h-to-*p* efficiently: the use of collections with accelerators within Nektar++

D. Moxey
College of Engineering, Maths & Physical Sciences, University of Exeter

C. Cantwell, S. J. Sherwin
Department of Aeronautics, Imperial College London

R. M. Kirby
Scientific Computing and Imaging Institute, University of Utah

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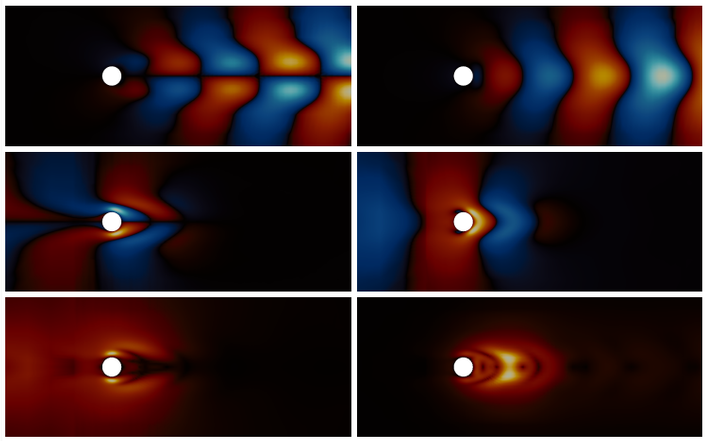
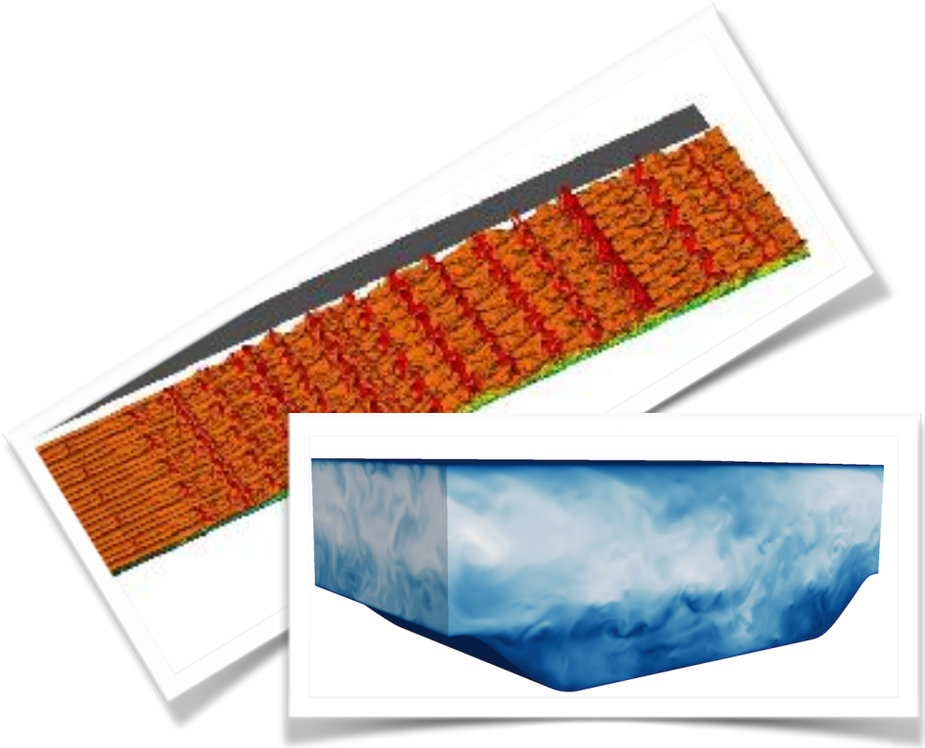
Outline

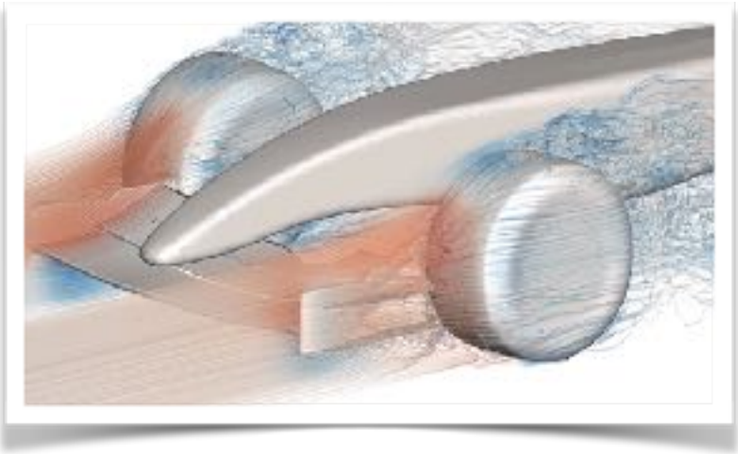
- Nektar++ & spectral/*hp* method
- Challenges for KNL
- Collections & `libxsmm`
- Summary

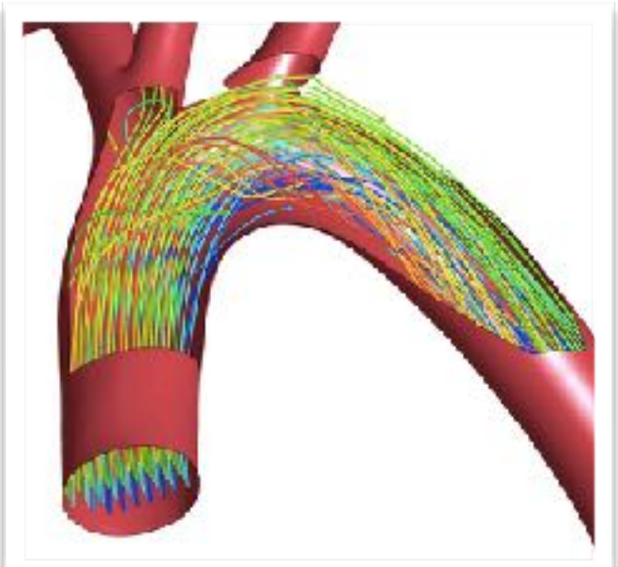
Nektar++ goals

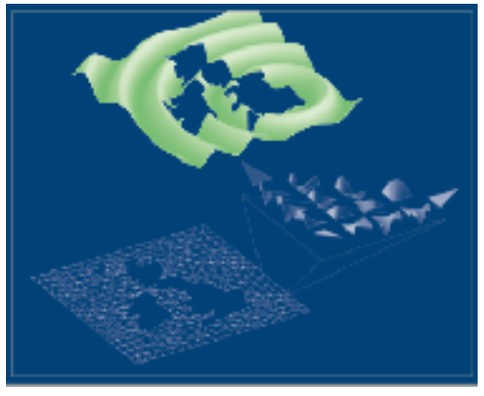
- Make it simpler/quicker to create high-order solvers for a range of fields and applications (including CG/DG/HDG)
- Support 1/2/3D and **unstructured hybrid meshes** for complex geometries: tets, prisms, etc.
- Scale to large numbers of processors
- Be efficient across a range of polynomial orders and core counts
- Bridge current and future hardware diversity

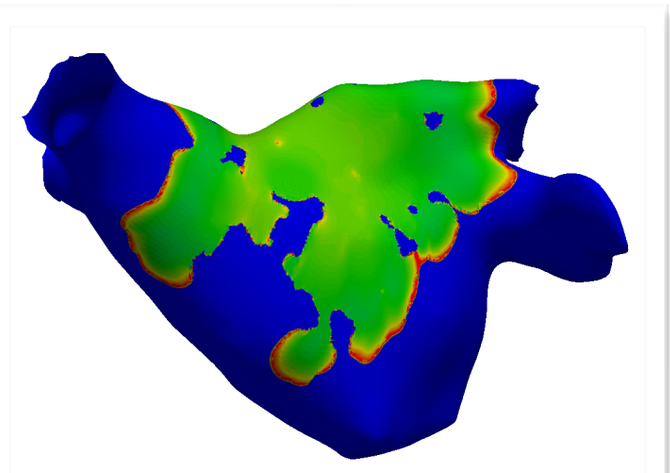


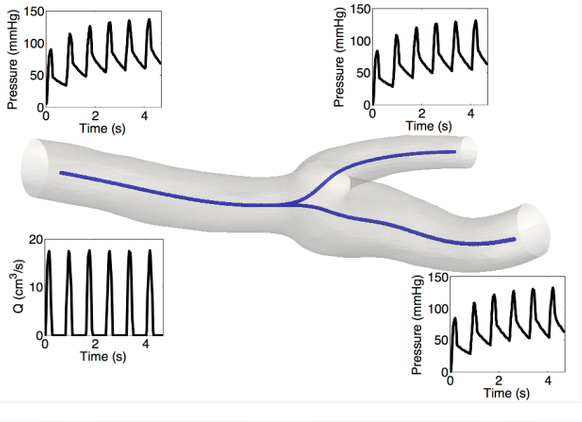











Pressure (mmHg)
150
100
50
0
0
2
4
Time (s)
Pressure (mmHg)
150
100
50
0
0
2
4
Time (s)
Q (cm3/s)
20
10
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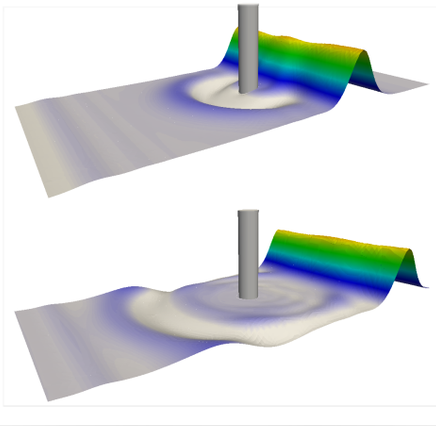
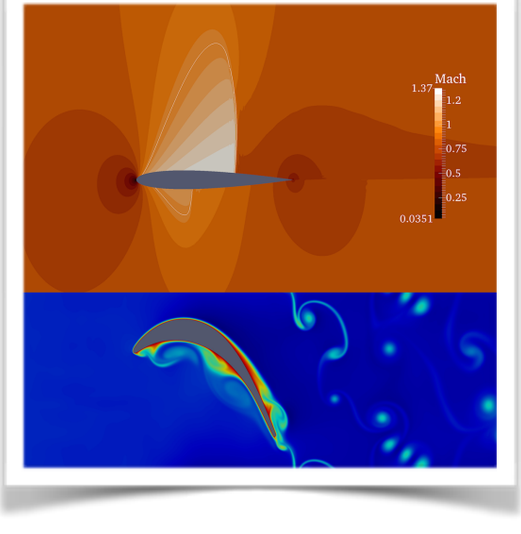
4
Time (s)
Pressure (mmHg)
150
100
50
0
0
2
4
Time (s)




