Performance-portable interfaces for applications in Scientific Computing

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(remotely for)
SIAM-AN20

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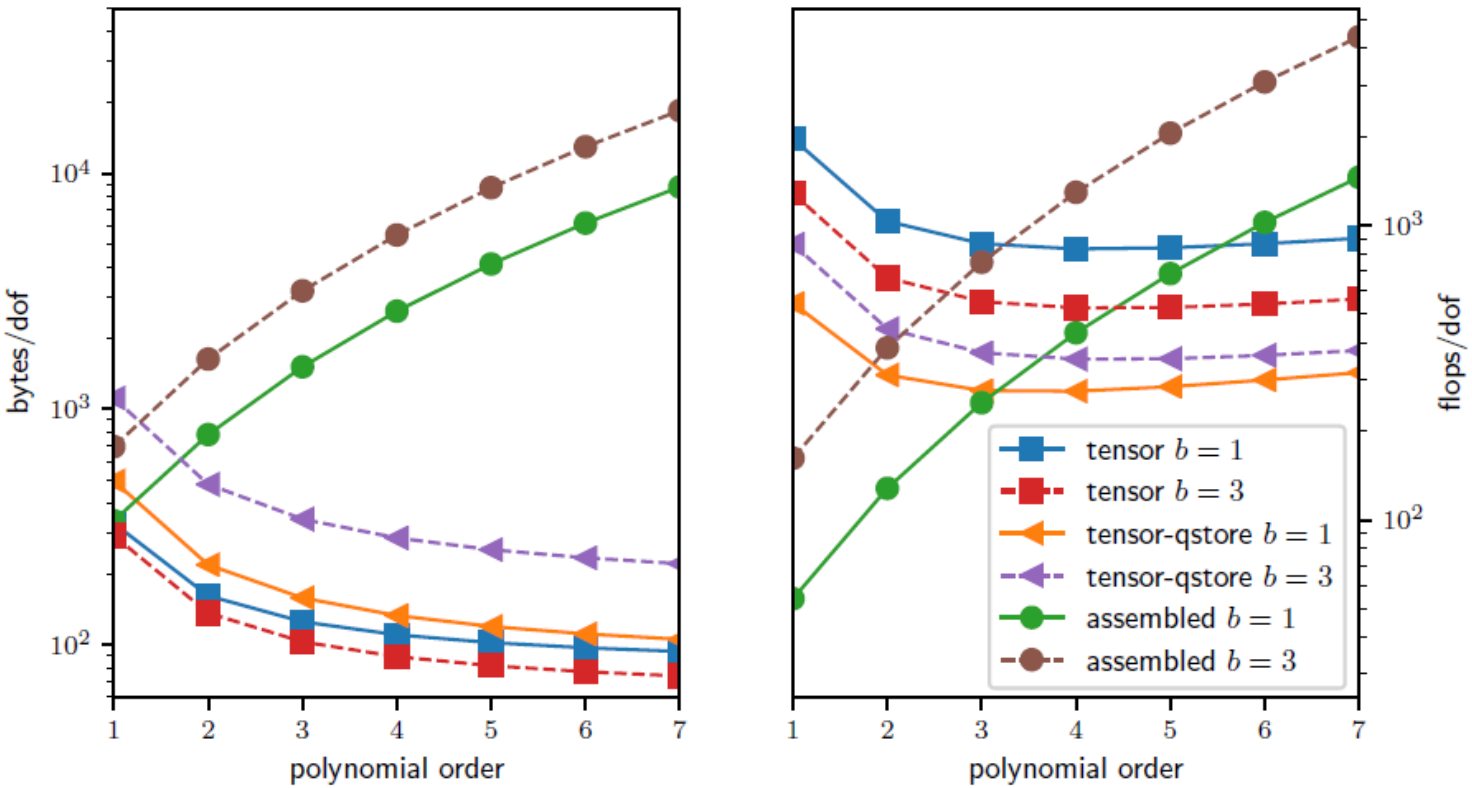
CEED
EXASCALE DISCRETIZATIONS

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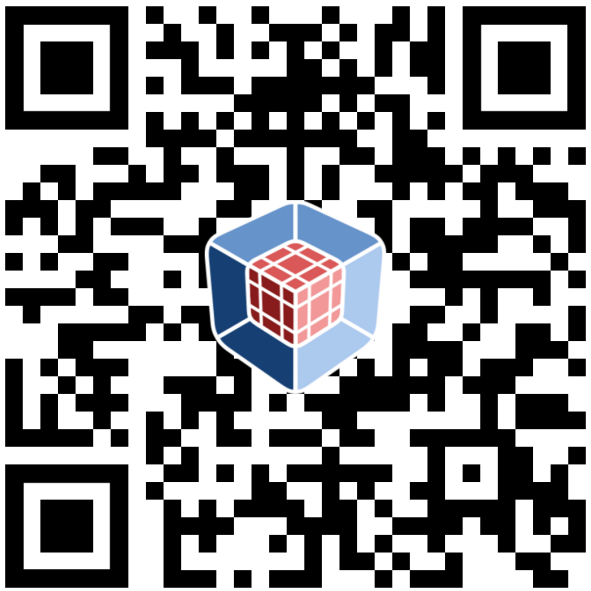
libCEED: the library within CEED (Center for Efficient Exascale Discretizations)

- 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), v0.6 (March 2020)



For latest release:

Kolev T., Fischer P., Abdelfattah A., Ananthan S., **Barra V.**, Beams N., Brown J. et al., *CEED ECP Milestone Report: Improve performance and capabilities of CEED-enabled ECP applications on Summit/Sierra* (2020, March 31st) DOI: `http://doi.org/10.5281/zenodo.3860804`

