Targeting the spectral/*hp* element method for exascale platforms

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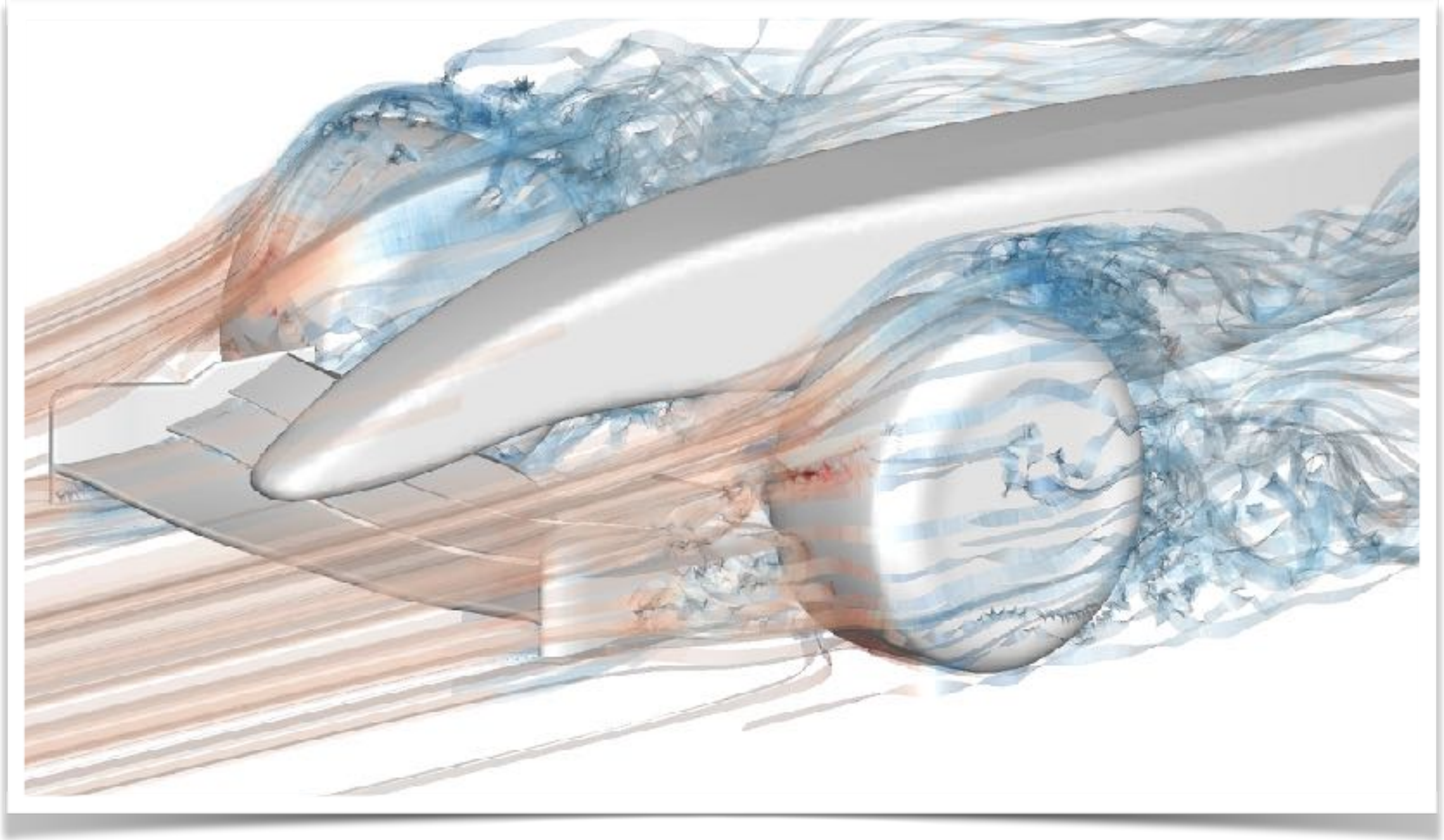
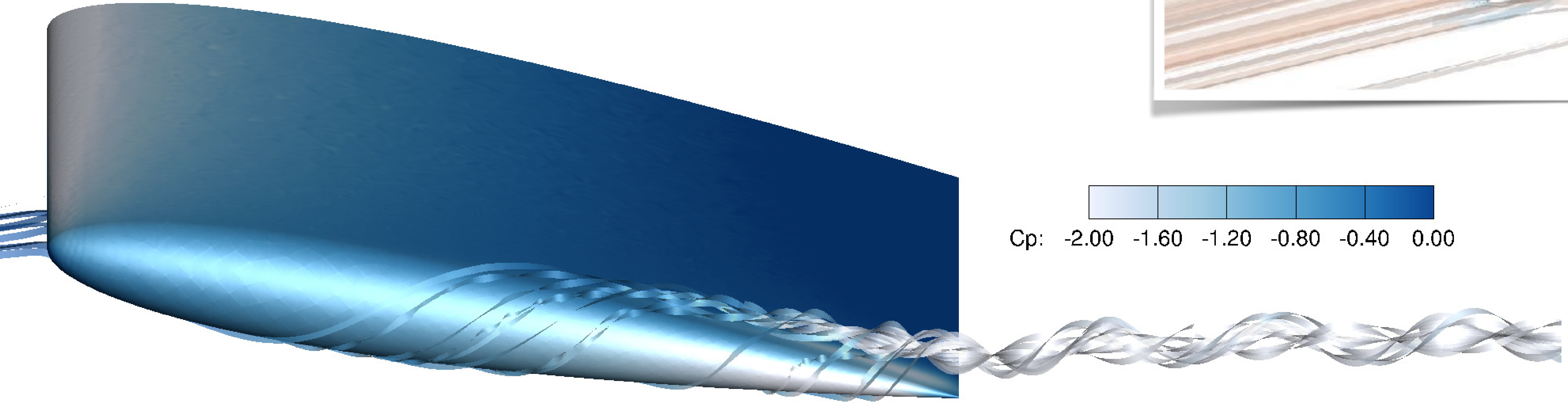
Outline

- Challenges for exascale: hardware landscape
- The spectral/*hp* element method
- Collections & `libxsmm`
- Summary

What CFD do we want to do at exascale?

- Industrial simulations at high Reynolds numbers
- Things that RANS struggles with: detachment, vortex interaction
- SVV-LES formulation of incompressible NS





Lombard, Moxey, Hoessler, Dhandapani, Taylor and Sherwin
Implicit large-eddy simulation of a wingtip vortex, AIAA Journal **54** (2), 2016

Why is exascale (CFD) hard?

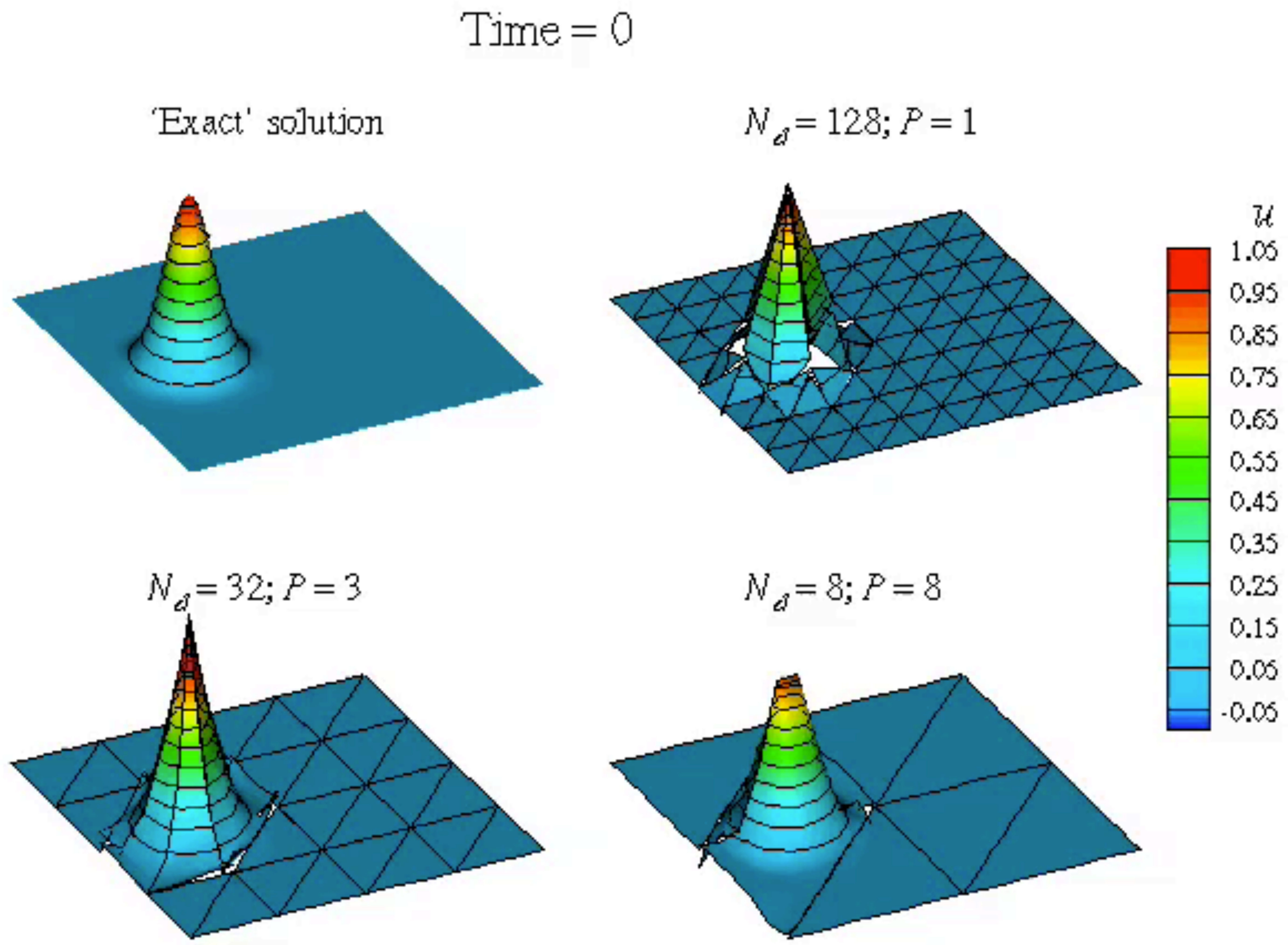
- Ideally: we want really fast single-core nodes with lots of memory bandwidth
- Instead, we get lots of FLOPS using many cores per node, lower clock speed

Main problem (asides from communication):

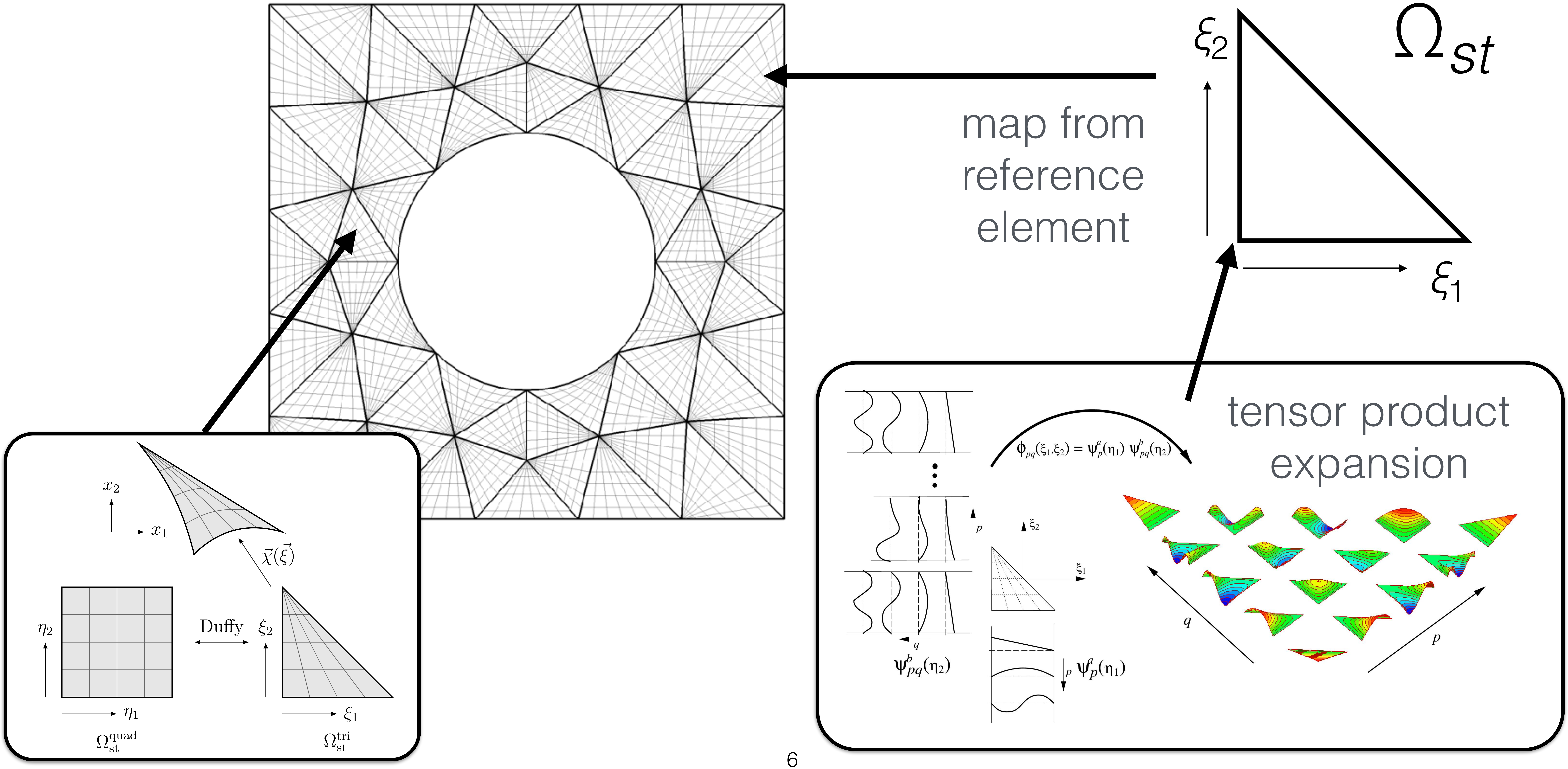
- Complicated memory hierarchies
- Very limited memory bandwidth

