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Fast Matrix-Free High-Order Discontinuous Galerkin Kernels: Performance Optimization and Modeling

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in collaboration with

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Outline

Application background

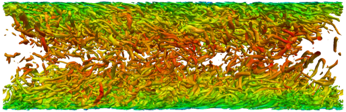
Matrix-free algorithm

Performance modeling

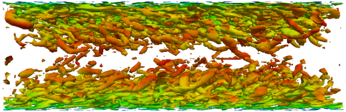
Summary

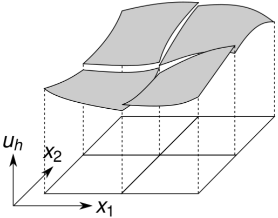
- Complex fluid dynamics simulations
- Code development based on `deal.II` library, `dealii.org`
- Main interest in incompressible flow at high Reynolds numbers $\rightarrow$ solutions smooth, but fine features $\rightarrow$ high resolution
- High-order polynomials within elements
- Fluxes at the element boundaries to weakly enforce continuity, allow for upwind fluxes similar to finite volumes
- Built-in numerical dissipation, in particular in underresolved scenarios
  - fewer degrees of freedom
  - particularly attractive for convection-dominated flows due to low dispersion errors

Visualization: turbulent flow in channel at $\mathrm{Re}_\tau = 590$, vortices visualized by lambda2-criterion DNS, 64^3 mesh with $k = 4$



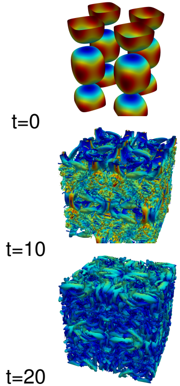
Implicit LES, 16^3 mesh with $k = 4$



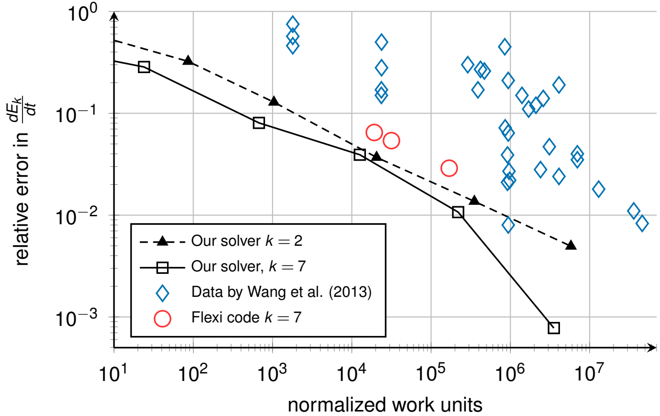


3D Taylor–Green vortex problem

Taylor–Green vortex at Re = 1600: iso-contours of q-criterion (value 0.1) colored by velocity magnitude



Opportunities with tuned implementation: We are **one order of magnitude faster** than all results from Wang et al. (2013), normalized run time



Wang, Fidkowski et al., High-order CFD methods: current status and perspective, *Int. J. Numer. Meth. Fluids* 72(8), 2013

Fehn, Wall, Kronbichler, Efficiency of high-performance discontinuous Galerkin spectral element methods for under-resolved turbulent incompressible flows, arXiv:1802.01439, 2018

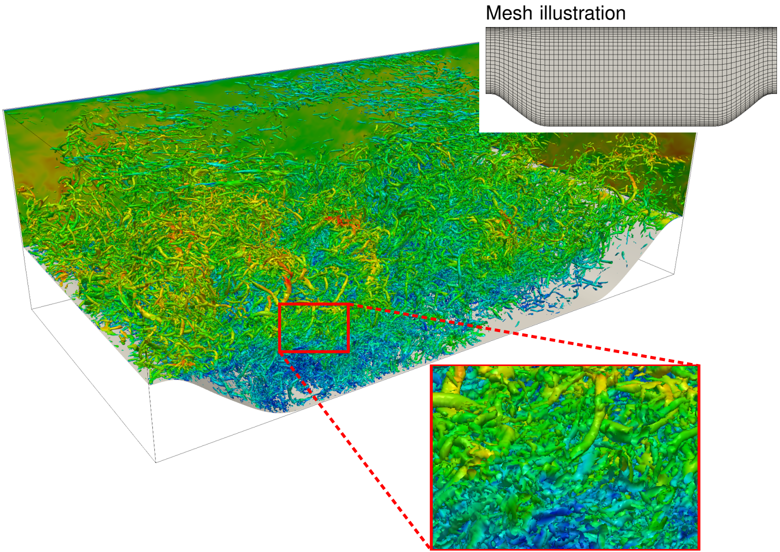
Compressible DG code Flexi: https://github.com/flexi-framework/flexi

