On Performance Portability for Unstructured High-order Finite Element Computations

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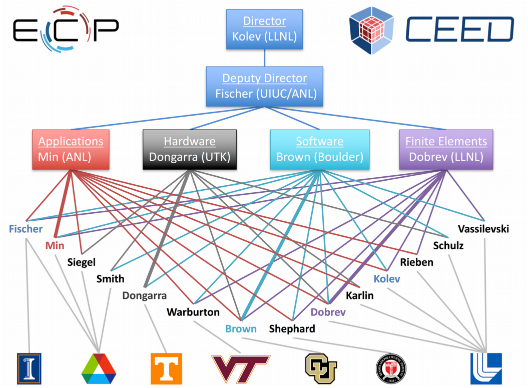
SIAM Annual Meeting, 2018-07-09

Goals & Team

- CEED is focused on the *development of next-generation discretization software and algorithms to enable efficient simulations for a wide range of science applications on future HPC systems*.
- Funding: $3.0M/year, 2 labs (LLNL, ANL), 5 universities



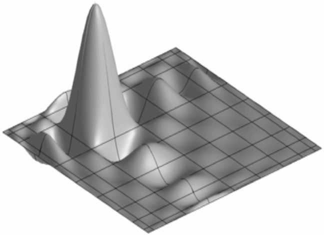
30+ researchers

EXASCALE COMPUTING PROJECT

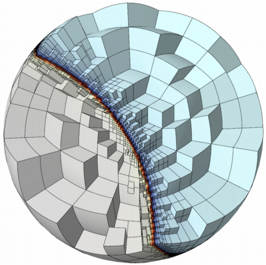
Co-design Motifs

- PDE-based simulations on **unstructured grids**
- **high-order** and **spectral** finite elements

  ✓ *any order space on any order mesh* ✓ *curved meshes,*
  ✓ *unstructured AMR* ✓ *optimized low-order support*

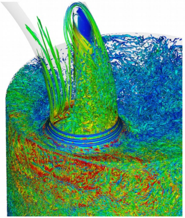


10th order basis function



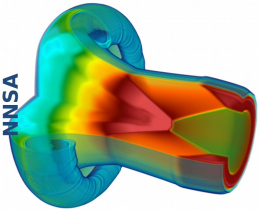
non-conforming AMR, 2nd order mesh

incompressible SEM / SC



6th order DNS turbulence (Nek)

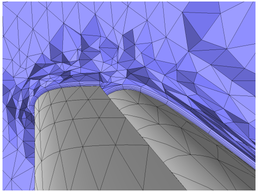
compressible FEM / NNSA



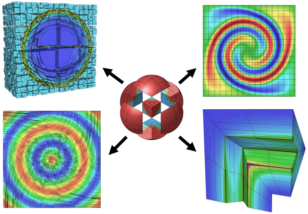
2nd order compressible shock hydro (MFEM)

High-Order Software Ecosystem

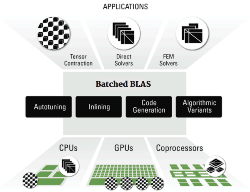
CEED
EXASCALE DISCRETIZATIONS



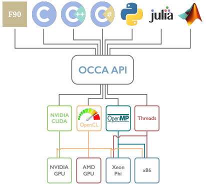
High-order Meshes



Unstructured AMR



Tensor contractions



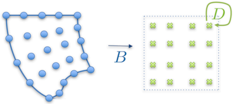
Performance portability

PETSc

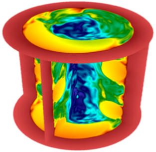
hypre
high performance preconditioners

Scalable matrix-free solvers

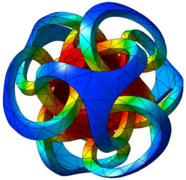
$$A = P^T G^T B^T D B G P$$



High-Order Operator Format



General Interpolation



High-Order Visualization

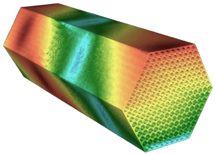
More info at: http://ceed.exascaleproject.org/fe