Therefore need algorithms with **high arithmetic intensities** that can actually use FLOPS available

Higher p means more work



Spectral/*hp* element method

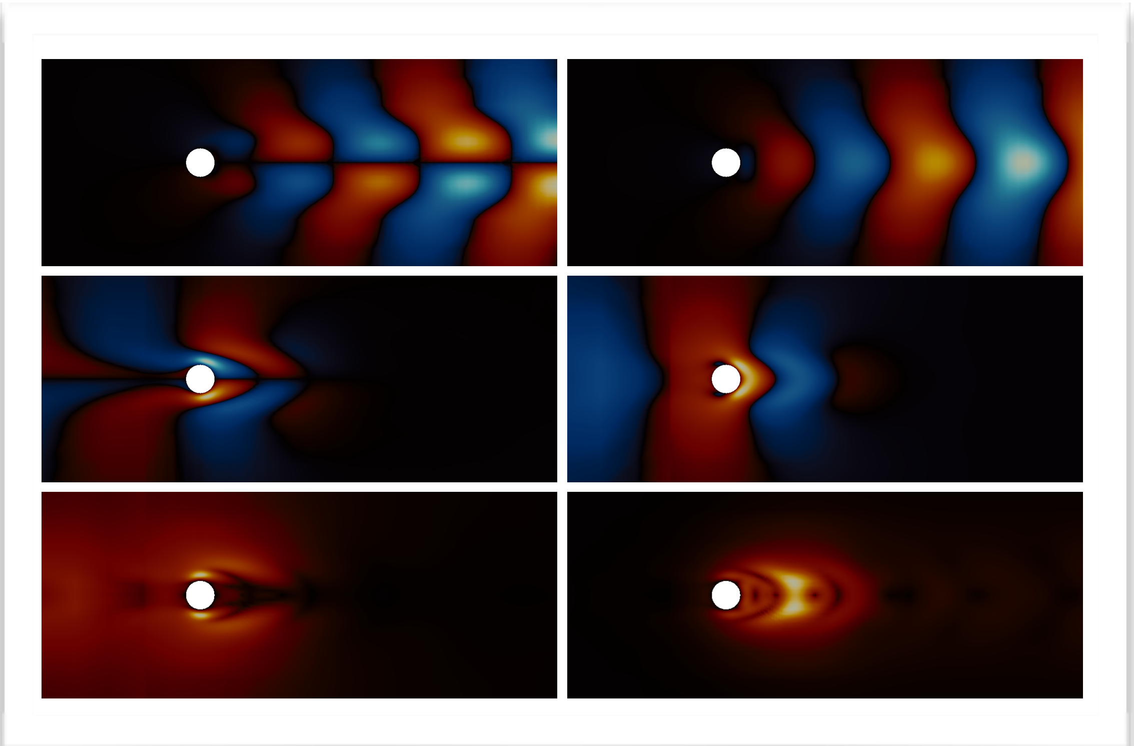


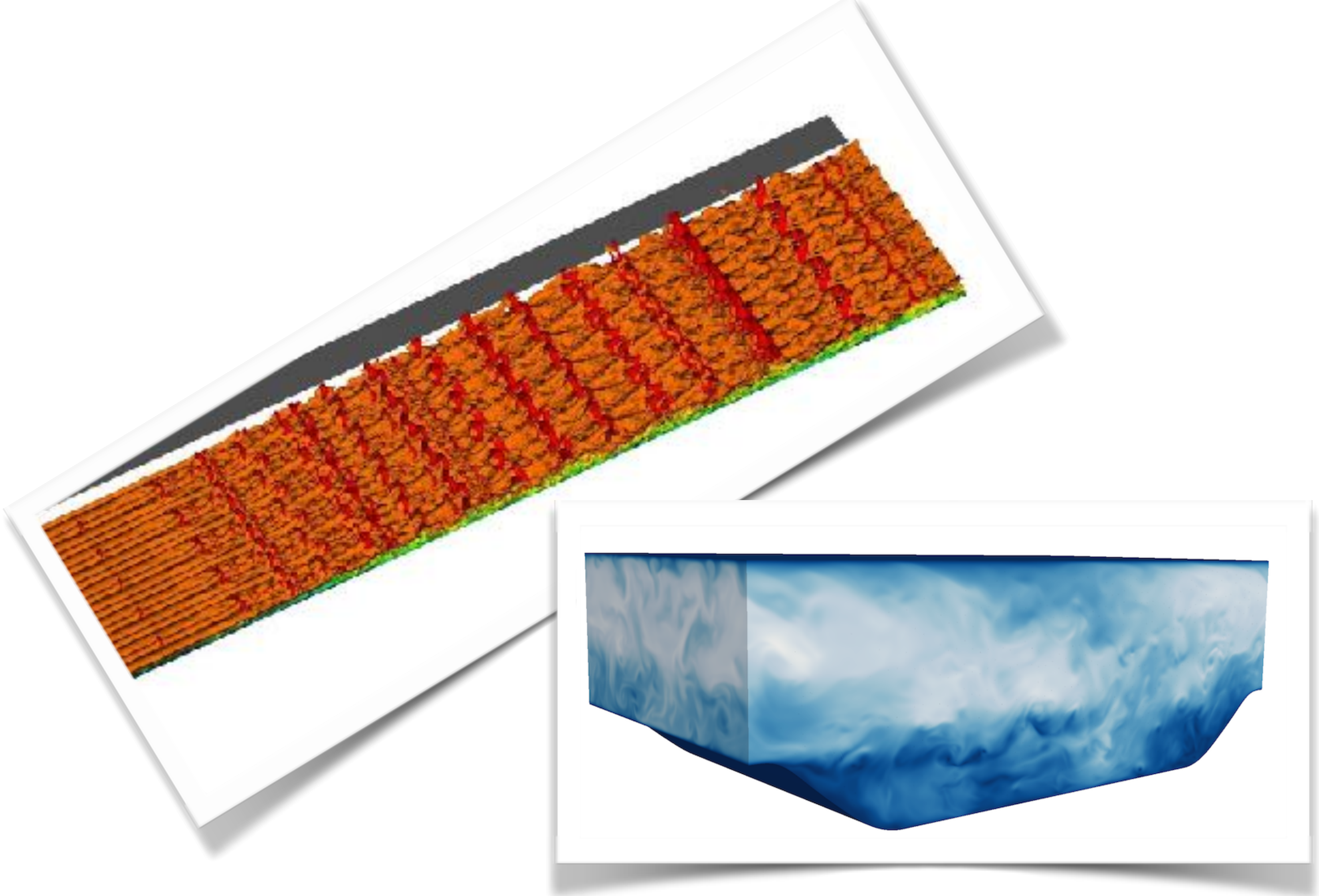
Nektar++ high-order framework

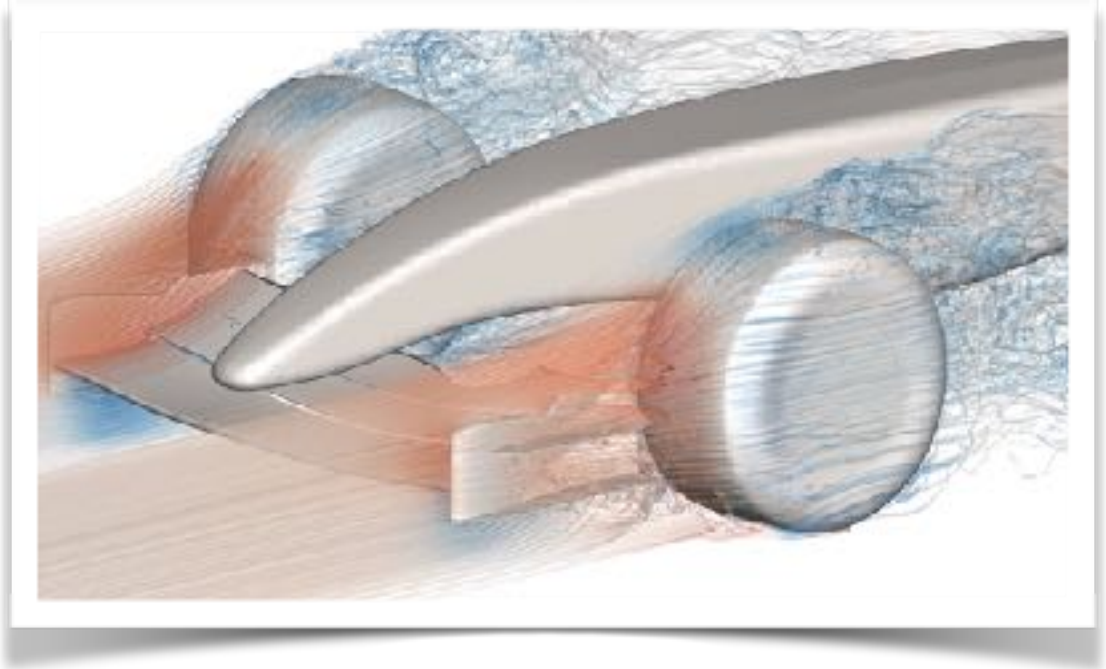
Framework for spectral(/hp) element method:

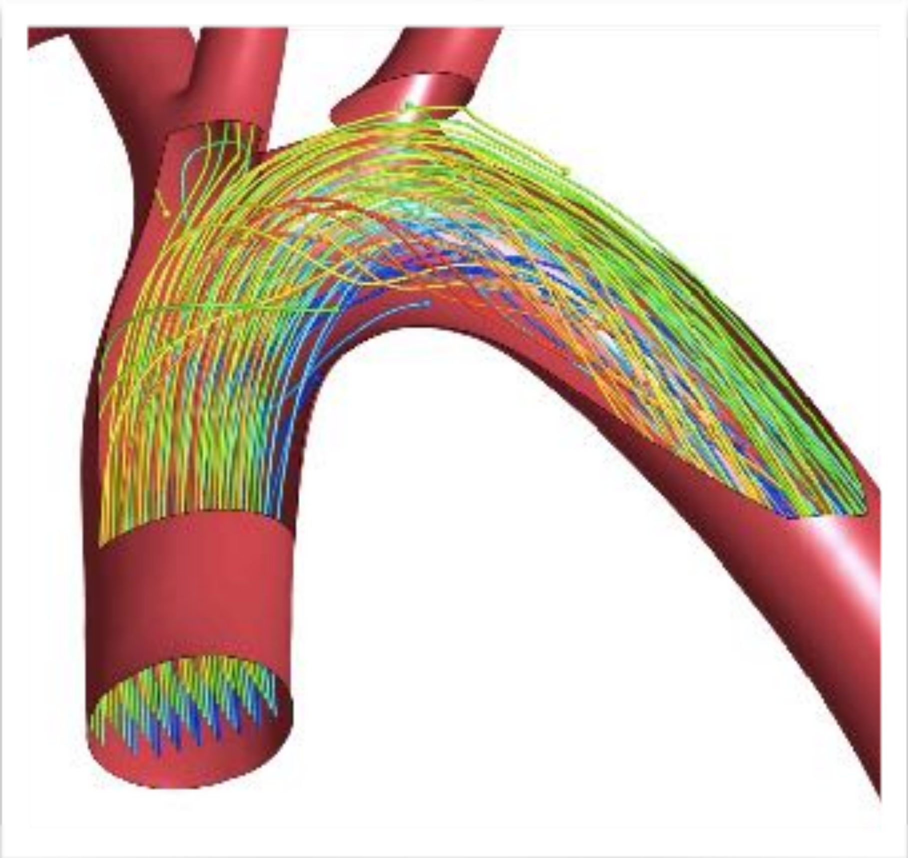
- Dimension independent, supports CG/DG/HDG
- Mixed elements (quads/tris, hexes, prisms, tets, pyramids) using hierarchical modal and classical nodal formulations
- Solvers for (in)compressible Navier-Stokes, advection-diffusion-reaction, shallow water equations, …
- Parallelised with MPI, tested scaling up to ~10k cores

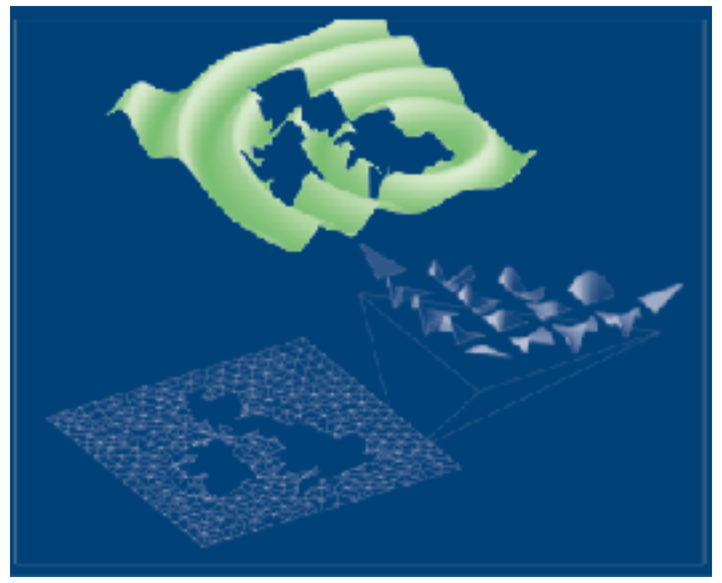
http://www.nektar.info/ nektar-users@imperial.ac.uk https://gitlab.nektar.info/

