Exploiting SIMD vectorisation for unstructured scale-resolving simulations

David Moxey
College of Engineering, Mathematics & Physical Sciences, University of Exeter

Roman Amici and Mike Kirby
Scientific Computing and Imaging Institute, University of Utah

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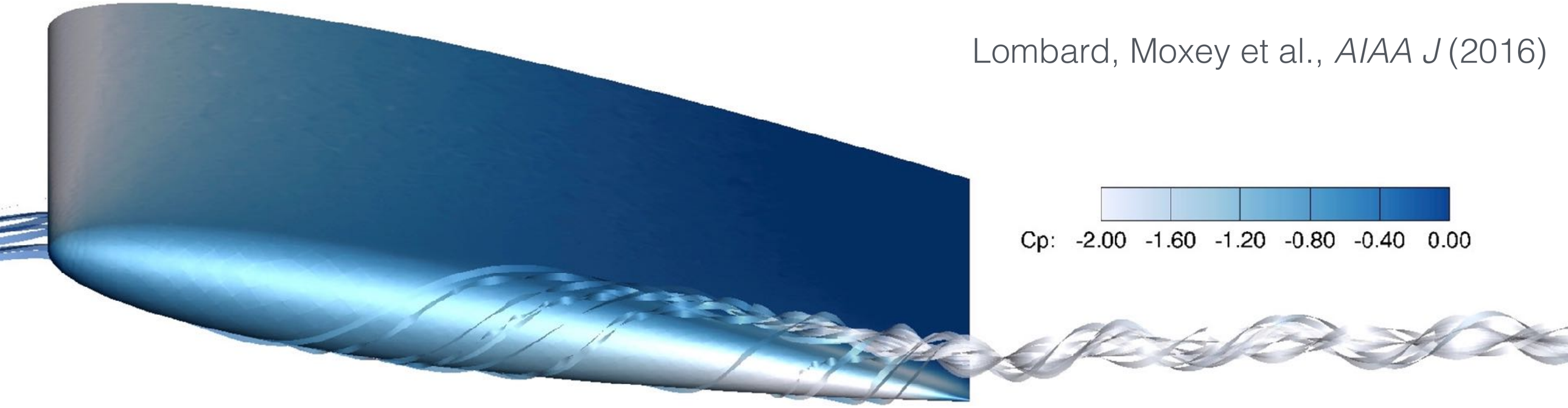


Lombard, Moxey et al., *AIAA J* (2016)

Increasing desire for **high-fidelity** CFD simulations in high-end aeronautics applications.

Want to accurately model 'difficult' features:

- strongly separated flows, vortex interaction;
- feature tracking and prediction.

Challenging with current RANS-based industry-standard tools.

Goal: develop methods and techniques for making LES affordable & routine.

Challenges

High order methods can provide a lot of benefits for these problems:

- ✓ very high accuracy over time/space;
- ✓ excellent for tracking transient structures;
- ✓ tuneable arithmetic intensity: overcome flops/byte barrier;
- ✓ geometric flexibility.

but there are also some challenges…

- ➤ implementation difficulty;
- ➤ extra work per degree of freedom means computational efficiency is important;
- ➤ other numerical challenges, e.g. scalable preconditioning;
- ➤ mesh generation.

The modern hardware landscape

- Peak FLOPS/s are increasing at around **50-60% per year**, but memory bandwidth only increasing at around **25% per year**[1].

- If we want the most out of our hardware, we need to fully exploit its architecture:

  - Many-core environment, perform multiple instructions per cycle: **SIMD vectorisation**;

  - Increase **arithmetic intensity** of algorithms: do as much work with data as possible.

[1] John McCalpin, *Memory bandwidth and system balance*, Supercomputing, 2016.

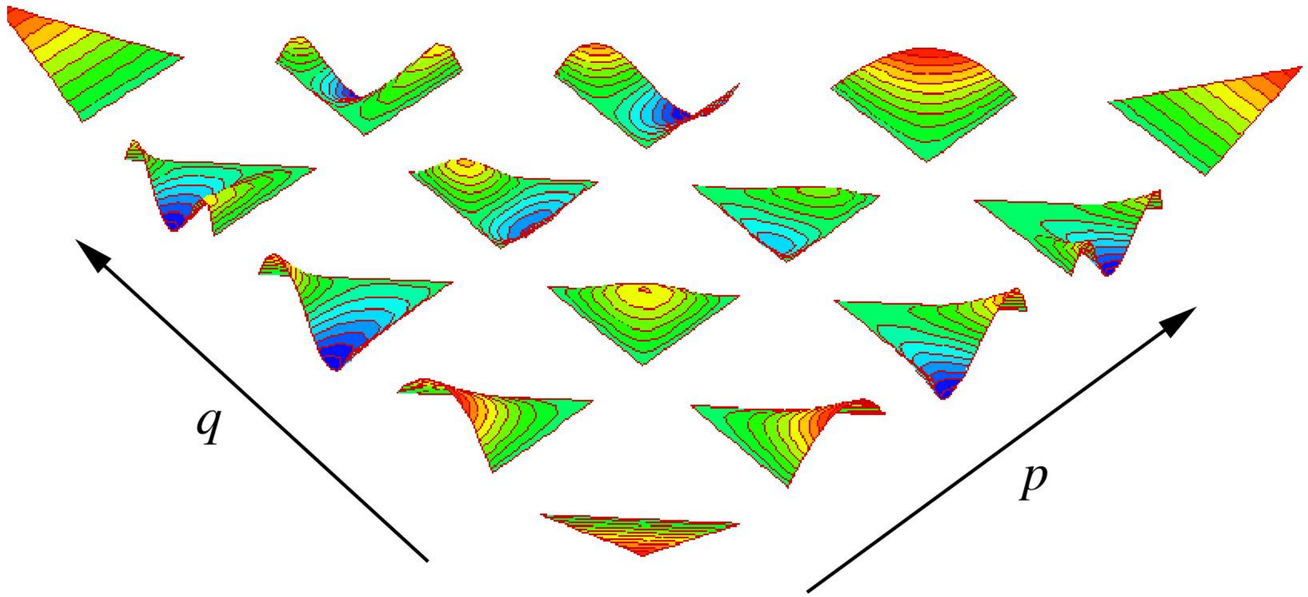
The modern hardware landscape

Tesla V100 Volta: ~7.8 TFLOP/s, ~300-900GB/s.
2,688 cores, 32 FP64 vector lanes.
32 FP64 FLOPS/cycle.

Xeon Platinum 8180M: ~1.7TFLOP/s, ~150GB/s.
28 physical cores, 8 FP64 vector lanes.
2 AVX512 + FMA units: 32 FLOPS/cycle.

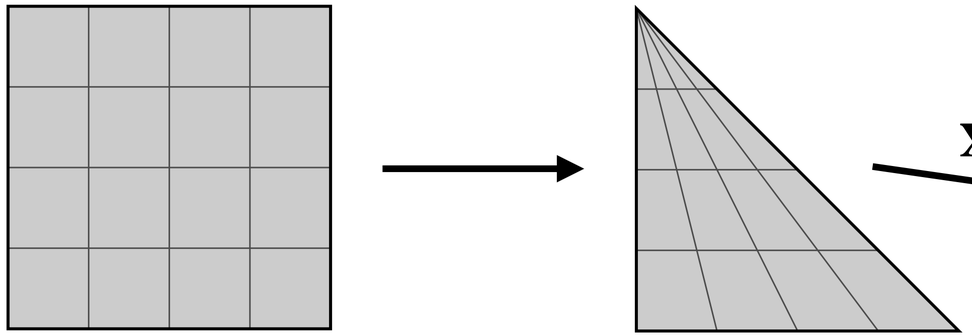
The spectral/*hp* element method

- Extend traditional FEM by adding higher order polynomials of degree *P* within each element.
- e.g. high-order triangle has (*P*+1)(*P*+2)/2 degrees of freedom at a given order *P*.
- Increased accuracy: more done per degree of freedom, increased **arithmetic intensity**.



