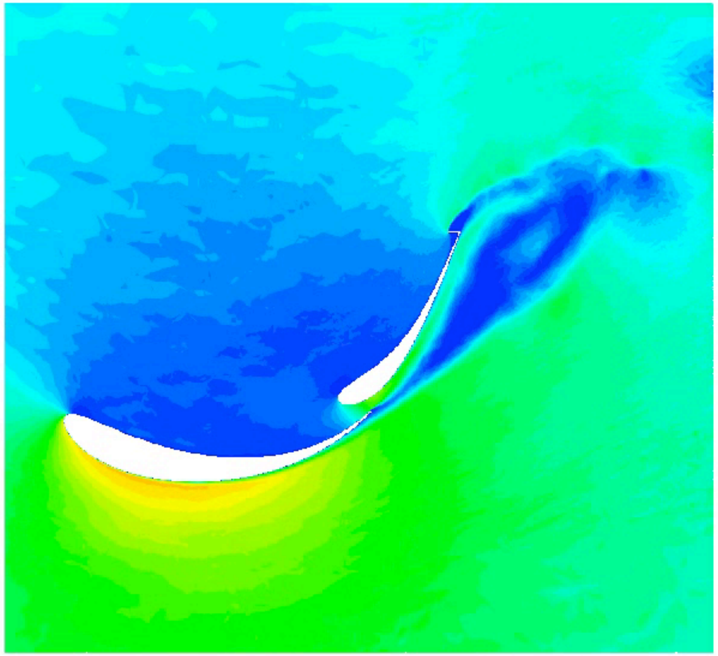
# Nektar++: A Progress Report

Spencer Sherwin, Chris Cantwell,
Dave Moxey, Mike Kirby
*Department of Aeronautics, Imperial College London*
*SCI Institute, University of Utah*



Dynamic pressure Re=100 000

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# Outline

- What are we doing?
- Optimizing our implementations
  - Variable p
  - Cloud computing

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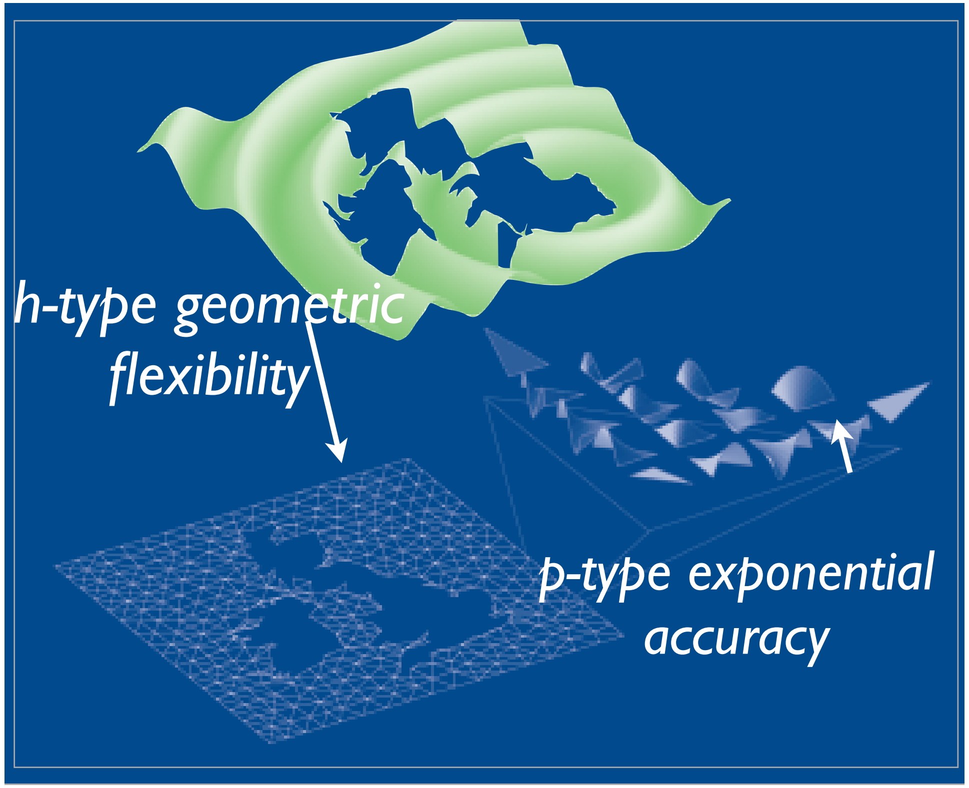
# Nektar++: An h to p finite element framework

*Provide an unified interface to an open environment which blends high- and low-order finite element methods.*

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NEKTAR++ SPECTRAL/HP ELEMENT FRAMEWORK

# Nektar++: www.nektar.info

Helmholtz problem: $$\nabla^2 u + \lambda u = f$$

$$\downarrow$$

Weak form + IBP: $$-(\nabla u, \nabla v) + \lambda(u, v) + (\nabla u, v)|_{d\Omega} = (f, v)$$

# Nektar++: www.nektar.info

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

Nektar++ is a spectral/hp element toolkit written in C++.