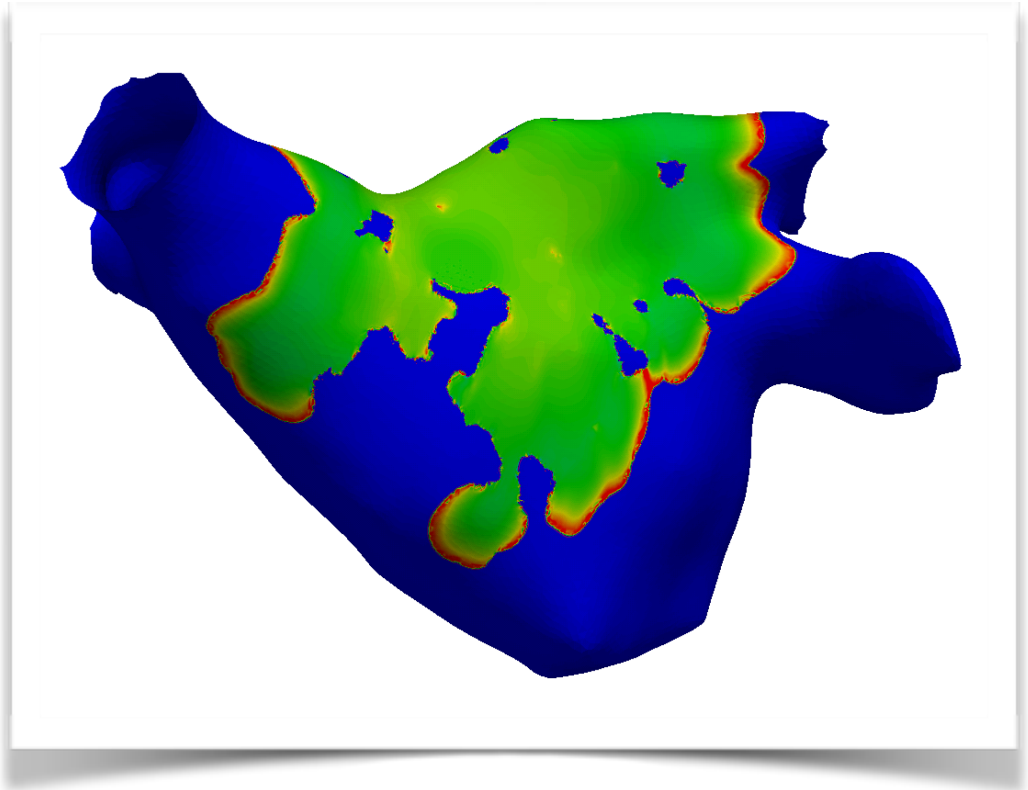


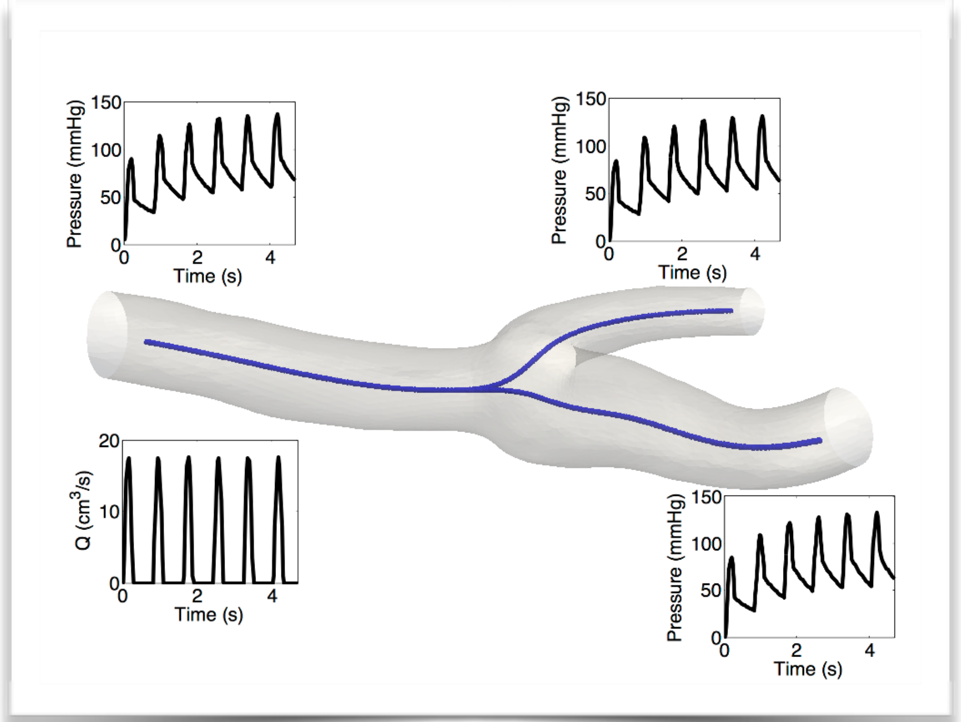











Pressure (mmHg)
150
100
50
0
2
4
Time (s)
Pressure (mmHg)
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Time (s)
Q (cm^3/s)
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Time (s)
Pressure (mmHg)
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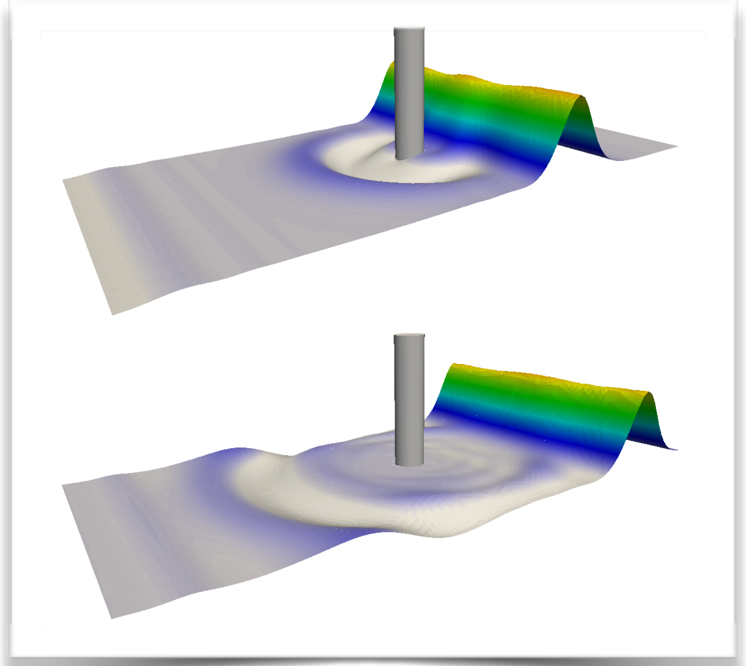
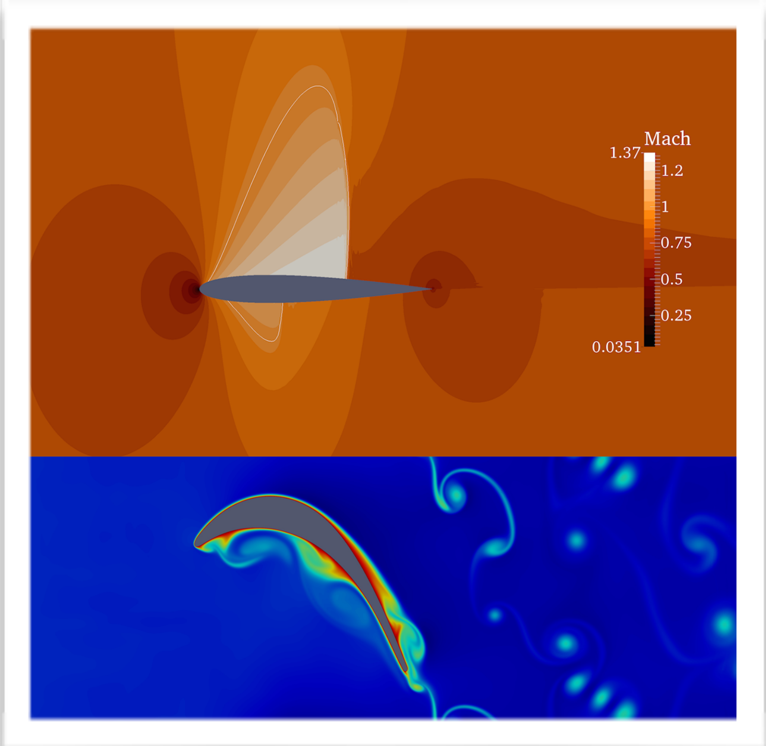
0
2
4
Time (s)




Mach
1.37
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0.75
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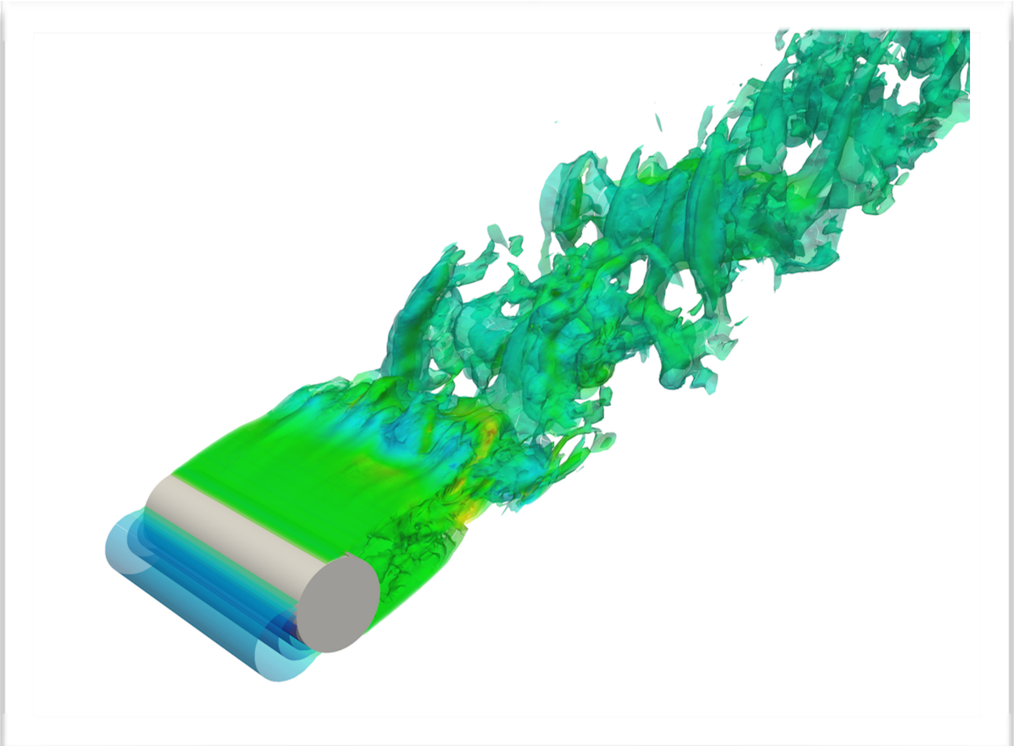
0.25
0.0351



Nektar++

- 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

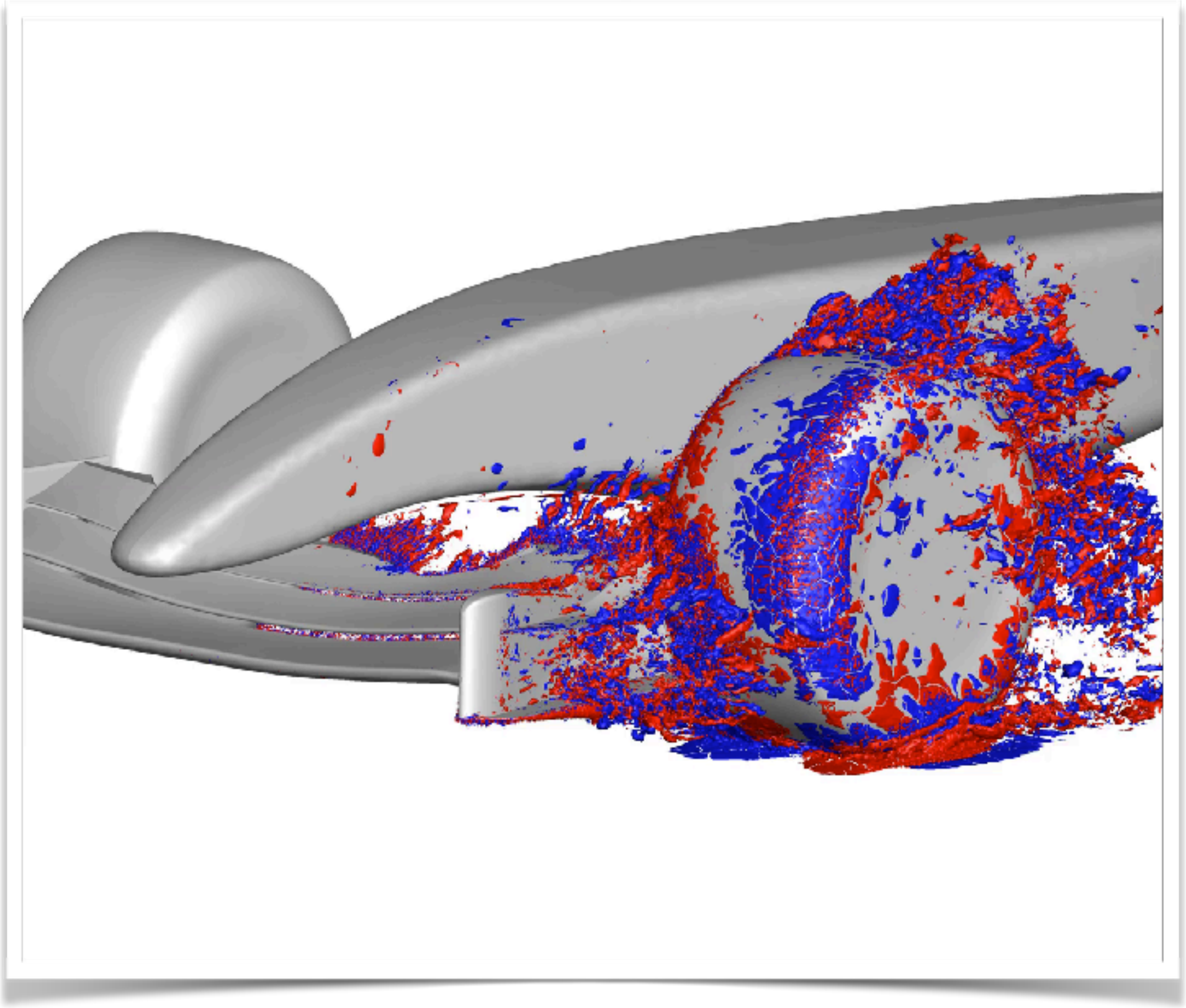
- Be efficient across a range of polynomial orders and core counts