spectral/*hp* element basis functions

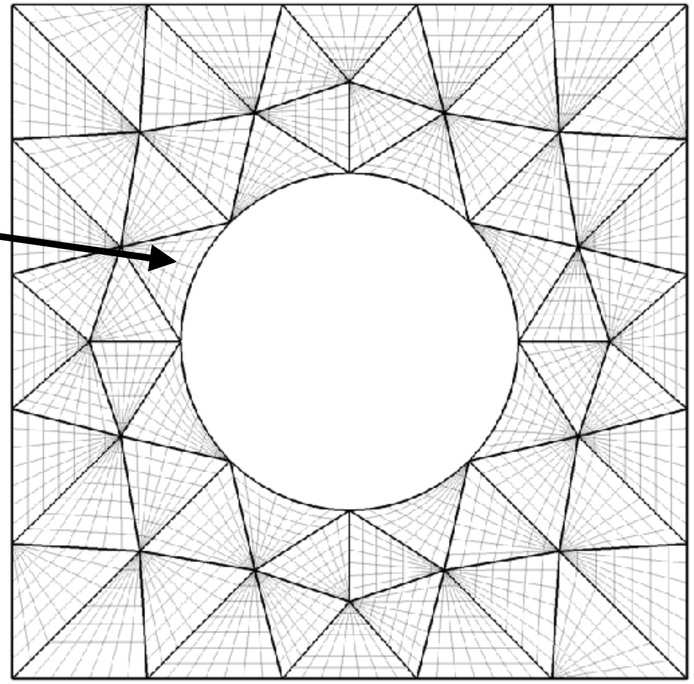
The spectral/*hp* element method



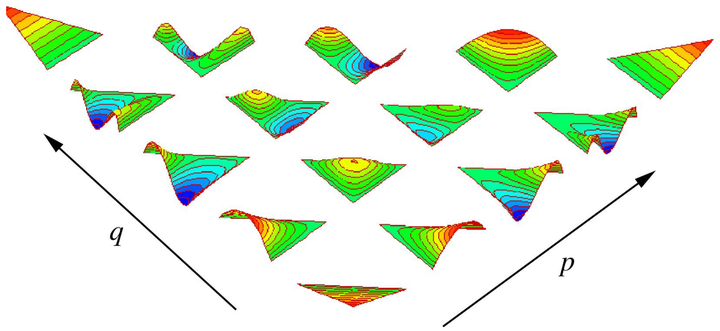
collapsed coordinates
$(\eta_1, \eta_2) \in [-1,1]^2$

reference element
$(\xi_1, \xi_2) \in \Omega_{st}$

$\mathbf{x} = \chi^e(\xi)$



(C^0) tensor product basis
$\phi_p^a(\eta_1)\,\phi_{pq}^b(\eta_2)$



"Defining" features of spectral/hp method

Generally *not* collocated

$$u(\xi_{1i}, \xi_{2j}) = \sum_{n=0}^{P^2} \hat{u}_n \phi_n(\xi) = \sum_{p=0}^{P} \sum_{q=0}^{Q} \hat{u}_{pq} \phi_p(\xi_{1i}) \phi_q(\xi_{2j})$$

quadrature points

modal coefficients

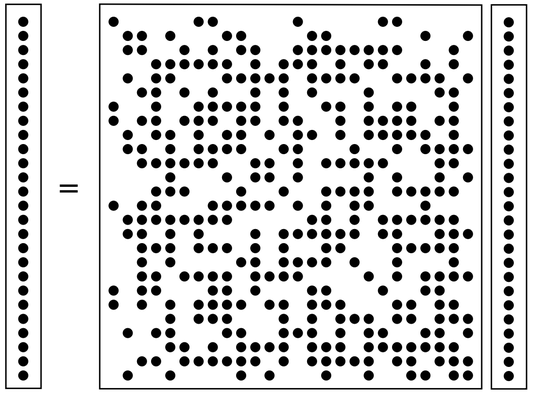
Uses tensor products of 1D basis functions, even for non-tensor product shapes

$$u(\xi_{1i}, \xi_{2j}, \xi_{3j}) = \sum_{p=0}^{P} \sum_{q=0}^{Q-p} \sum_{r=0}^{R-p-q} \hat{u}_{pqr} \phi_p^a(\xi_{1i}) \phi_{pq}^b(\xi_{2j}) \phi_{pqr}^c(\xi_{3k})$$

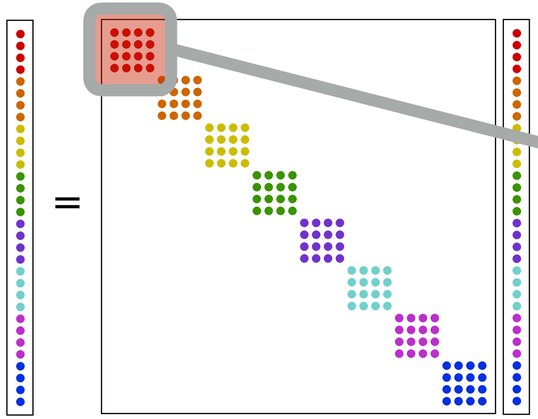
basis function indexing harder

Implementation choices

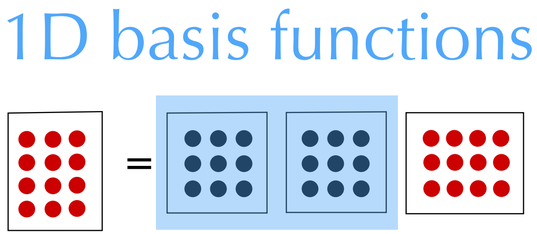
Finite element operation evaluations (e.g. mass matrix) form bulk of simulation cost; can be done in several ways.



Global matrix
assemble a sparse matrix



Local evaluation
create elemental dense matrices + assembly map



Matrix free
no local matrices at all
sum factorisation speedup

increasing arithmetic intensity

Sum-factorisation

Key to performance at high polynomial orders: complexity $\mathrm{O}(P^{2\mathrm{d}})$ to $\mathrm{O}(P^{\mathrm{d}+1})$

$$\sum_{p=0}^{P}\sum_{q=0}^{Q}\hat{u}_{pq}\phi_p(\xi_{1i})\phi_q(\xi_{2j}) = \sum_{p=0}^{P}\phi_p(\xi_{1i})\left[\sum_{q=0}^{Q}\hat{u}_{pq}\phi_q(\xi_{2j})\right]$$