ECP EXASCALE COMPUTING PROJECT

CEED Software Products

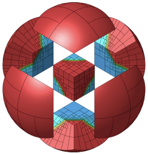
CEED's library model enables ECP apps to easily take advantage of the new discretization technologies

- state-of-the art CEED **discretization libraries**
  - ✓ *better exploit the hardware to deliver significant performance gain over conventional methods*
  - ✓ *based on MFEM/Nek, low & high-level APIs*



nek5000.mcs.anl.gov

High-performance spectral elements



mfem.org

Scalable high-order finite elements

CEED's proxies and general purpose libs target ECP vendors, STs, broader community

- **Ceedlings** - CEED kernels, bake-off probs & miniapps
  - ✓ *main tools to engage vendors & external projects*
- CEED **broadly applicable libraries**

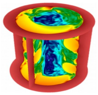
MAGMA

icl.cs.utk.edu/magma

LAPACK for GPUs, multi/many-core

libocca.org

Lightweight performance portability



GSLIB

PUMi

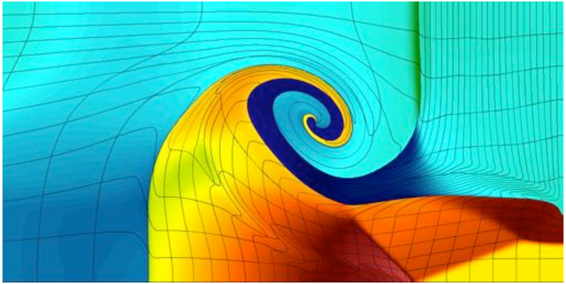
Parallel Unstructured Mesh Infrastructure

Holmes

PETSc

Main deliverable: all CEED software freely available on GitHub at https://github.com/CEED
New releases: mfem-3.3, gslib, Laghos and NekCEM ceedling, …

Applicable to variety of physics

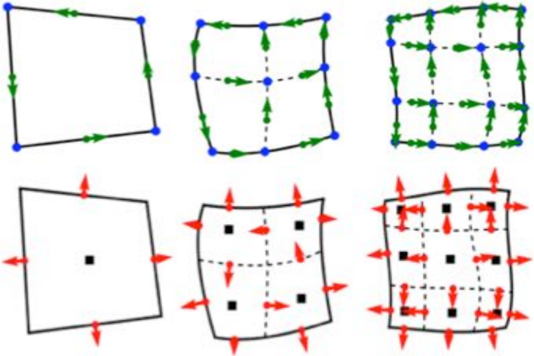


Compressible flow (ALE, 8th order)

$$H(grad) \xrightarrow{\nabla} H(curl) \xrightarrow{\nabla\times} H(div) \xrightarrow{\nabla\cdot} L_2$$

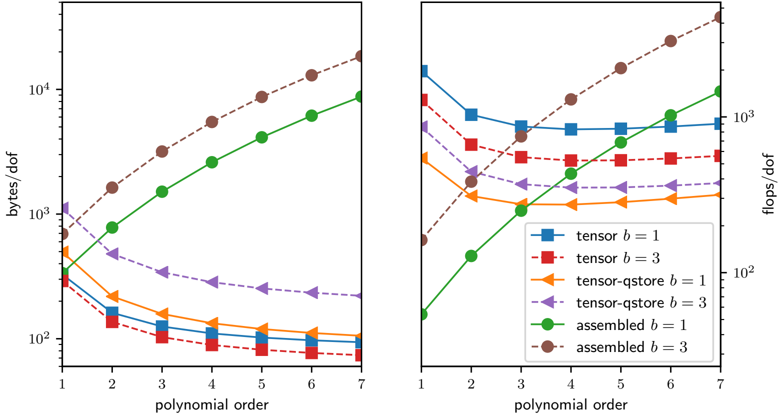
$H(grad)$	$H(curl)$	$H(div)$	L_2
“nodes”	"edges"	"faces"	"zones"
High-order kinematics	High-order MHD	High-orde rad. diff.	High-order thermodynamics