Mach
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1.2
1
0.75
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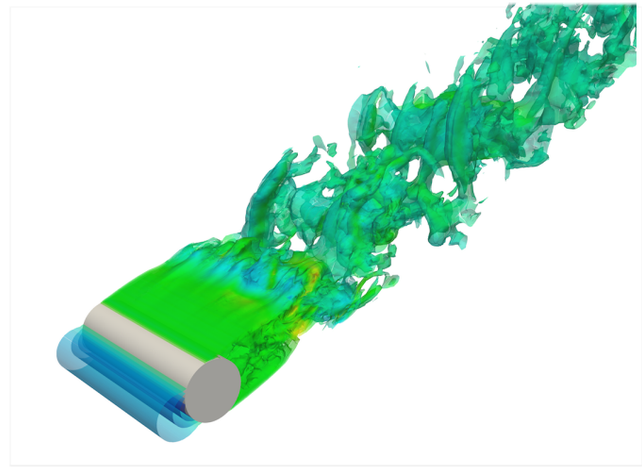
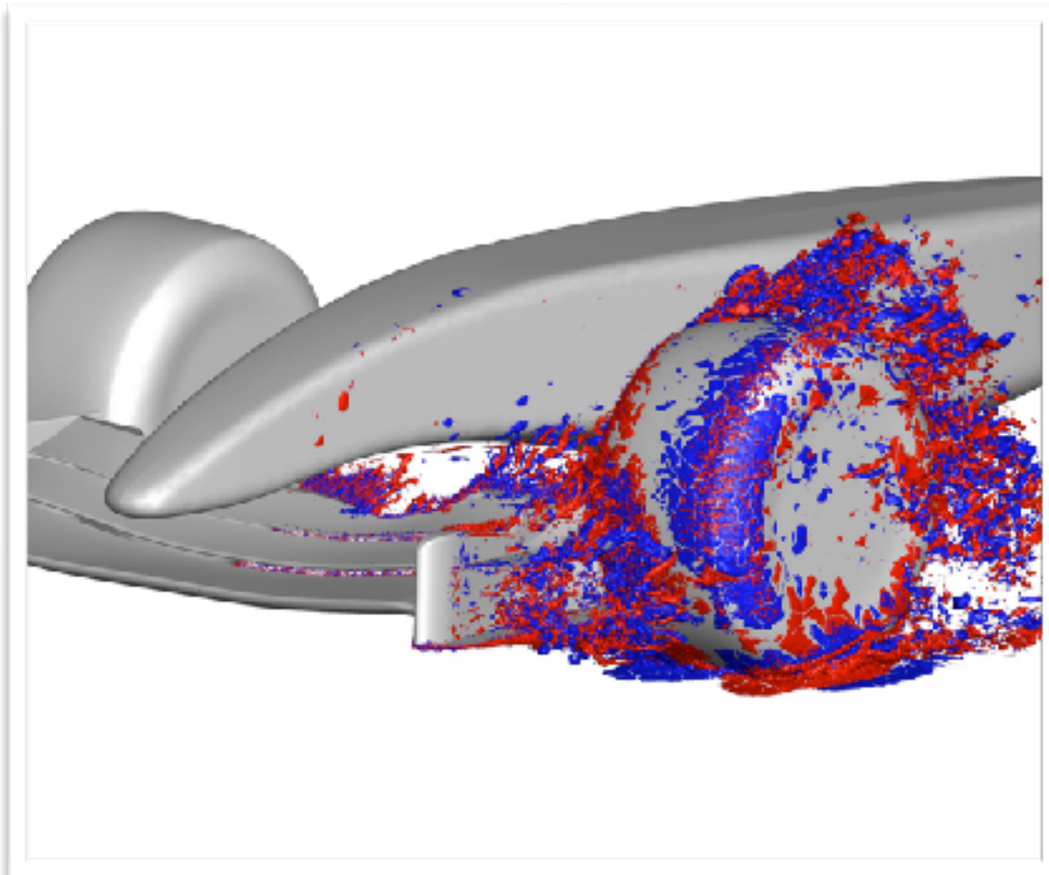
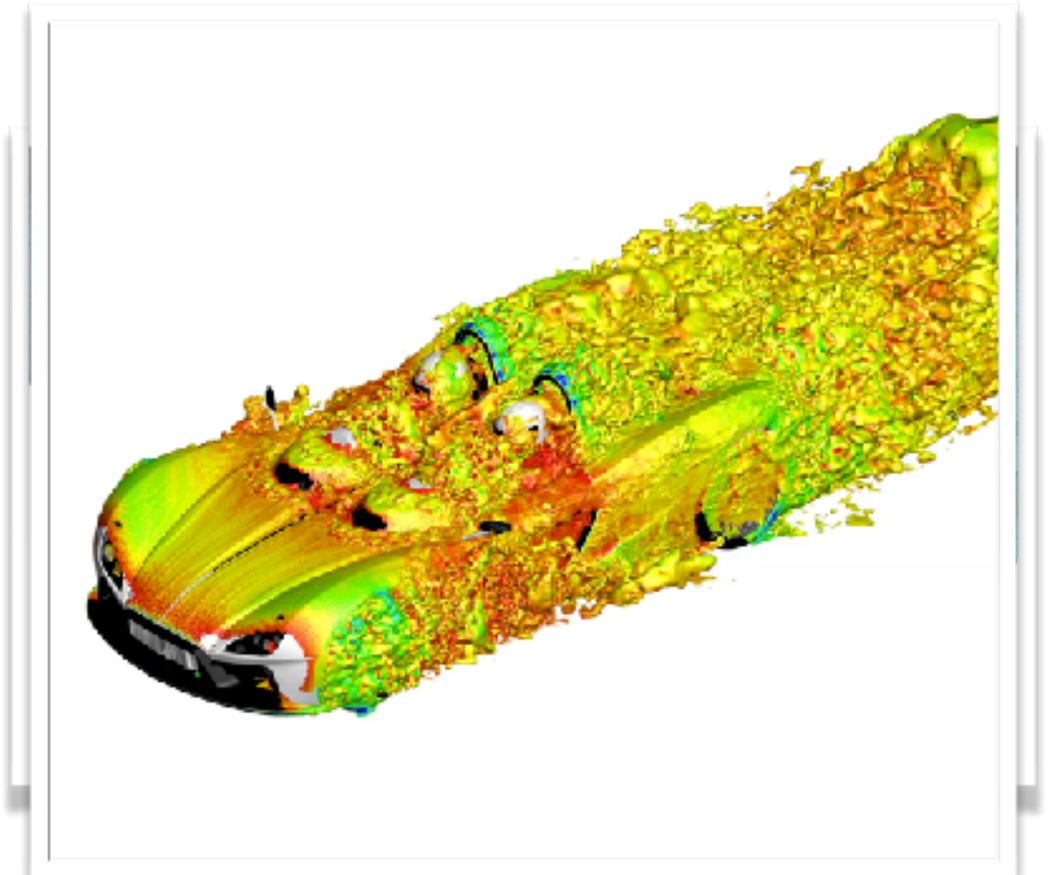
0.25
0.0351



Unstructured simulations

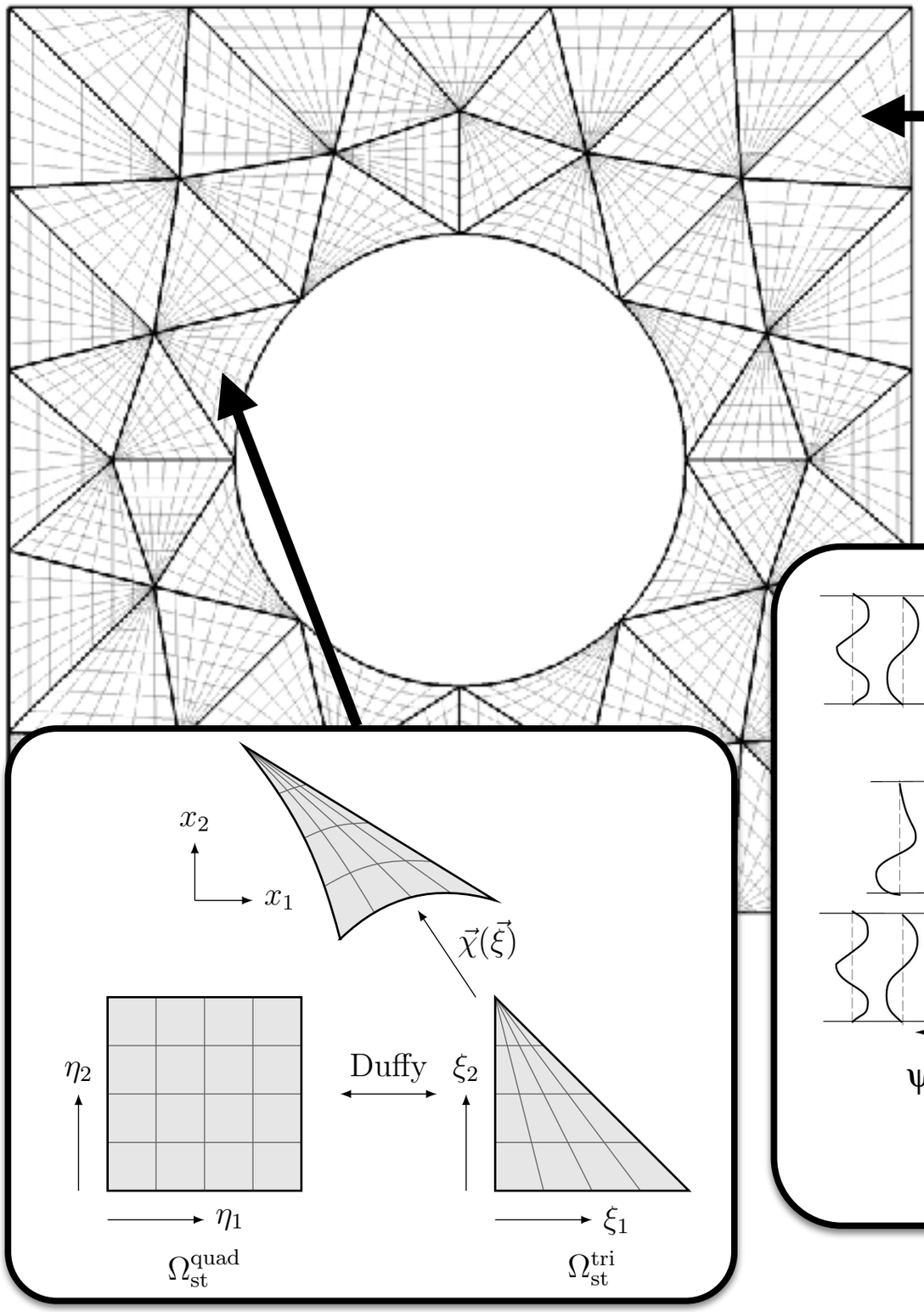
Common knowledge that hexes yield best performance