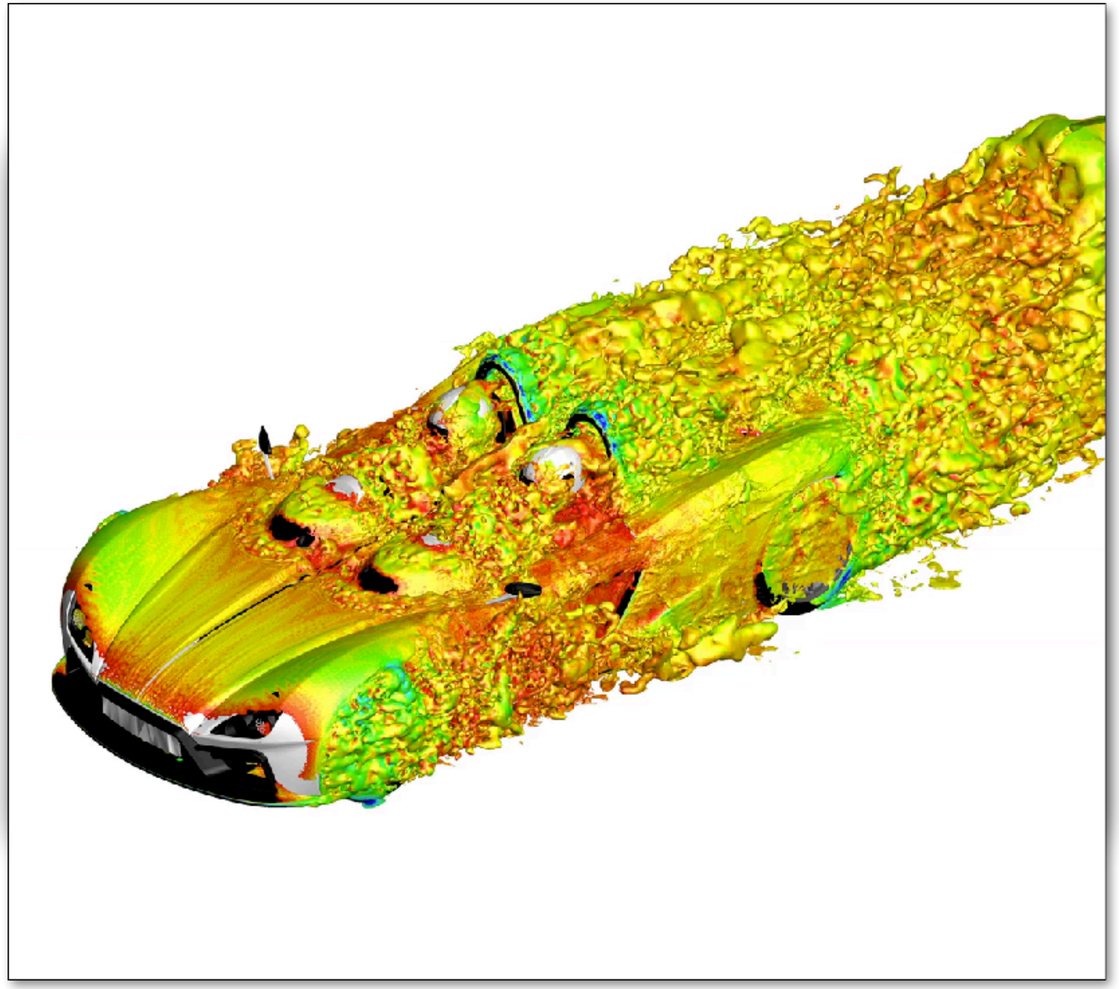
store this

Works in essentially the same way for more complex indexing for e.g. triangles:

$$\sum_{p=0}^{P}\sum_{q=0}^{Q-p}\hat{u}_{pq}\phi_p^a(\xi_{1i})\phi_{pq}^b(\xi_{2j}) = \sum_{p=0}^{P}\phi_p^a(\xi_{1i})\left[\sum_{q=0}^{Q-p}\hat{u}_{pq}\phi_{pq}^b(\xi_{2j})\right]$$

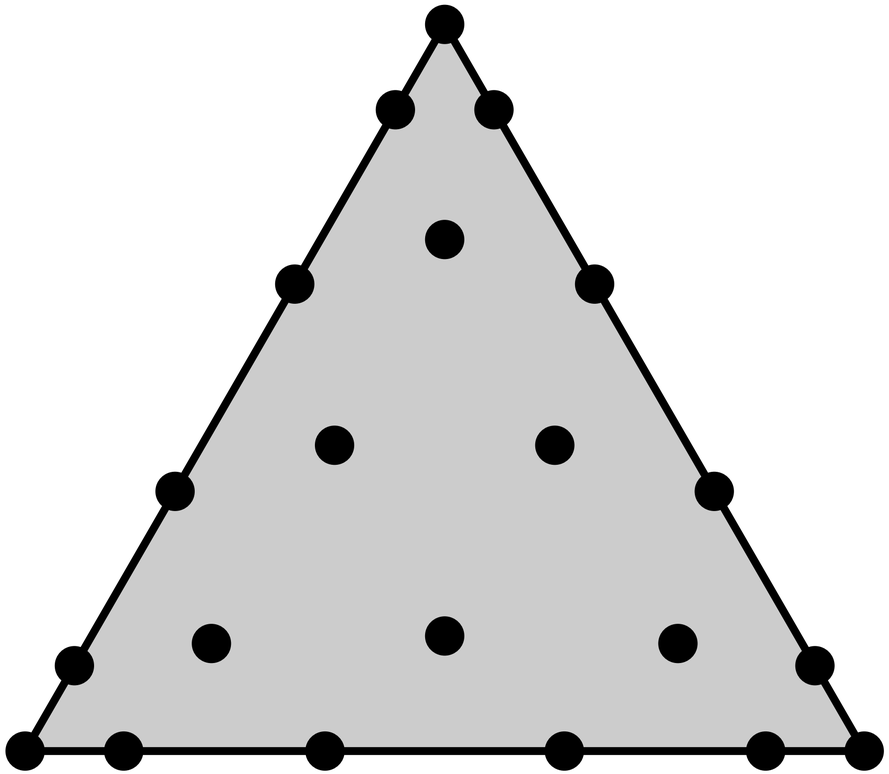
store this

Unstructured simulations



- Common knowledge: hex/quad elements yield best performance.
- However complex geometries presently require meshes of ‘unstructured’ elements: tets, prisms, etc.
- Potentially use tensor-product basis on unstructured elements, enable matrix-free operators + sum factorisation.

Unstructured elements



P5 triangle, Fekete points

- Unstructured elements generally make use of Lagrange basis functions.
- Combine this with a suitable set of cubature points: either collocated or not.
- However this loses tensor-products structure: i.e. no sum factorisation possible.

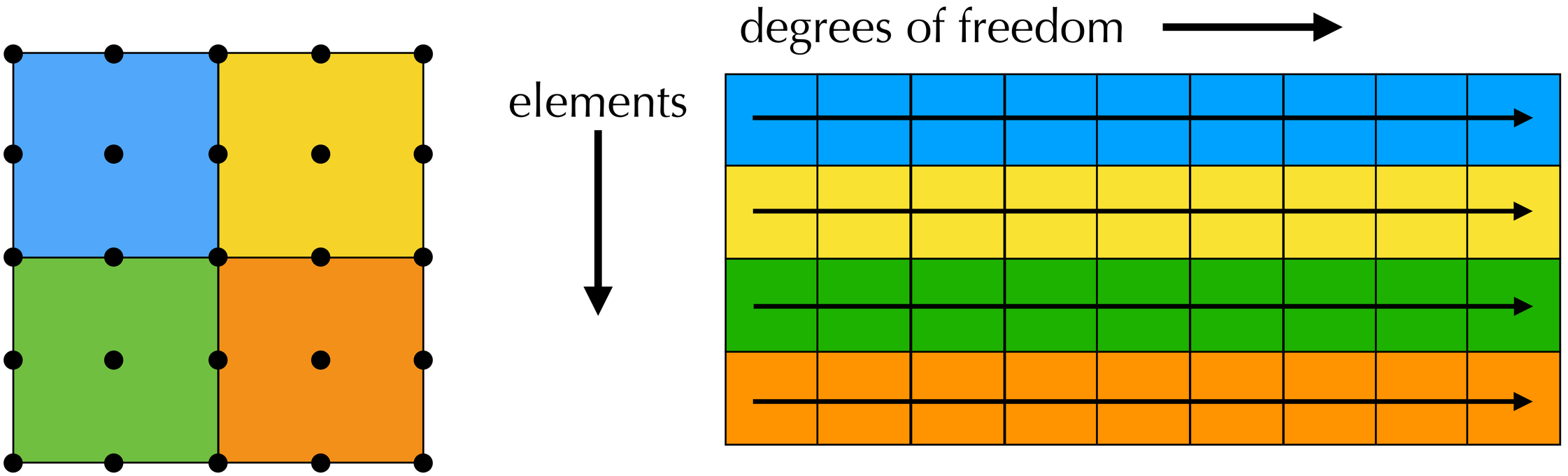
Key questions

- Under spectral/*hp* approach, sum-factorisation matrix-free operators are certainly possible for any element type. Some questions:
  - How much performance do we lose relative to hex/quad?
  - How should SIMD be used?
- Developed a benchmarking utility for Helmholtz operator to test viability of this approach: used for implicit solve in incompressible N-S equations.