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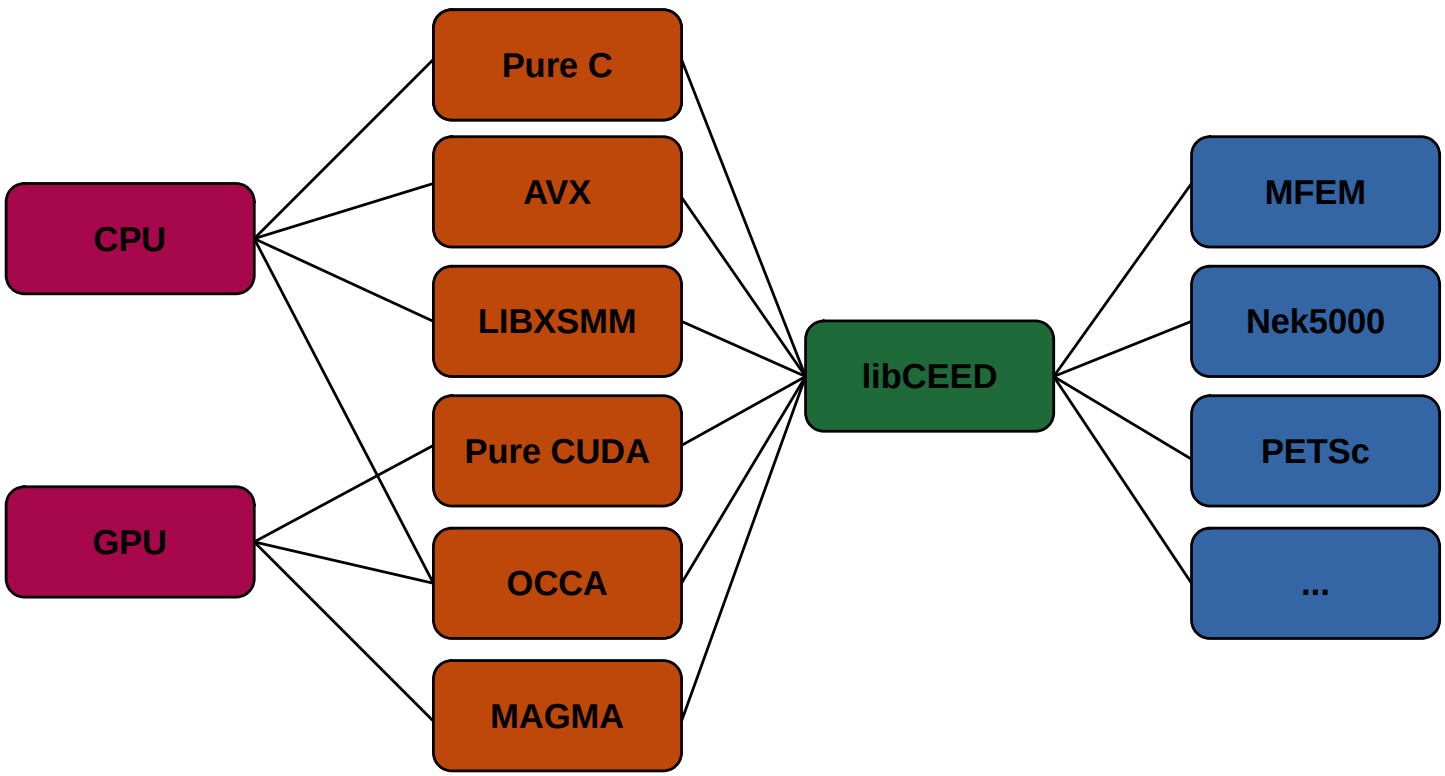
libCEED backends



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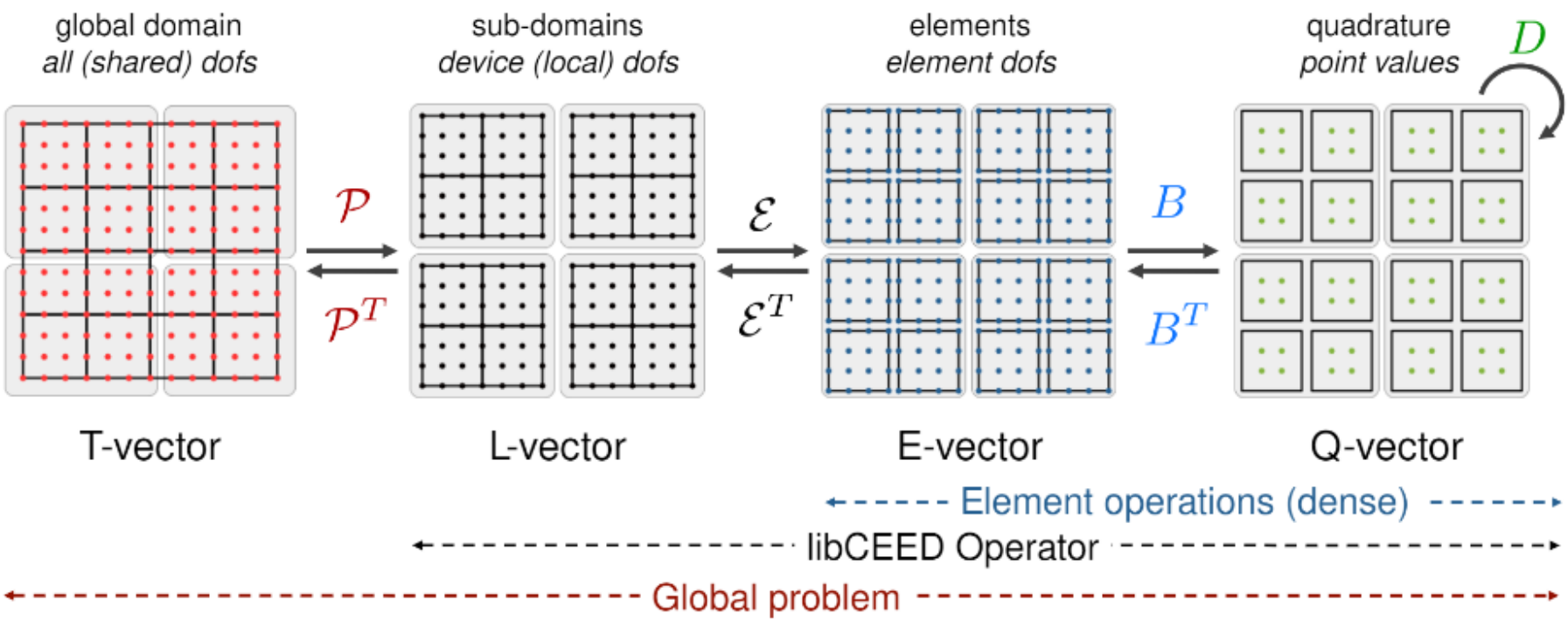
libCEED decomposition

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



Point-wise QFunctions

User-defined QFunctions:

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

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or from libCEED's Gallery:

$$\nabla \cdot (\nabla u)$$

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

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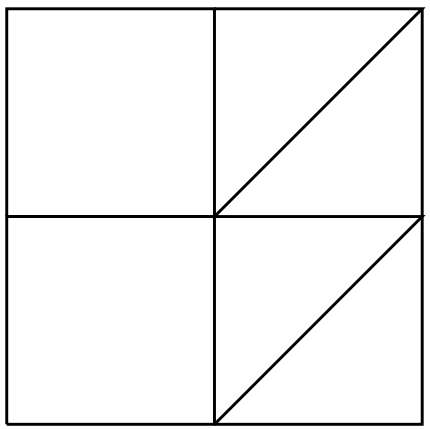