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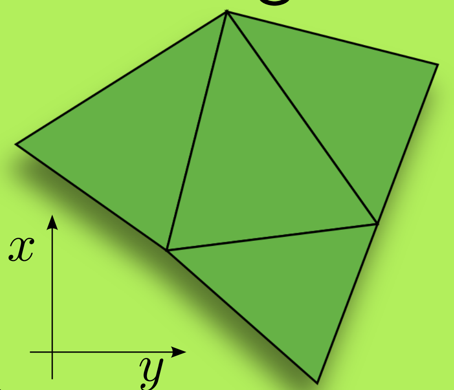
MultiRegions




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

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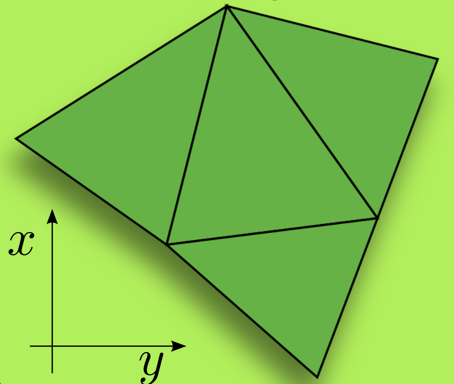
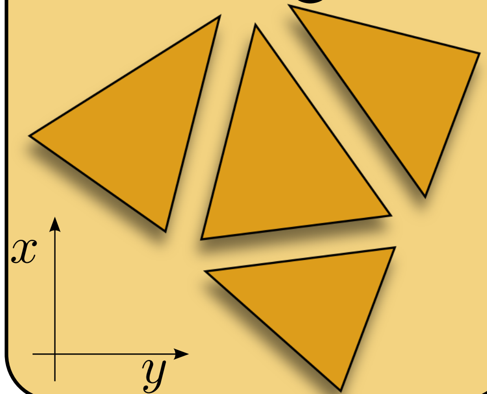



LocalRegions




$$\mathbf{f}[i] = \boxed{\int_\Omega \Phi_i(x) f(x)\,dx} = \boxed{\sum_e^{N^{el}} \sum_p \int_{\Omega^e} \phi_p(x) f(x)\,dx}$$

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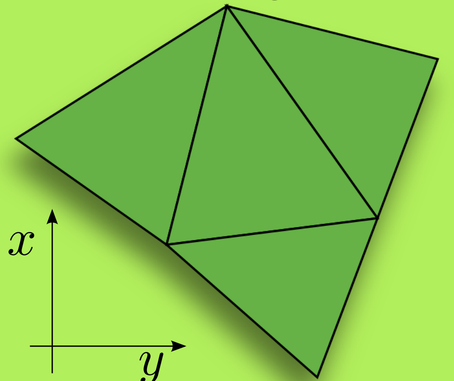
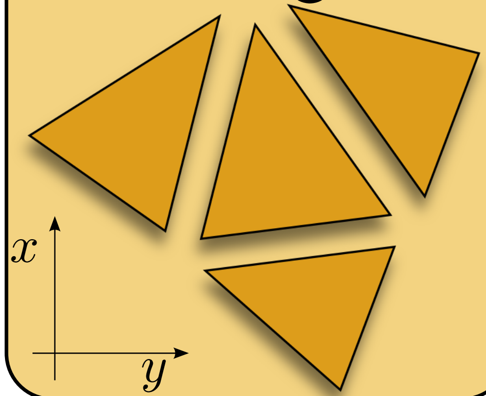
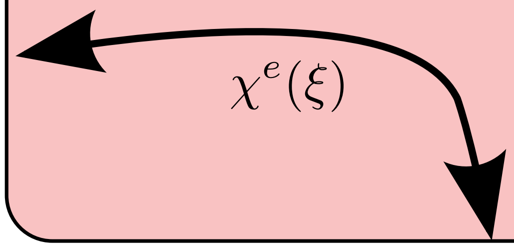
MultiRegions