$$\nabla^2 u - \lambda u = f(x) \quad \rightarrow \quad (\mathbf{L} + \lambda \mathbf{M})\hat{\mathbf{u}} = \hat{\mathbf{f}}$$

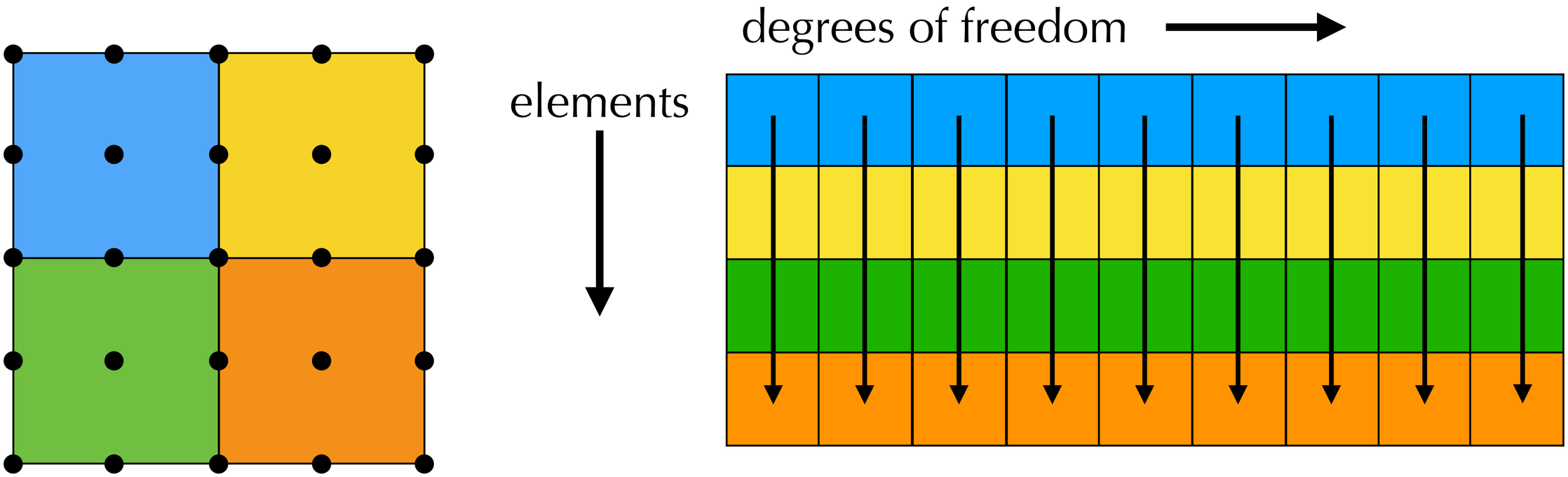
Data layout

Natural to consider data laid out element by element



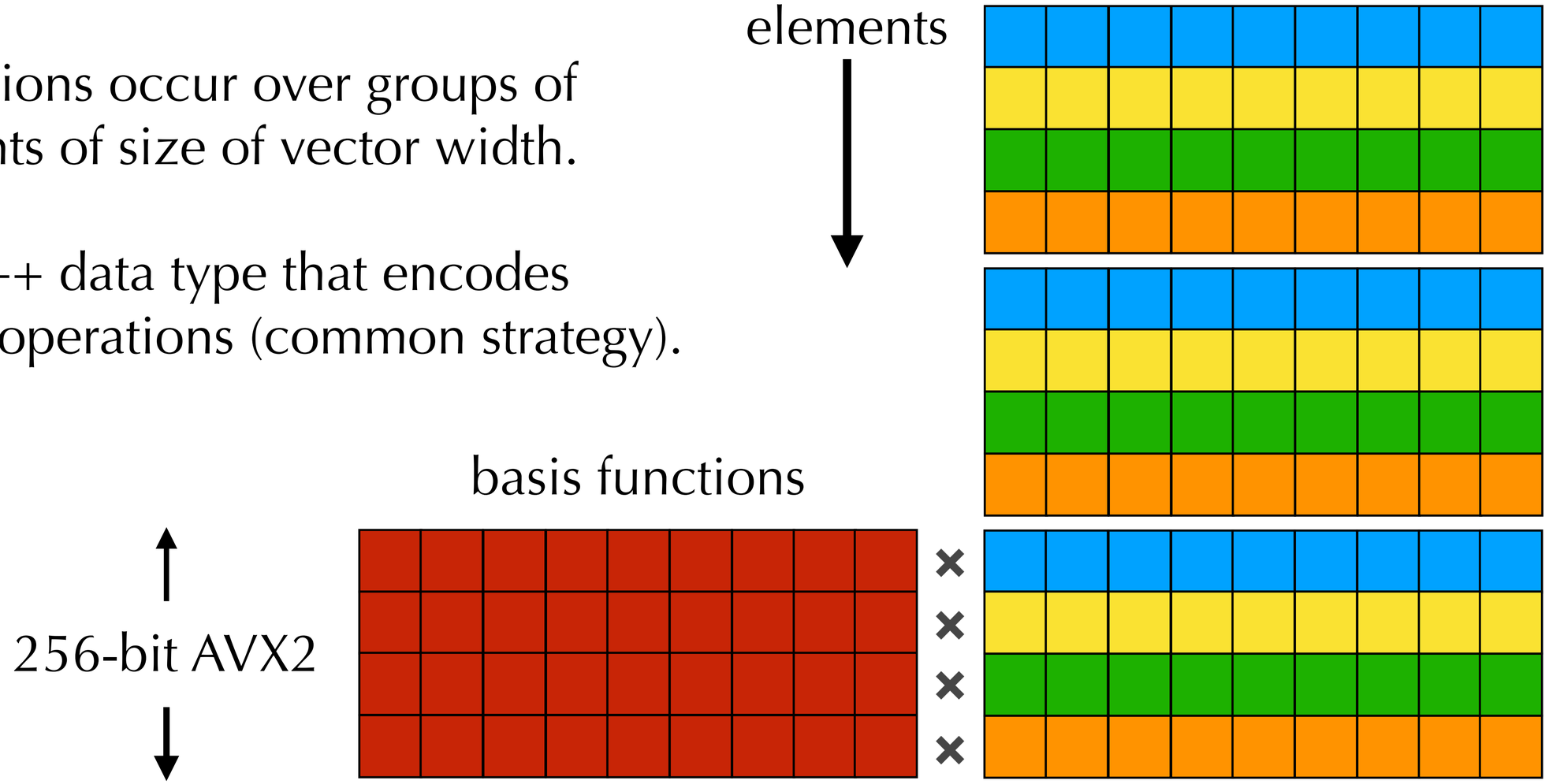
Data layout

Exploit vectorisation by grouping DoFs by vector width



Data layout

- Operations occur over groups of elements of size of vector width.
- Use C++ data type that encodes vector operations (common strategy).



Implementation particulars

- Hand-written kernels for each element type to implement three key components: **interpolation**, **derivatives** and **inner products/integration**.
- Written using C++: templating on (potentially heterogeneous) polynomial order and quadrature order.
- Also templates on **affine elements** (spatially-constant Jacobian) vs. **curvilinear** (spatially-varying); no consideration for Cartesian meshes.
- Templating gives *significant* improvements in runtime performance, particularly for complex loop structures found in this regime.