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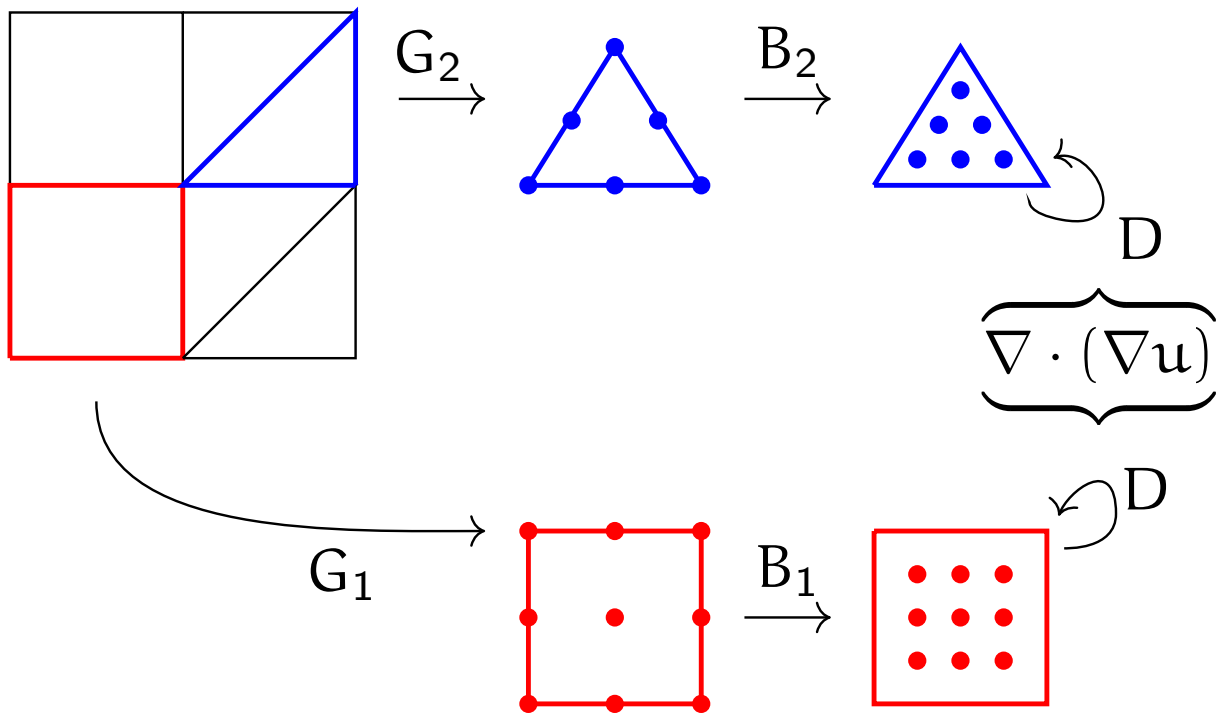
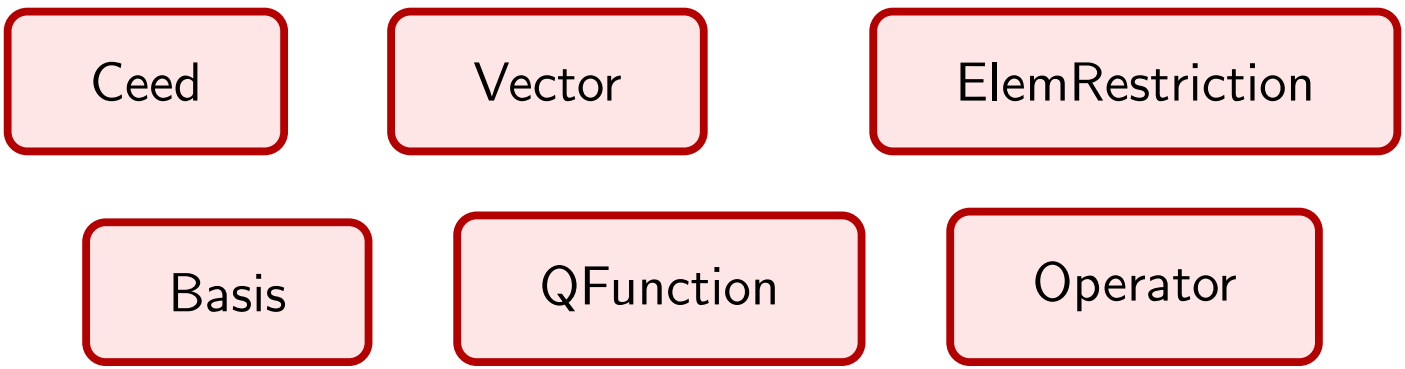


libCEED's Python interface

Classes:



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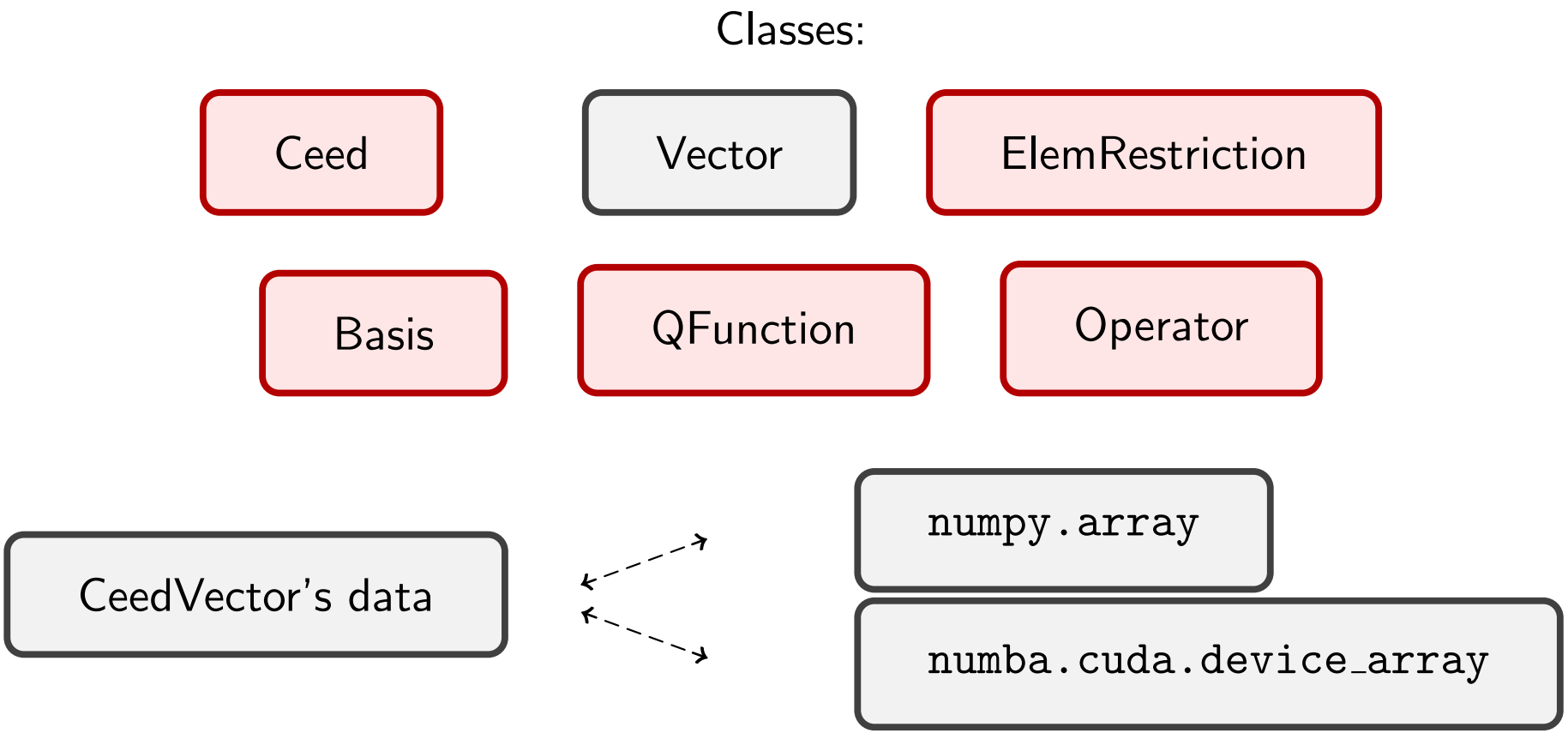
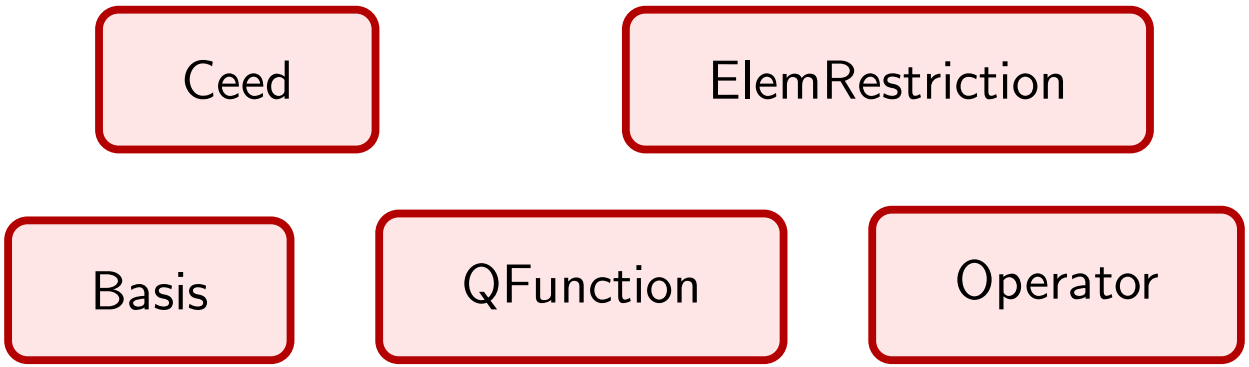


libCEED's Python interface



More details:

Barra V., Brown J., Thompson J., Dudouit Y., *High-performance operator evaluations with ease of use: libCEED's Python interface*, Proceedings of the SciPy 2020 conference (2020, July 12) url: `http://conference.scipy.org/proceedings/scipy2020/libceed-paper.html`

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Docs and tutorials

More info on our Python interface and interactive Jupyter notebook tutorials can be found at:

`https://hub.gke.mybinder.org/user/ceed-libceed-tyuu81m6/lab`

Our (very first!) user manual can be found at:

`https://libceed.readthedocs.io`

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Performance on Skylake: AVX

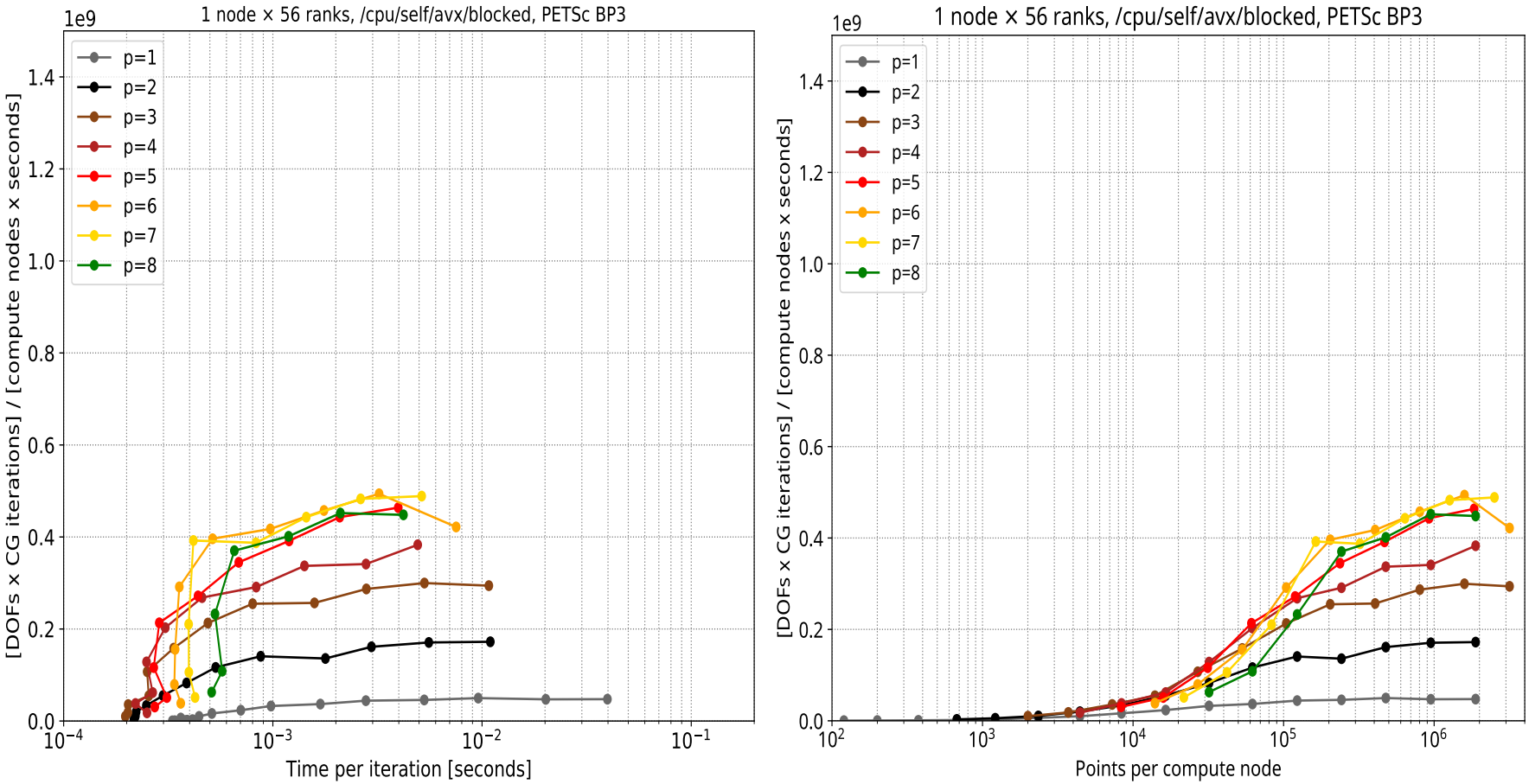

Figure: Skylake (2x Intel Xeon Platinum 8180M CPU 2.50GHz) with gcc-8 compiler. AVX blocked backend: in (a) w.r.t. time ; in (b) w.r.t. problem size ($q = P + 2$, $P = p + 1$)

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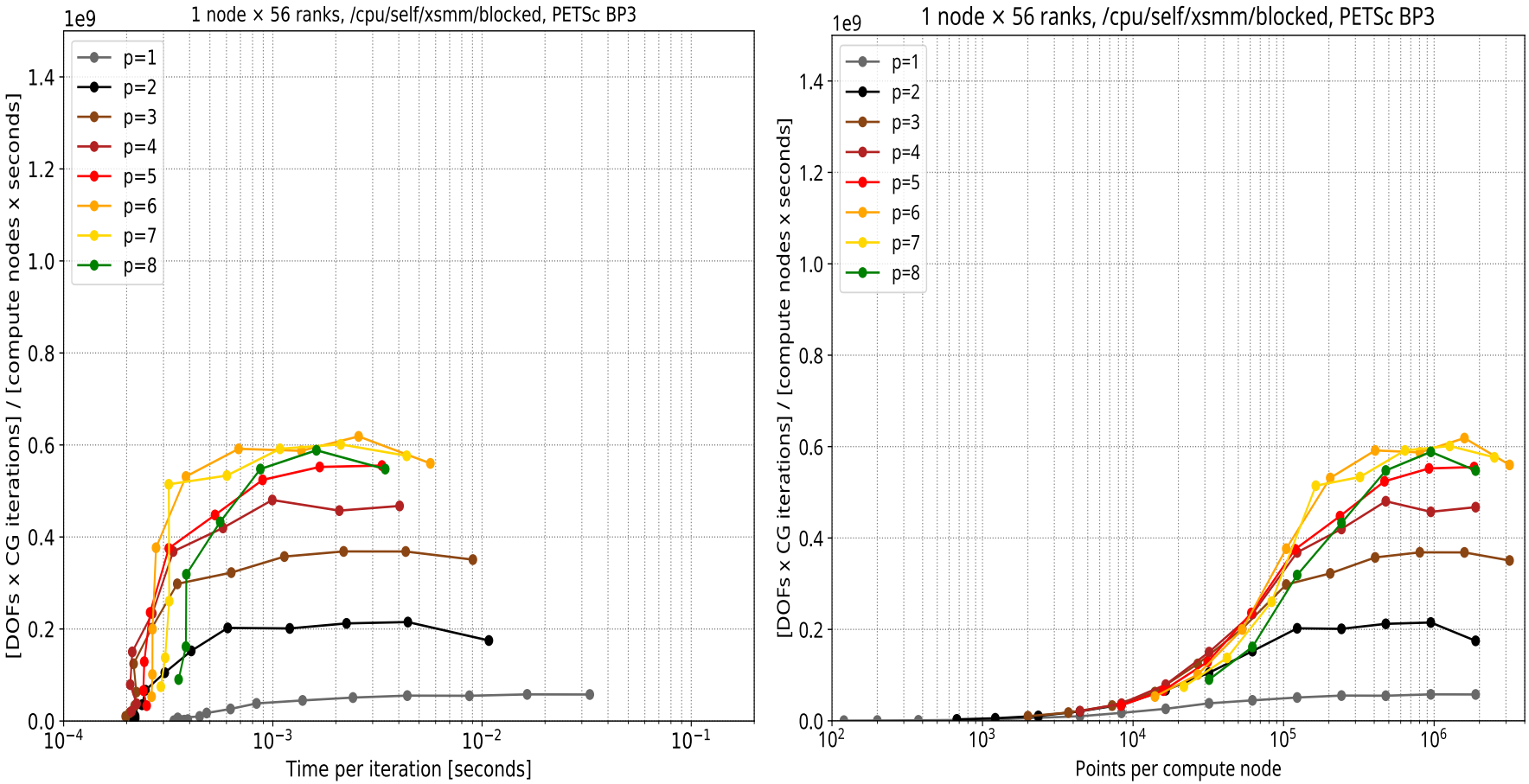
Performance on Skylake: libXSMM



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Performance on an AMD EPYC: libXSMM

