Library Interface Design and Performance Portability

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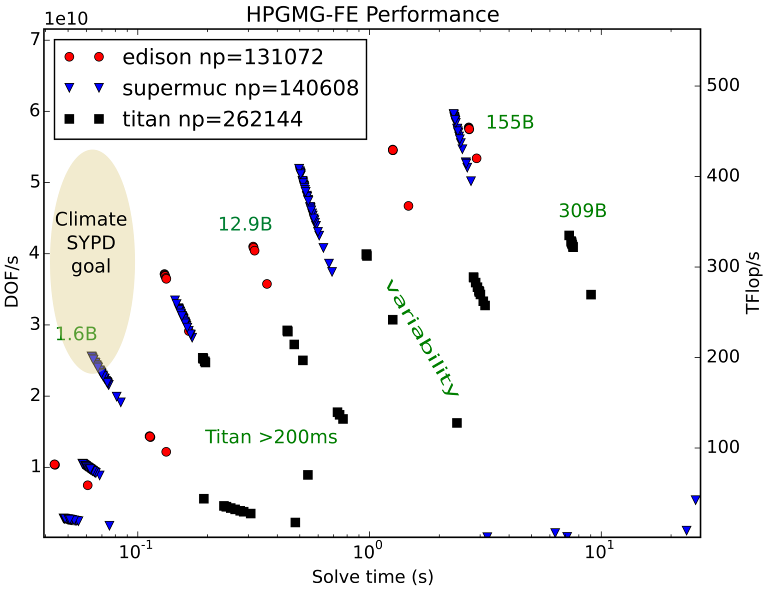
This talk: `https://jedbrown.org/files/20190225-PerfPortability.pdf`

What is performance portability?

- Performs well across range of architectures and problem configurations with modest development and maintenance effort.
- All architectures require massive parallelism
  - 28-core Xeon: dual-issue FMA with 16-lane registers, 6-cycle latency: 5376 in-flight flops
  - About 4x more for V100
- Architectural differences
  - Persistent cache on CPU, big register space on GPU
  - Programming model expression of coalesced loads (e.g., CUDA vs OpenMP/OpenACC)
  - Tolerance for lane divergence (SIMT versus masked SIMD); what does compiler need to know/use?
- Problem configurations: time to solution requirements (problem sizes)
  - constitutive models, etc.