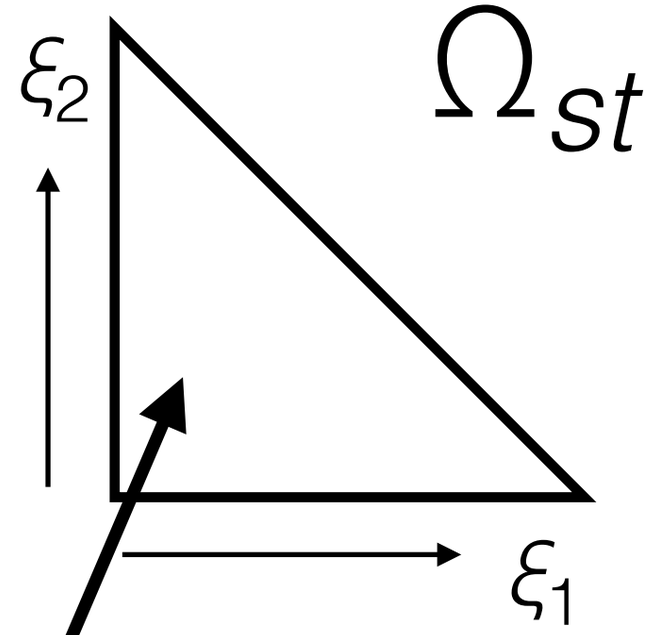


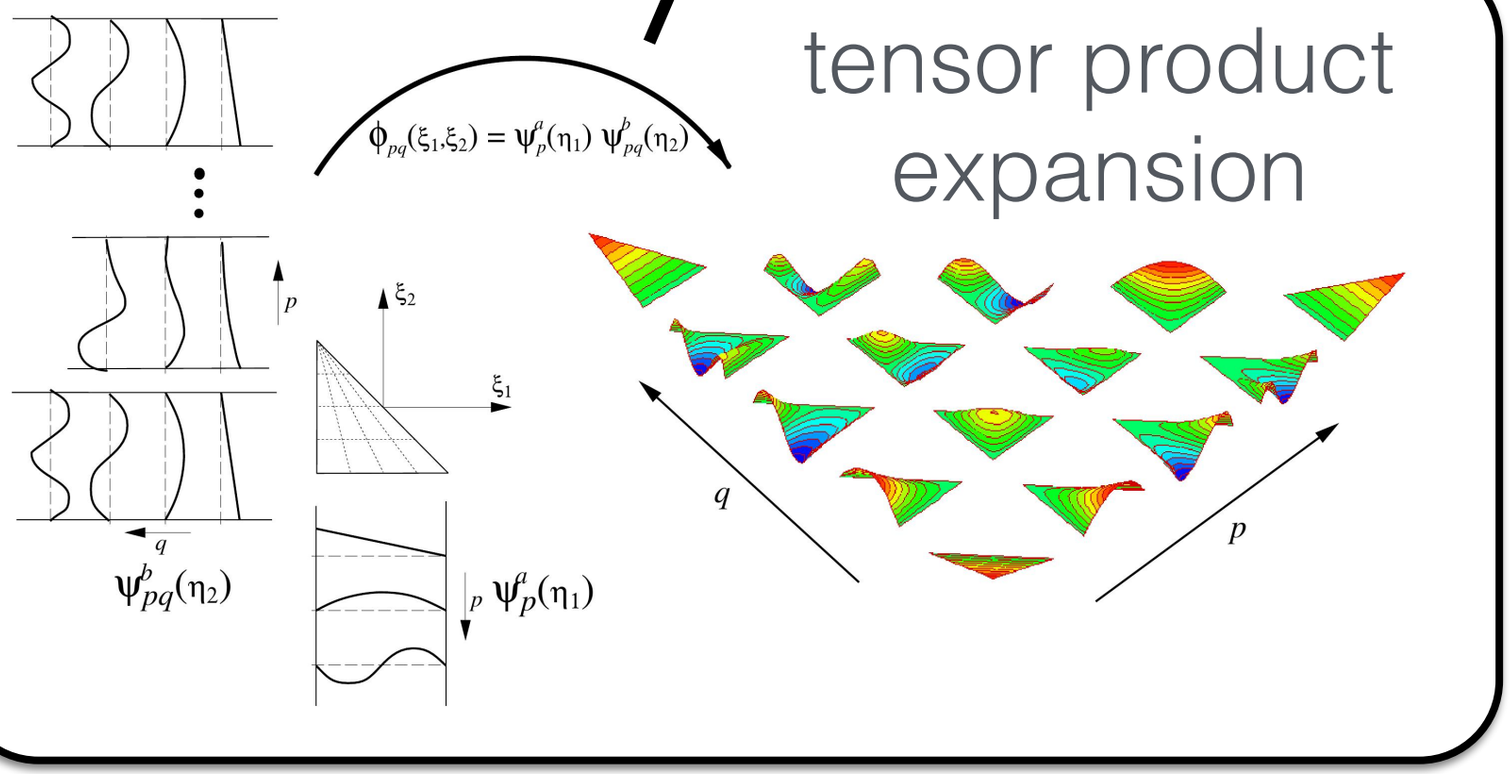
Complex geometries presently **require** unstructured meshes - how to improve performance?

Spectral/*hp* element method



map from reference element



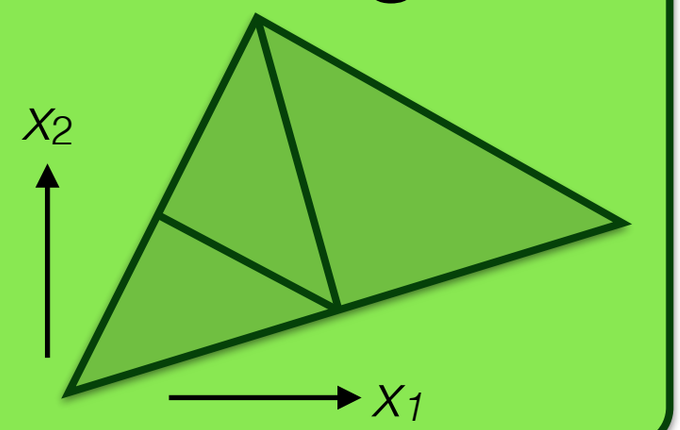


Framework design

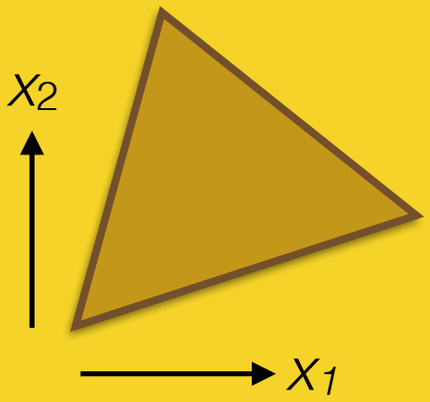
$$u^{\delta} = \sum_i \hat{u}_i \Phi_i(x)$$

$$u_e^{\delta} = \sum_p \hat{u}_p \phi_p(x)$$

MultiRegions



LocalRegions



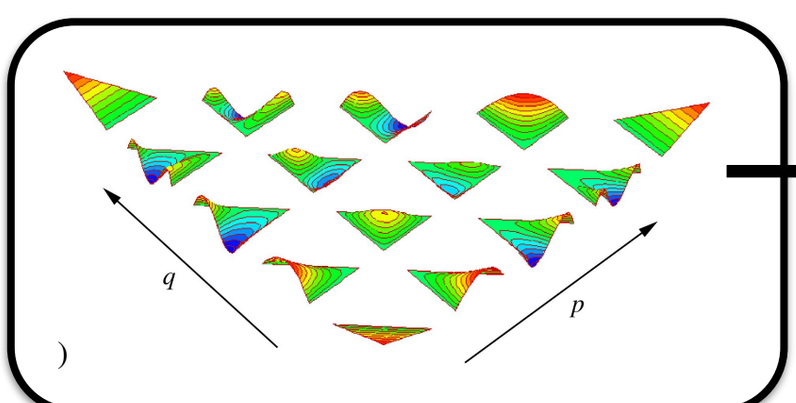
SpatialDomains

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

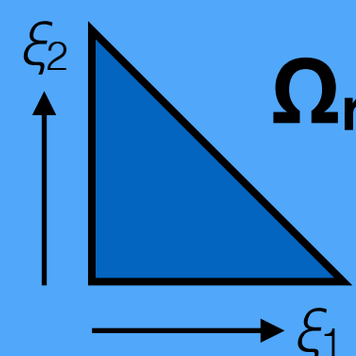
$$\frac{\partial x_i}{\partial \xi_j} \quad \frac{\partial \xi_i}{\partial x_j}$$

$$\mathrm{f}[i] = \int_{\Omega} f(x)\Phi_i(x)\,dx$$

$$\mathrm{f}[i] = \sum_{e=1}^{N_{\mathrm{el}}} \int_{\Omega^e} f(x)\psi_i^e(x)\,dx$$