de Rham complex



Linear, quadratic and cubic finite element spaces on curved meshes

Performance of assembled versus unassembled

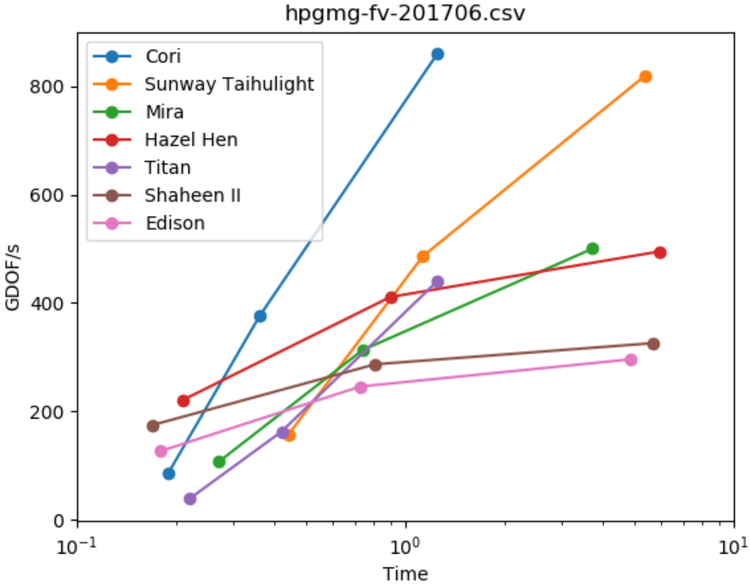


- Arithmetic intensity for Q_p elements
  - $< \frac{1}{4}$ (assembled), ≈ 10 (unassembled), ≈ 5 to 10 (hardware)
- store Jacobian information at Gauss quadrature points, can use AD

Performance versatility: $n_{1/2}$ and $t_{1/2}$

- Suppose a linear scaling algorithm
- Let $r(n)$ be the performance rate (e.g., DOF/second or GF/s) for local problem size $n = N/P$
- Let $r_{\max} = \max_n r(n)$ be the peak attainable performance
- $n_{1/2} = \min\{n : r(n) \geq \frac{1}{2} r_{\max}\}$
  - Local problem sizes $n < n_{1/2}$ will not yield acceptable efficiency
- $t_{1/2} = 2n_{1/2}/r_{\max}$
  - Time to solution less than $t_{1/2}$ is not feasible with acceptable efficiency

2017 HPGMG performance spectra



CEED Bake-Off Problems

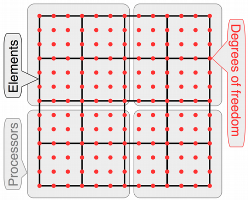
BP1: Solve {Bu=f}, where {B} is the mass matrix.

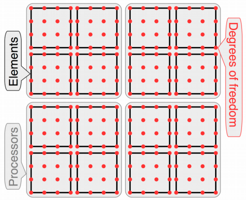
BP2: Solve the vector system $\{Bu_i=f_i\}$ with {B} from BP1.

BP3: Solve {Au=f}, where {A} is the Poisson operator.

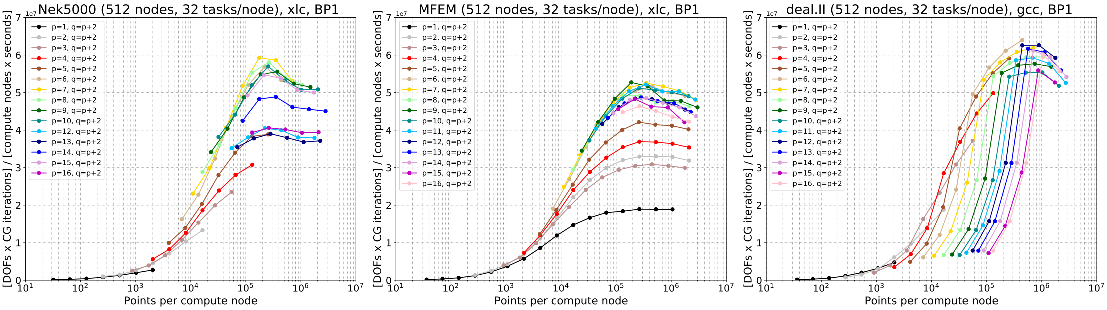
BP4: Solve the vector system $\{Au_i=f_i\}$ with {A} from BP3.

