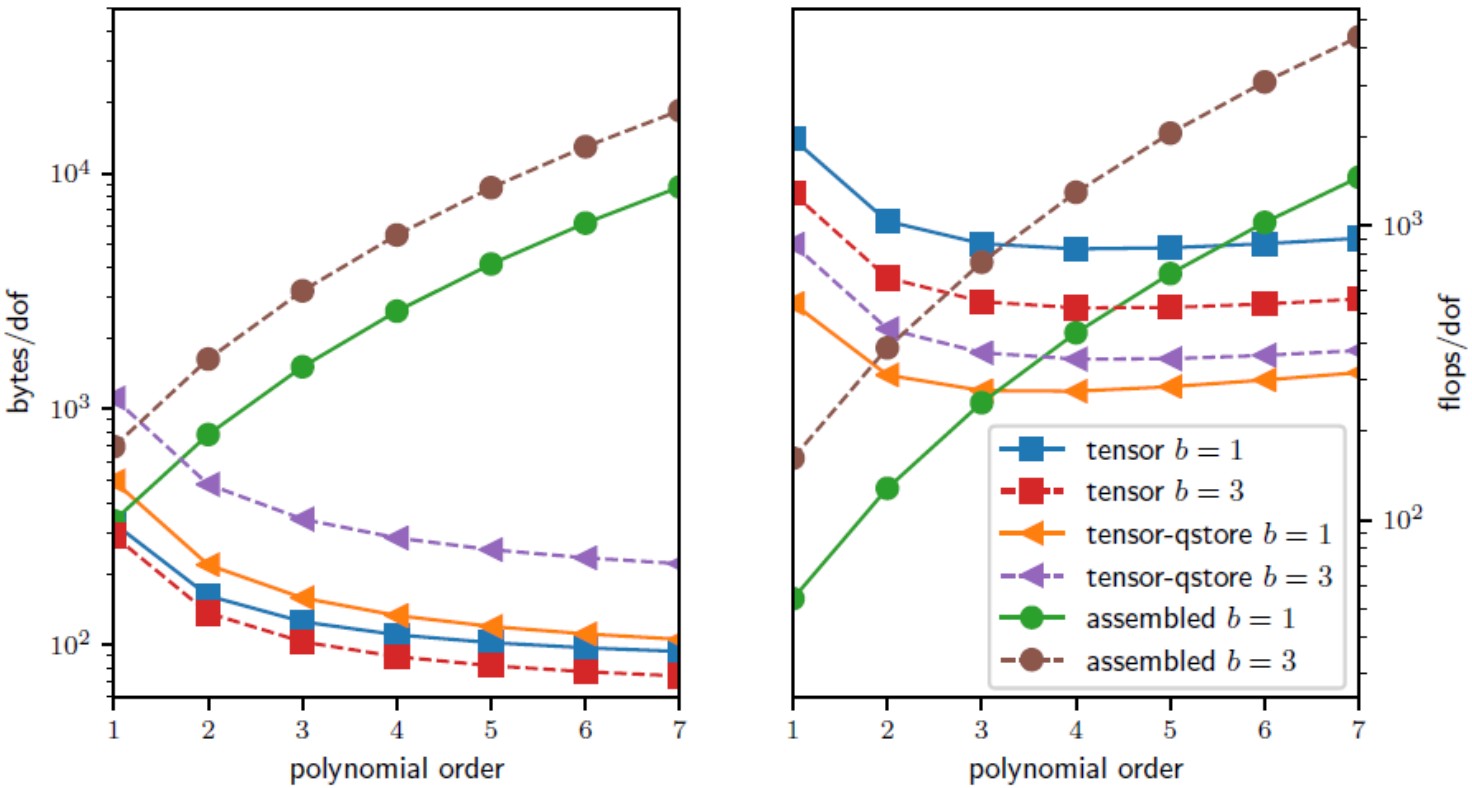
Motivation: Why matrix-free? And why high-order?