Tests

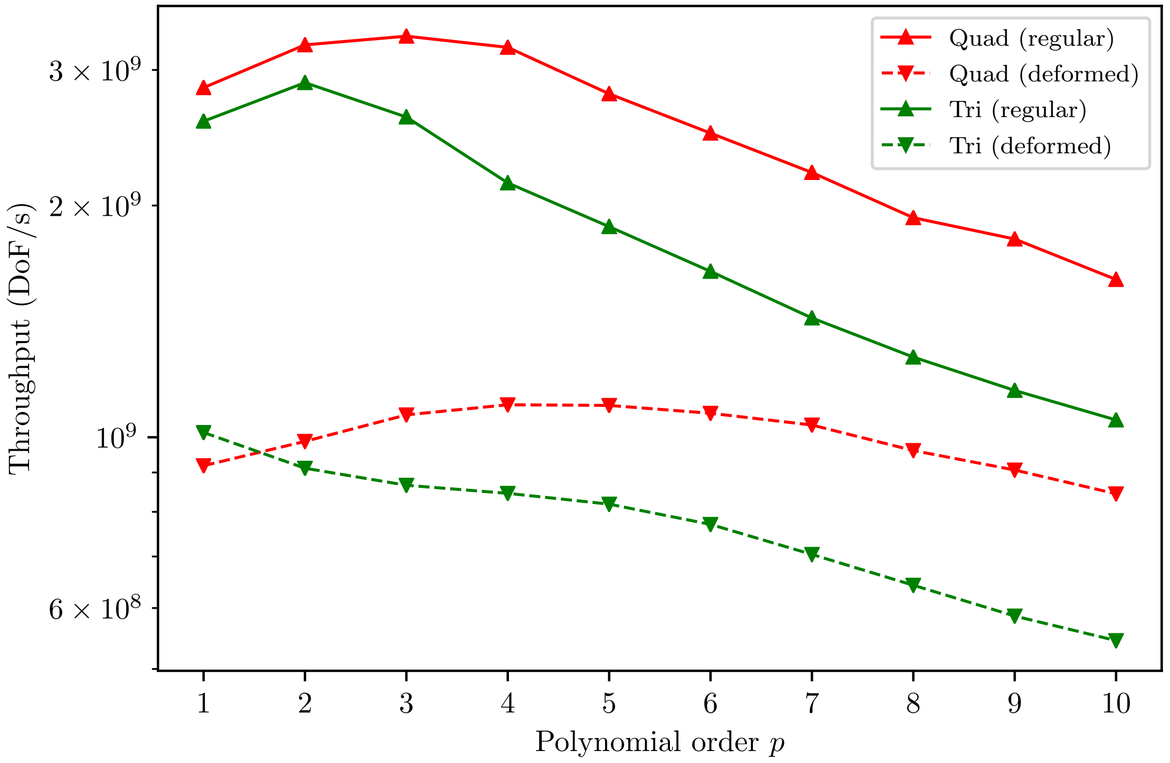
- Benchmarking of Helmholtz operator performed on two architectures with varying SIMD widths.

	Broadwell (AVX2)	Skylake (AVX512)
Model	E5-2697 v4	Xeon Gold 6130
Clock speed(s)	2.3 / 2.0 GHz standard / AVX2	2.1 / 1.7 / 1.3 GHz standard / AVX / AVX512
Cores / sockets	18 / 2	16 / 2
Max node GFLOP/s	1,152	870 (AVX2) 1,331 (AVX512)

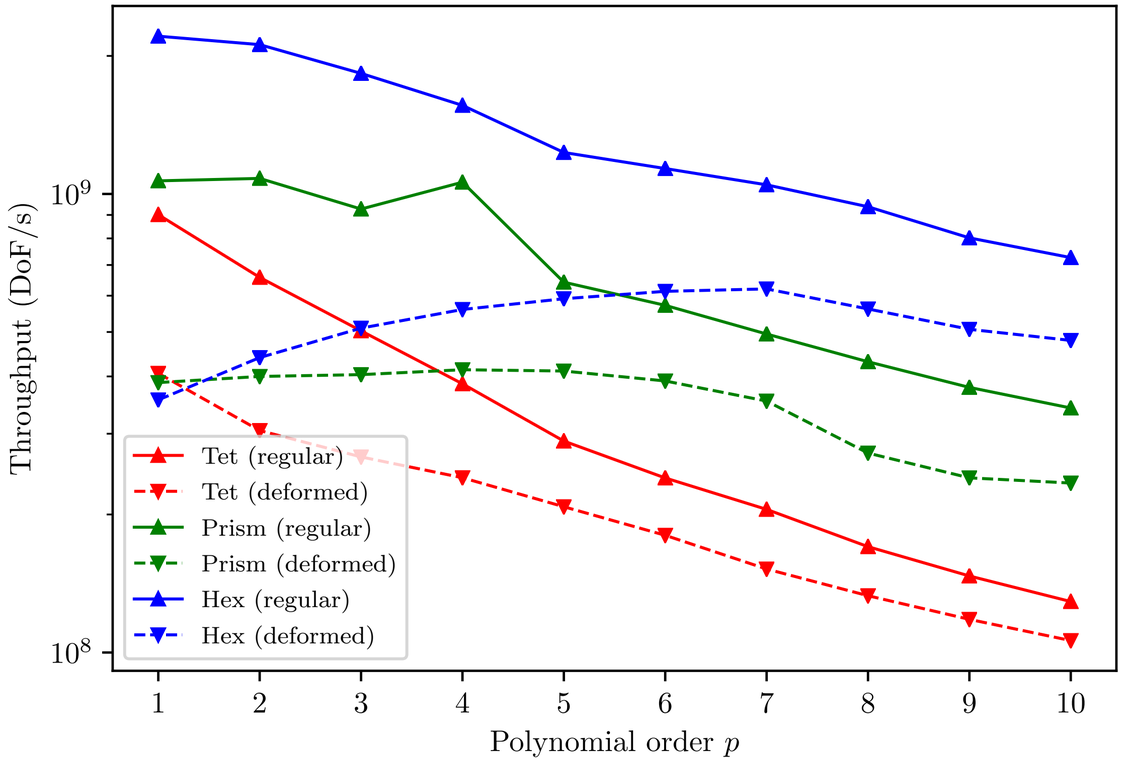
Assessing performance

- Various techniques used to assess kernel performance:
  - **Throughput**: number of local DoF/s processed, for a mesh whose sizes exceeds available cache.
  - GFLOP/s gives some indication of capabilities, provided we are not memory-bound.
  - Better is **roofline analysis**: where do we sit in terms of memory bandwidth to arithmetic intensity?
- Note all results for local elemental operation evaluation only: C^0 work in progress.

Throughput (AVX2, Broadwell)