High-order geometry example: Flow over periodic hills

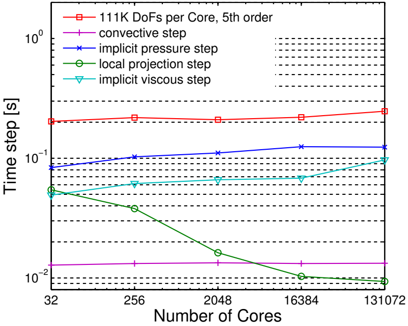
- High order usually includes high-order geometry: manifold descriptions
- Support for unstructured and adaptive meshes through `deal.II` and `p4est` libraries

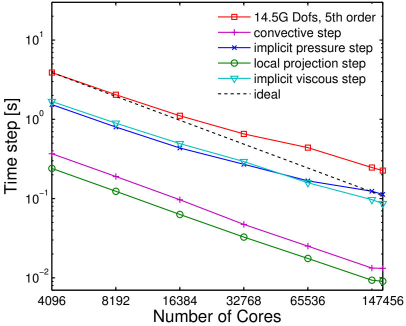
- Computations with up to 800m DoFs and 9m time steps

Krank, Kronbichler, Wall, Direct numerical simulation of flow over periodic hills up to $\mathrm{Re}_\tau = 10,595$, submitted, 2017



Implementation: Scales to 147k cores





Weak and strong scaling on SuperMUC (9 216 nodes with 16 Sandy Bridge cores each)

- Very good scaling to largest size. Algorithmic components:
  - Explicit convective step (typical explicit time stepping)
  - Solution of pressure Poisson equation (**geometric multigrid**)
  - Projection step + Helmholtz equation: CG solver preconditioned by inverse mass matrix

Krank, Fehn, Wall, Kronbichler, A high-order semi-explicit discontinuous Galerkin solver for 3D incompressible flow with application to DNS and LES of turbulent channel flow. *J. Comput. Phys.*, 348, 2017

Symmetric interior penalty discretization of the Laplacian $\nabla^2 u$:

$$\sum_{K \in \text{cells}} (\nabla \varphi_i, \nabla u)_K - \left\langle \varphi_i, \frac{\mathbf{n} \cdot (\nabla u^- + \nabla u^+)}{2} \right\rangle_{\partial K} - \left\langle \mathbf{n} \nabla \varphi_i, \frac{u^- + u^+}{2} \right\rangle_{\partial K} + \langle \varphi_i, \tau(u^- - u^+) \rangle_{\partial K}$$

Notation in face integrals $\langle \cdot, \cdot \rangle_{\partial K}$

- u^- is solution inside element K
- u^+ is solution on neighbor over the face
- At boundary, u^+ from b.c., e.g. $u^+ = -u^-$

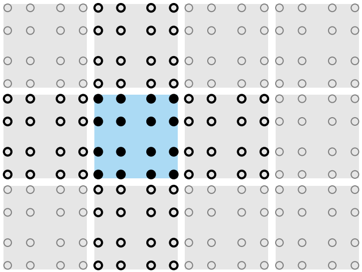
Matrix-vector product $v = Au$
Entry v_i generated by testing with φ_i