- Range of polynomial orders: {p=1, 2,...,8}, at least.
- Cover range of sizes: from 1 element/MPI rank up to the memory limit.
- BP1 and BP2 are relevant for many hyperbolic substeps in transport problems. BP3 and BP4 reflect pressure, momentum, and diffusion updates in fluid/thermal transport.
- Vector forms BP2 and BP4 reveal benefits of increased *data reuse* and of *amortized communication overhead.*
- Benchmark repo: https://github.com/CEED/benchmarks





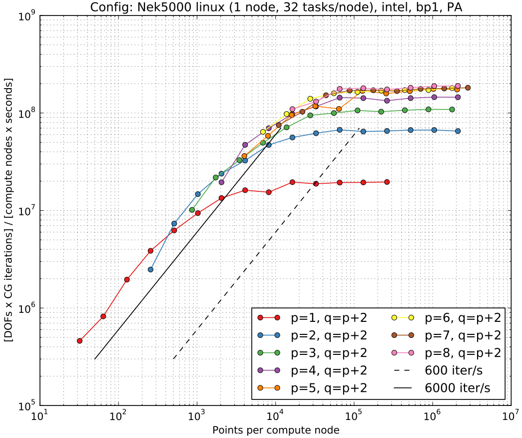
BP terminology: T- and E-vectors of HO dofs

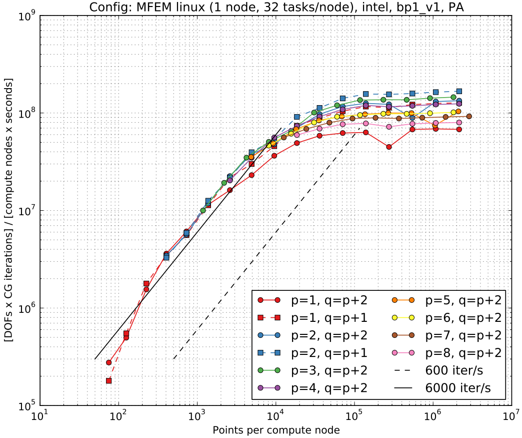


(a) BP1 Nek5000 (b) BP1 MFEM (c) BP1 deal.II

Figure: BP1 results of Nek5000 (left), MFEM (center), and deal.ii (right) on BG/Q with varying polynomial order ($p = 1, \ldots, 16$) with the number of quadrature points ($q = p + 2$). The number cpu cores $P = 8,192$.