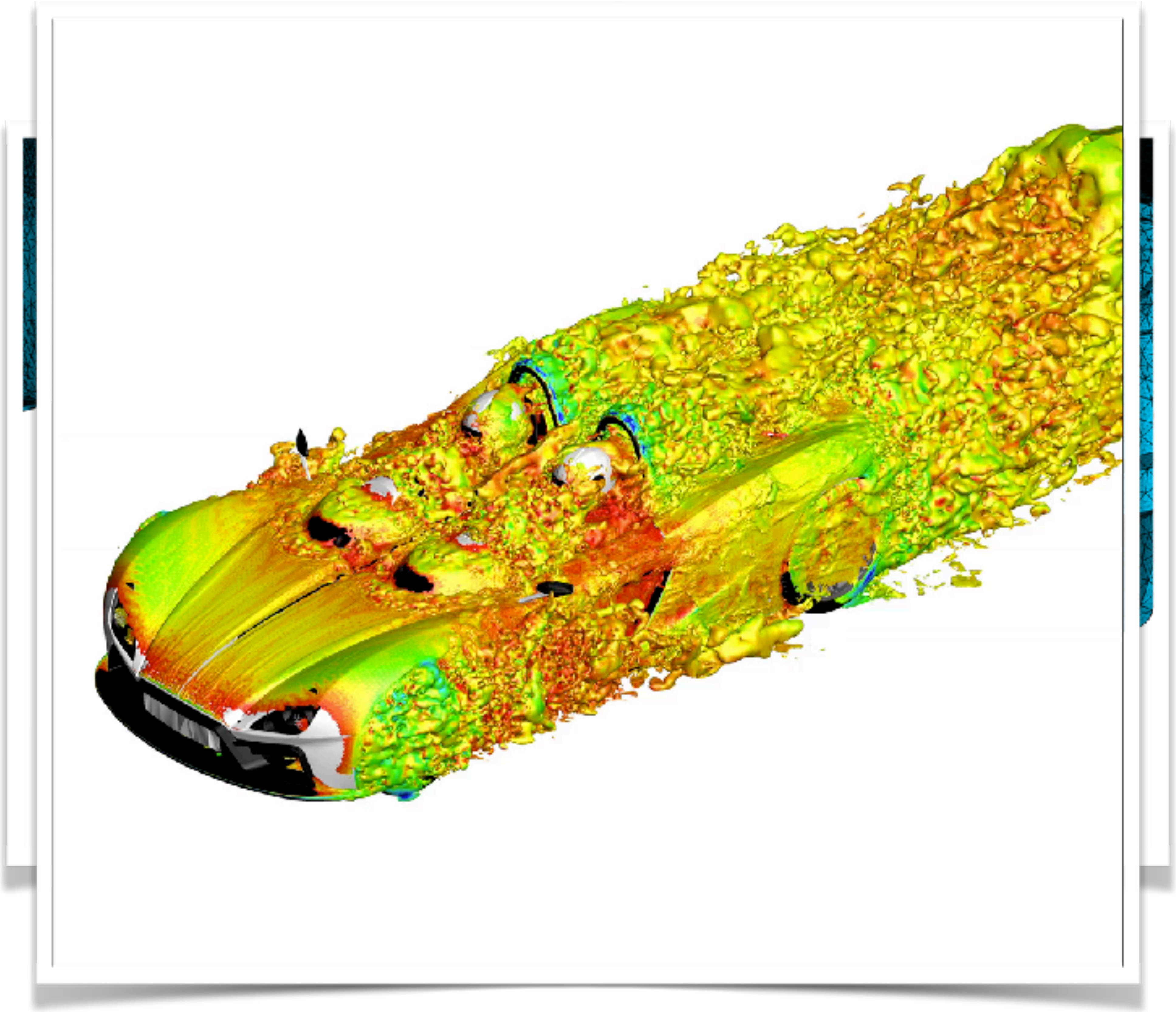
- Bridge current and future hardware diversity

Unstructured simulations

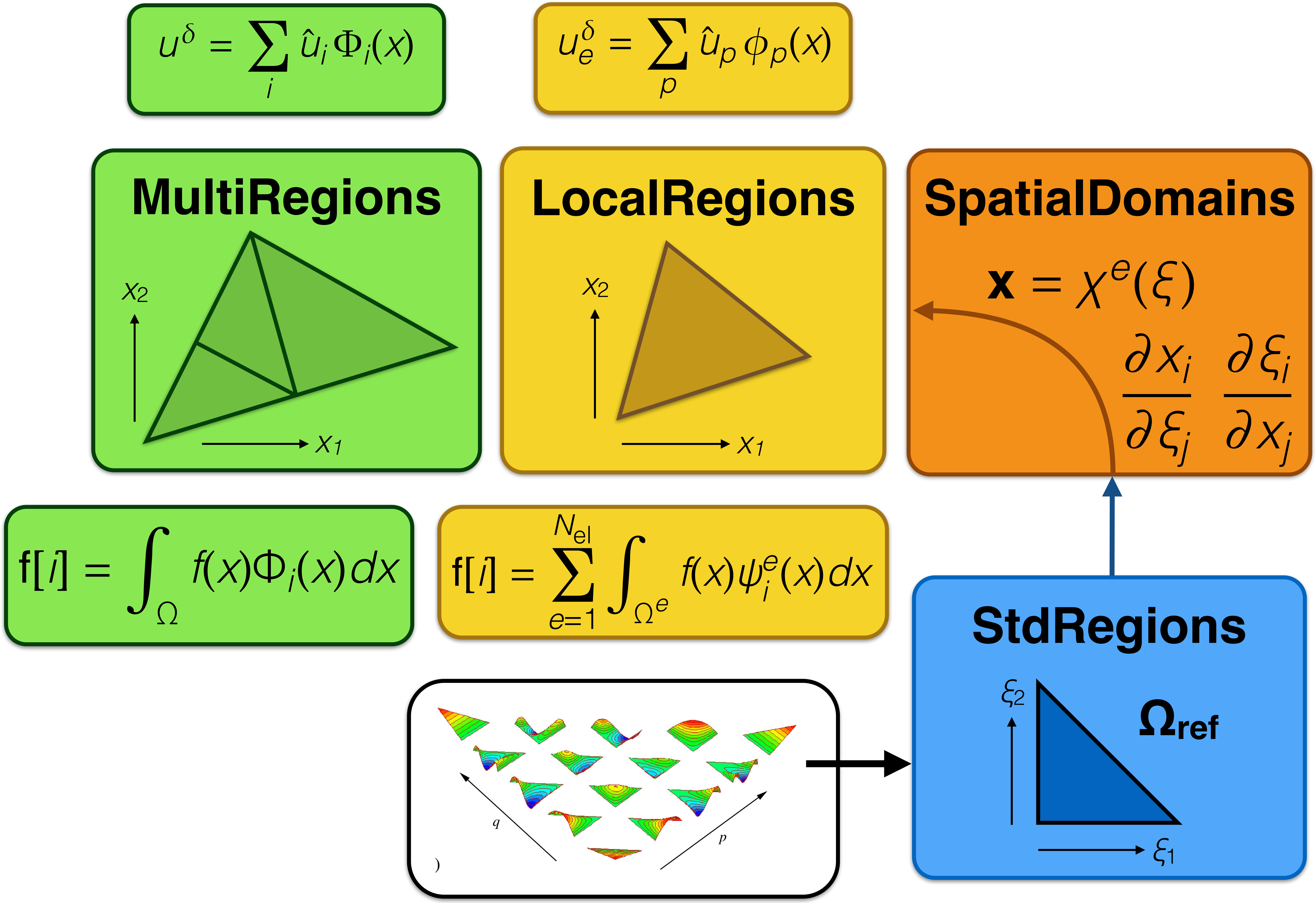
Commonly known that hexes yield best performance because they have *tensor product* structure

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





Framework design



"Defining" features of spectral/*hp*

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

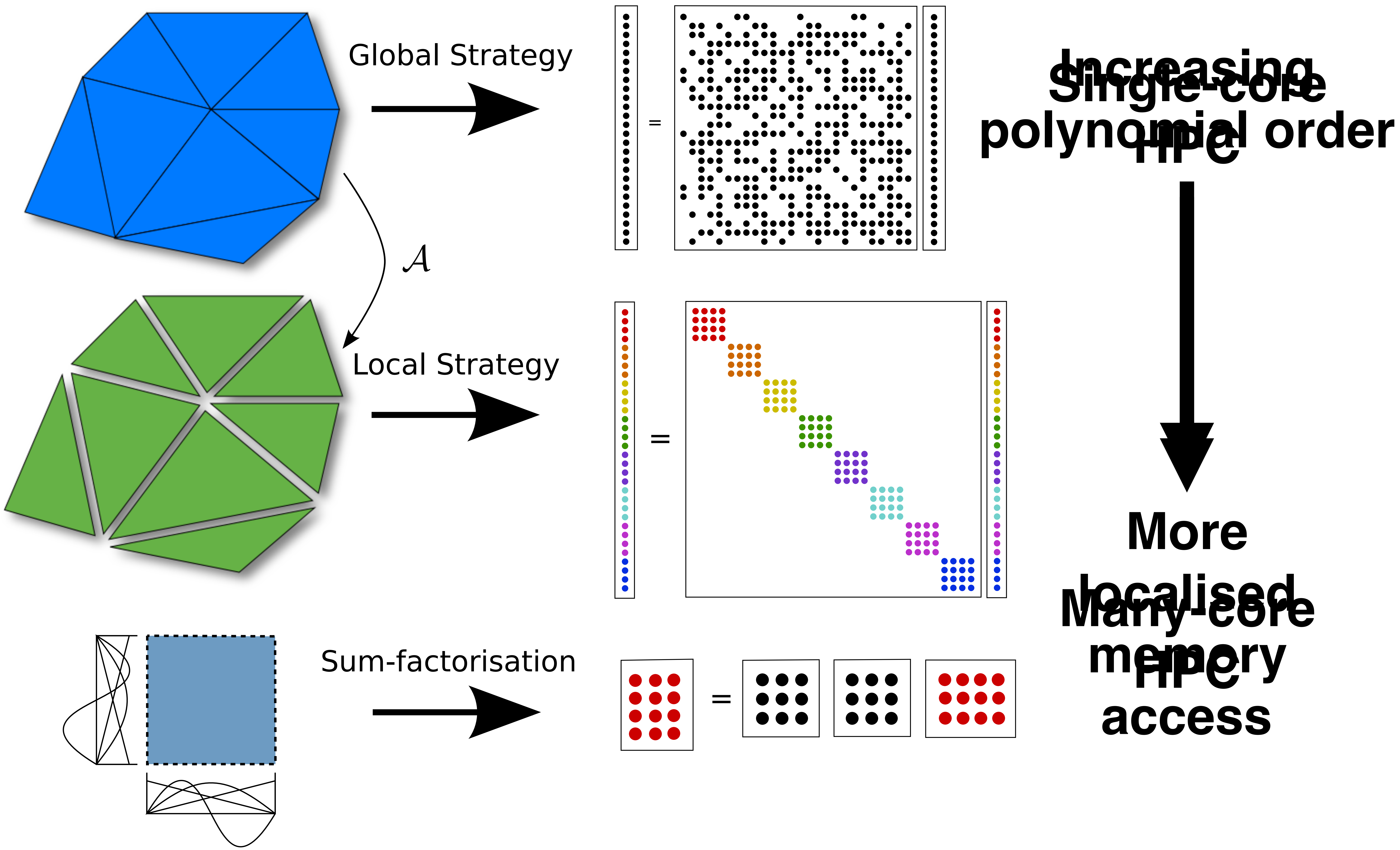
$$\sum_{p=1}^{P}\sum_{q=1}^{Q}\hat{u}_{pq}\phi_p(\xi_{1i})\phi_q(\xi_{2j}) = \sum_{p=1}^{P}\phi_p(\xi_{1i})\left[\sum_{q=1}^{Q}\hat{u}_{pq}\phi_q(\xi_{2j})\right]$$

store this

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

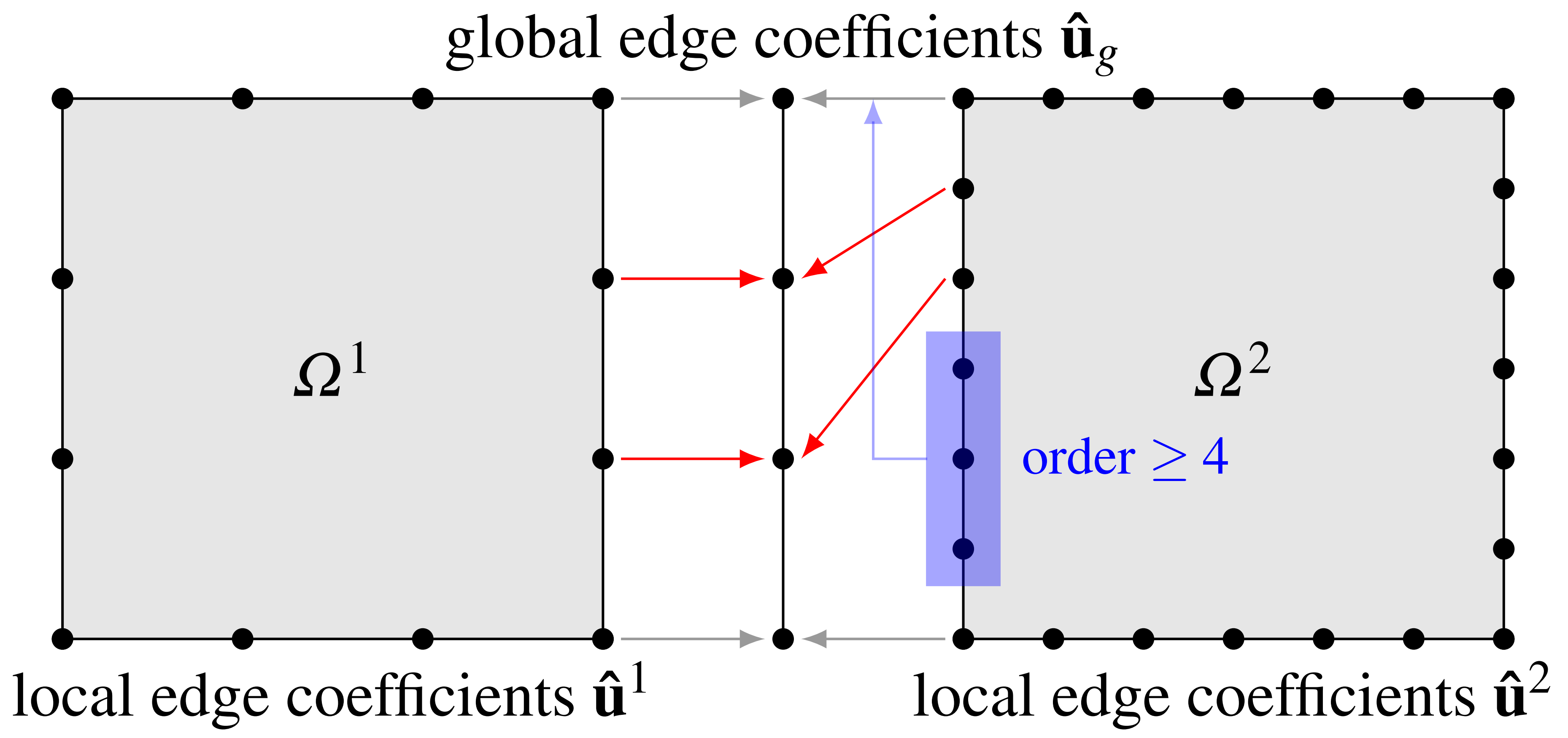
Key point: **We can still do this** for tris, tets, prisms...
but have to cope with harder indexing and smaller matrices