LocalRegions




SpatialDomains

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$$= \sum_e \sum_p \int_{\Omega^e} \phi_p(\chi^e(\xi)) f(\chi^e(\xi)) J^e \, d\xi$$

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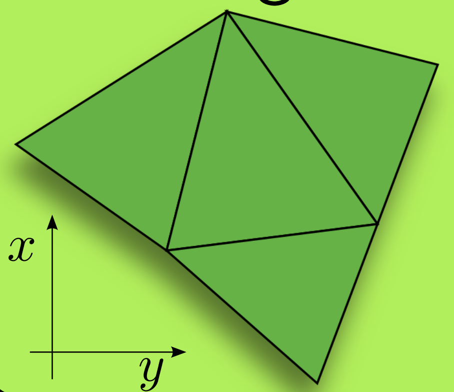
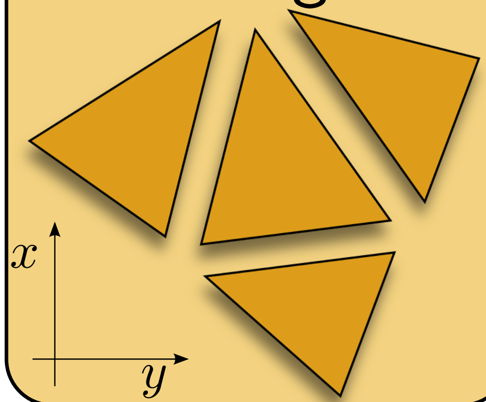
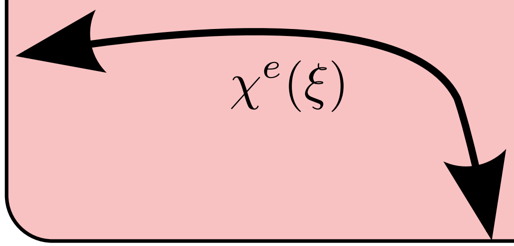
## MultiRegions



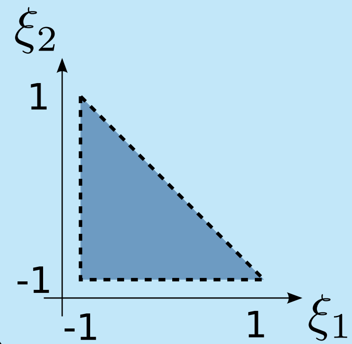

## LocalRegions




## SpatialDomains




## StdRegions




$$\mathbf{f}[i] = \int_\Omega \Phi_i(x) f(x)\,dx = \sum_e^{N^{el}} \sum_p \int_{\Omega^e} \phi_p(x) f(x)\,dx$$

$$= \sum_e \sum_p \int_{\Omega^e} \phi_p(\chi^e(\xi)) f(\chi^e(\xi)) J^e\,d\xi$$

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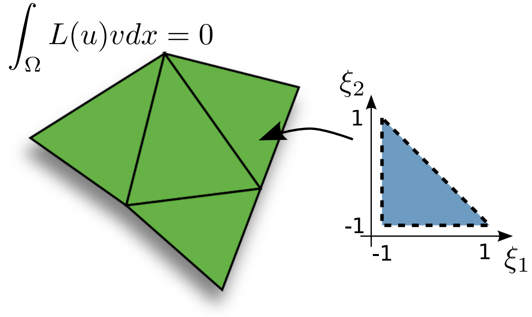
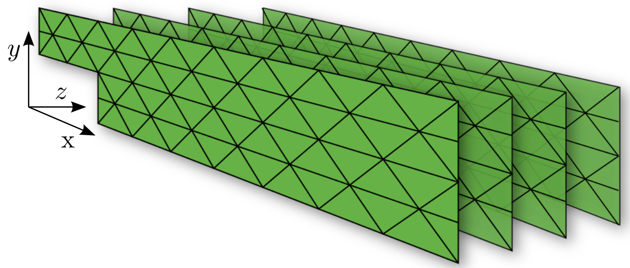