HPGMG-FE on Edison, SuperMUC, Titan

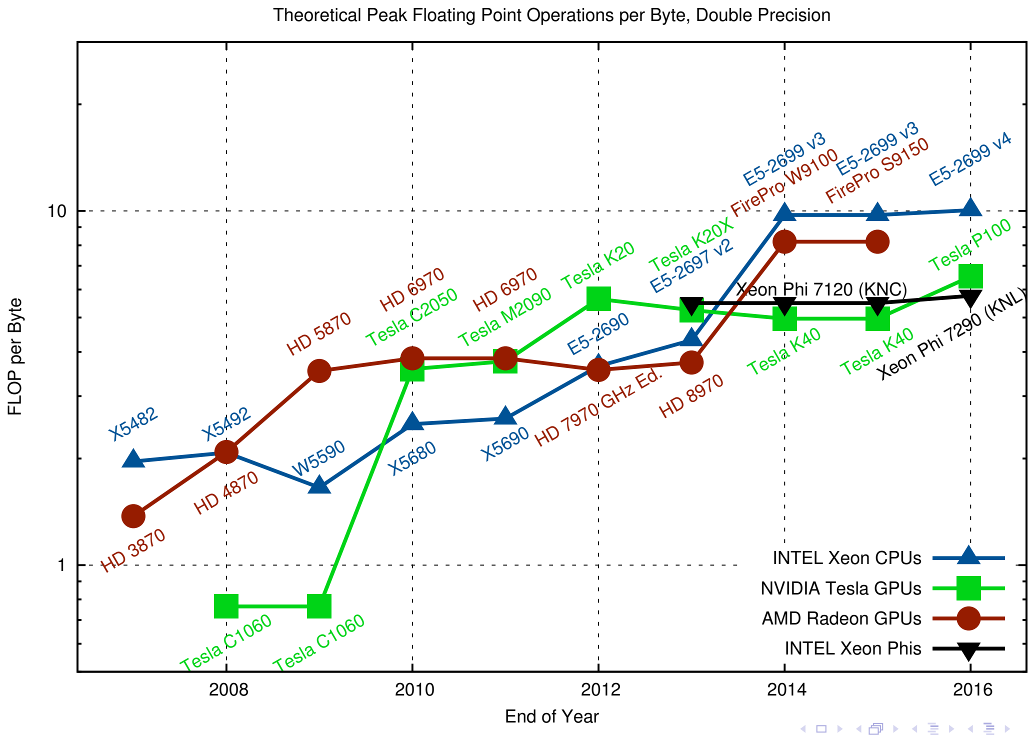


Modest development and maintenance effort

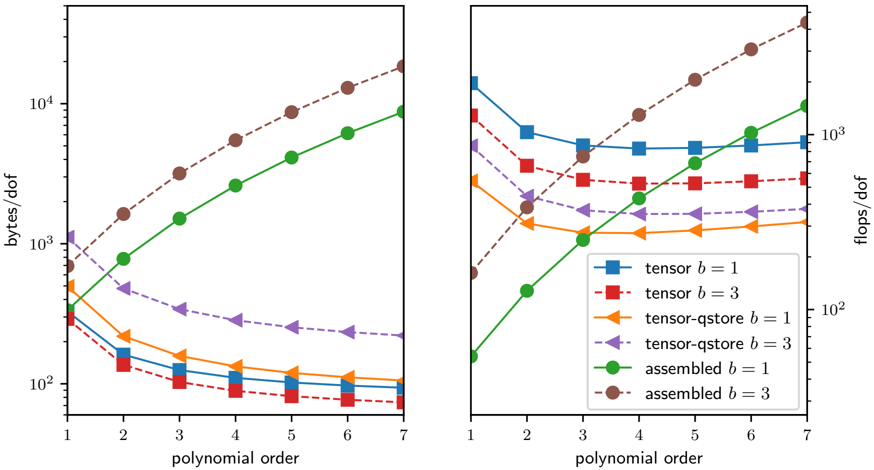
- Some custom code may be needed; how to leverage?
- Granularity of extensibility
  - BLAS/LAPACK: Users compose large dense linear algebraic operations
  - BLIS: Users implement packing schemes; reuse “microkernel”
  - Users implement different PDE, discretization, and constitutive models
  - FEniCS: domain-specific language for finite element
- Maintenance
  - Interface stability for the extensible parts
  - Ability to rapidly affect “infrastructure” (turtles all the way down?)

Approaches

Type of software	Expressive	Interoperable/Environment	Contributors	New architecture	Packaging/Distribution
Library (LAPACK, FFTW, BLIS @MS129 ↓)	$-$	$+$	$+$	0	$+$
Dynamic/extensible Library (libCEED)	0	$+$	$+$	plugin	if stable ABI
Template Library (Kokkos @MS129)	0	0	0	$+$	recompile
DSL/code generation/JIT (Firedrake)	$+$	$-$	0	$+$	?
New Language (Chapel)	$+$	$-$	$-$	?	?


Theoretical Peak Floating Point Operations per Byte, Double Precision
FLOP per Byte
End of Year
10
1
2008
2010
2012
2014
2016
X5482
X5492
W5590
X5680
X5690
E5-2690
E5-2697 v2
E5-2699 v3
E5-2699 v3
E5-2699 v4
HD 3870
HD 4870
HD 5870
HD 6970
HD 6970
HD 7970 GHz Ed.
HD 8970
FirePro W9100
FirePro S9150
Tesla C1060
Tesla C1060
Tesla C2050
Tesla M2090
Tesla K20
Tesla K20X
Tesla K40
Tesla K40
Tesla P100
Xeon Phi 7120 (KNC)
Xeon Phi 7290 (KNL)
INTEL Xeon CPUs
NVIDIA Tesla GPUs
AMD Radeon GPUs
INTEL Xeon Phis