StdRegions



"Defining" features

Generally *not* collocated

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

quadrature points

modal coefficients

Uses tensor products of 1D basis functions, *even for non-tensor product shapes*, but indexing harder

$$u(\xi_{1i}, \xi_{2j}, \xi_{3k}) = \sum_{p=1}^{P} \sum_{q=1}^{Q-p} \sum_{r=1}^{R-p-q} \hat{u}_{pqr} \phi^a_p(\xi_{1i}) \phi^b_{pq}(\xi_{2j}) \phi^c_{pqr}(\xi_{3k})$$

Sum-factorisation

Essential for performance at high polynomial orders

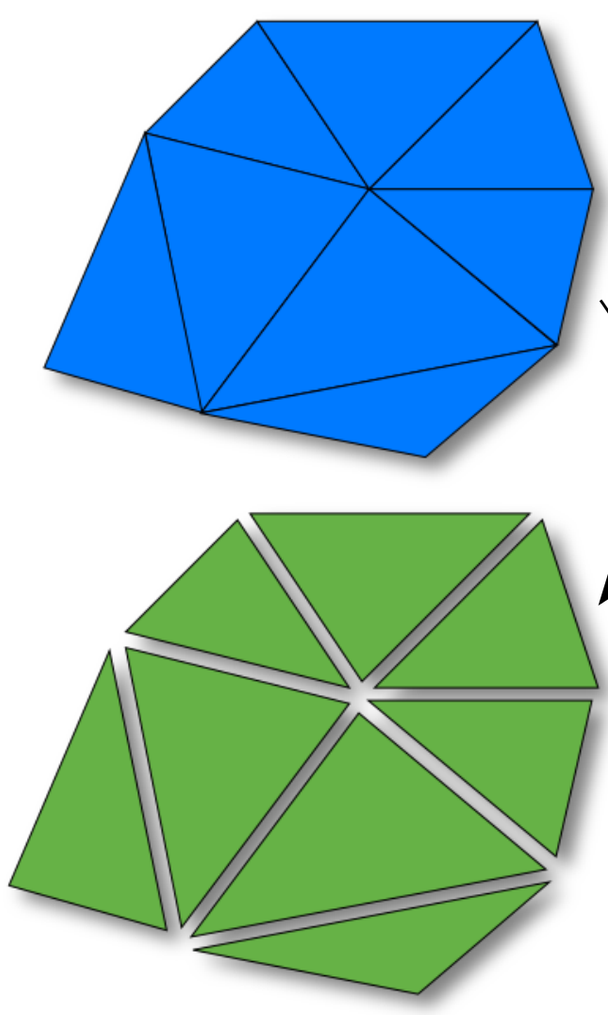
$$\sum_{p=1}^{P}\sum_{q=1}^{Q}\hat{u}_{pq}\phi_p(\xi_{1i})\phi_q(\xi_{2j}) = \sum_{p=1}^{P}\phi_p(\xi_{1i})\left[\sum_{q=1}^{Q}\hat{u}_{pq}\phi_q(\xi_{2j})\right]$$

store this

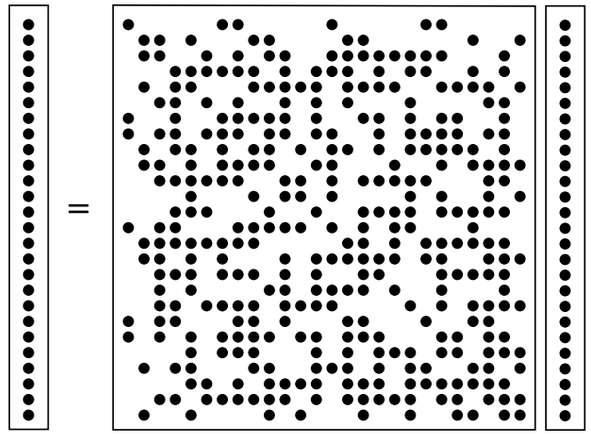
2D: $O(P^4) \rightarrow O(P^3)$ 3D: $O(P^6) \rightarrow O(P^4)$

We **can also do this** for tris, tets, prisms... but have to cope with harder indexing and smaller matrices

Implementation choices

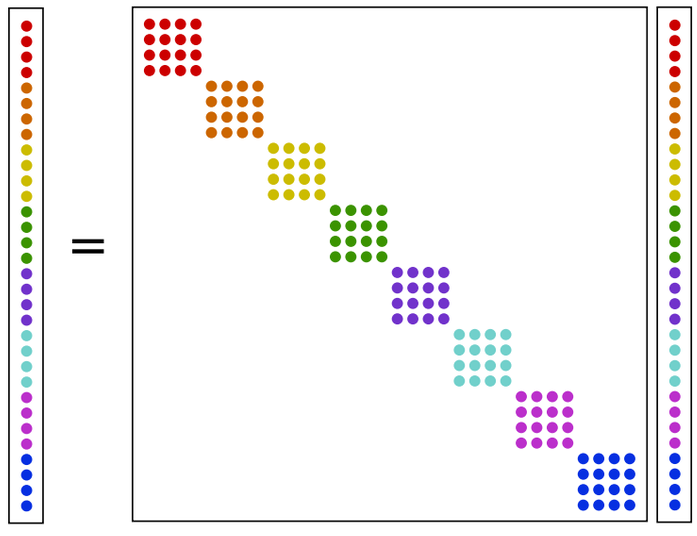


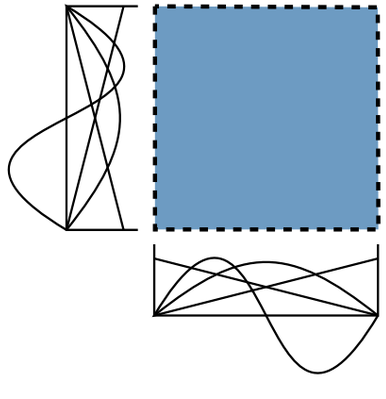
Global Strategy



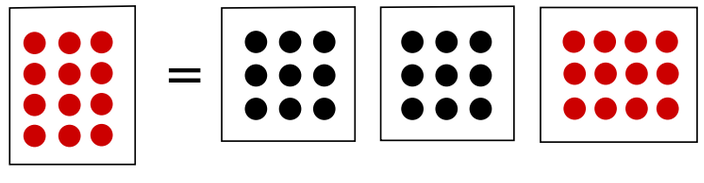
$\mathcal{A}$

Local Strategy





Sum-factorisation



Increasing polynomial order

More localised memory access

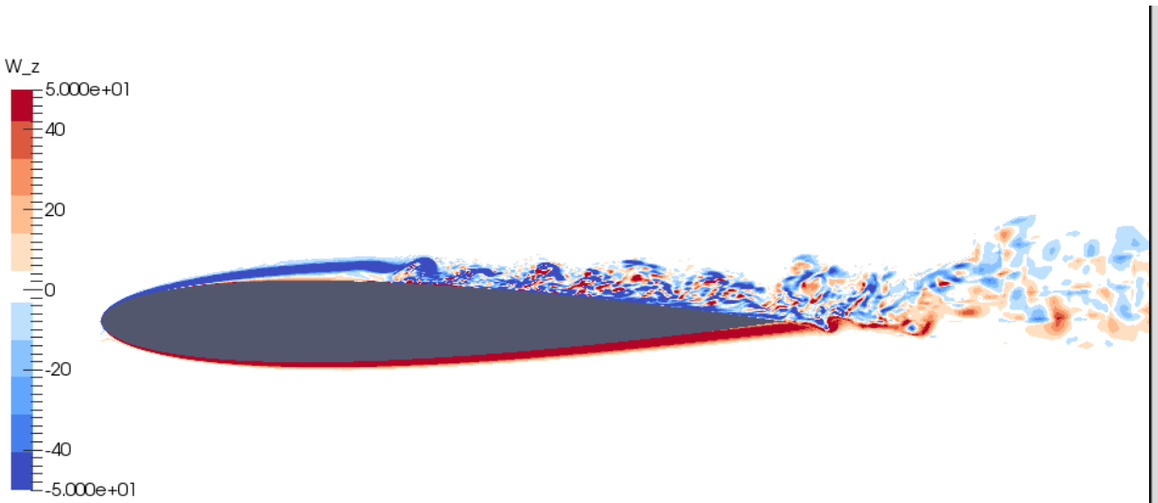
h-to-*p* efficiently

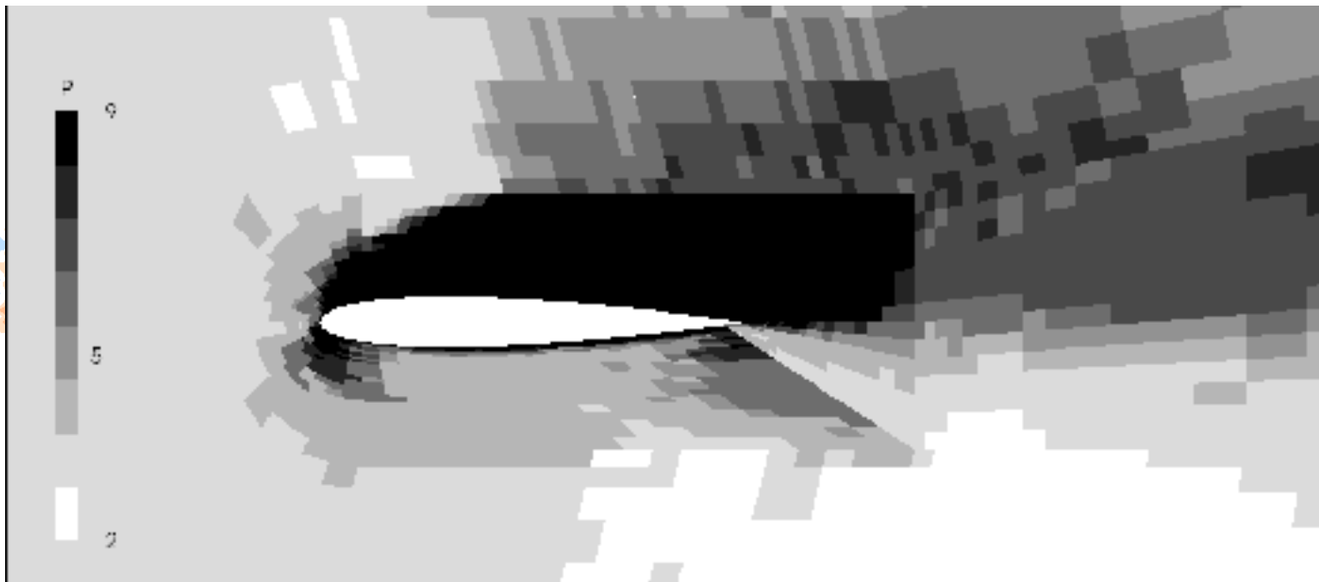
Why do we care about having *all* these approaches?