BP1 on KNL: Nek5000 and MFEM





Nek5000 $n_{1/2} = 15k, t_{1/2} = 150\mu s$

MFEM $n_{1/2} = 10k, t_{1/2} = 400\mu s$

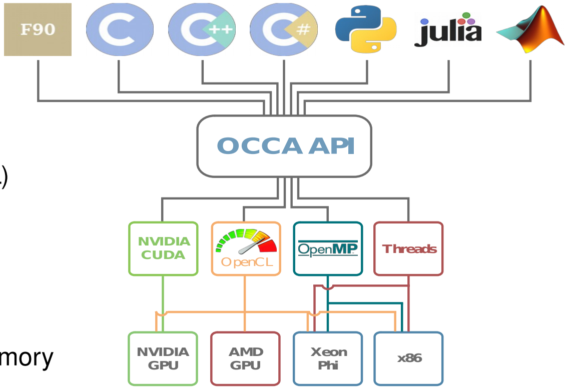
- BG/Q has similar performance

Lightweight Performance Portability

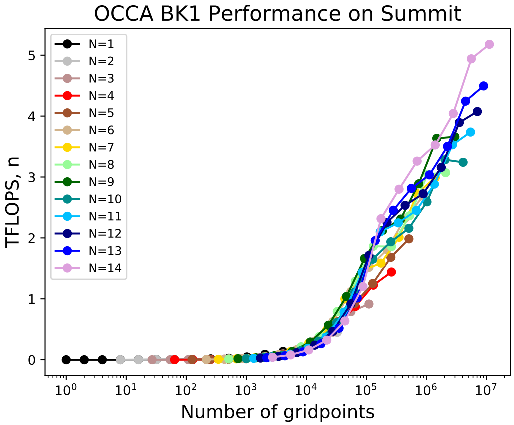
CEED/OCCA is an open-source library that provides an unified API for programming different types of devices, including CPUs, GPUs, Intel's Xeon Phi, FPGAs.

Features:

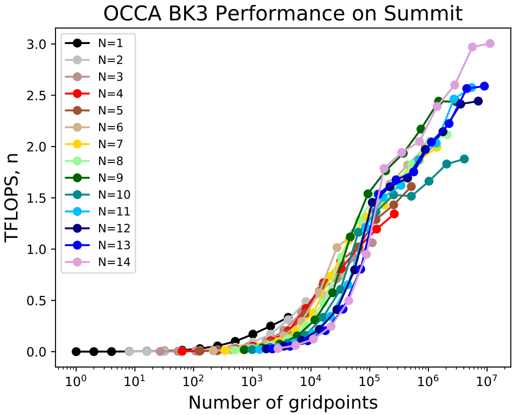
- Supported on many languages, such as C++, C, and Fortran
- *JIT compilation for kernels*
- Single kernel language for all backends (OKL)
- Currently supports Serial, OpenMP, CUDA, and OpenCL backends. Works with MPI
- MIT License, http://www.libocca.org
- Extensible backend API, allowing for future features. For example, support for unified memory in CUDA and mapped memory in OpenCL



OCCA performance on Summit (V100)



(a) BK1 Summit



(b) BK3 Summit

Figure: BK1 and BK3 V100 performance: TFLOPS versus problem size n for different polynomial orders, N. Operating on E-vectors (does not include element restriction $\mathscr{E}, \mathscr{E}^T$)

Batched Computing Technology

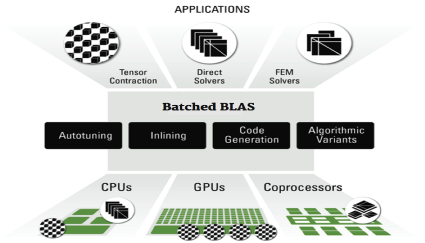
- Matrix-free basis evaluation needs efficient tensor contractions, e.g.,

$$C_{i1,i2,i3} = \sum_k A_{k,i1} B_{k,i2,i3}$$

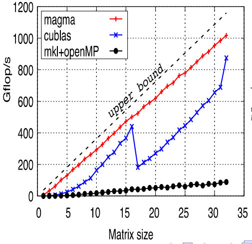
- **CEED/MAGMA** designed batched methods to split the computation in many small high-intensity GEMMs, grouped together (batched) for efficient execution:

Batch_{ $C_{i3} = A^T B_{i3}$, for range of i3 }

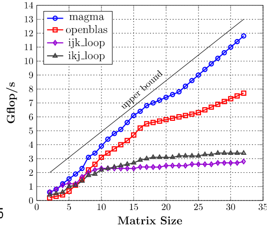
- Developed techniques needed for autotuning, code inlining, code generation (reshapes, etc.), algorithmic variants for different architectures.
- Achieve 90+% of theoretically derived peaks.
- Significantly outperform vendor libraries.
- Released through MAGMA.