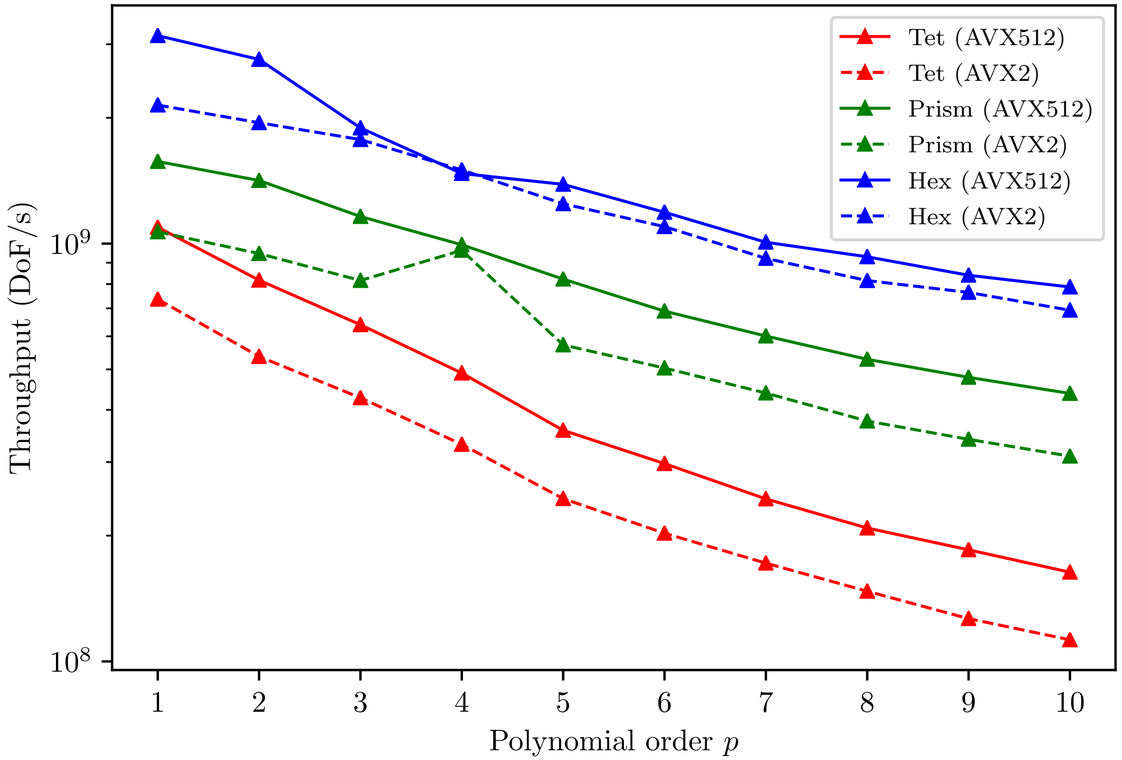


2D: Quads, triangles

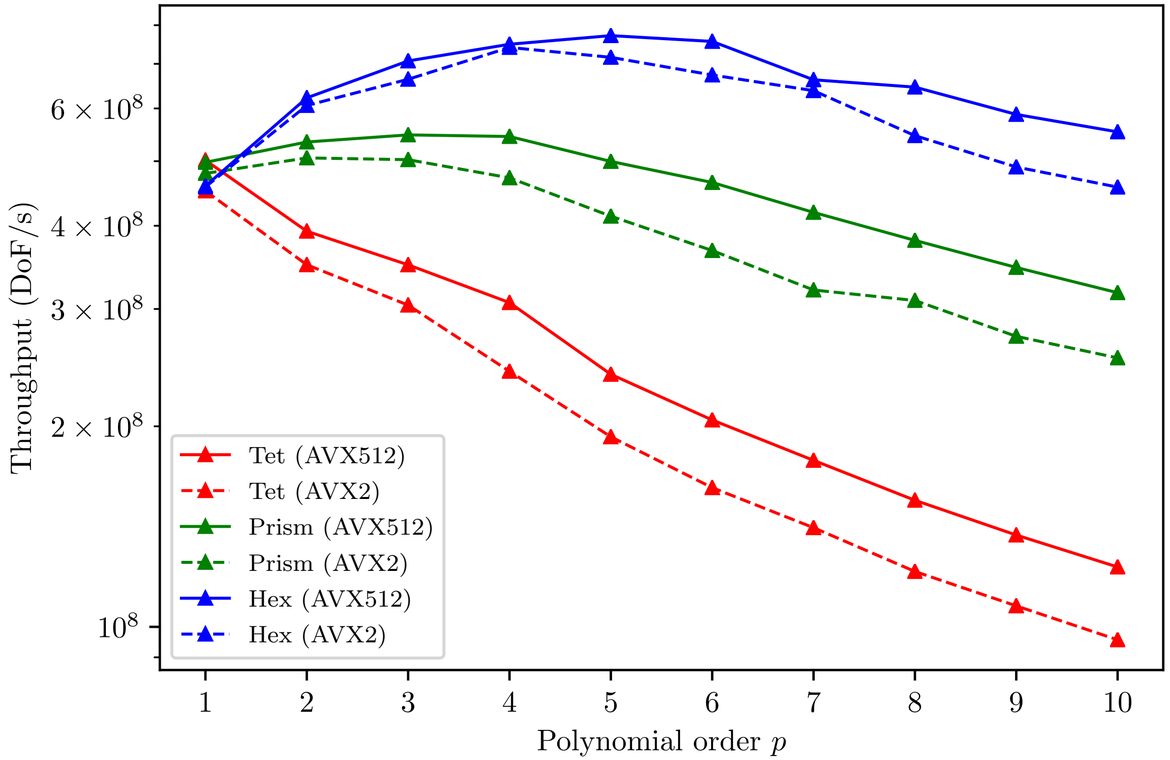


3D: Hexahedra, prisms, tetrahedra

Throughput (AVX512/AVX2, Skylake)



3D: ‘Regular’ elements



3D: ‘Deformed’ elements

Some clear trends

- This behaves pretty much as you might anticipate:
  - For regular elements, clear hierarchy of element type/dimension, where throughput is lost as dimension/complexity of indexing increases.
  - Regular elements outperform deformed elements due to increased memory bandwidth.
  - Relative performance gap between deformed elements decreases at moderate polynomial orders.

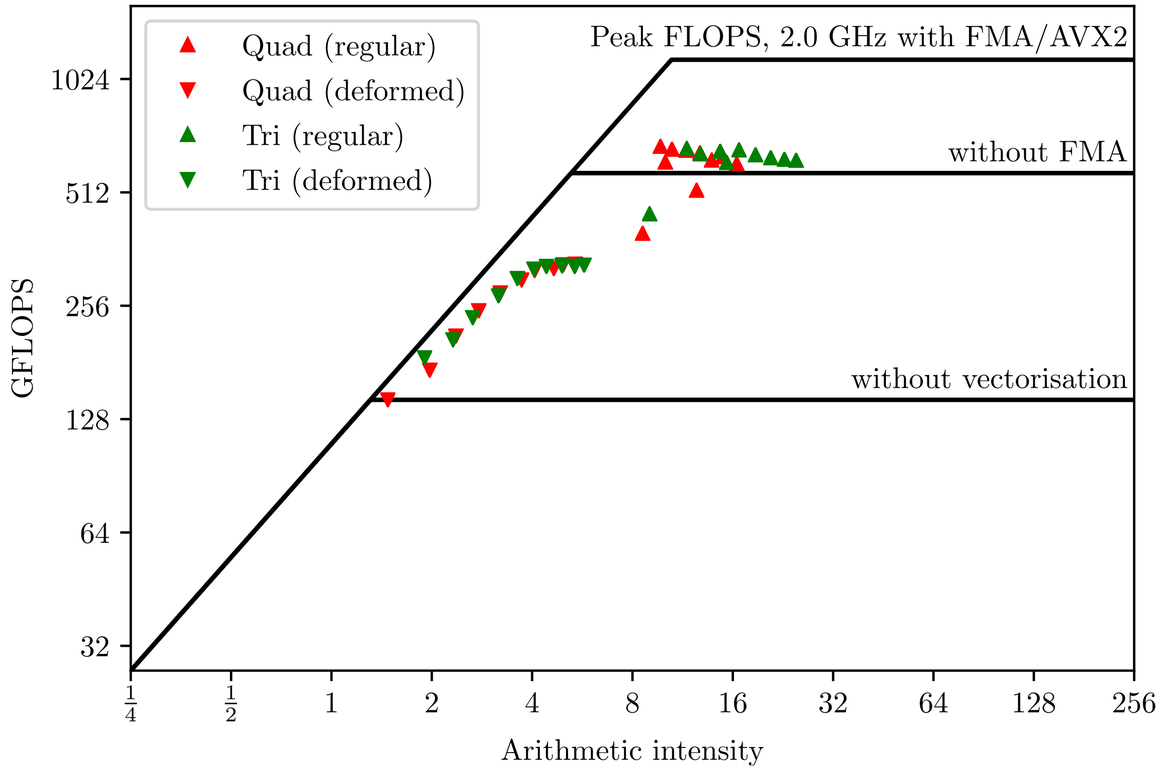
Roofline model

- Roofline modelling should give better indication of ability of kernel to hit peak computational performance:

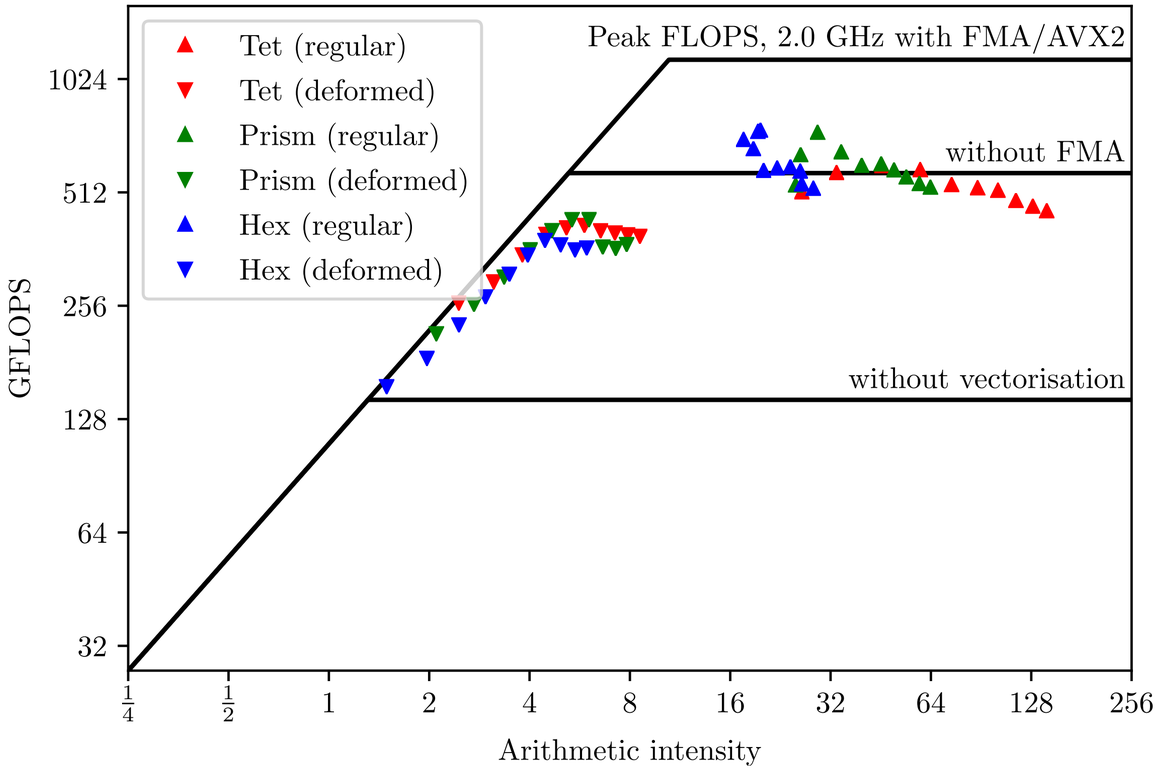
$$\text{Max GFLOPS/s} = \min(\text{peak GFLOPS/s}, \text{peak memory bandwidth} \times \alpha)$$

- Profiled on Broadwell architecture using `likwid` performance profiling tools; hardware counters observed for GFLOPS/s and memory transfer.