- Approach performance varies wildly depending on many factors that are not *a priori* determinable

- Allow us to explore the space of flops/byte ratio

- Also important for e.g. variable-*p* simulations





Challenges for KNL

- Nektar++ written in C++ (surprise!), uses abstraction, inheritance and OO heavily
  - ✔ Great for writing code & rapid prototyping
  - ✘ Hard to make it highly performant
  - ✘ Also hard to track/control memory usage

- Handing memory
  - ➡ DRAM vs. MCDRAM or host vs. device
  - ➡ Making this transparent to solver developers

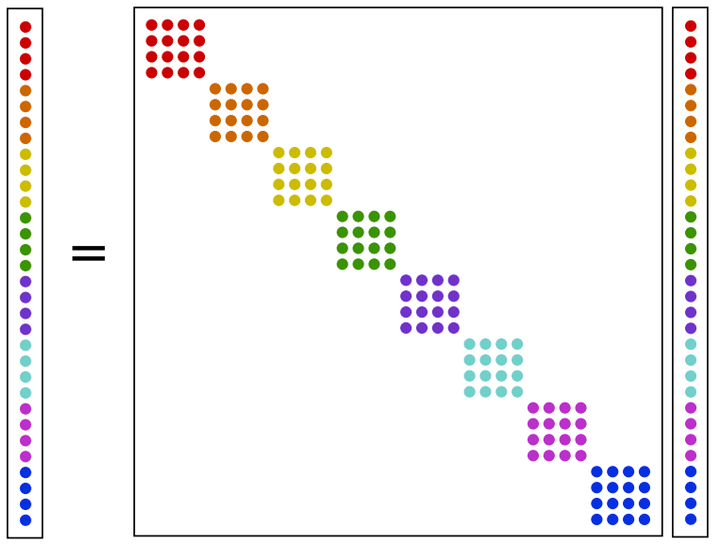
- Threading and SIMD vectorisation

Collections

- Reformulate implementation choices into kernel operations over multiple elements
- Group geometric terms $\frac{\partial x_i}{\partial \xi_j}$
- Focus around key components of Laplacian:
  - ➡ Backward transformation: $u_e^\delta = \sum_p \hat{u}_p \phi_p(x)$
  - ➡ Inner product: (Φ_i, Φ_j)
  - ➡ Derivatives: $\partial u / \partial x_i$
  - ➡ Inner product w.r.t. derivative: $(\Phi_i, \nabla \Phi_j)$

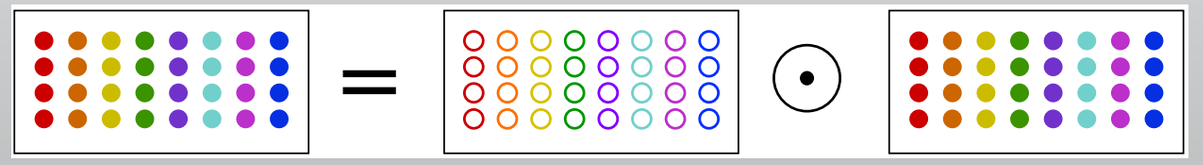
Schemes

Local Matrix

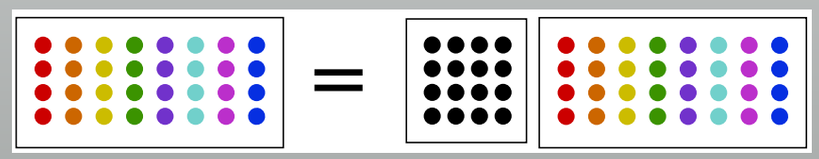


StdMat (standard matrix)

1. Apply Jacobian **(L1)**

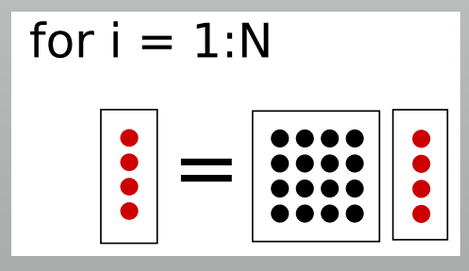


2. Multiply by ref. matrix **(L3)**



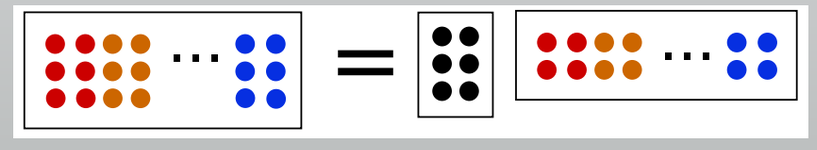
IterPerExp

1. Apply Jacobian **(L1)**
2. Apply local sum fact. **(N x L3)**

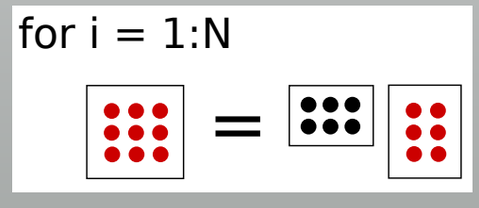


SumFac

1. Apply Jacobian **(L1)**
2. Mult. first dimension **(L3)**



3. Mult. second dimension **(N x L3)**

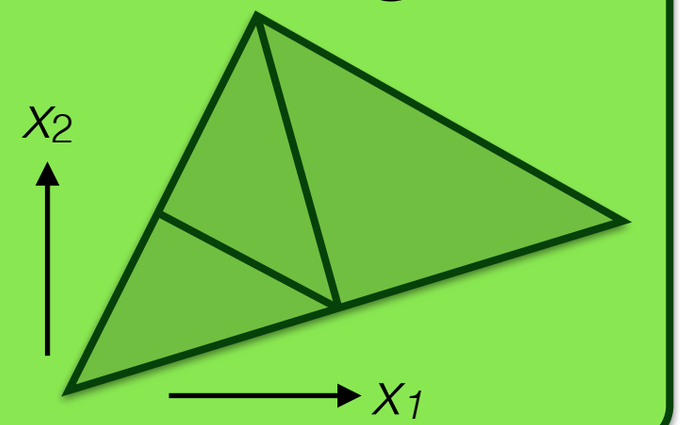


Collections

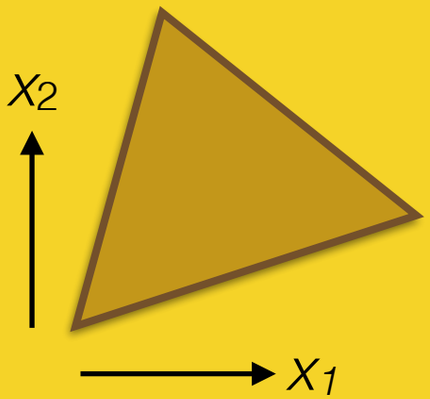
$$u^{\delta} = \sum_i \hat{u}_i \Phi_i(x)$$

$$u_e^{\delta} = \sum_p \hat{u}_p \phi_p(x)$$

MultiRegions



LocalRegions

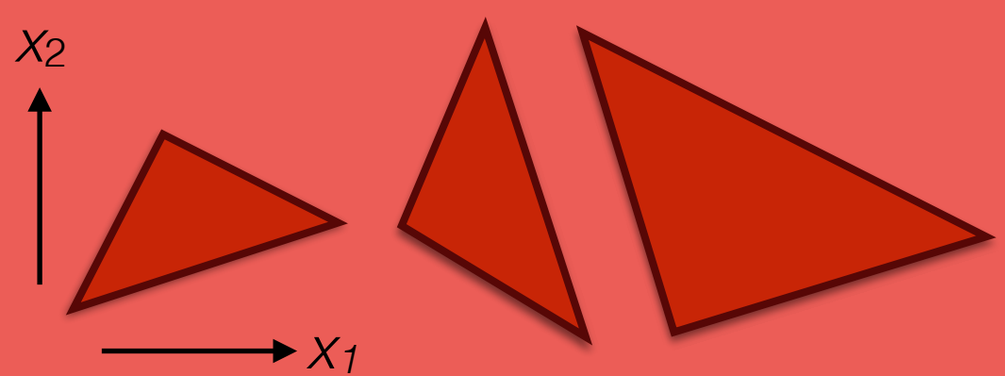


SpatialDomains

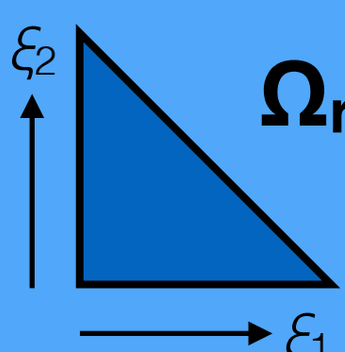
$$\mathbf{x} = X^e(\xi)$$

$$\frac{\partial x_i}{\partial \xi_j} \quad \frac{\partial \xi_i}{\partial x_j}$$