Batched DGEMMs on GPU (P100, 100K)

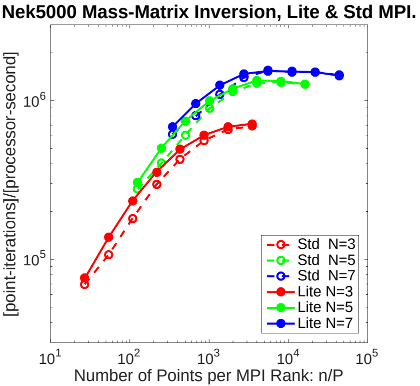


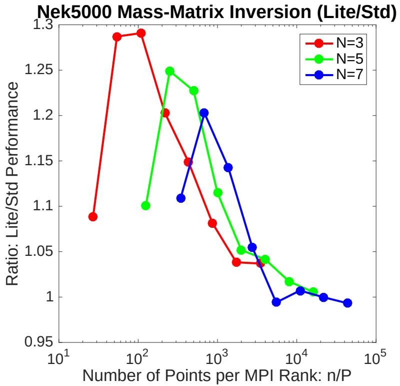
Batched DGEMMs on ARM (Tegra X1 : 4-core Cortex A57)



MPICH CH4: lightweight device layer

- CH4: faster offload, better fast path/inlining/IPO





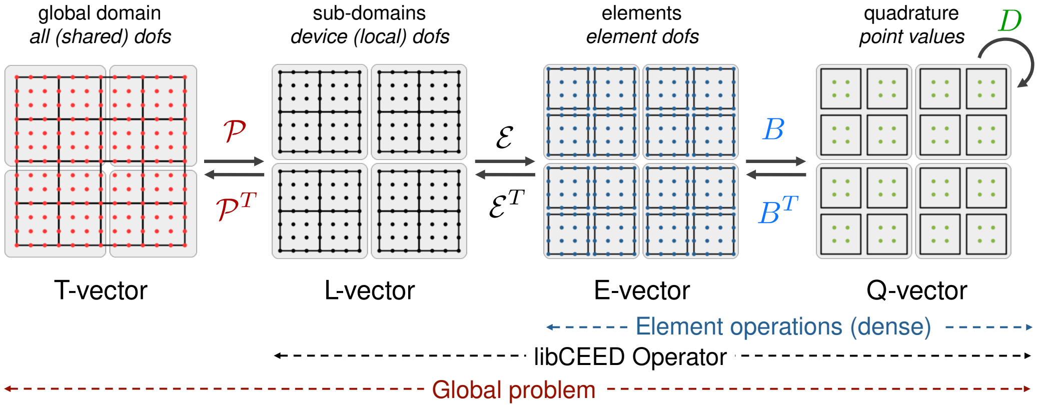
libCEED: Code for Efficient Extensible Discretization

- BSD-2 license, C library with Fortran interface
- Releases: v0.1 (January), v0.2 (March), v0.3 (imminent)
- Purely algebraic interface
- Extensible backends
  - CPU: reference, vectorized
  - OCCA (just-in-time compilation): CPU, OpenMP, OpenCL, CUDA
  - MAGMA
- Platform for collaboration with vendors
- Minimal assumptions about execution environment, parallel decomposition
- Primary target: high order finite element methods
  - $H^1, H(\mathrm{div}), H(\mathrm{curl})$
  - also of interest to spectral difference, etc.
  - Exploit tensor product structure when possible

ECP EXASCALE COMPUTING PROJECT

CEED EXASCALE DISCRETIZATIONS

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



Quadrature Function

$$v^T F(u) \sim \int_\Omega v \cdot f_0(u, \nabla u) + \nabla v : f_1(u, \nabla u) \qquad v^T J w \sim \int_\Omega \begin{bmatrix} v \\ \nabla v \end{bmatrix}^T \begin{bmatrix} f_{0,0} & f_{0,1} \\ f_{1,0} & f_{1,1} \end{bmatrix} \begin{bmatrix} w \\ \nabla w \end{bmatrix}$$

$$u_e = B \mathcal{E}_e u \qquad \nabla u_e = \frac{\partial X}{\partial x} B_\nabla \mathcal{E}_e u$$

$$J w = \sum_e \mathcal{E}_e^T \begin{bmatrix} B \\ B_\nabla \end{bmatrix}^T \underbrace{\begin{bmatrix} I & \\ & \left(\frac{\partial X}{\partial x}\right)^T \end{bmatrix} W_q \begin{bmatrix} f_{0,0} & f_{0,1} \\ f_{1,0} & f_{1,1} \end{bmatrix} \begin{bmatrix} I & \\ & \left(\frac{\partial X}{\partial x}\right) \end{bmatrix}}_{\text{coefficients at quadrature points}} \begin{bmatrix} B \\ B_\nabla \end{bmatrix} \mathcal{E}_e w$$