Matrix-free algorithm: loop over cells K

- Extract local vector values on cell: $u_K = P_K u$
- Compute cell integral $(\nabla \varphi_i, \nabla u)$ from local interpolation of u_K, $i = 1, \ldots, (k+1)^d$
- Loop over all faces, $f = 1, \ldots, 2d$:
  - Load neighboring values $u^+_{K,f}$
  - Compute face integral contributions and add to cell integral
- Write contribution back into vector

Kronbichler, Kormann, A generic interface for parallel finite element operator application. *Comput. Fluids* 63 (2012)
Kronbichler, Kormann, Fast matrix-free evaluation of discontinuous Galerkin finite element operators. arXiv:1711.03590 (2017)

Illustration for $k = 3$ (4th order) in 2D



- ○ Degrees of freedom in mesh
- **o** Read access element i, j
- ● Read + write access element i, j

Basic matrix version:

$$v_{i,j} = A^{0,0} u_{i,j} + A^{+,0} u_{i+1,j} + A^{-,0} u_{i-1,j} + A^{0,+} u_{i,j+1} + A^{0,-} u_{i-1,j-1}$$

Full matrix complexity $(k+1)^{2d}$: Very inefficient at high degree k in 3D

Tensor product of 1D matrices

$$A^{0,0} = A^{0}_{1\mathrm{D}} \otimes M_{1\mathrm{D}} + M_{1\mathrm{D}} \otimes A^{0}_{1\mathrm{D}}$$

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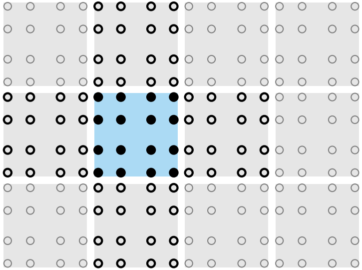

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More efficient evaluation with sum factorization

$$v_{i,j} = \left(A^0_{1\text{D}} U_{i,j} + A^+_{1\text{D}} U_{i+1,j} + A^-_{1\text{D}} U_{i-1,j}\right) M^{\mathrm{T}}_{1\text{D}} + M_{1\text{D}} \left(U_{i,j} A^{0,\mathrm{T}}_{1\text{D}} + U_{i,j+1} A^{+,\mathrm{T}}_{1\text{D}} + U_{i,j-1} A^{-,\mathrm{T}}_{1\text{D}}\right)$$

$U_{i,j}$ column-major matrification of $u_{i,j}$

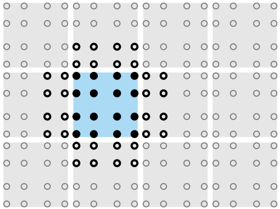
Complexity: $d(k+1)^{d+1}$

Initial optimization: Choice of basis

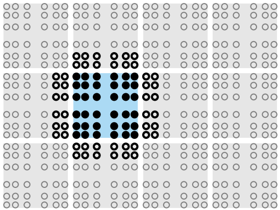
Evaluation of $v_{i,j} = \left(A^0_{1D} U_{i,j} + A^+_{1D} U_{i+1,j} + A^-_{1D} U_{i-1,j}\right) M^T_{1D} + M_{1D} \left(U_{i,j} A^{0,T}_{1D} + U_{i,j+1} A^{+,T}_{1D} + U_{i,j-1} A^{-,T}_{1D}\right)$

- Choice 1 (spectral elements): Use basis where M is diagonal
  - Full neighbor pulled in (possible indirect addressing)
  - Interpolation matrix from neighbor with $(k+1)^d$ points
  - Total number of tensor product interpolations: 6 in 2D, 9 in 3D
- Choice 2: Basis with two 1D shape functions have $\phi_i(0) \neq 0$ and $\phi_i'(0) \neq 0$ (Hermite)
  - Coupling matrices cheaper
  - Cheaper despite additional mass matrices
  - Total number of tensor product interpolations: 4 in 2D, 8 in 3D