Collections

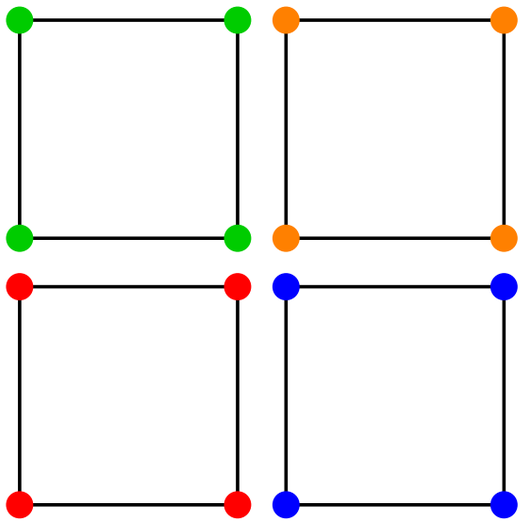


StdRegions

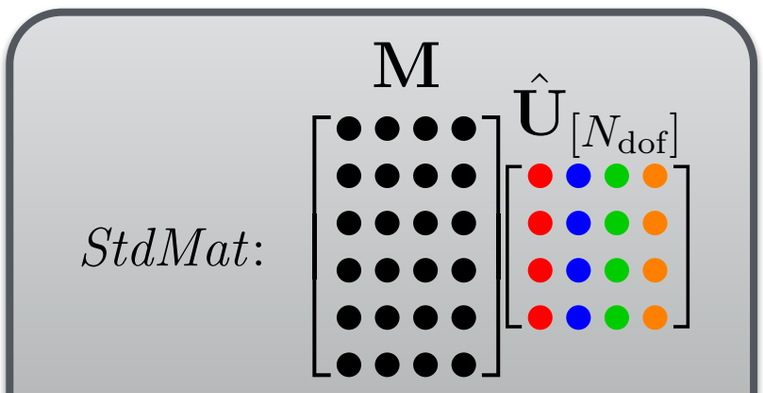


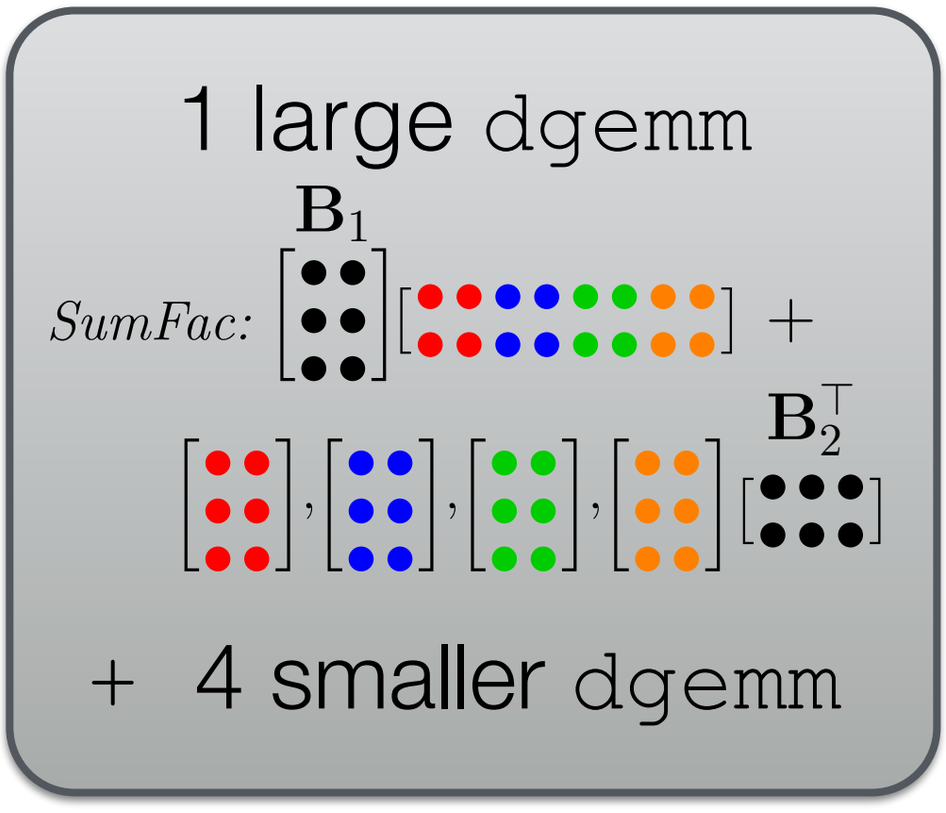
Collections

Use BLAS calls throughout



4 quad mesh





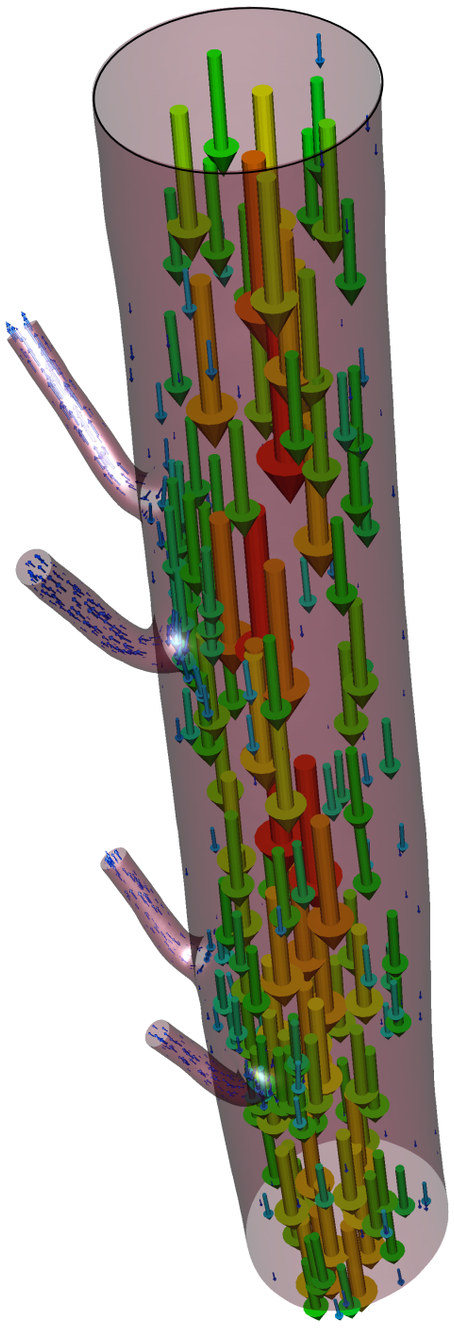
Can also do this for non-TP elements:
data ordering harder, matrices smaller (bad for BLAS)