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)

[Courtesy: Jed Brown]

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libCEED backends

`/cpu/self/ref/*`:	with `*` reference serial and blcoked implementations
`/cpu/self/avx/*`:	AVX (Advanced Vector Extensions instruction sets) with `*` reference serial and blocked implementations
`/cpu/self/xsmm/*`:	LIBXSMM (Intel library for small dense/sparse mat-multiply) with `*` reference serial and blocked implementations
`/*/occa`:	OCCA (just-in-time compilation) with `*`: CPU, GPU, OpenMP (Open Multi-Processing: API), OpenCL (framework for CPUs, GPUs, etc.)
`/gpu/magma`:	CUDA MAGMA (dense Linear Algebra library for GPUs and multicore architectures) kernels
`/gpu/cuda/*`:	CUDA with `*`: `ref` (reference pure CUDA kernels), `reg` (CUDA kernels using one thread per element), `shared`, optimized CUDA kernels using shared memory `gen`, optimized CUDA kernels using code generation

Same source code can call multiple CEEDs with different backends. On-device operator implementation with unique interface

Tensor contractions

Let $\{x_i\}_{i=0}^{p}$ denote the LGL nodes with the corresponding interpolants $\{\psi_i^p\}_{i=0}^{p}$. Choose a quadrature rule with nodes $\{q_i^Q\}_{i=0}^{Q}$ and weights $\{w_i^Q\}$. The basis evaluation, derivative, and integration matrices are $B_{ij}^{Qp} = \psi_j^p(q_i^Q)$, $D_{ij}^{Qp} = \partial_x \psi_j^p(q_i^Q)$, and $W_{ij}^{Q} = w_i^Q \delta_{ij}$. In 3D:

$$\mathbf{B} = B \otimes B \otimes B \tag{13}$$
$$\mathbf{D}_0 = D \otimes B \otimes B \tag{14}$$
$$\mathbf{D}_1 = B \otimes D \otimes B \tag{15}$$
$$\mathbf{D}_2 = B \otimes B \otimes D \tag{16}$$
$$\mathbf{W} = W \otimes W \otimes W \tag{17}$$

These tensor-product operations cost $2(p^3Q + p^2Q^2 + pQ^3)$ and touch only $O(p^3 + Q^3)$ memory. In the spectral element method, when the same LGL points are reused for quadrature (i.e., a collocated method with $Q = p + 1$), then $\mathbf{B} = \mathbf{I}$ and $\mathbf{D}$ reduces to $O(p^4)$.

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libCEED API for operator composition

Creation of QFunctions and CEED operators:

```
CeedQFunctionCreateInterior(ceed, 1, Mass, Mass_loc, &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);
CeedOperatorSetField(op_mass, "v", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
```

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CeedOperatorSetField(op_mass, "v", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
```

$$f(\mathbf{u}, \mathbf{p}; \Theta) \rightleftharpoons f(u, p; \mathbf{\Theta})$$

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CeedOperatorSetField(op_mass, "u", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
CeedOperatorSetField(op_mass, "weights", Erestrictudi, CEED_NOTRANSPOSE, basisx, weights);
CeedOperatorSetField(op_mass, "v", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
```

$$f(\mathbf{u}, \mathbf{p}; \Theta) \rightleftharpoons f(u, p; \mathbf{\Theta})$$