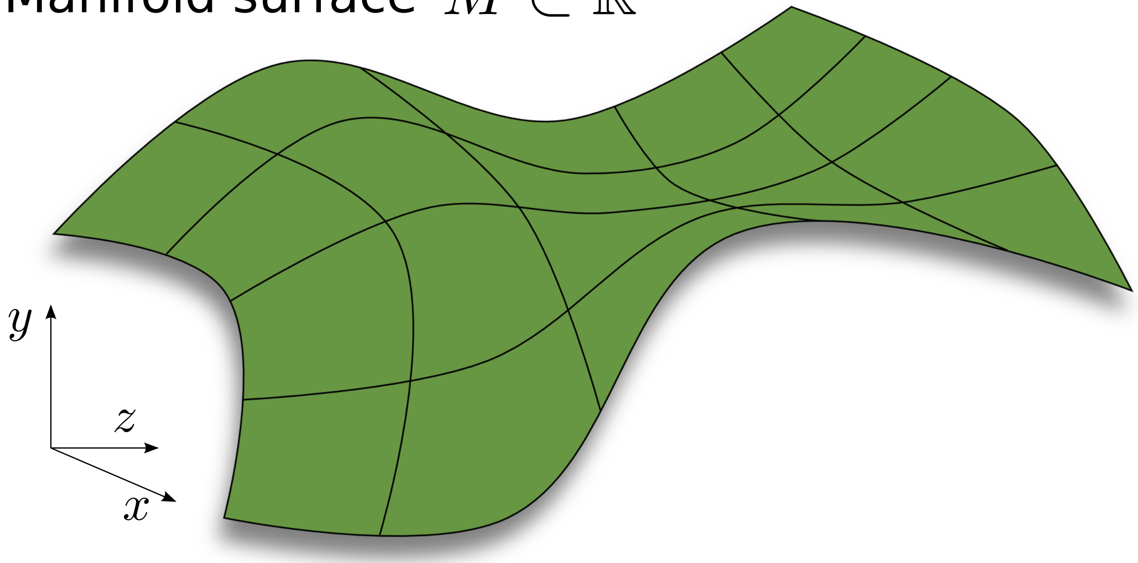

# Mathematical Construction

Expose different discretisations (CG, DG) by combining and reusing low-level elemental mathematical constructs.