- B and B_∇ are tensor contractions – independent of element geometry
- Choice of how to order and represent gathers $\mathcal{E}$ and scatters $\mathcal{E}^T$
- Who computes the metric terms and other coefficients?
- Similar for Neumann/Robin and nonlinear boundary conditions

Quadrature Functions

- Multiple inputs and outputs
- Independent operations at each of `Q` quadrature points
- Ordering and number of elements not specified

```c
int L2residual(void *ctx, CeedInt Q,
               const CeedScalar *const in[],
               CeedScalar *const out[]) {
  const CeedScalar *u = in[0], *rho = in[1], *target = in[2];
  CeedScalar *v = out[0];
  for (CeedInt i=0; i<Q; i++)
    v[i] = rho[i] * (u[i] - target[i]);
  return 0;
}
```

Element restriction $\mathcal{E}_e$

- Conforming homogeneous mesh: boolean matrix with homogeneous block size
- Non-conforming mesh: anchored rows have linear combination
- Nek5000-style E-vector: indexed identity
- libCEED backends are allowed to reorder, compress, etc.
- May be applied all at once or in batches

libCEED Operator

$$A = \mathscr{P}^T \underbrace{\mathscr{E}^T B D B \mathscr{E}}_{\text{CeedOperator}} \mathscr{P}$$

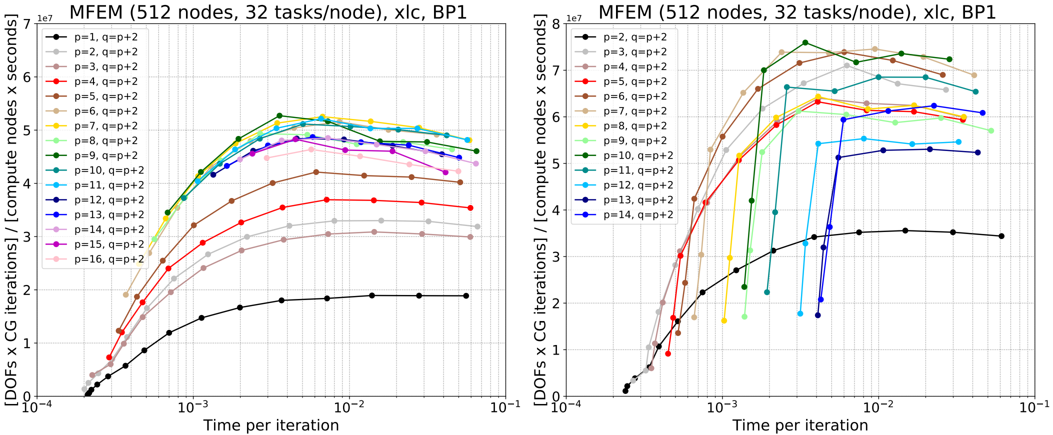
- element restriction $\mathscr{E}$, basis B, quadrature function D

```
CeedOperatorCreate(ceed, qf_L2residual, &op);
CeedOperatorSetField(op, "u", E, Basis, CEED_VECTOR_ACTIVE);
CeedOperatorSetField(op, "rho", CEED_RESTRICTION_IDENTITY,
                     CEED_BASIS_COLOCATED, rho);
CeedOperatorSetField(op, "target", CEED_RESTRICTION_IDENTITY,
                     CEED_BASIS_COLOCATED, target);
CeedOperatorSetField(op, "v", E, Basis, CEED_VECTOR_ACTIVE);
```