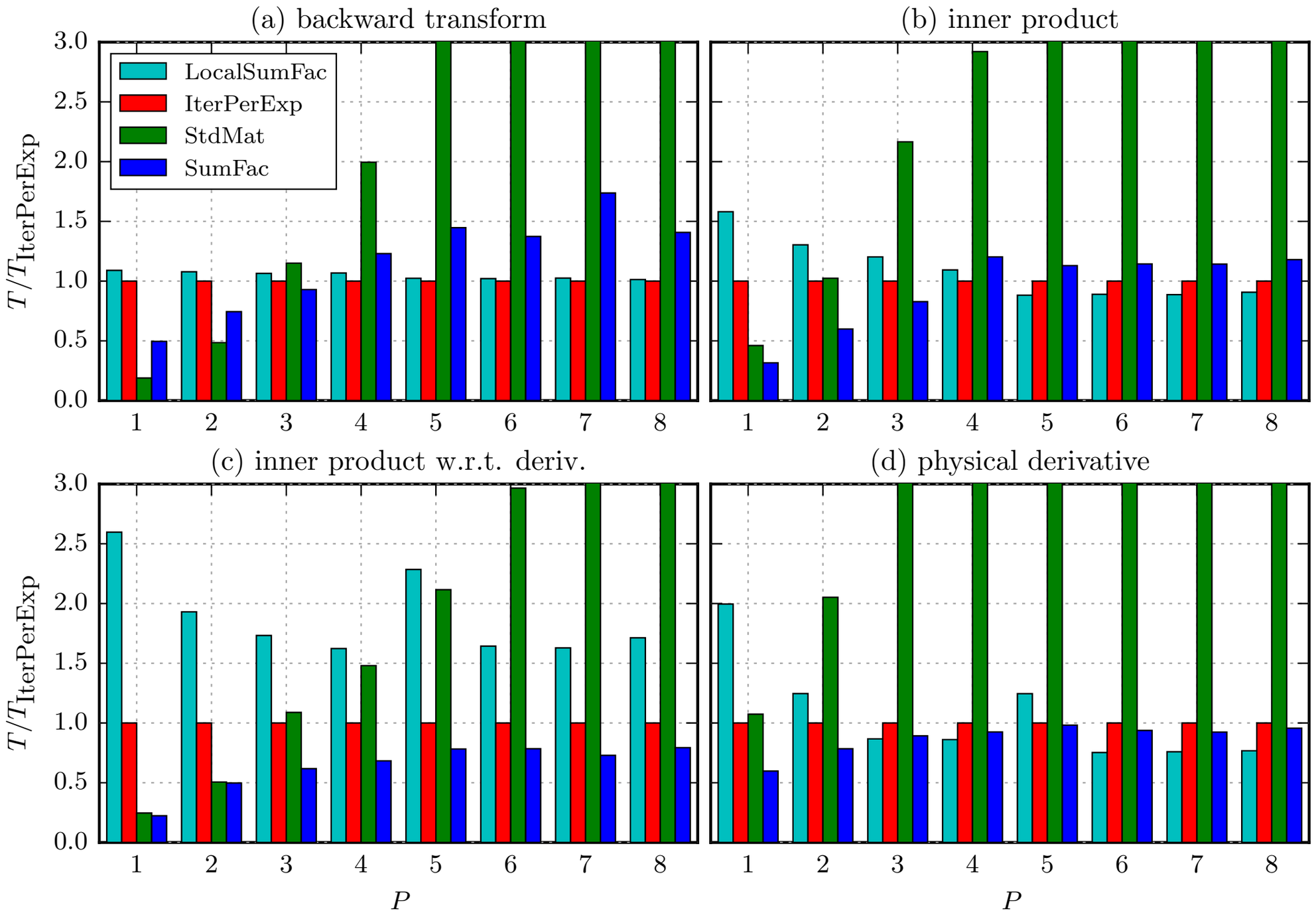
Test case

Intercostal pair

21k prisms

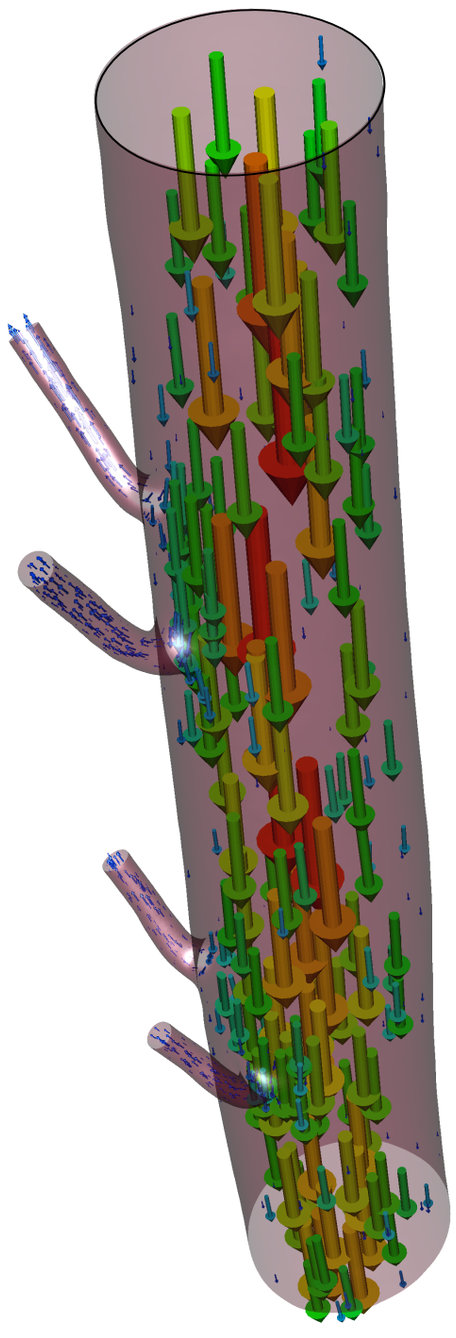
41k tets

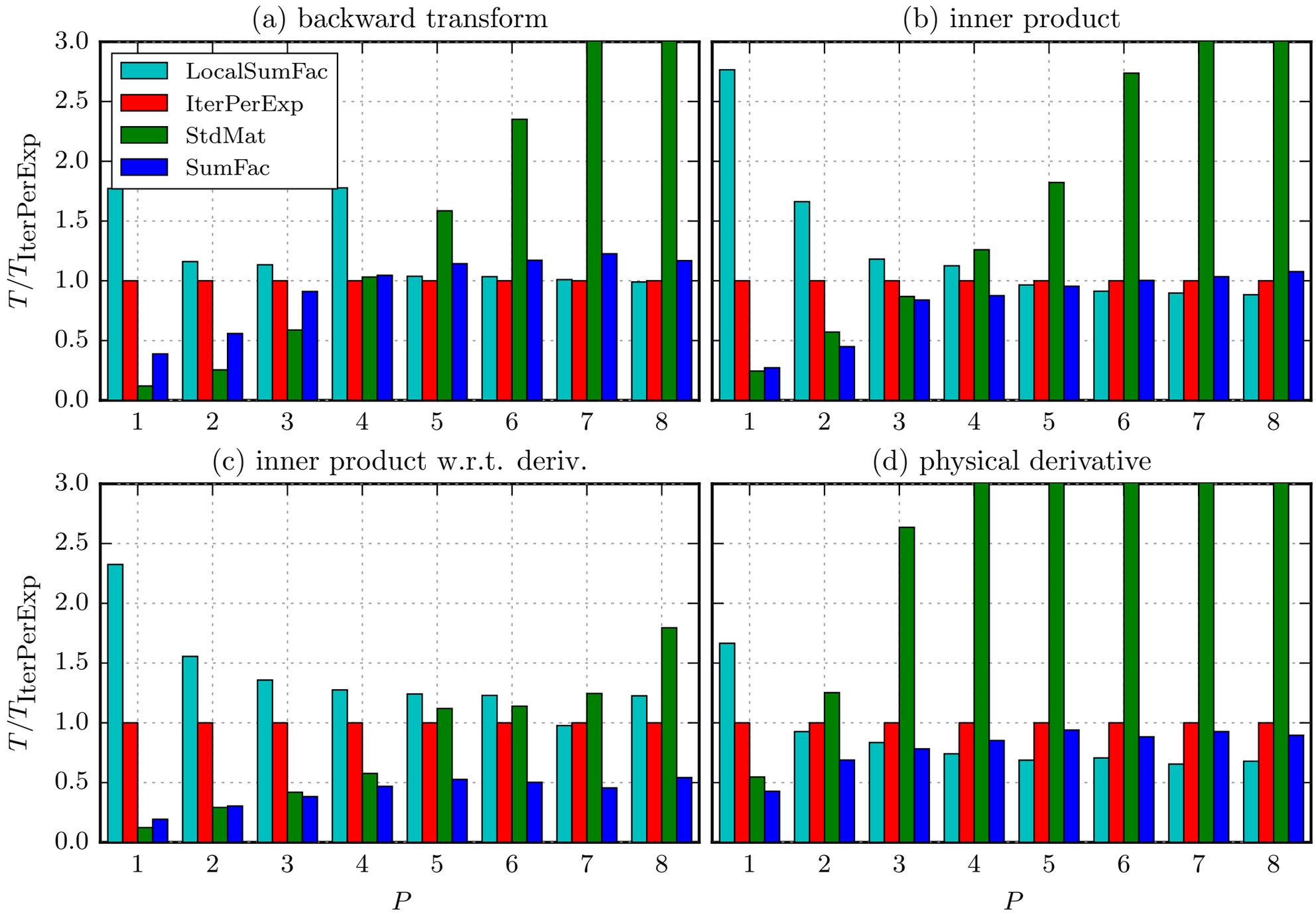




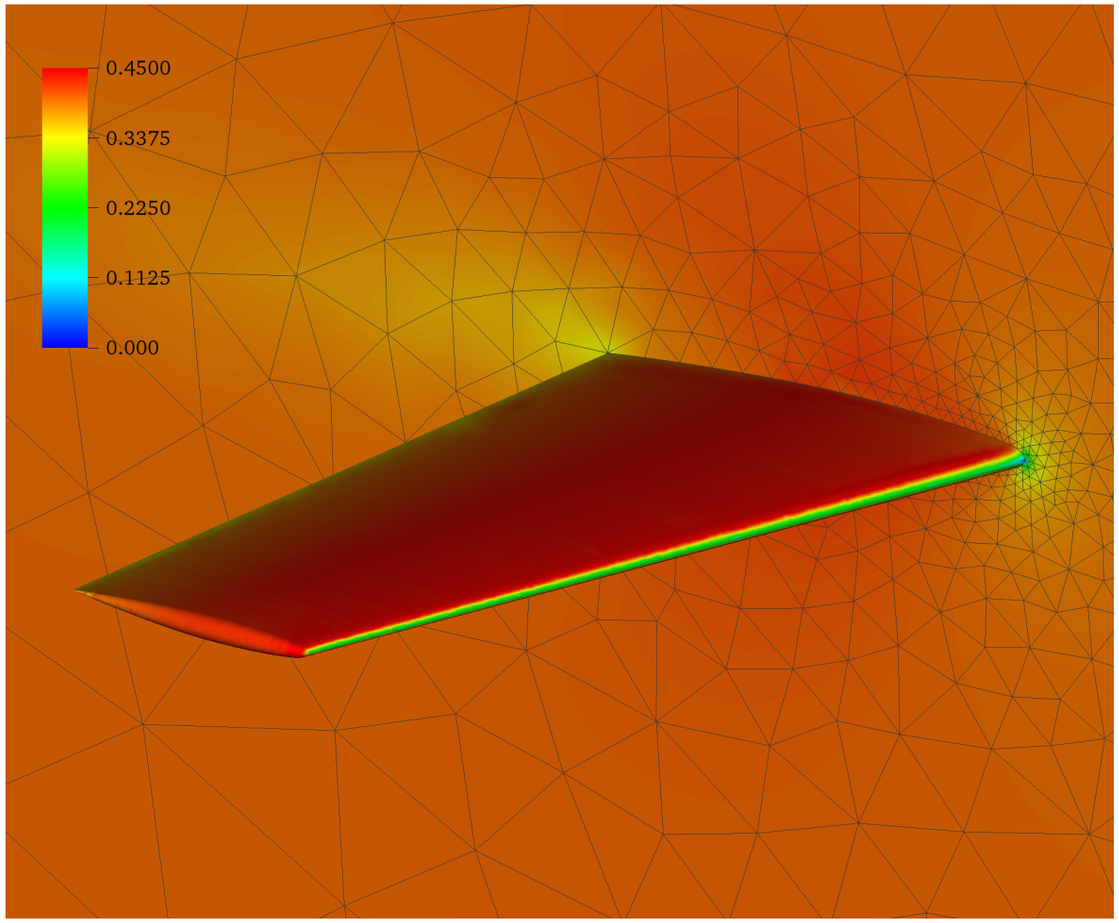
Test case

Intercostal pair
21k prisms
41k tets





Example: ONERA M6 wing



		Scheme timings [s]			
Machine	Operator	*LocalSumFac*	*IterPerExp*	*StdMat*	*SumFac*
`cx2`	BwdTrans	0.00213393	0.00209944	**0.000202192**	0.000534608
	IProductWRTBase	0.00245141	0.00200234	**0.000233064**	0.000521411
	IProductWRTDerivBase	0.0266448	0.017248	**0.00201284**	0.00298702
	PhysDeriv	0.00485056	0.00492247	0.00389733	**0.00319892**
`ARCHER`	BwdTrans	0.000643393	0.000638955	**2.36882e-05**	4.74285e-05
	IProductWRTBase	0.000754697	0.000712303	**2.78743e-05**	0.000150587
	IProductWRTDerivBase	0.00827777	0.00530682	**0.00019947**	0.000643919
	PhysDeriv	0.00075556	0.000595179	**0.000287773**	0.000318533

	Wall-time per timestep [s]		
Machine	*LocalSumFac*	Auto-tuned collections	Improvement
`ARCHER`	1.308	0.744	43%
`cx2`	0.356	0.135	62%