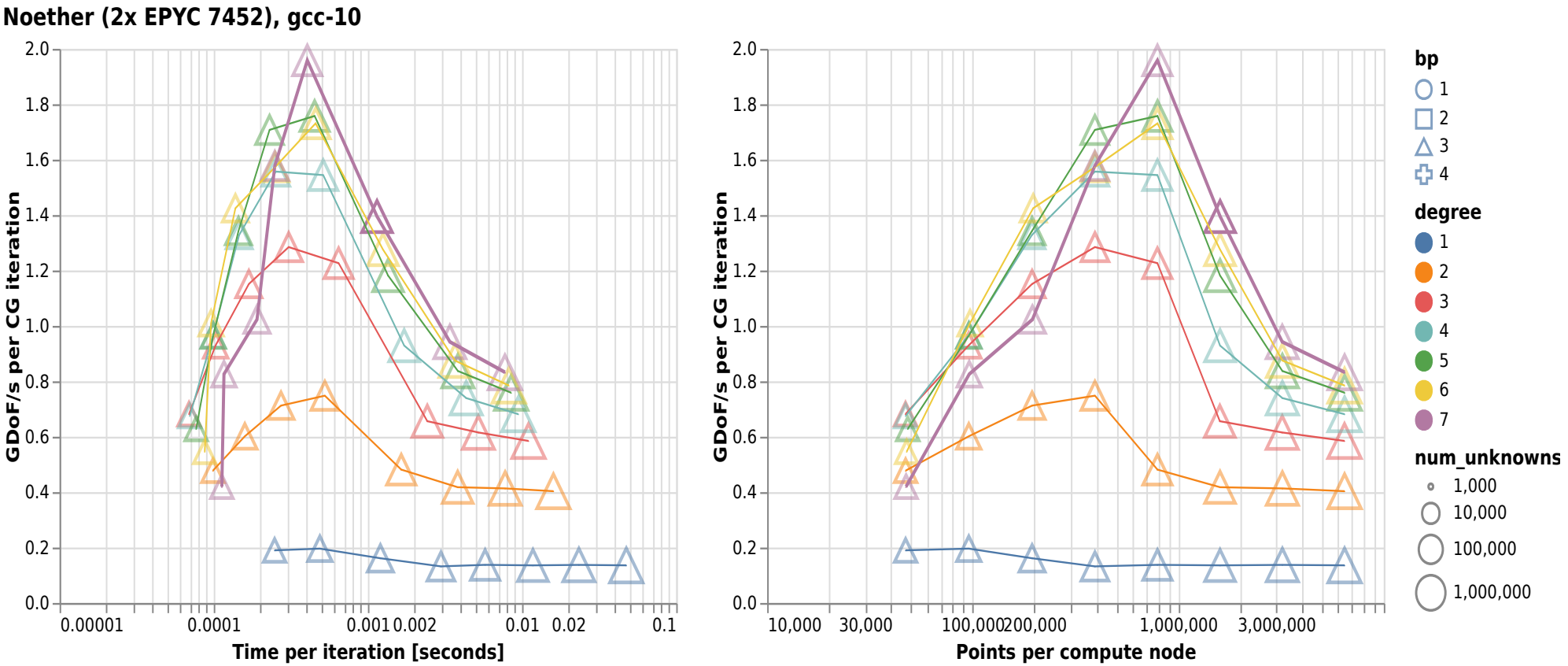

Figure: 2x AMD EPYC 7452 (32-core) with gcc-10 compiler. LIBXSMM blocked backend ($q = P + 2$, $P = p + 1$) with respect to time (left) and problem size (right)

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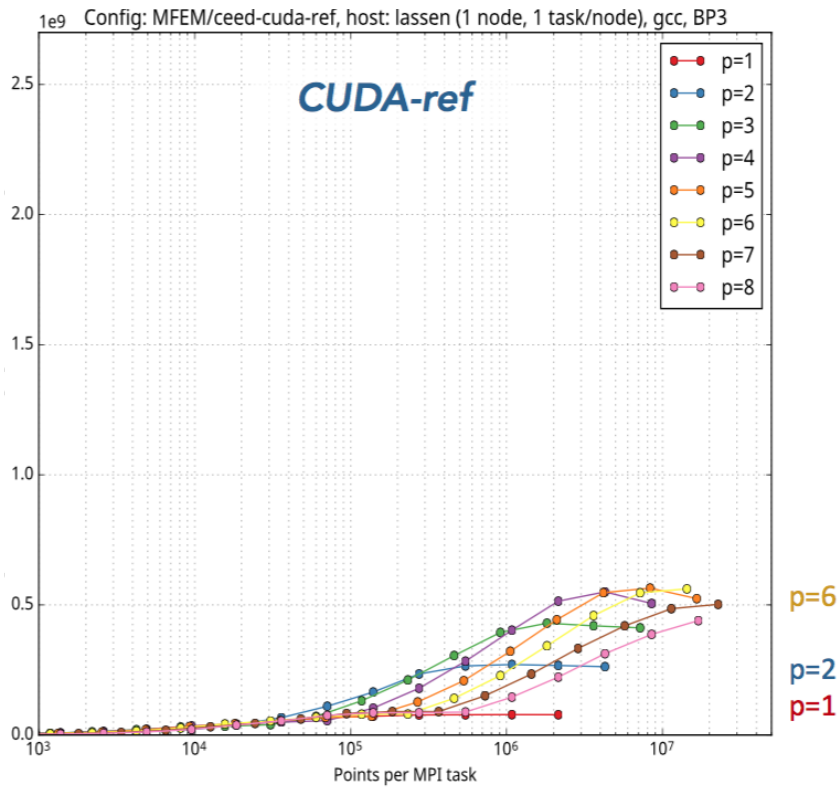
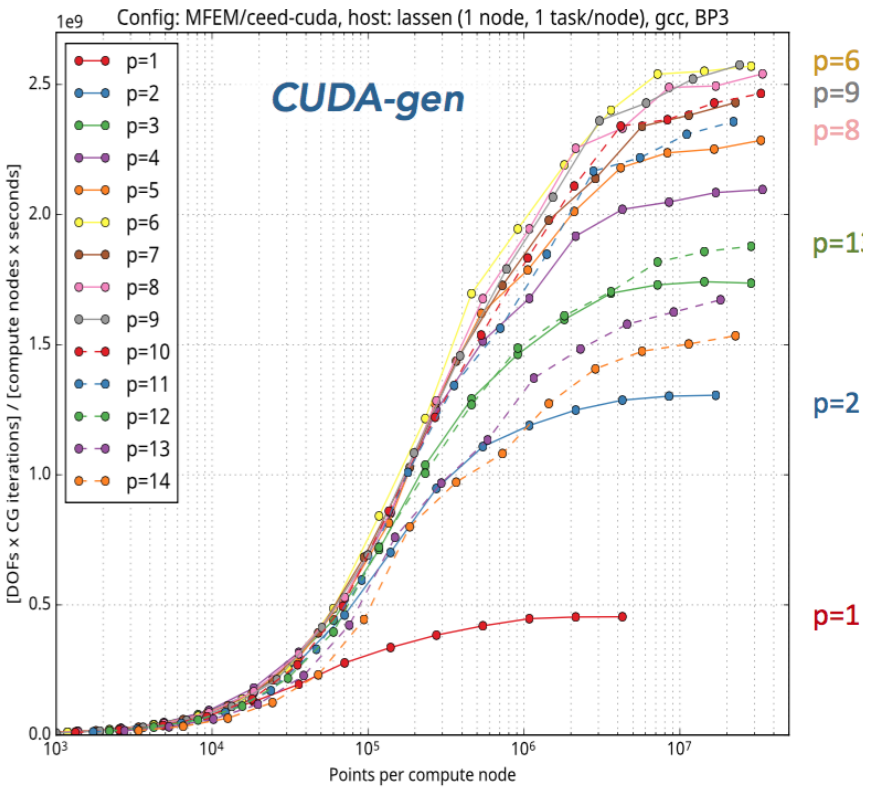
Preliminary GPU results: MFEM + libCEED





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

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A miniapp: a compressible Navier-Stokes solver

Compressible Navier-Stokes equations in conservative 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

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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 (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

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

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where

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

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

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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 $\mathbf{X} = (X, Y, Z) \in \mathbf{I} = [-1, 1]^3$.