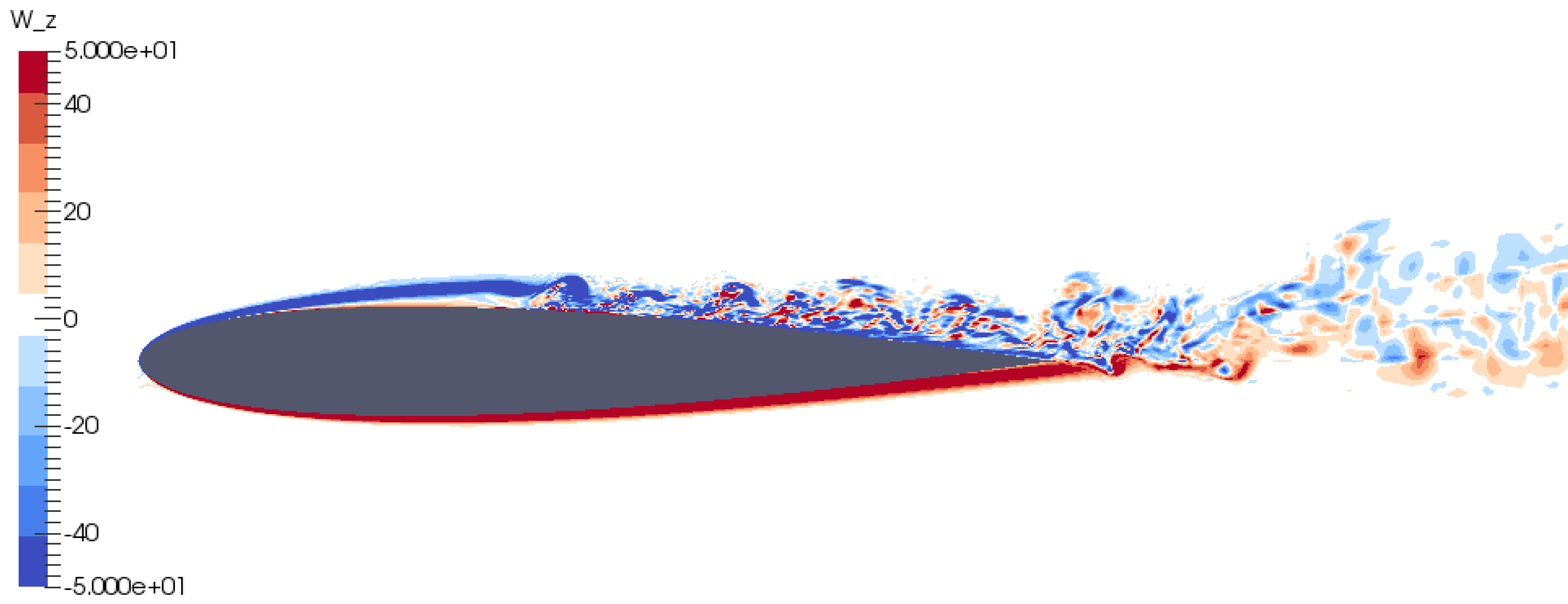
Implementation choices

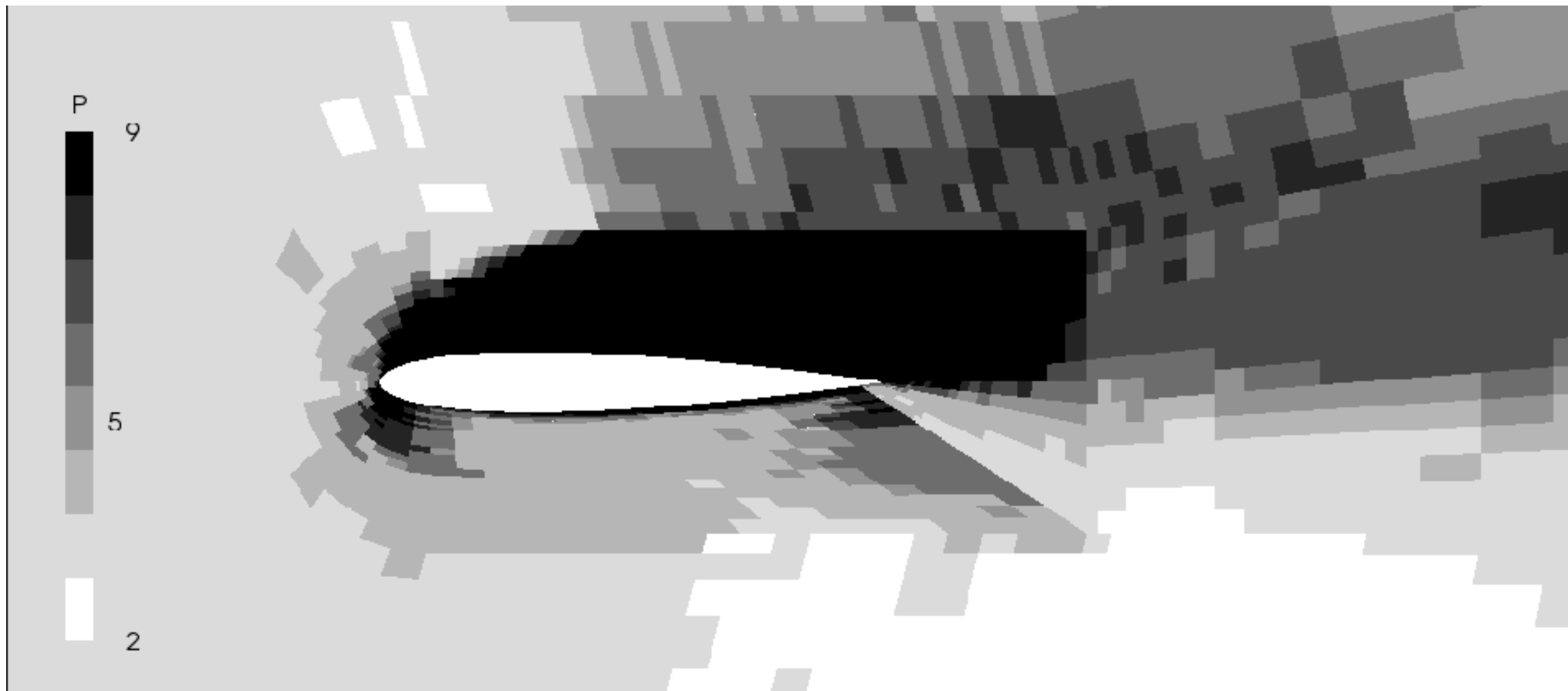


h-to-*p* efficiently

- 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





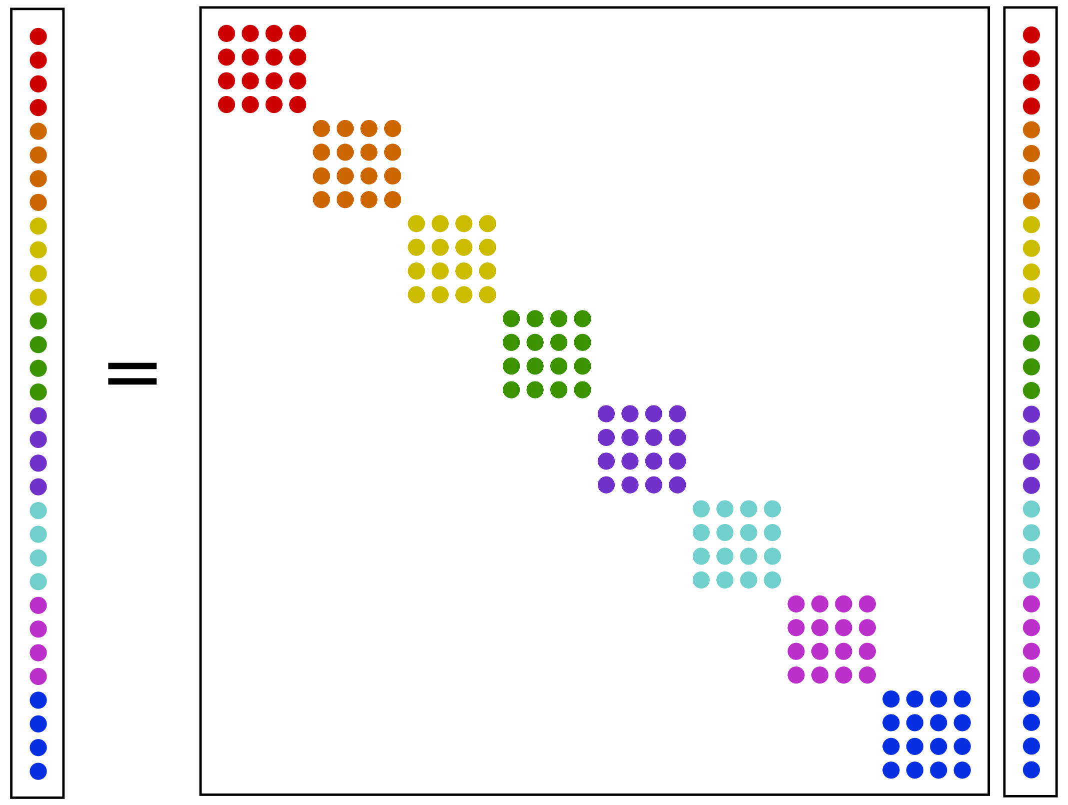


Collections

- Reformulate implementation choices into kernel operations over multiple elements
- Group geometric terms $\dfrac{\partial x_i}{\partial \xi_j}$
- 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: $(\Phi_i, \nabla\Phi_j)$

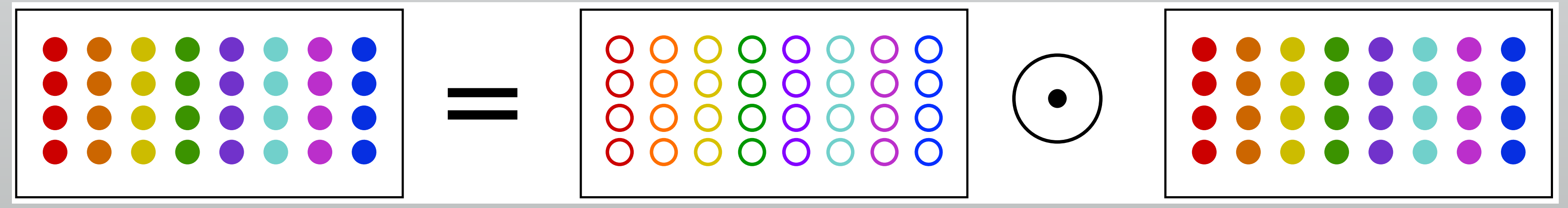
Schemes

Local Matrix

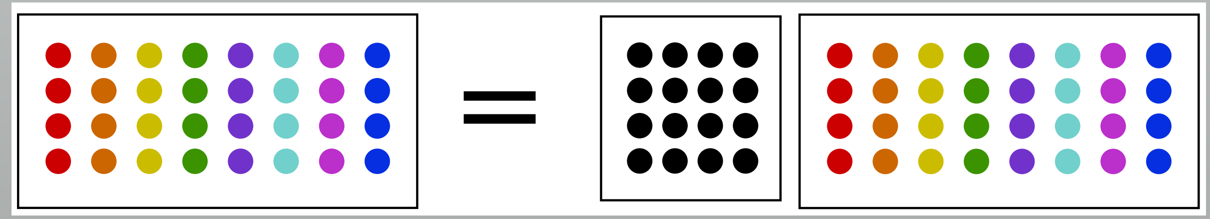


StdMat (standard matrix)