Vectorization techniques

- Vectorize within a single high-order element
  - Minimal working set (as small as one element)
  - Specialized implementation for different degree/# quadrature points
  - Hard to avoid cross-lane operations at modest degree
  - Nek5000
- Vectorize across elements in batches `[i,j,k,e]`
  - Working set has at least vector length number of elements (e.g., 8)
  - Generic implementation is easy to optimize; no cross-lane operations
  - HPGMG-FE, Deal.II (Kronbichler and Kormann), MFEM (new)

MFEM vectorization performance



(a) Cetus internal vectorization

(b) Cetus external vectorization

Figure: Internal versus external element vectorization for BP1.

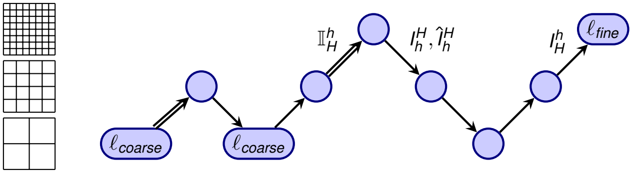
HPGMG: a benchmark for supercomputers

- `https://hpgmg.org`
- Mark Adams, Sam Williams (finite-volume), Jed (finite-element), John Shalf, Brian Van Straalen, Erich Strohmeier, Rich Vuduc
- Annual BoFs at Supercomputing since 2014
- Implementations

  Finite Volume memory bandwidth intensive, simple data dependencies, 4th order

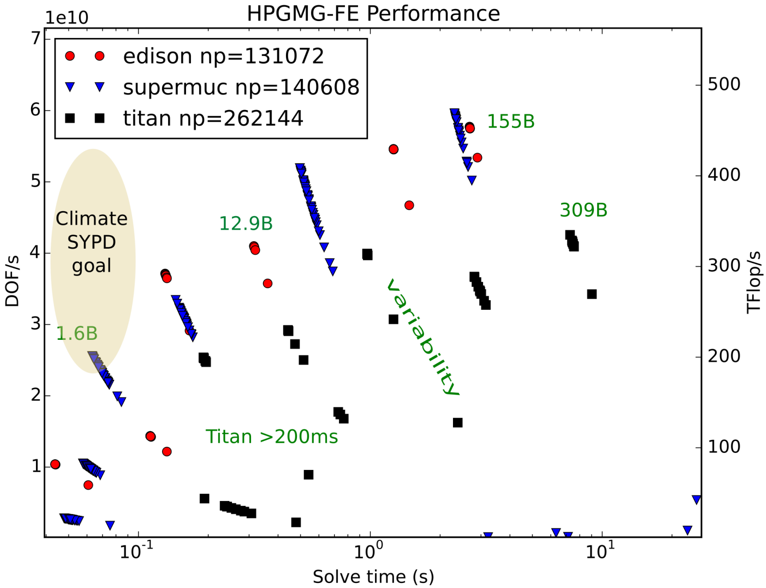
  Finite Element compute- and cache-intensive, vectorizes, overlapping writes
- Full multigrid, well-defined, scale-free problem
- Matrix-free operators, Chebyshev smoothers

Full Multigrid (FMG): Prototypical Fast Algorithm



- start with coarse grid
- truncation error within one cycle
- about five work units for many problems
- no “fat” left to trim – robust to gaming
- distributed memory – restrict active process set using Z-order
  - $\mathcal{O}(\log^2 N)$ parallel complexity stresses network
- scale-free specification
  - no mathematical reward for decomposition granularity
  - don’t have to adjudicate “subdomain”

HPGMG-FE on Edison, SuperMUC, Titan



Outlook

- libCEED is interested in contributors and friendly users
- GPU performance optimizations in progress
- Cache versus vectorization tradeoffs
  - Backends should automatically choose internal versus external vectorization
  - Choice depends on architecture, element size, number of fields
- Throughput versus latency optimizations
- Even/odd performance optimization
- Incorporate algorithmic differentiation
- Developing exchange/storage interfaces for high-order fields
- Many other activities to improve high order ecosystem