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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 $\psi_{kji} = h_i(X) h_j(Y) h_k(Z)$.

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

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

Strong and weak formulations

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

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Weak form:

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Explicit time discretization:

$$\mathbf{q}_N^{n+1} = \mathbf{q}_N^n + \Delta t \sum_{i=1}^{s} b_i k_i\,, \tag{7}$$

adaptive Runge-Kutta-Fehlberg (RKF4-5) method

Implicit time discretization:

$$\begin{aligned} \mathbf{f}(\mathbf{q}_N) &\equiv \mathbf{g}(t^{n+1}, \mathbf{q}_N, \dot{\mathbf{q}}_N) = 0\,, \\ \dot{\mathbf{q}}_N(\mathbf{q}_N) &= \alpha\mathbf{q}_N + \mathbf{z}_N \end{aligned} \tag{8}$$

α-method

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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

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

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

where P_0 is the atmospheric pressure.

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

Density current

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

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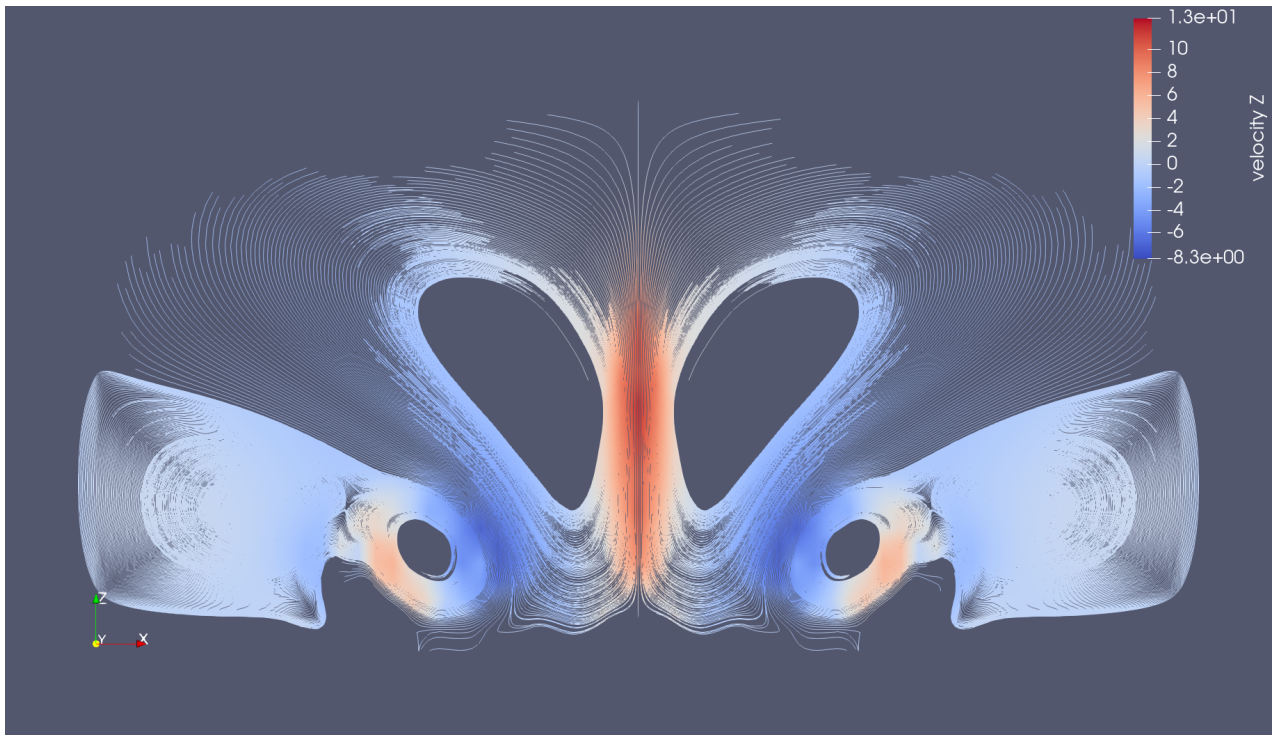
Recent Developments: Implicit time-stepping



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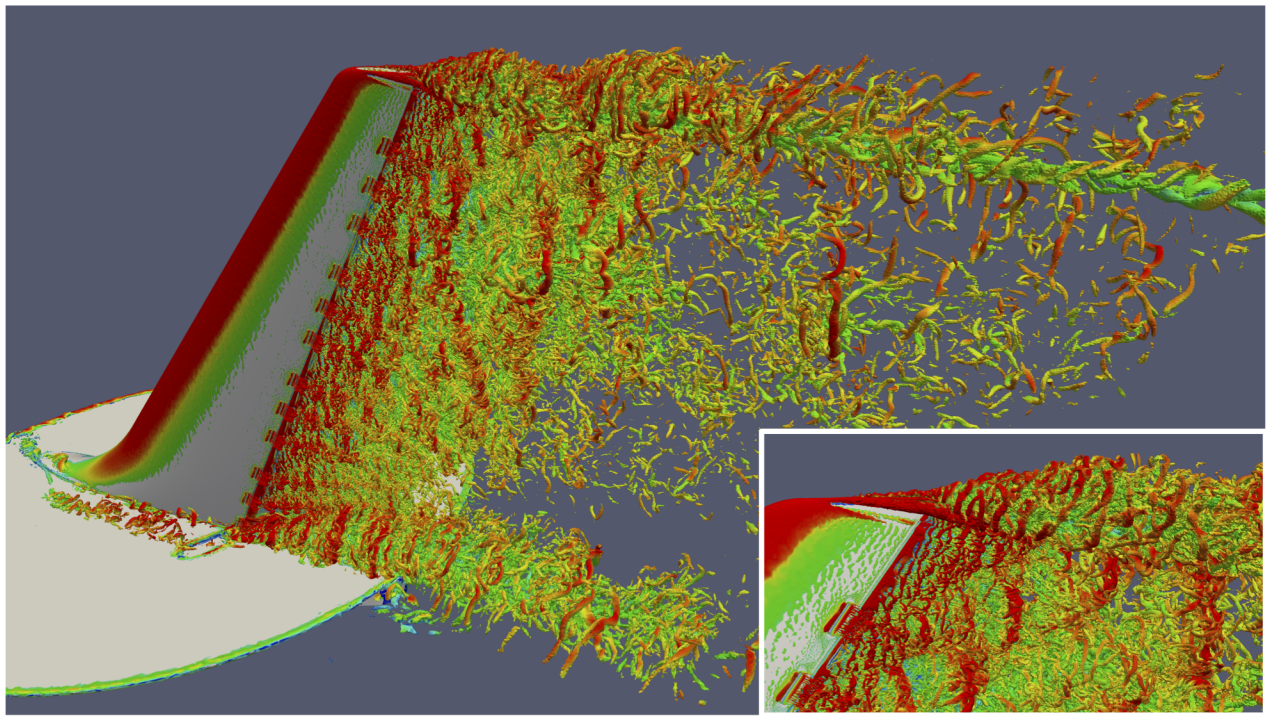
Recent Developments: PHASTA Integration