1. Apply Jacobian **(L1)**

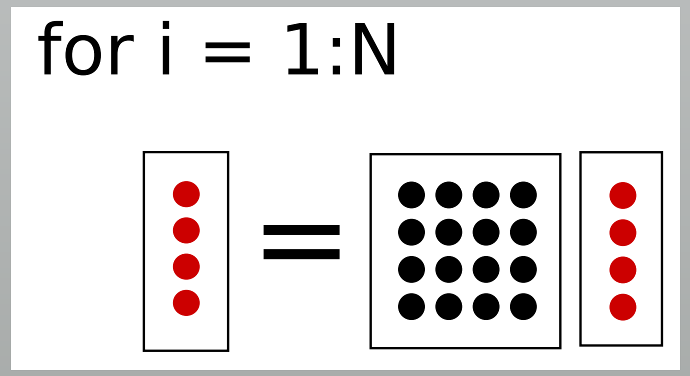


2. Multiply by ref. matrix **(L3)**



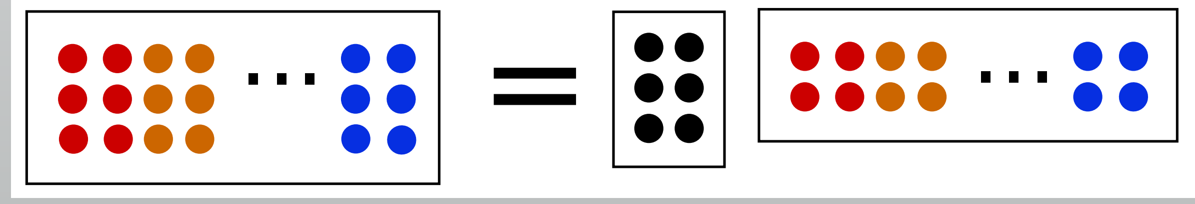
IterPerExp

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

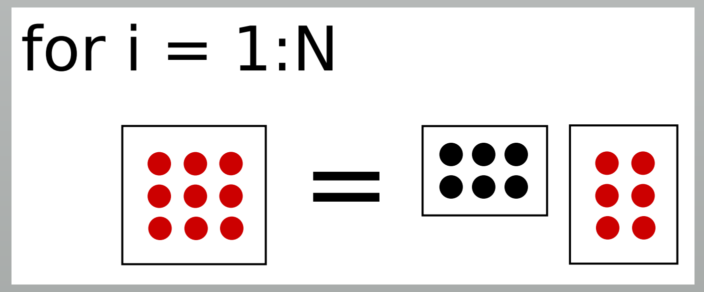


SumFac

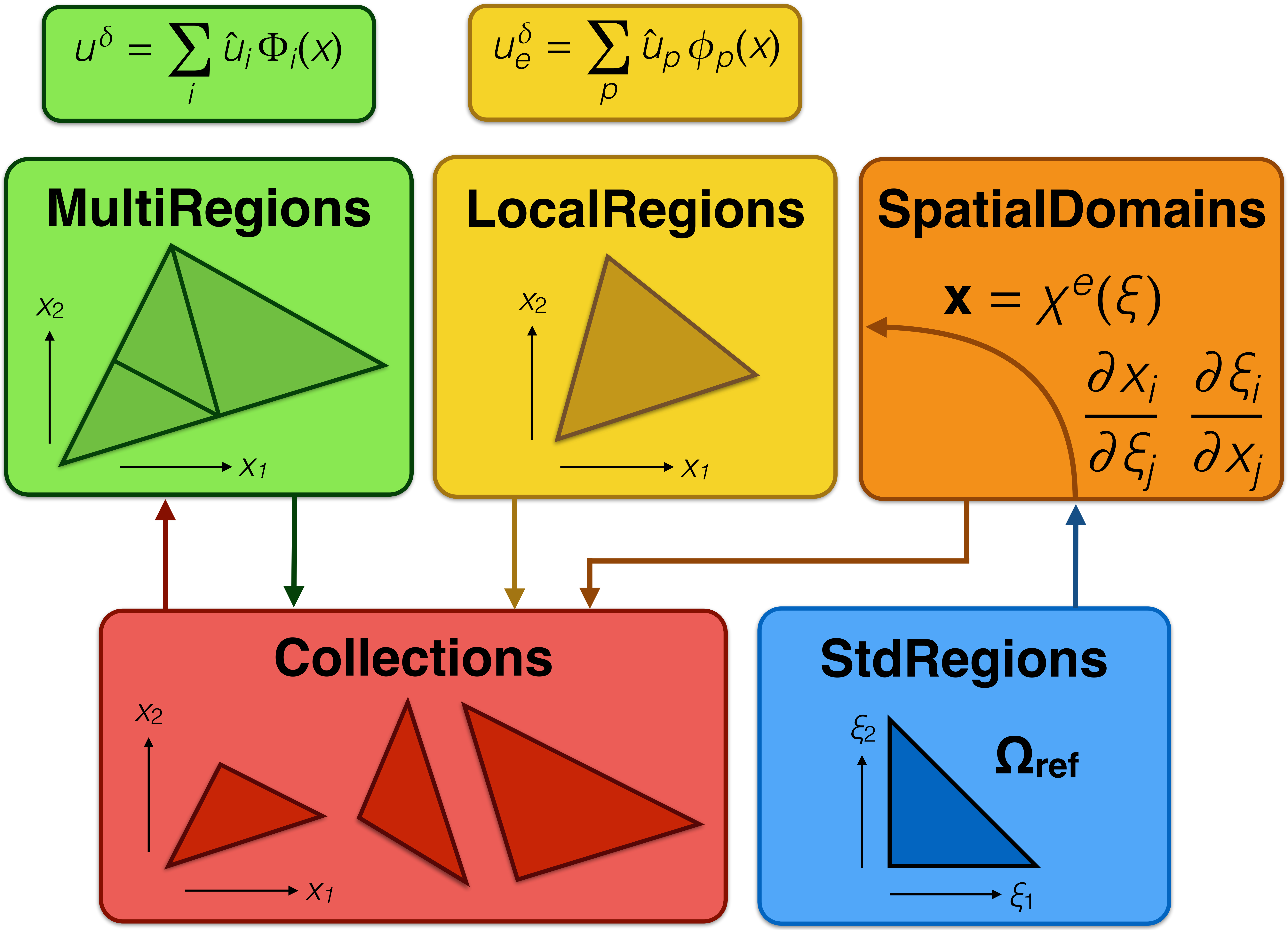
1. Apply Jacobian **(L1)**
2. Mult. first dimension **(L3)**