Performance of assembled versus unassembled

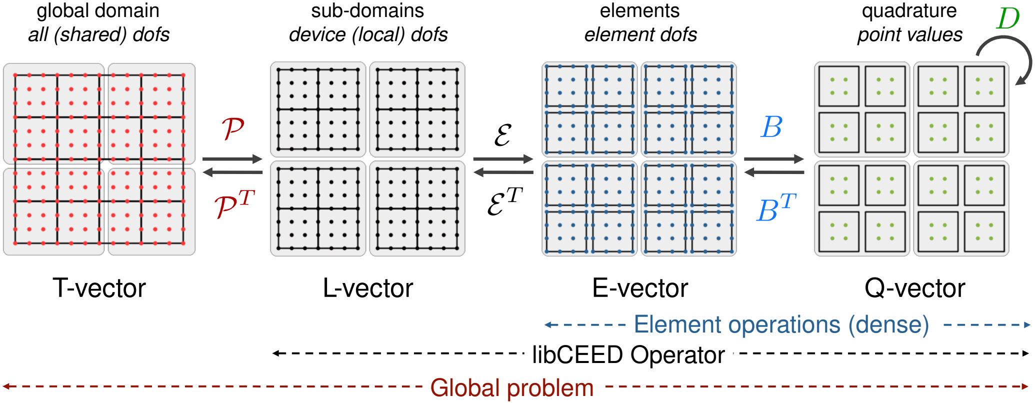


- Arithmetic intensity for Q_p elements
  - $< \frac{1}{4}$ (assembled), ≈ 10 (unassembled), ≈ 5 to 10 (hardware)
- store Jacobian information at Gauss quadrature points, can use AD

libCEED: Code for Efficient Extensible Discretization

- BSD-2 license, C library with Fortran interface
- Releases: v0.1 — v0.3 (2018); v0.4 to be released in March
- Purely algebraic interface
- Extensible backends
  - CPU: reference, blocked/vectorized, libXSMM
  - OCCA (just-in-time compilation): CPU, OpenMP, OpenCL, CUDA
  - MAGMA
  - CUDA using NVRTC (Steven Roberts & Yohann Dudouit, to be merged soon)
- 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

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



Quadrature Function

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

$$u = B_I \mathscr{E}_e u_L \qquad \nabla u = \frac{\partial X}{\partial x} B_\nabla \mathscr{E}_e u_L$$

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

- B and B_∇ are tensor contractions – independent of element geometry
- Choice of how to order and represent gathers $\mathscr{E}$ and scatters $\mathscr{E}^T$
- 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

```
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];
  #pragma omp simd
  for (CeedInt i=0; i<Q; i++)
    v[i] = rho[i] * (u[i] - target[i]);
  return 0;
}
CeedQFunctionAddInput(qf, "u", 1, CEED_EVAL_INTERP);
CeedQFunctionAddInput(qf, "rho", 1, CEED_EVAL_INTERP);
CeedQFunctionAddInput(qf, "target", 1, CEED_EVAL_INTERP);
CeedQFunctionAddOutput(qf, "v", 1, CEED_EVAL_INTERP);
```

Building Operators

$$v^T F(u) \sim \int_\Omega v \cdot f_0(u, \nabla u) + \nabla v : f_1(u, \nabla u)$$

$$u = B_I \mathcal{E}_e u_L \quad \nabla u = \frac{\partial X}{\partial x} B_\nabla \mathcal{E}_e u_L$$

- `CeedOperatorCreate(ceed,` f`, &op);`
- `CeedOperatorSetField(op, "velocity",` $\mathcal{E}$`,` B`,` u_L`);`
- Apply: implementation handles batching, work buffers, and calling $f(u, \nabla u)$.
- User links to interface library
- Backend implementation switchable at run-time
- Two-phase implementation enables connectivity analysis and JIT

libCEED Operator

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

- quadrature function D
- For each field: element restriction $\mathscr{E}$, basis B, where to find vector