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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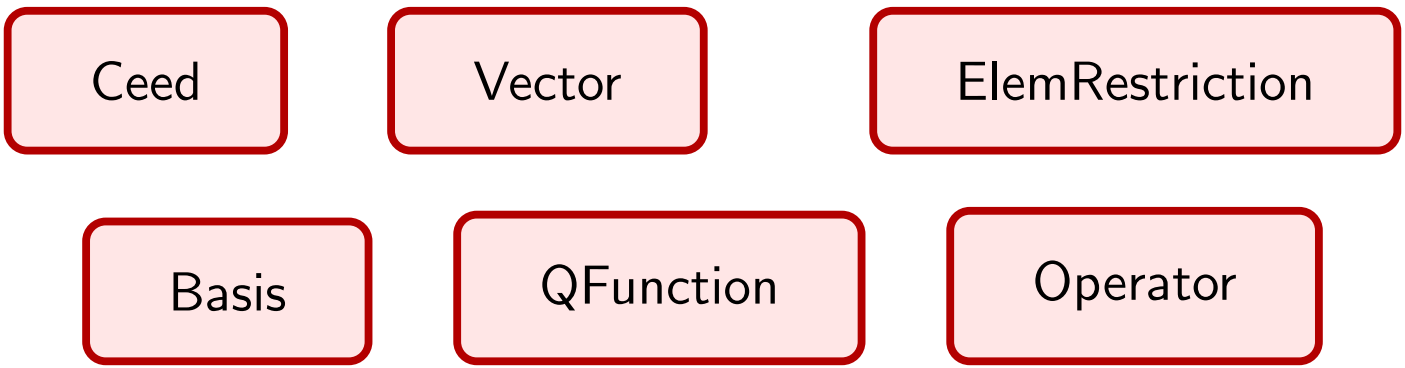
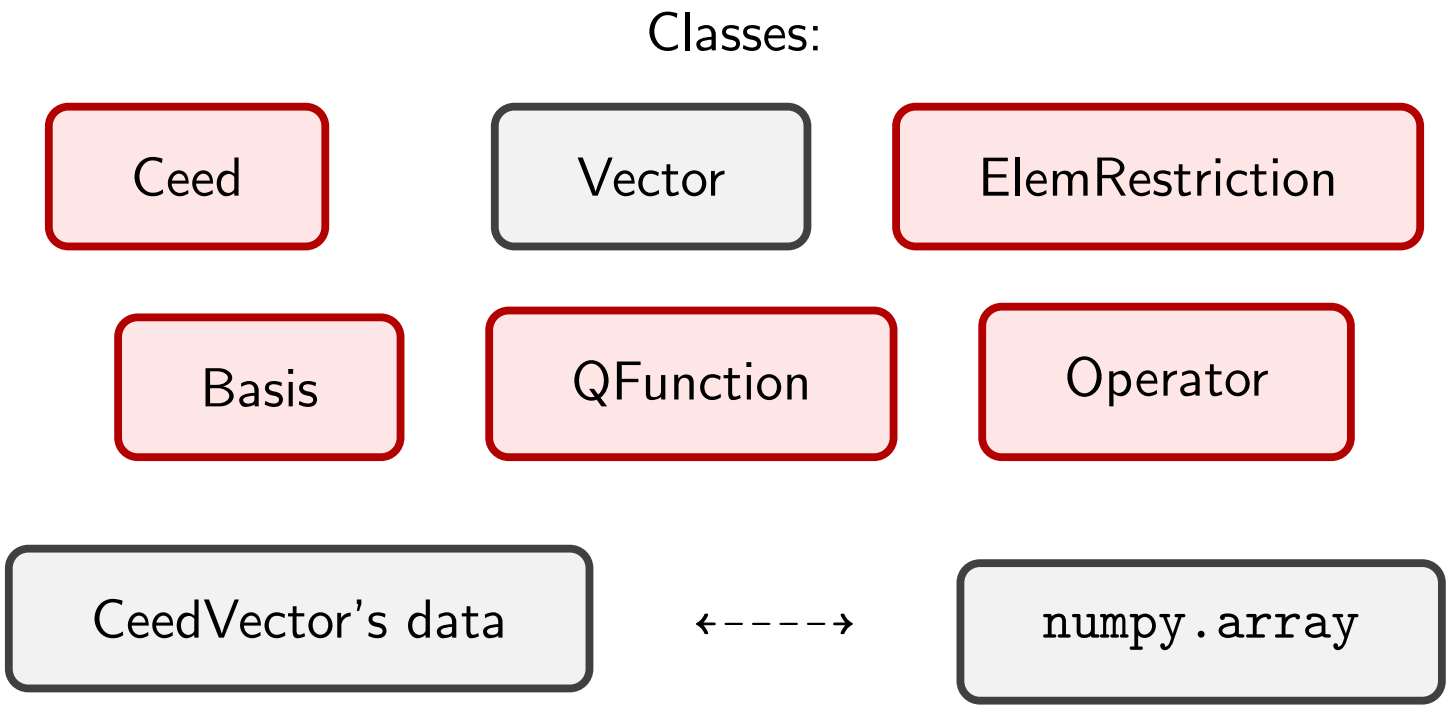
libCEED's Python interface

Classes:

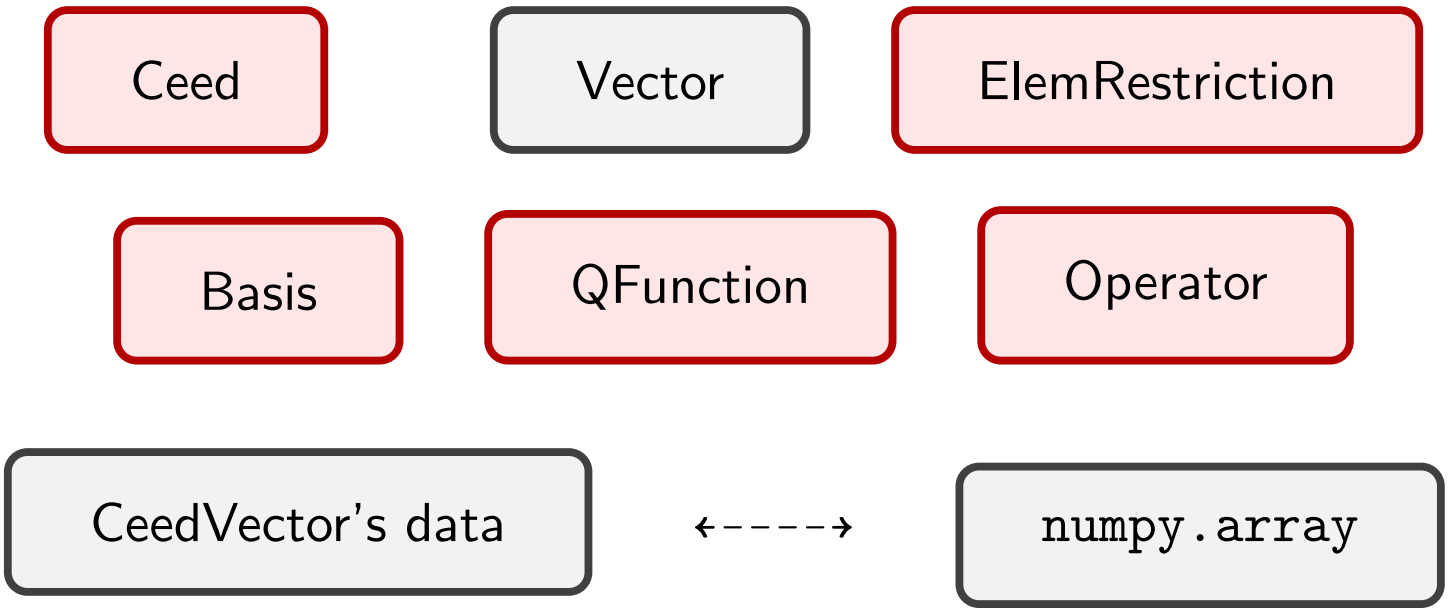


libCEED's Python interface



libCEED's Python interface

Classes:




```
import libceed
ceed = libceed.Ceed()
n = 10
x = ceed.Vector(n)

print(x)
```

or

```
import libceed
ceed = libceed.Ceed()
x = ceed.Vector(size=10)

print(x)
```

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Python interface (some examples)

Vector

```
import libceed
ceed = libceed.Ceed('/gpu/cuda/gen')
x = ceed.Vector(size=10)

a = np.arange(1, 4, dtype="float64")
x.set_array(a, cmode=libceed.USE_POINTER)
b = x.get_array_read()
print(b)
```

```
import libceed
ceed = libceed.Ceed('/cpu/self')
u = ceed.Vector(size=10)

u.set_value(0)
print(u)
```

Python interface (some examples)

Vector

```
import libceed
ceed = libceed.Ceed('/gpu/cuda/gen')
x = ceed.Vector(size=10)

a = np.arange(1, 4, dtype="float64")
x.set_array(a, cmode=libceed.USE_POINTER)
b = x.get_array_read()
print(b)
```

```
import libceed
ceed = libceed.Ceed('/cpu/self')
u = ceed.Vector(size=10)

u.set_value(0)
print(u)
```

Elemrestriction

```
ne = 8
x = ceed.Vector(ne+1)
y = ceed.Vector(2*ne)
r = ceed.ElemRestriction(ne, 2, ne+1, 1, ind, cmode=libceed.USE_POINTER)
r.apply(x, y)
r.T.apply(y, x)
```

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C interface Vs Python interface