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

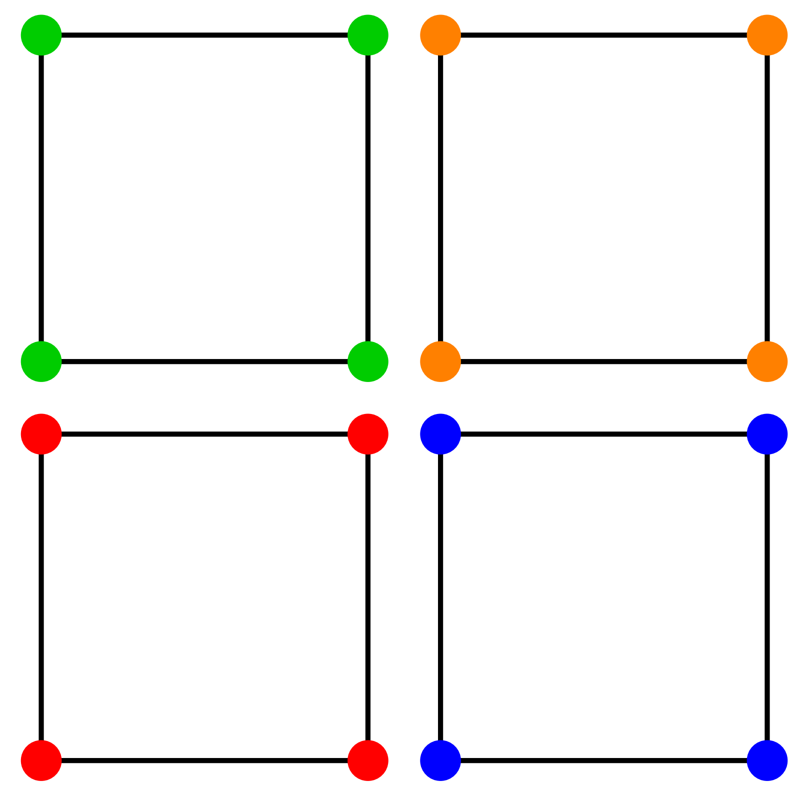


Collections

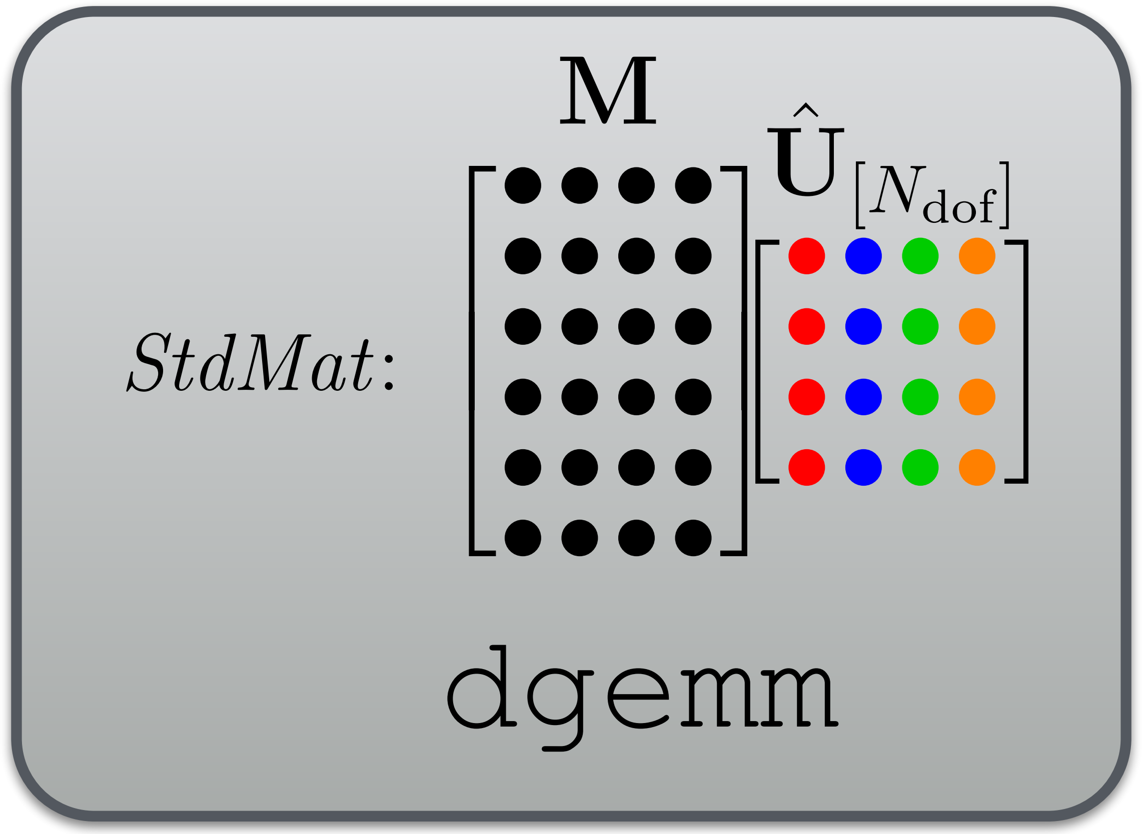


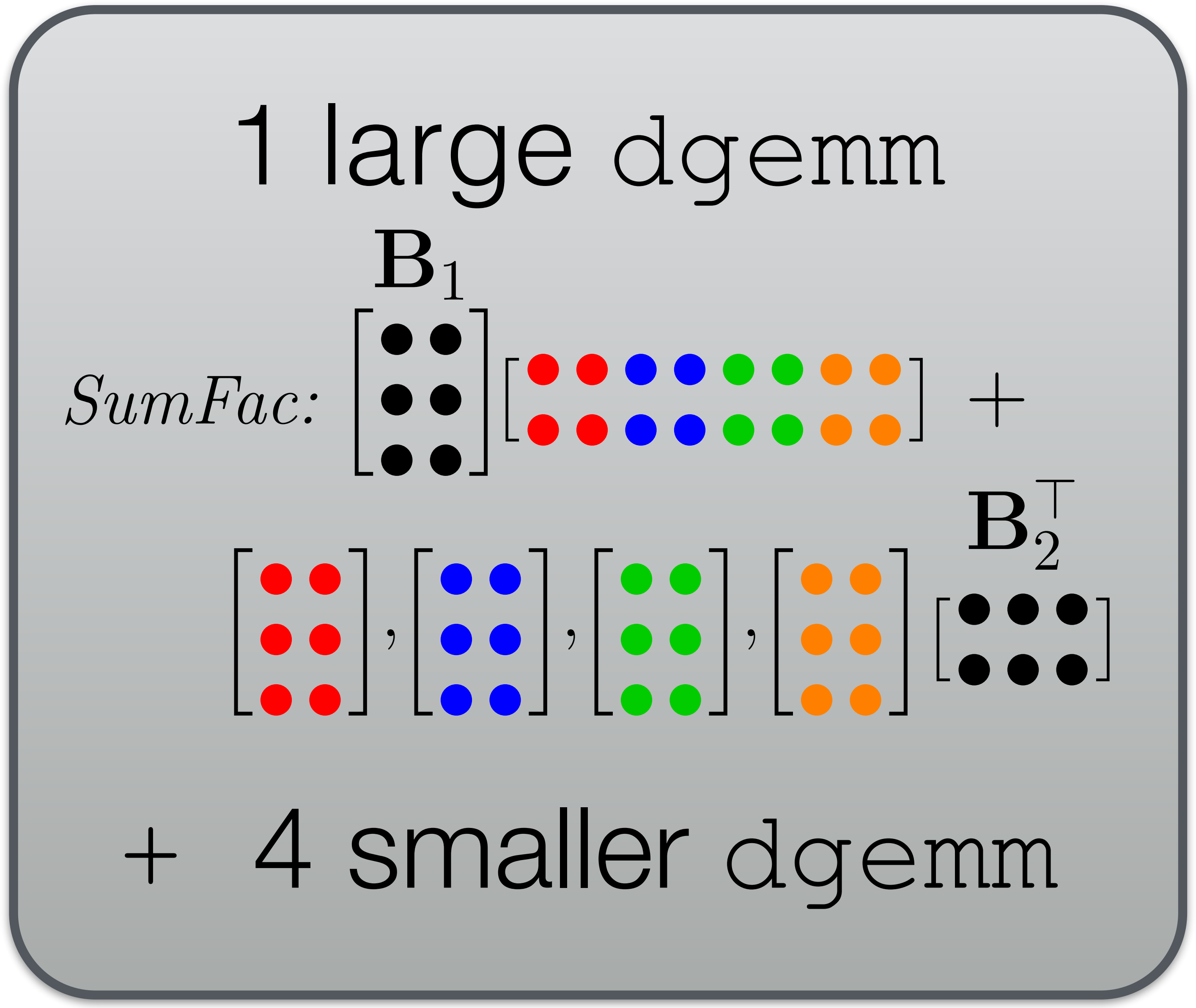
Collections

Use BLAS calls throughout



4 quad mesh

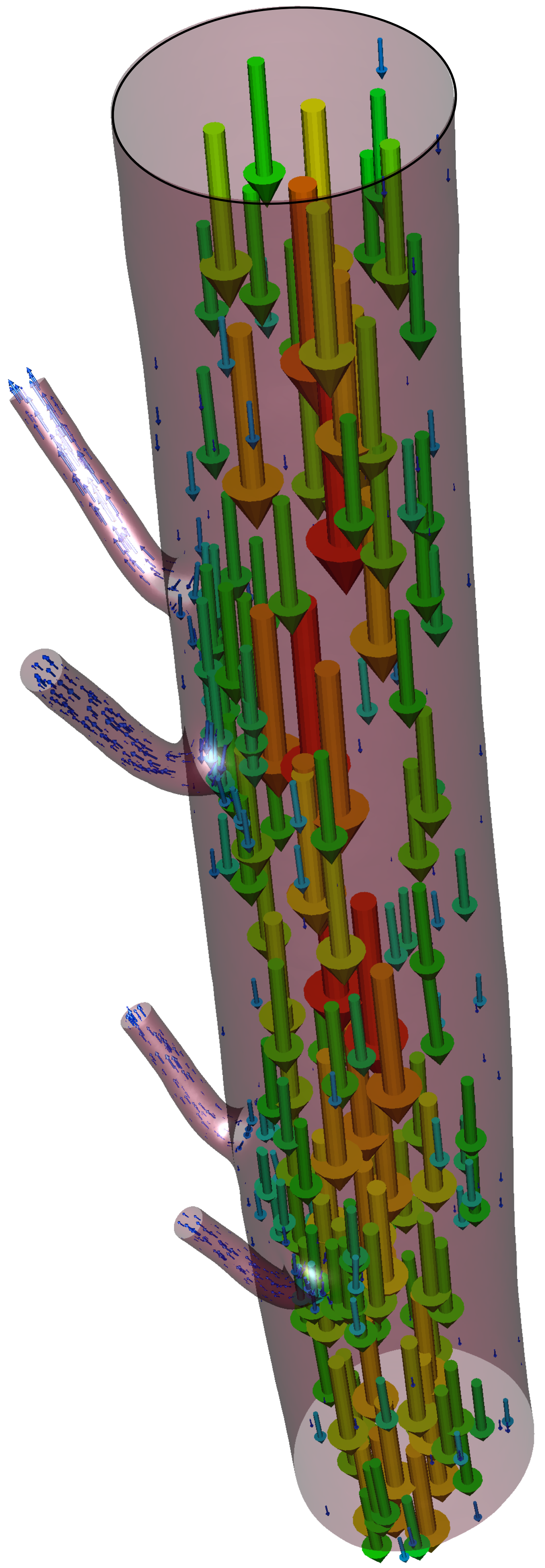


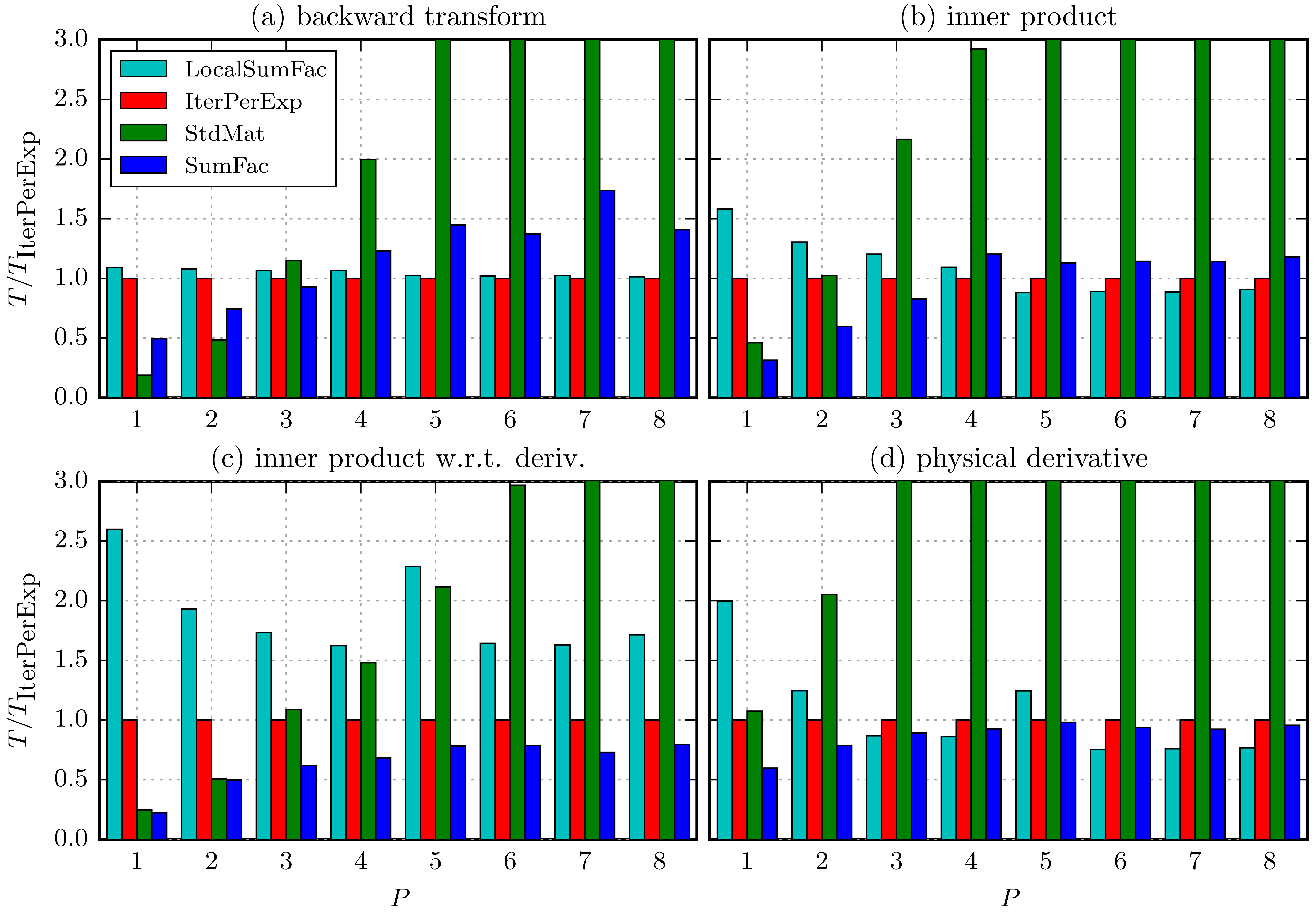


Can also do this for non-TP elements:
data ordering harder, matrices smaller (bad for BLAS)

Test case

Intercostal pair
21k prisms
41k tets





Test case

Intercostal pair
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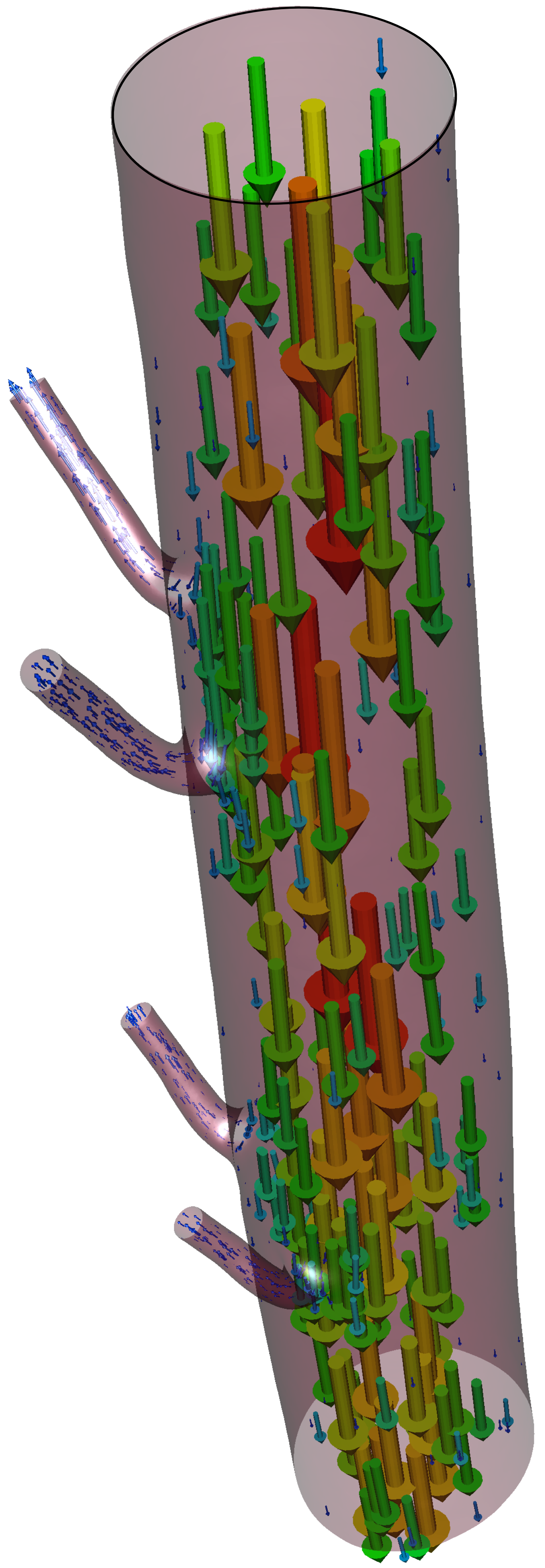
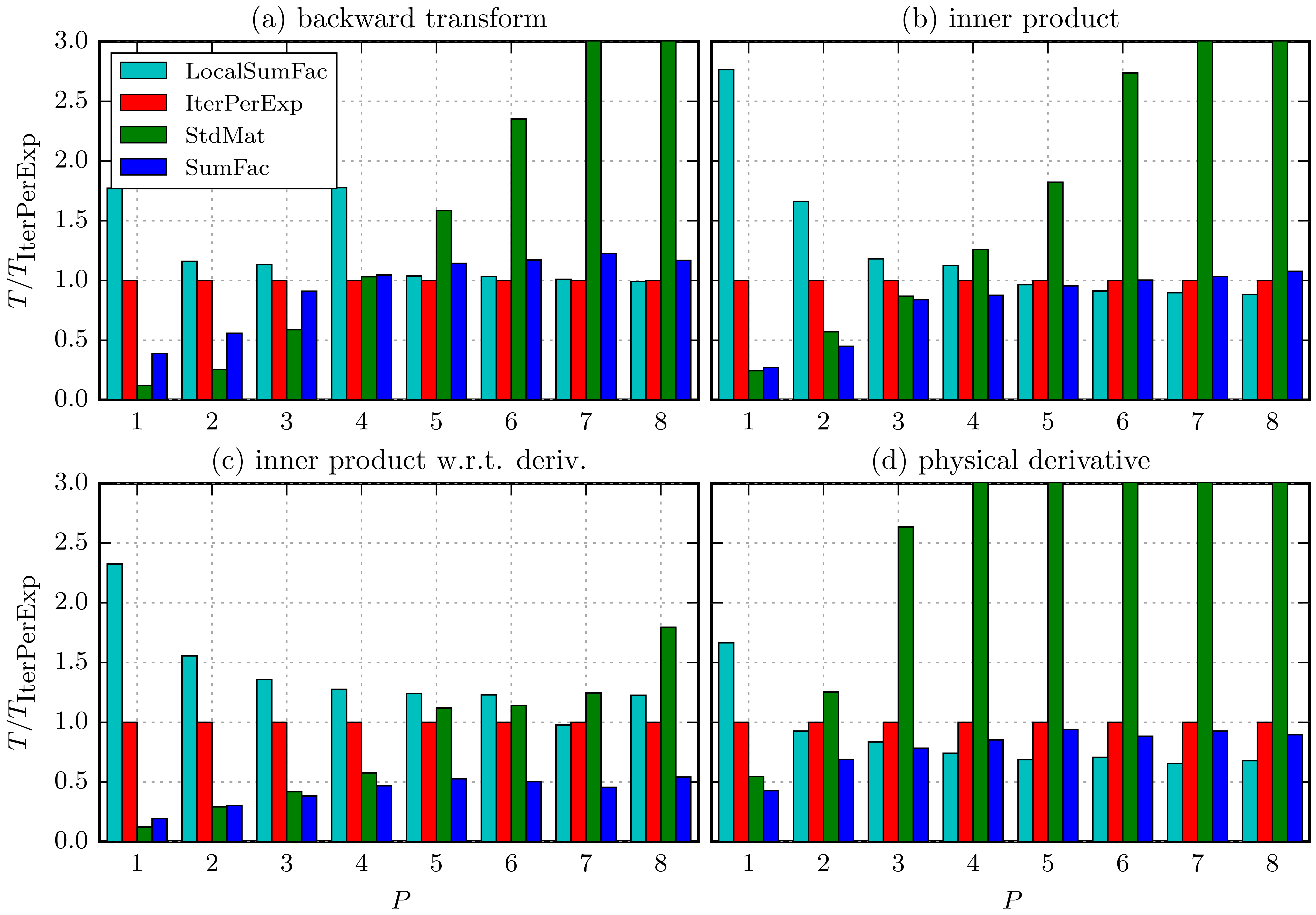
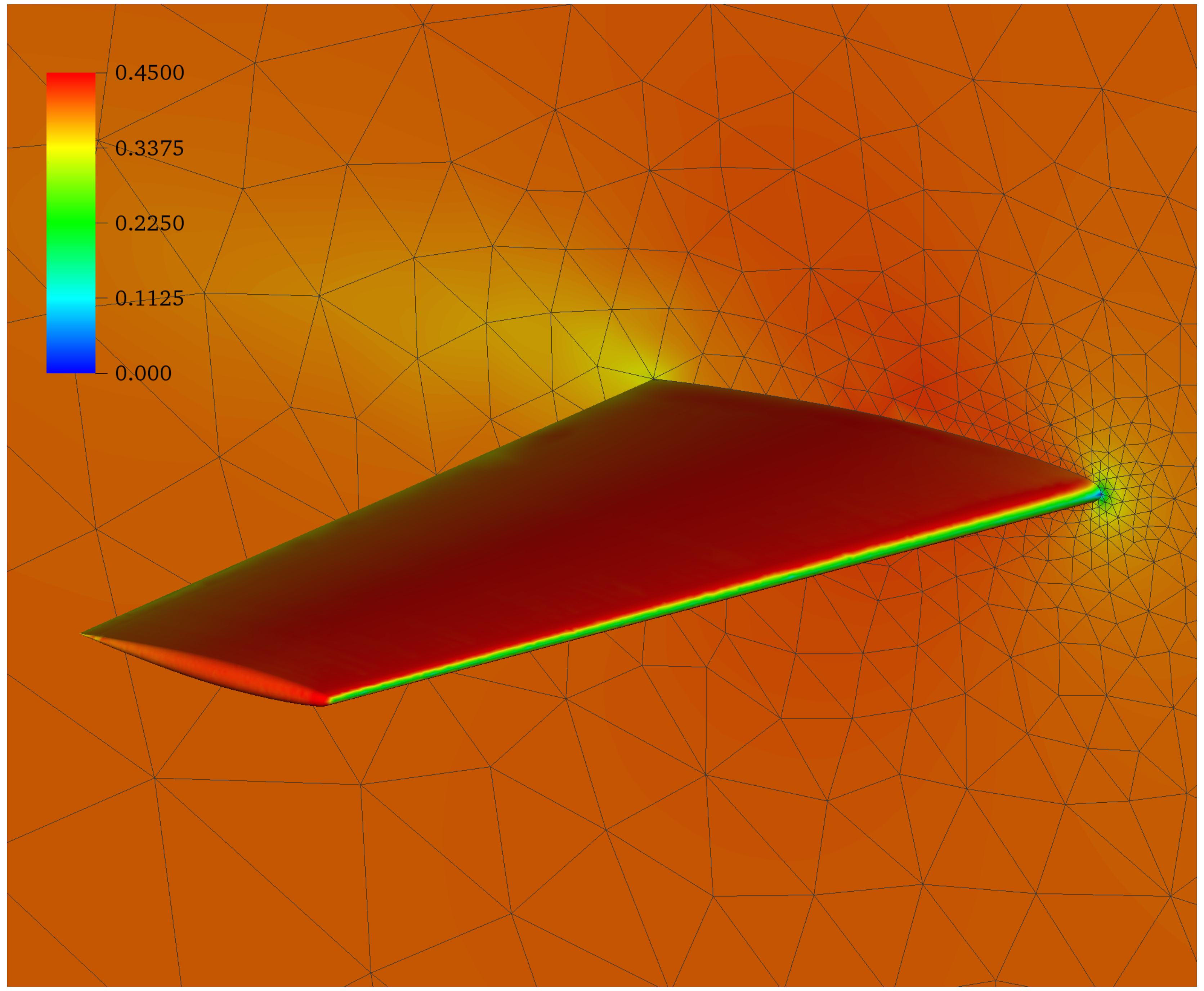