Data access Hermite basis $k = 3$



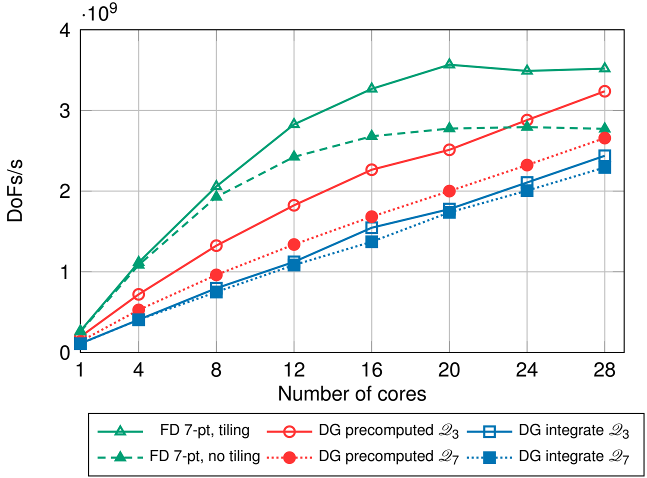
Data access Hermite-like $k = 5$



Choice 2 gives (much) better performance

Comparison to finite differences: throughput

Evaluation on Cartesian mesh on 2 $\times$ 14 core Intel Broadwell Xeon E5-2690 v4



Upper performance limit: 4.7 DoFs/s (read input vector from RAM at 112 GB/s, read + write output vector)

DG operator evaluation almost *for free* because **additional arithmetics on cacheable data**, mostly hidden behind transfer on otherwise memory-starved system

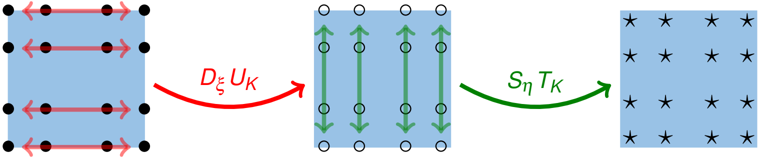
Tuned finite difference stencils with tiling together with K.-R. Wichmann, W. A. Wall

- Final stencil only separable into precomputed 1D matrices A^0_{1D}, A^+_{1D}, A^-_{1D}, M_{1D} for axis-aligned (Cartesian) meshes and constant coefficients
- Want to address numerical integration for general geometries and nonlinear operators
- Sum factorization not in final matrix but for transformation between vector entries and quadrature points (established by spectral element community)

Generic matrix-free implementation with integration

Efficient matrix-free implementation using deal.II[1] [2] `www.dealii.org`

General layout for interpolation into quadrature points:



Vector values u_K on nodes

$\frac{\partial}{\partial \xi} u^h$ on quadrature points

$$\frac{\partial}{\partial \xi} u^h(\xi_q, \eta_q)\Big|_{\text{q\_points}} = (D_\xi \otimes S_\eta)\mathbf{u}_K$$

Dense matrix-matrix multiply $D_\xi \; \mathbf{U}_K \; S_\eta^\mathrm{T}$

Evaluation cost: $\mathcal{O}((k+1)^4)$ per element (degree k in 3D)

Naive evaluation: $\mathcal{O}((k+1)^6)$

[1] Kronbichler, Kormann, A generic interface for parallel cell-based finite element operator application, *Comput. Fluids* 63 (2012)

[2] Kronbichler, Kormann, Fast matrix-free evaluation of discontinuous Galerkin finite element operators, arXiv:1711.03590 (2017)

Performance characterization with DG operator evaluation

Objective assessment much less mature than in finite difference or lattice Boltzmann communities

- What is the expected number of arithmetic operations?
  - Sum factorization most beneficial on quad/hex elements
  - Evaluation without sum factorization is too much work for $k \geq 3$ (except triangles)
  - Evaluate the geometry on the fly or load precomputed data?
  - Which basis and what evaluation techniques appropriate?
- What is the expected memory transfer?
  - Some projects separate face integrals into global data structure $\rightarrow$ several sweeps through data for a single operator evaluation
  - Some projects split loops in quadrature into global loops
- Must use implementation-independent **throughput metric: degrees of freedom per second (DoFs/s)**
- No DG cross-project benchmarking yet (?) corresponding recent CEED initiative for FEM `http://ceed.exascaleproject.org/bps`

Performance expectations

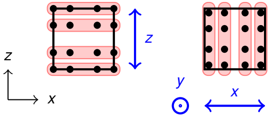
- **Ideal memory access:** A single load to source, a single store (or load+store with read-for-ownership)
- **Arithmetics:** Around 120–250 operations per DoF
- **Balance:** 5–10 FLOPs/Byte

Must consider both compute and memory access!