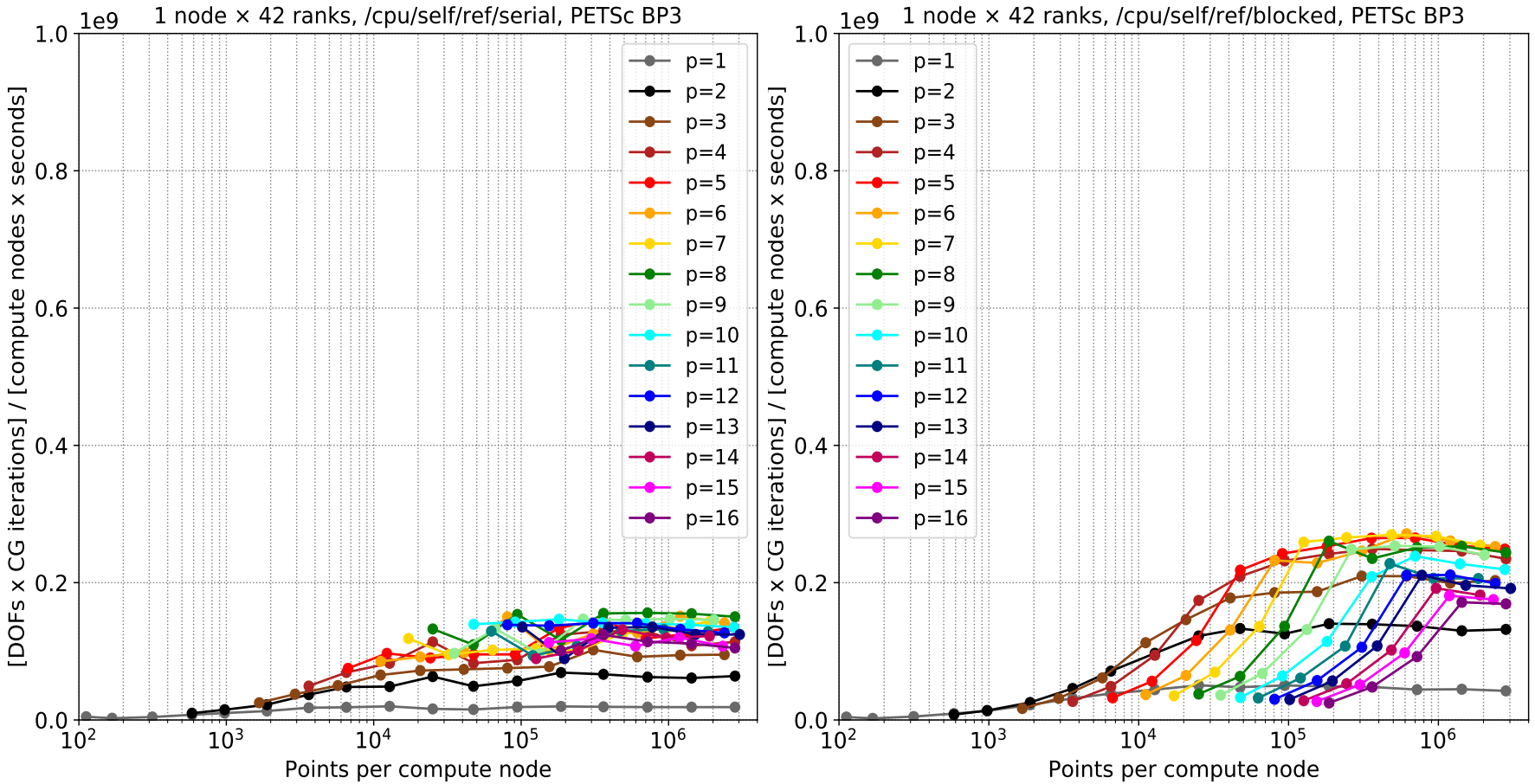
```
CeedQFunctionCreateInterior(ceed, 1, Mass, Mass_loc, &qf_mass);
CeedQFunctionAddInput(qf_mass, "u", 5, CEED_EVAL_INTERP);
CeedQFunctionAddInput(qf_mass, "weights", 1, CEED_EVAL_NONE);
CeedQFunctionAddOutput(qf_mass, "v", 5, CEED_EVAL_INTERP);

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,
CEED_BASIS_COLLOCATED, weights);
CeedOperatorSetField(op_mass, "v", Erestrictu, CEED_TRANSPOSE, basisu, CEED_VECTOR_ACTIVE);
```

```
qf_mass = ceed.QFunction(1, qfs.apply_mass, os.path.join(file_dir,
"test-qfunctions.h:apply_mass"))
qf_mass.add_input("u", 5, libceed.EVAL_INTERP)
qf_mass.add_input("weights", 1, libceed.EVAL_NONE)
qf_mass.add_output("v", 5, libceed.EVAL_INTERP)

op_mass = ceed.Operator(qf_mass)
op_mass.set_field("u", Erestrictu, basisu, libceed.VECTOR_ACTIVE, libceed.TRANSPOSE)
op_mass.set_field("weights", Erestrictudi, libceed.BASIS_COLLOCATED, weights)
op_mass.set_field("v", Erestrictu, basisu, libceed.VECTOR_ACTIVE, libceed.TRANSPOSE)
```

Performance w. r. t. size on Summit: ref (non optimized)



(a) (b)

Figure: OLCF Summit (2x IBM POWER9) with gcc-9 compiler. Backends: in (a) ref serial; in (b) ref blocked ($q = P + 2$, $P = p + 1$)

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