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



[Ref: `phasta.scigap.org`]

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Recent Developments: Stabilization methods

We have added Streamline Upwind (SU) and Streamline Upwind/Petrov-Galerkin (SUPG) stabilization methods to our Navier-Stokes example.

For the advection case:

Not stabilized version.

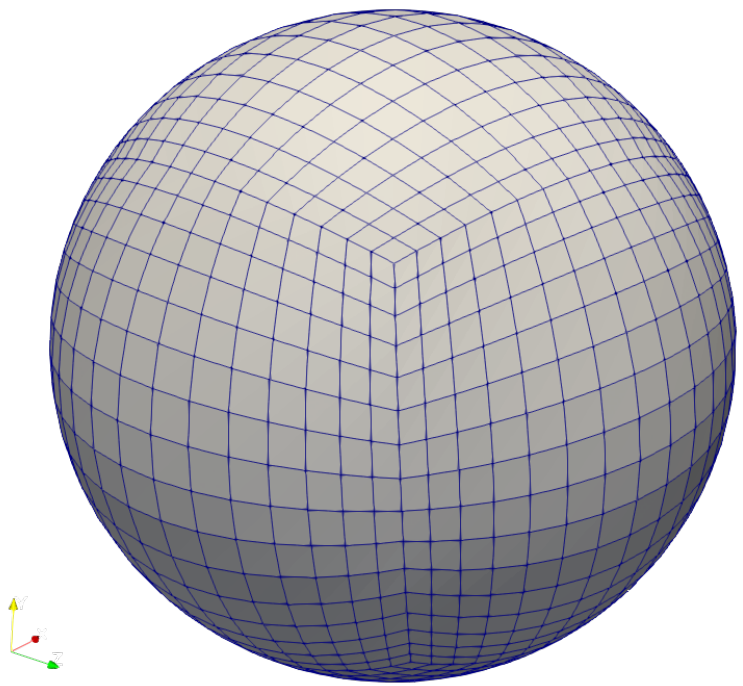
Stabilized version.

Recent Developments: BPs on the cubed-sphere

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

$$\frac{\partial \mathbf{u}}{\partial t} = -(\omega + f)\hat{k} \times \mathbf{u} - \nabla\left(\frac{1}{2}|\mathbf{u}|^2 + g(h + h_s)\right) \tag{10a}$$

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h_0 + h)\mathbf{u} \tag{10b}$$



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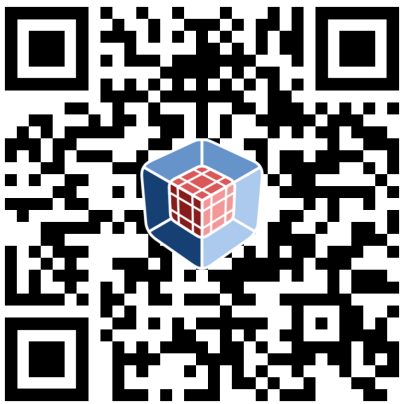
Conclusions

- 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
  - Full compressible Navier-Stokes equations
- We have included implicit time-stepping and SU/SUPG stabilization methods



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Outlook

Ongoing and future work:

- Algorithmic differentiation of Q-Functions
- Ongoing work on CUDA and HIP optimizations
- Complete SWE solver on the cubed-sphere
- We always welcome contributors and users
  `https://github.com/CEED/libCEED`

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

Thank you!

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libCEED backends

`/cpu/self/ref/*`:	with `*` reference serial and blocked 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:

$$\mathbf{B} = B \otimes B \otimes B \tag{11}$$

$$\mathbf{D}_0 = D \otimes B \otimes B \tag{12}$$

$$\mathbf{D}_1 = B \otimes D \otimes B \tag{13}$$

$$\mathbf{D}_2 = B \otimes B \otimes D \tag{14}$$

$$\mathbf{W} = W \otimes W \otimes W \tag{15}$$

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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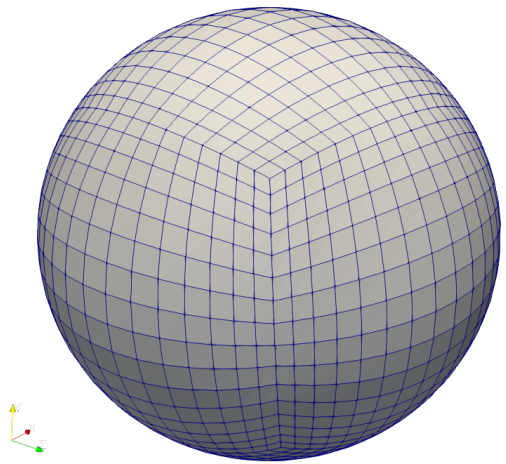
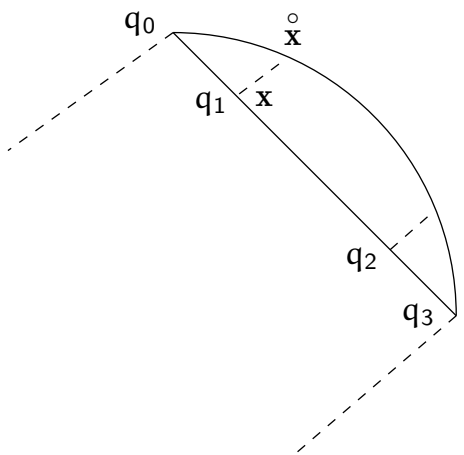
Geometry on the sphere





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

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

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

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