Only cell integrals, only compute phase of 3D Laplacian, 2×14 core Intel Broadwell E5-2690 v4, 2.9 GHz (incl AVX-2 turbo)

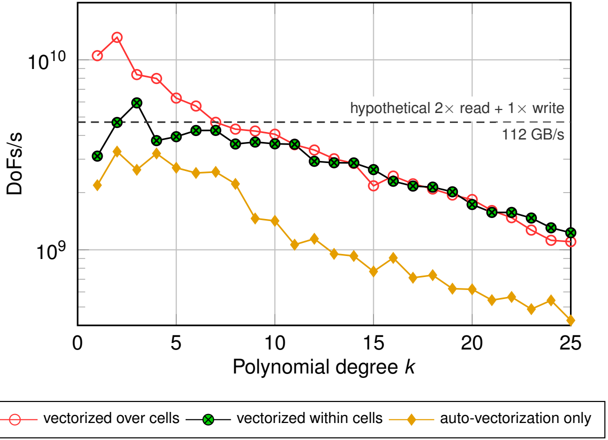
Forced vectorization within cells, 4-times blocking in z

Values in nodes   Values in q-points



Vectorize over several cells

50	54	58	62	51	55	59	63
34	38	42	46	35	39	43	47
18	22	26	30	19	23	27	31
2	6	10	14	3	7	11	15
48	52	56	60	49	53	57	61
32	36	40	44	33	37	41	45
16	20	24	28	17	21	25	29
0	4	8	12	1	5	9	13



Conclusion: Must explicitly vectorize

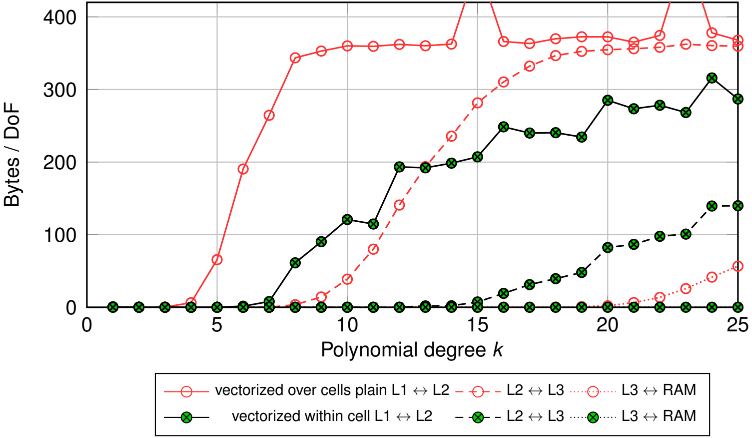
Doesn’t vectorization over cells drown caches?

Yes, but there are outer level caches...

Higher degree: more cache access → more arithmetics → **no big impact** for $k < 20$ on Broadwell (or $k < 12$ on KNL)

Cache transfer analysis with the Likwid tool `github.com/RRZE-HPC/likwid` (hardware performance counters)

Performance can be improved by tiling within tensor product, see Kronbichler & Kormann, arXiv:1711.03590