Example: ONERA M6 wing



Machine	Operator	Scheme timings [s]			
		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

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

Compressible Euler flow
Fully explicit, $P = 2$, 960 cores, ~150k tets
Inner product w.r.t derivative very important

Runtime improvement: 40-60% ↑

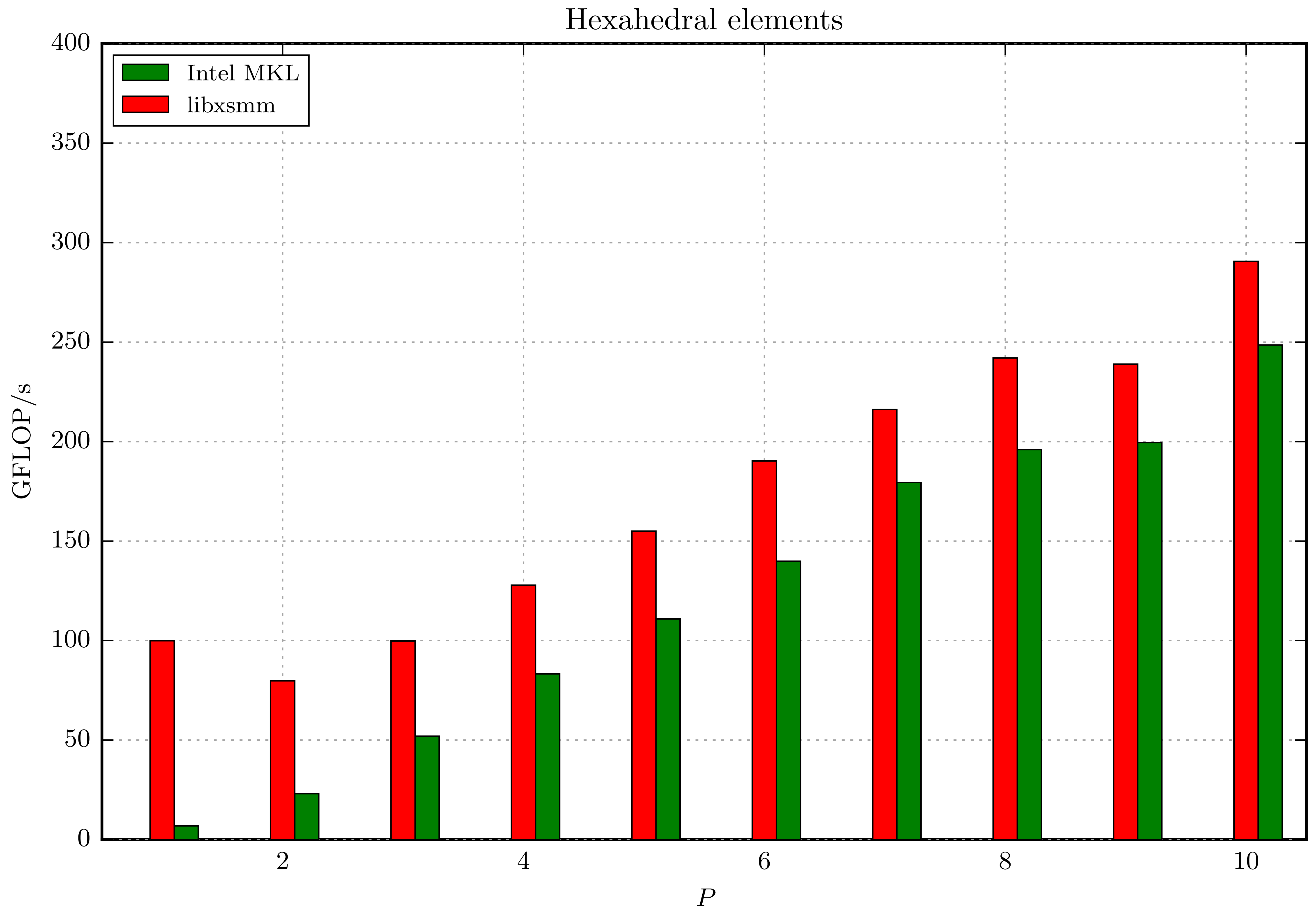
Implementation challenges: KNL + many-core

- 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
  - ➡ e.g. on KNL, DRAM vs. MCDRAM or host vs. device
  - ➡ Making this transparent to solver developers
- Threading and SIMD vectorisation

Work in progress: `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)

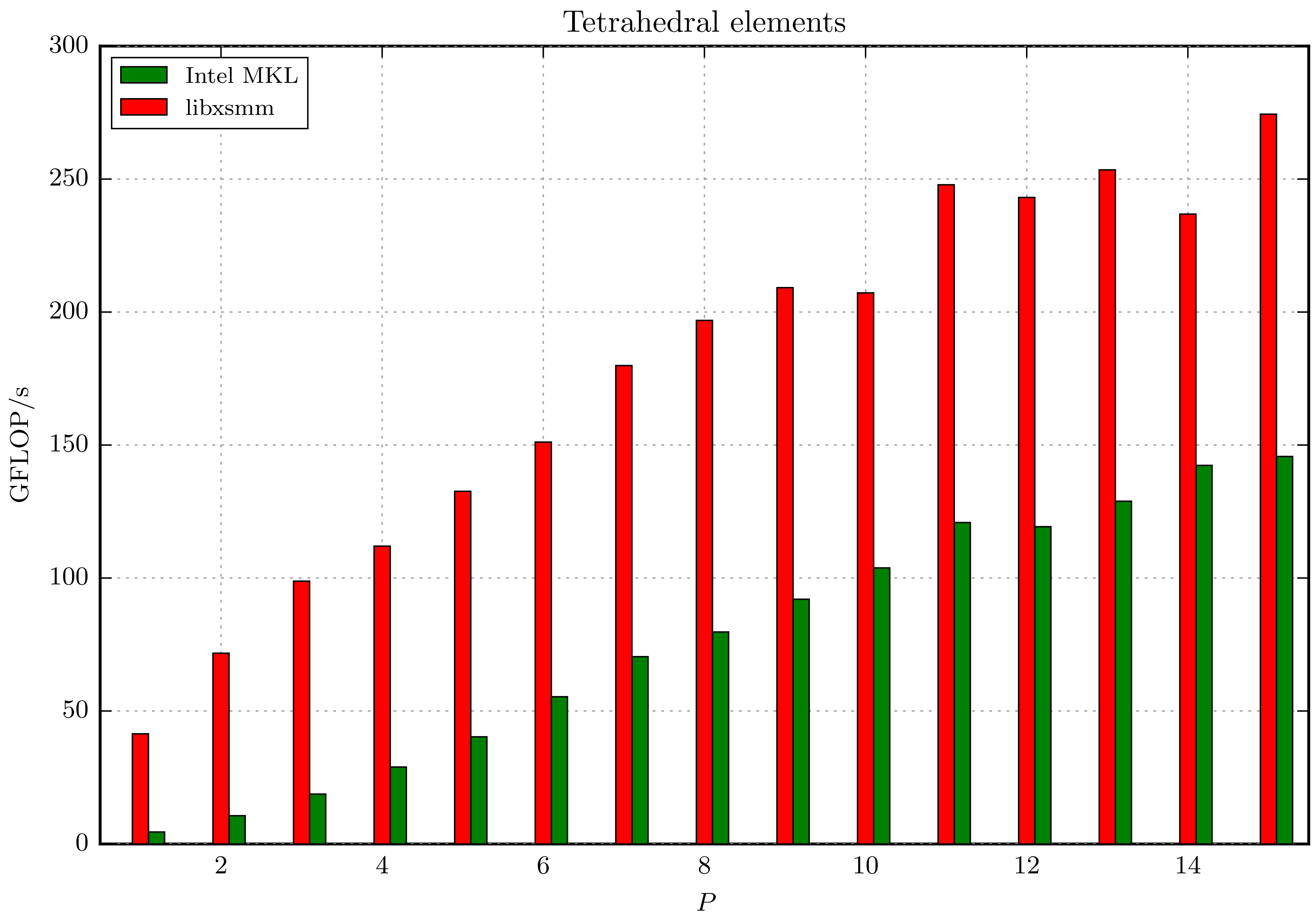
GFLOP/s performance



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

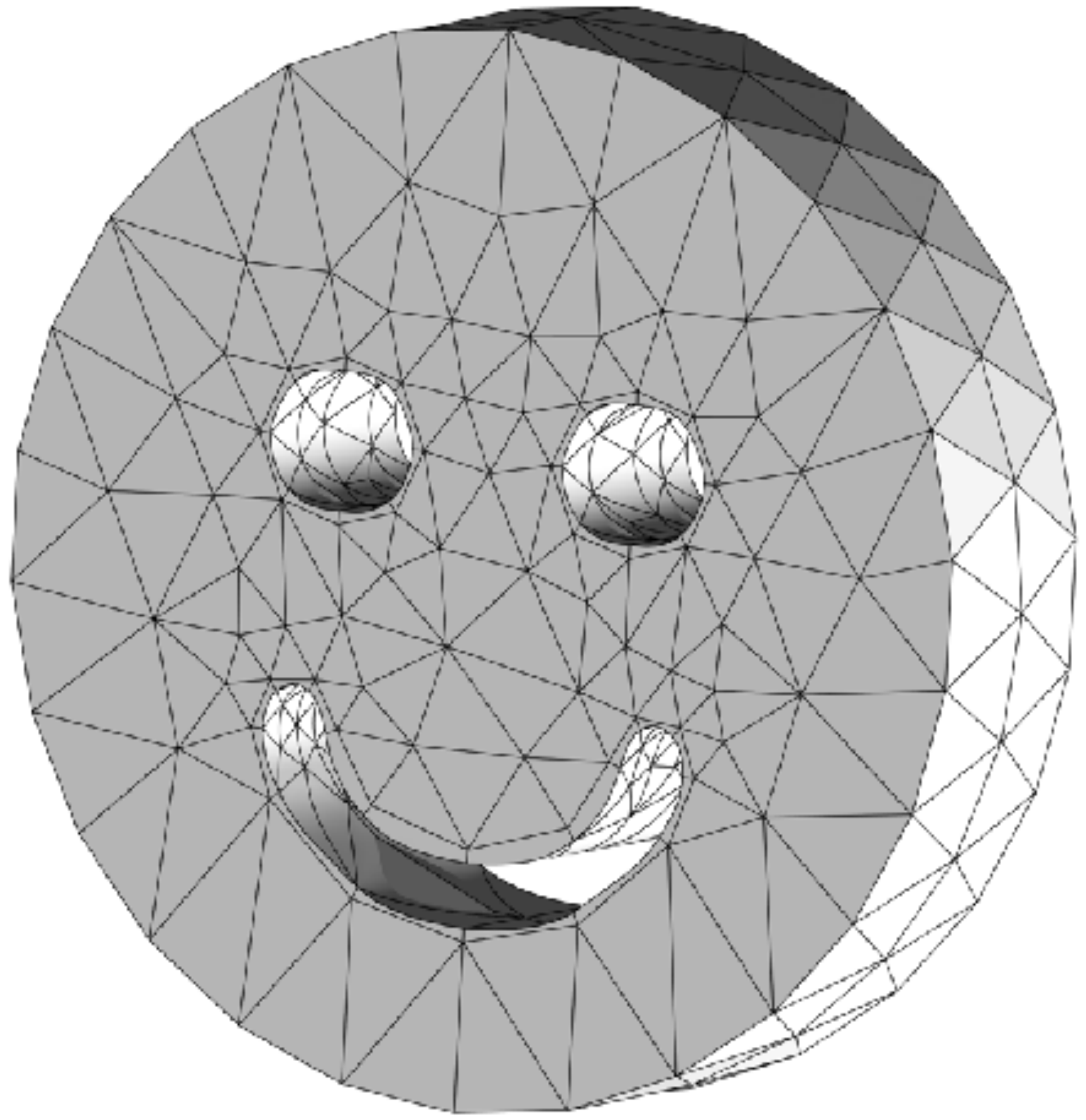
- Collections have sped up our code and made us think much harder about memory & hardware, particularly for current hardware such as KNL

- 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!



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