Runtime improvement: 40-60%

Compressible Euler flow

Fully explicit, $P = 2$, 960 cores, ~150k tets

Inner product w.r.t derivative very important

libxsmm

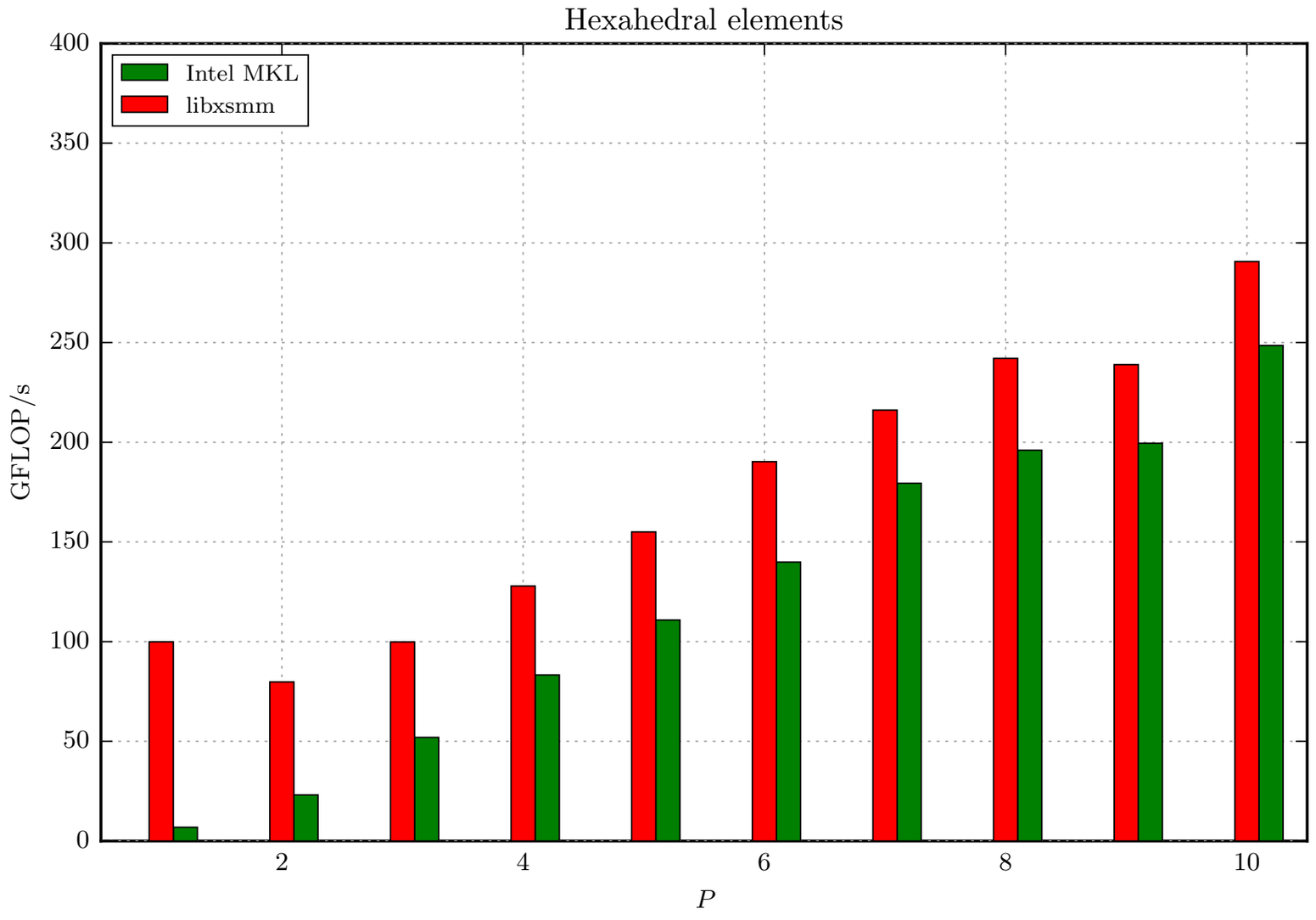
- Most of the matrix-matrix multiplies done in collections are small, at least in one rank

- libxsmm yields encouraging performance gains over standard MKL/BLAS, particularly for non-TP elements

- **Challenge:** our existing calls frequently use transposes - need to reorder/pretranspose

  ➡ This is very challenging for non-tensor product elements (tris/tets/etc)

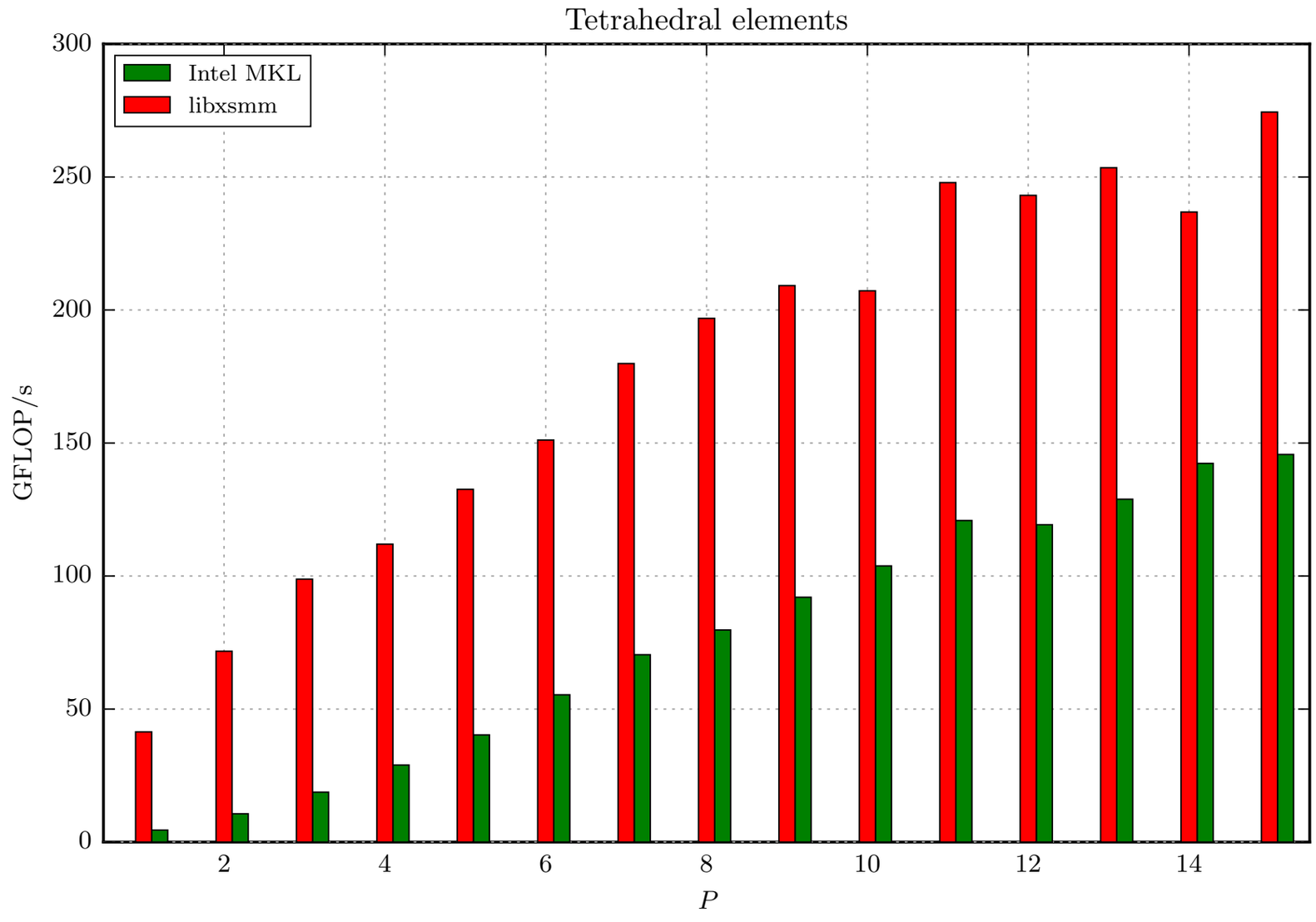
GFLOP/s performance



2 x Intel E5-2670v3
theoretical peak ~1TFLOP/s

~20-40% improvements
in both flops & runtime
over MKL

GFLOP/s performance



Higher performance gains
Recovers hex performance

Requires us to
reorder local coefficients

Summary

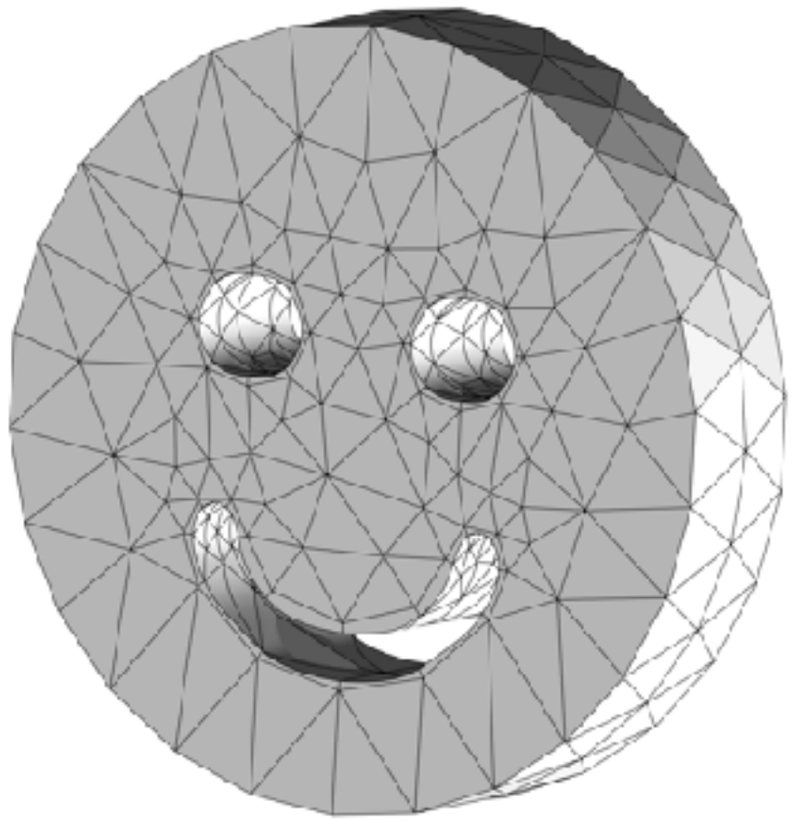
- Collections have sped up our code and made us think much harder about memory & hardware, particularly for KNL architecture

- Transition to kernels easier to consider threading, vectorisation & tuning, but keeping transparency

- `libxsmm` looks encouraging for maximising hardware potential, particularly for non-TP elements

- Still need to tackle memory management, particularly for KNL & non-CPU architectures

Thanks for listening!



https://davidmoxey.uk/ @davidmoxey

d.moxey@imperial.ac.uk

www.nektar.info