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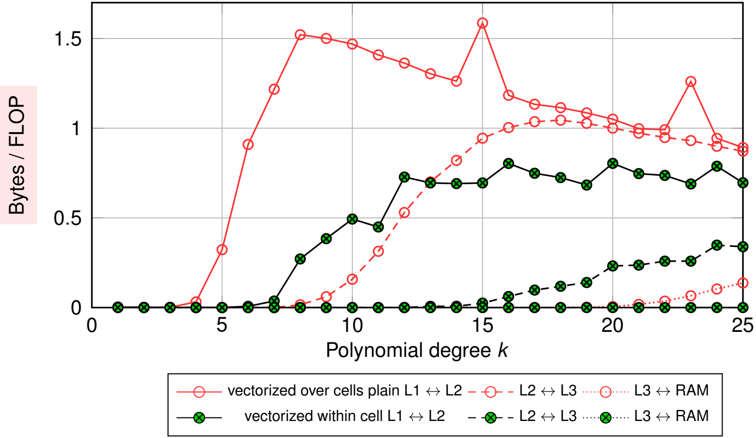
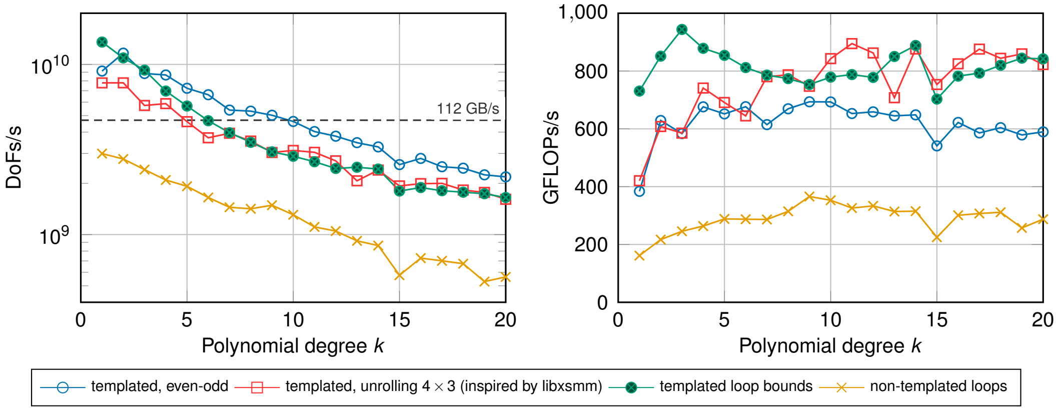


Test of throughput on 2 × 14 core Intel Broadwell E5-2690 v4, 2.9 GHz (incl AVX-2 turbo), 1,299 GFLOPs/s arithmetic peak

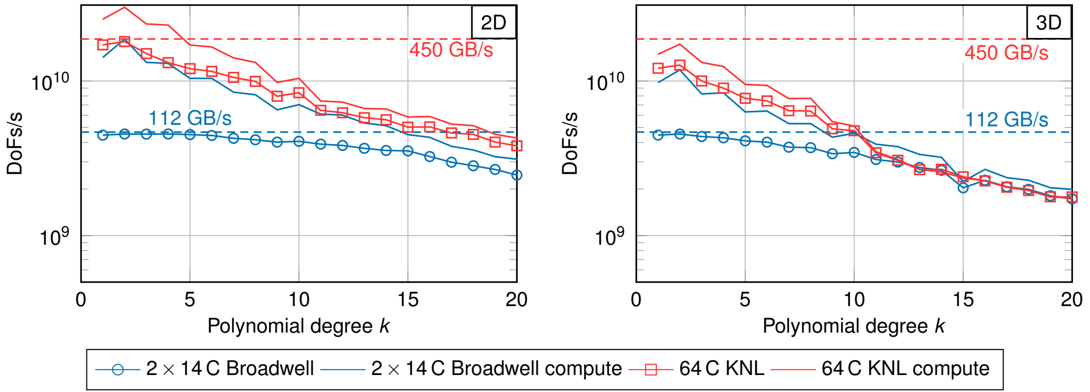


Favorite method: even-odd decomposition[3], compile-time loop bounds

[3] Kopriva, *Implementing spectral methods for partial differential equations*, Springer, 2009