Roofline results



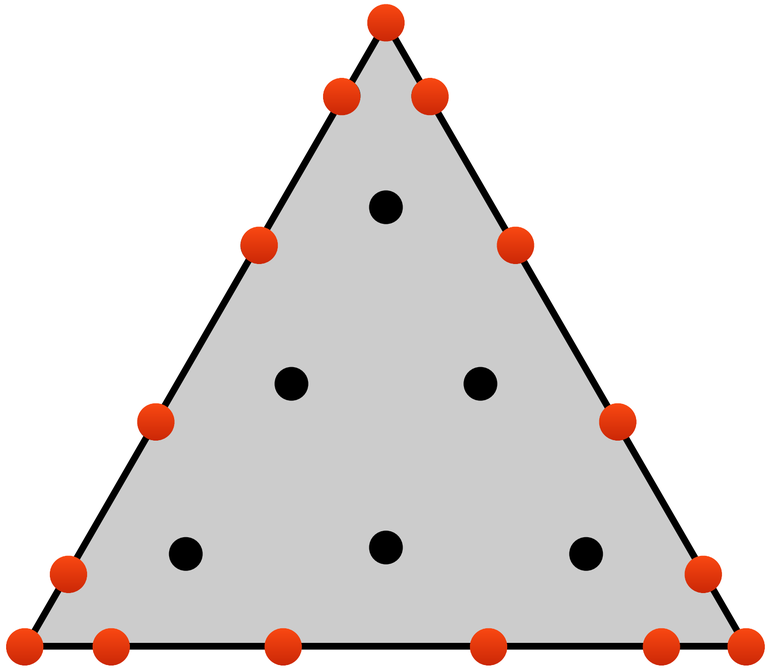
2D: Quads, triangles



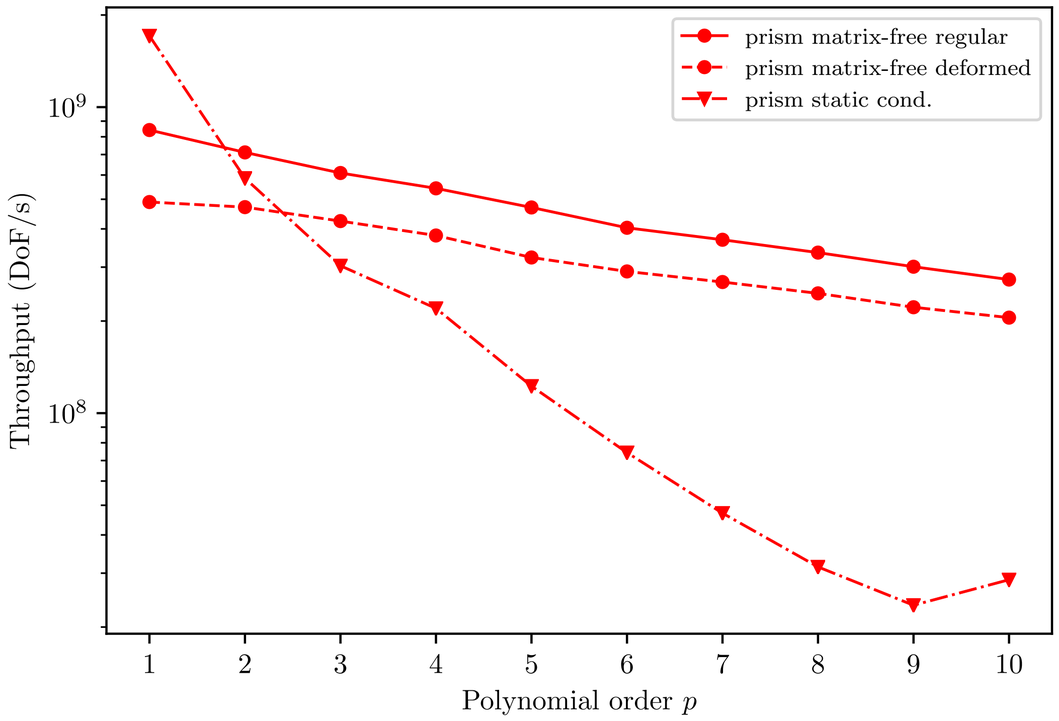
3D: Hexahedra, prisms, tetrahedra

Some comparisons: static condensation

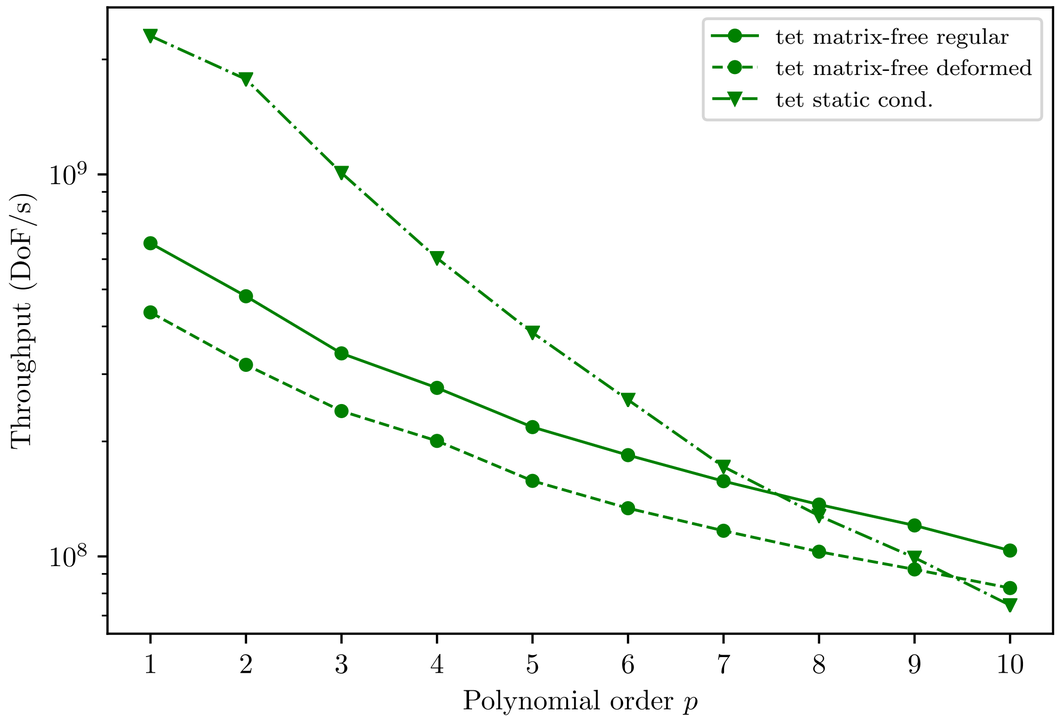
- A common strategy to improve performance when considering high-order elements is **static condensation** (or substructuring).
- Reorder degrees of freedom so that all boundary DoF are first, followed by interior.
- Use Schur complement to form a smaller system to solve on the boundary.
- Loses all tensor product structure, need to use local matrix approach.



Throughput against static condensation



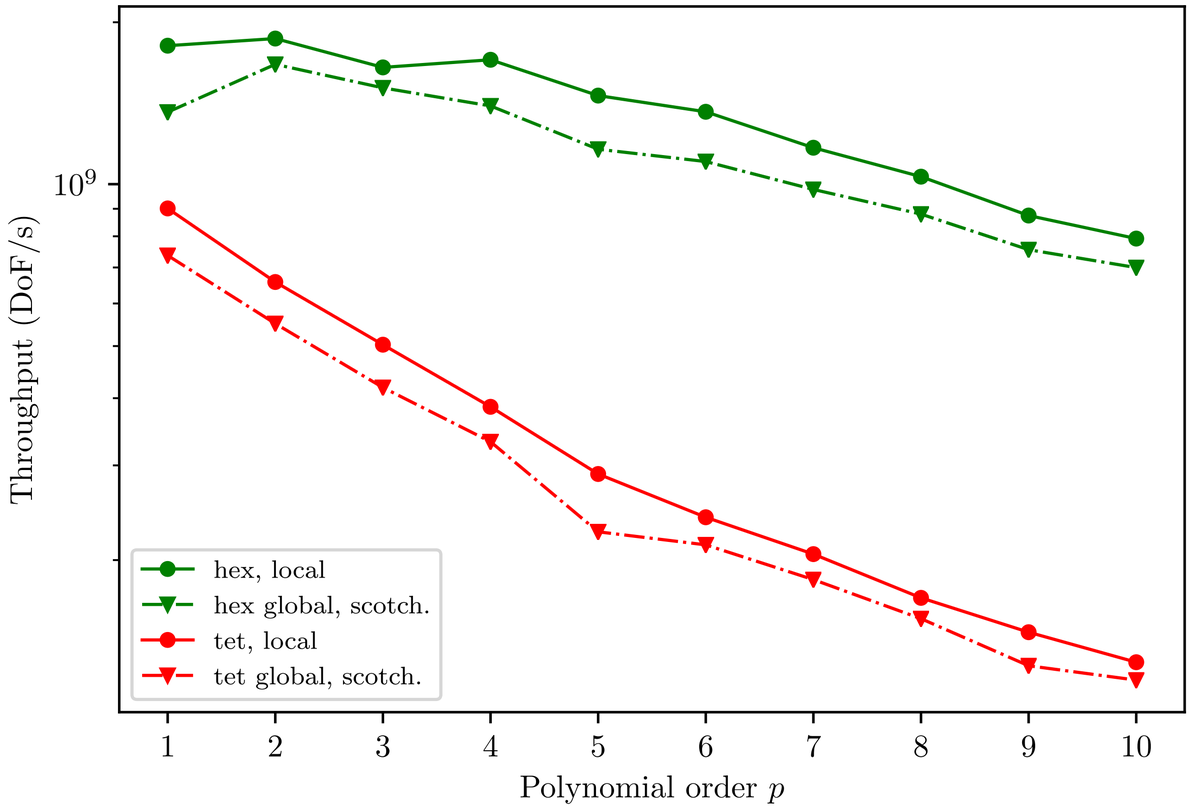
Prisms



Tetrahedra

Work in progress: C^0 operators

- Throughput reduces as expected when taking into account more expensive global assembly.
- However for a constant DoF problem (i.e. change mesh size as a function of polynomial order), cost at higher orders is reduced relative to increased memory requirements.



Summary

- Efficient matrix-free implementations of key finite element operators are certainly achievable on modern architectures for ‘unstructured’ elements.
- Inevitable drop in performance from quads/hexahedra: complexity of indexing, additional cache pressure, etc.
- However relative performance of e.g. hex/prism and quad/tri is actually pretty good, particularly for deformed elements; important for e.g. boundary layer problems with large proportion of BL prisms.
- Future directions: revisit elemental basis formulations.

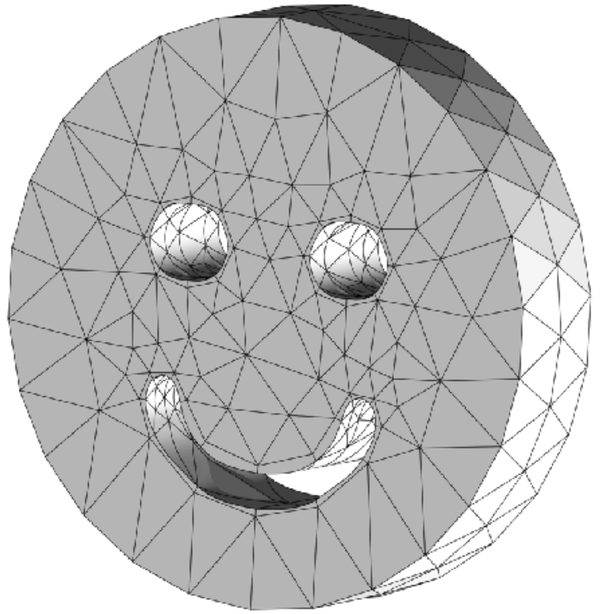
Thanks for listening!

https://davidmoxey.uk/

d.moxey@exeter.ac.uk

www.nektar.info

https://prism.ac.uk/



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Nektar++: enhancing the capability and application of high-fidelity spectral/*hp* element methods

David Moxey[1], Chris D. Cantwell[2], Yan Bao[3], Andrea Cassinelli[2], Giacomo Castiglioni[2], Sehun Chun[4], Emilia Juda[2], Ehsan Kazemi[4], Kilian Lackhove[6], Julian Marcon[2], Gianmarco Mengaldo[7], Douglas Serson[2], Michael Turner[2], Hui Xu[5,2], Joaquim Peiró[2], Robert M. Kirby[8], Spencer J. Sherwin[2]