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

CeedOperatorApply(op, u, v, &request);
```

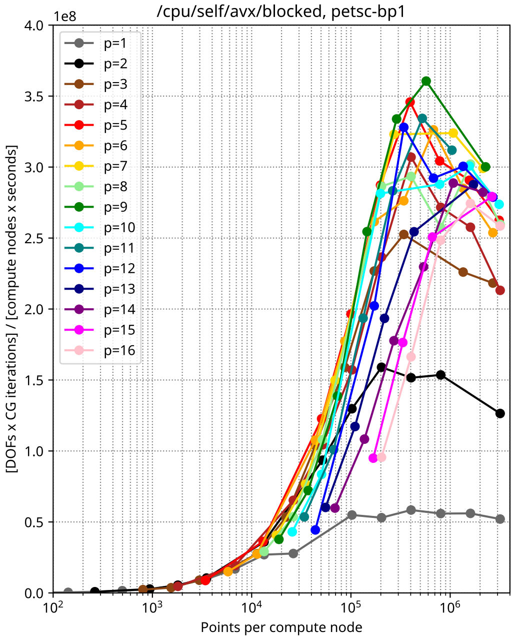
Element restriction $\mathcal{E}_e$

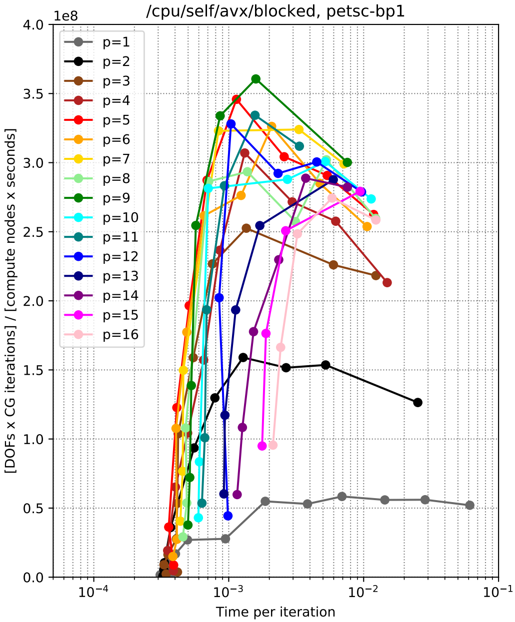
- Conforming homogeneous mesh: boolean matrix with homogeneous block size
- Non-conforming mesh: anchored rows have linear combination
- Nek5000/DG-style E-vector: indexed identity
- libCEED backends are allowed to reorder, compress, etc.
- May be applied all at once or in batches
- CeedOperator implementation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

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
- $t_{1/2} = 2 n_{1/2} / r_{\max}$
  - Time to solution less than $t_{1/2}$ is not feasible with acceptable efficiency

Performance spectra