Cell integrals with vector transfer

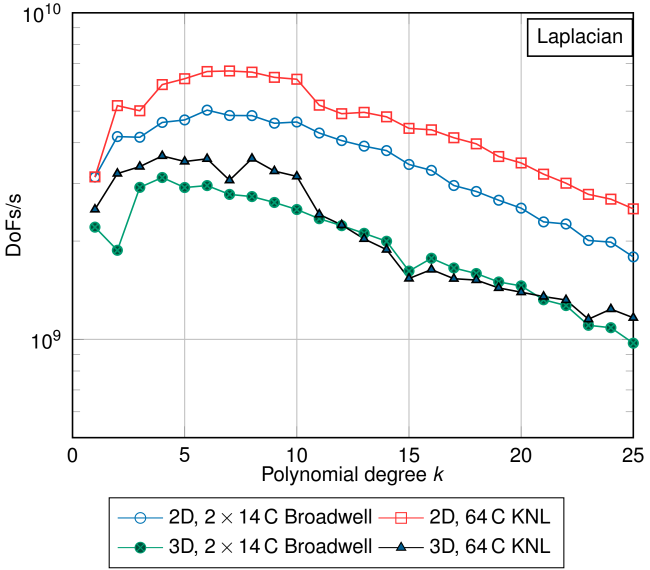
Compare 2×14 core Intel Broadwell E5-2690 v4 (at 2.9 GHz) and 64 core Intel Knights Landing 7210 (at 1.1 GHz), problem size 8M to 56M



Both KNL and Broadwell reach $> 50\%$ of arithmetic peak for instruction mix with 35% FMA, 30% add, 35% multiply

Arithmetics including face integrals

- Face integrals constitute significant portion of arithmetics
  - 80% at $k = 1$
  - 52% at $k = 5$
  - 35% at $k = 11$
- Involve additional gather access into neighbors for vectorization over cells not displayed here

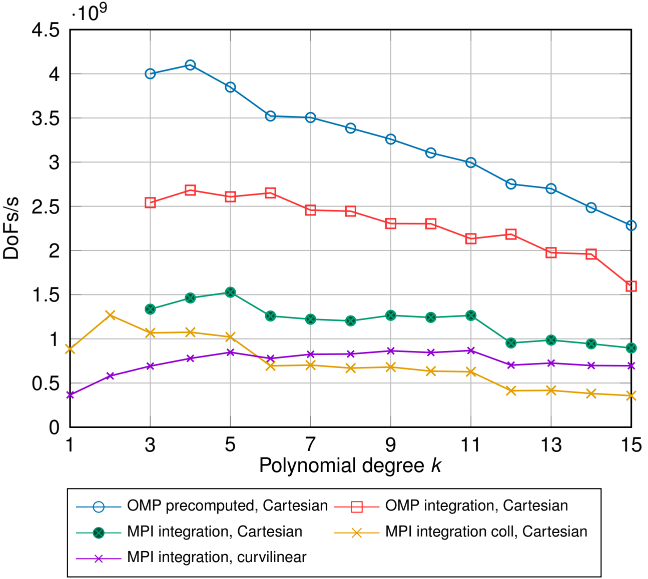


Throughput of operator evaluation: 3D DG-SIP Laplacian

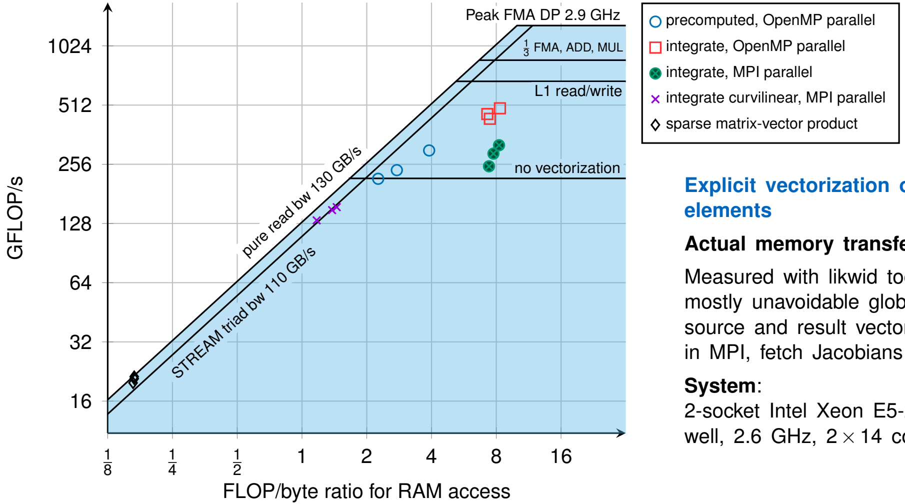
Two parallelization options:

- OpenMP: direct access to neighbors in shared memory
- MPI: Must explicitly send data, pack & unpack and MPI routines take around 35% of time at $k = 6$
- Shared memory model clearly better

System: 2×14 core Intel Broadwell E5-2690 v4, utilize streaming stores



Performance characterization by roofline



Explicit vectorization over several elements

Actual memory transfer

Measured with likwid tool; transfers mostly unavoidable global data: Fetch source and result vectors, pack/unpack in MPI, fetch Jacobians (curvilinear)

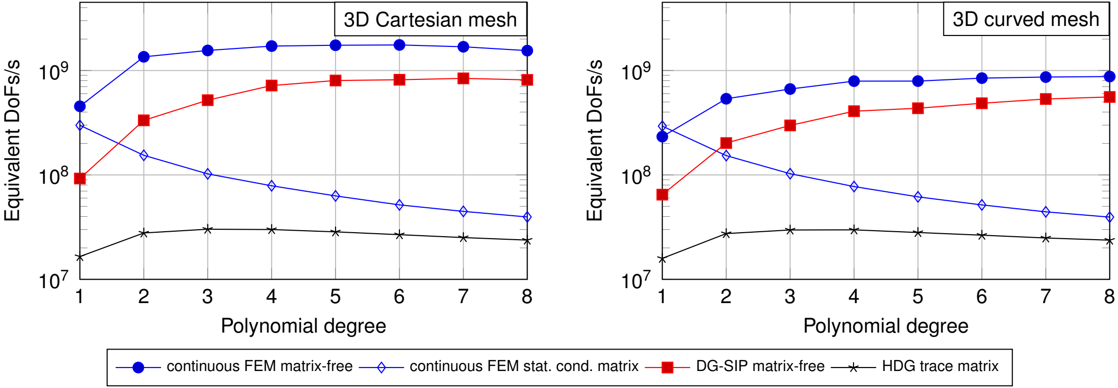
System:
2-socket Intel Xeon E5-2690 v4 (Broadwell, 2.6 GHz, 2×14 cores)

Arithmetic balance for polynomial degrees $k = 3, 5, 9$

Comparison to other schemes

Continuous finite elements, DG-SIP, hybridizable discontinuous Galerkin (HDG) representing efficient sparse matrix-based scheme

Throughput measured using run time against $n_{\text{cells}}(k+1)$ "equivalent" DoFs to make different discretizations comparable[4]



[4] Kronbichler, Wall, A performance comparison of continuous and discontinuous Galerkin methods with fast multigrid solvers, *arXiv:1611.03029* (2016)

Summary

- Comprehensive approach to tuning – not just FLOPs or GB/s but
  - choose mathematical formulation considering both data access and computations
  - apply arithmetic optimizations such as even-odd decomposition guided by throughput, not GFLOPs/s
  - vectorization over cells very efficient on Intel machines (but **not** on GPUs, see Ljungkvist & Kronbichler, 2017)
- Realization by matrix-free approach with sum factorization on hexahedra is highly efficient! Reaches 3 billions DoFs/s = finite different performance
- Challenge 1: Memory transfer of geometry
- Challenge 2: BLAS-1 vector operations take large share of time
  - More than 60% in conjugate gradient solver with simple precond.
  - More than 30% in Chebyshev smoother with multigrid

Need programming model that interleaves global operations as much as possible

Ljungkvist, Kronbichler, Multigrid for matrix-free finite element computations on graphics processors. Technical Report IT-2017-006, Uppsala University, 2017