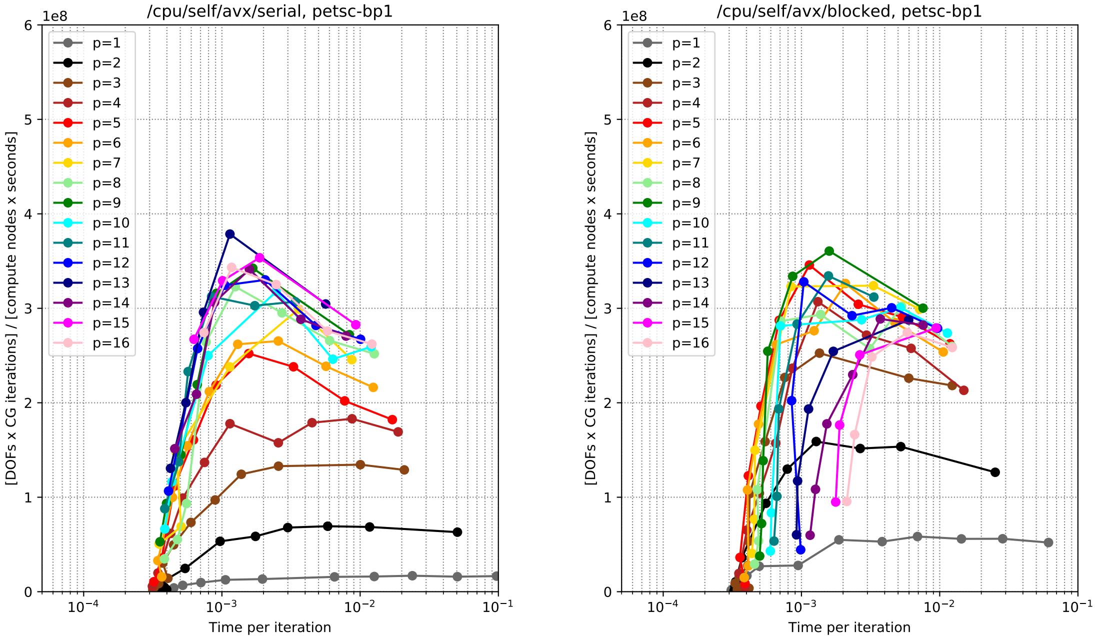




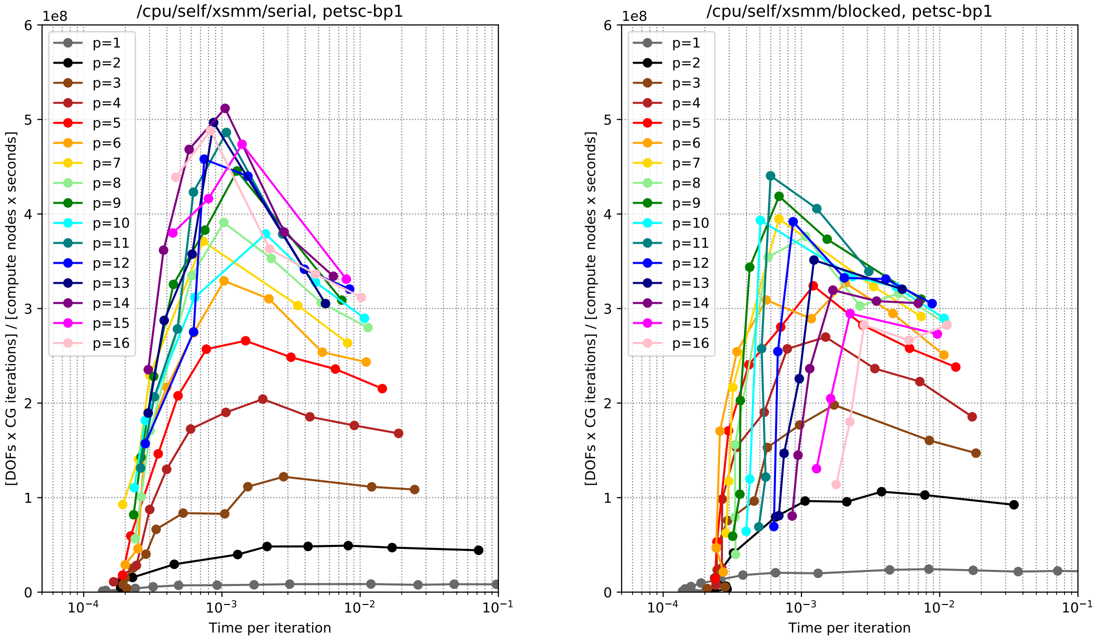
Vectorization techniques

- 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)

AVX internal vs external vectorization



libXSMM internal vs external vectorization



Outlook

- `spack install ceed` works; next release in March
- libCEED is interested in contributors and friendly users
- Need consistent strategy for JIT of Q-functions
  - How much fusion and inlining?
- Performance optimizations in progress
  - Backends should automatically choose internal versus external vectorization
  - Choice depends on architecture, element size, number of fields, problem size
  - Even/odd decomposition (symmetry)
- Mixed topology (works, but needs flattening)
- Hanging node interpolation (can be done in $\mathscr{P}$)