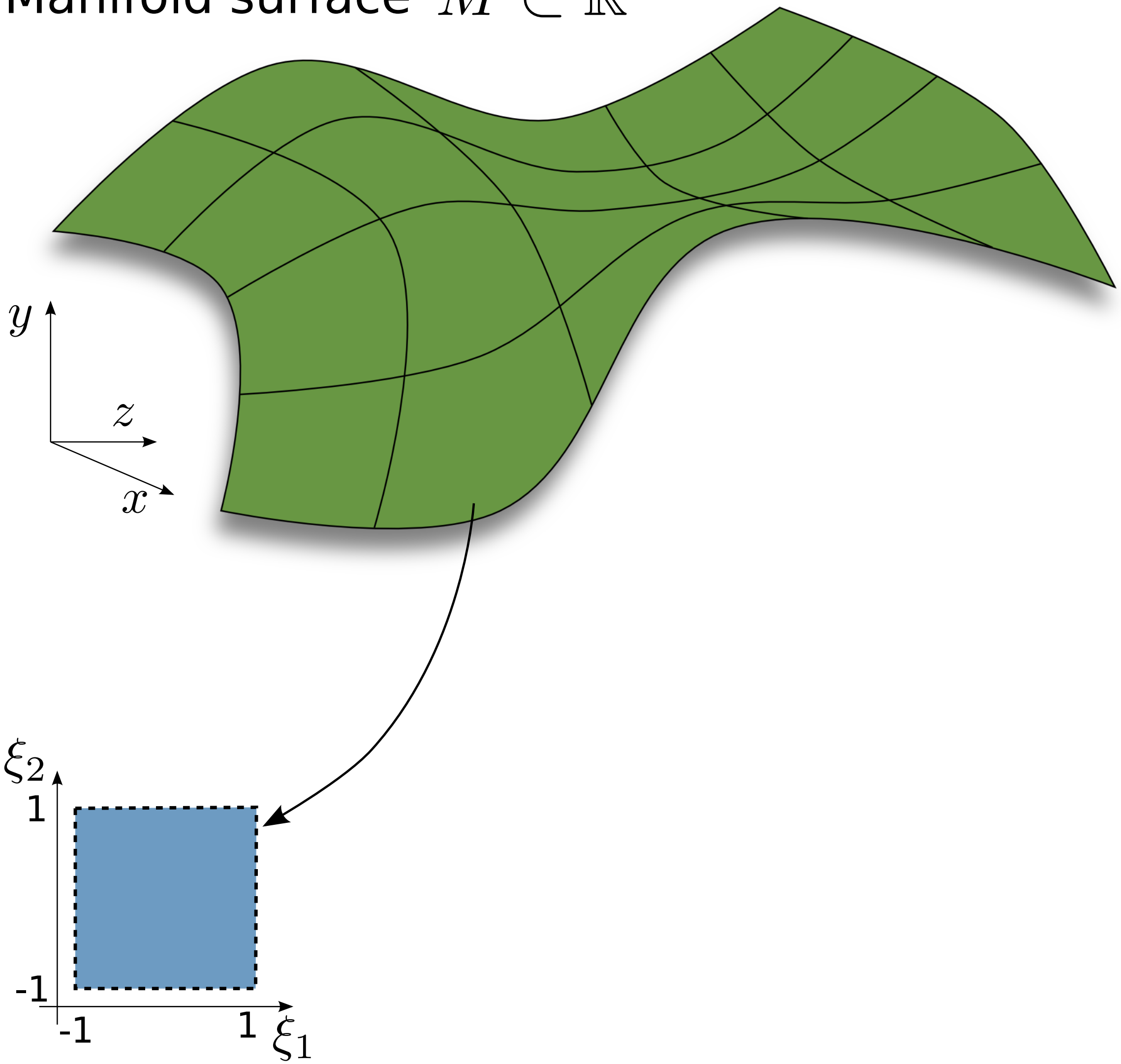



Retain and exploit domain symmetries and embeddings (homogeneous, cylindrical, manifold)

Manifold surface $M \subset \mathbb{R}^3$



Manifold surface $M \subset \mathbb{R}^3$




e.g. Laplace operator generalises to Laplace-Beltrami

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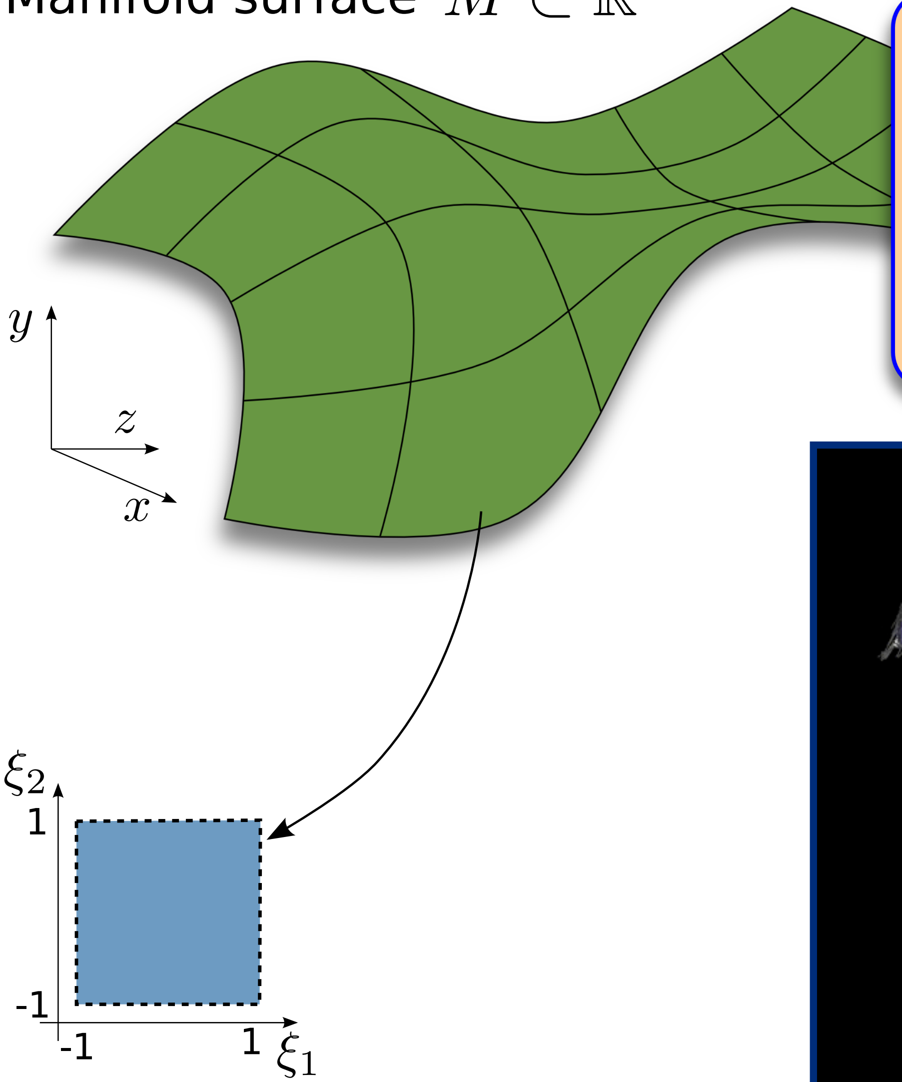
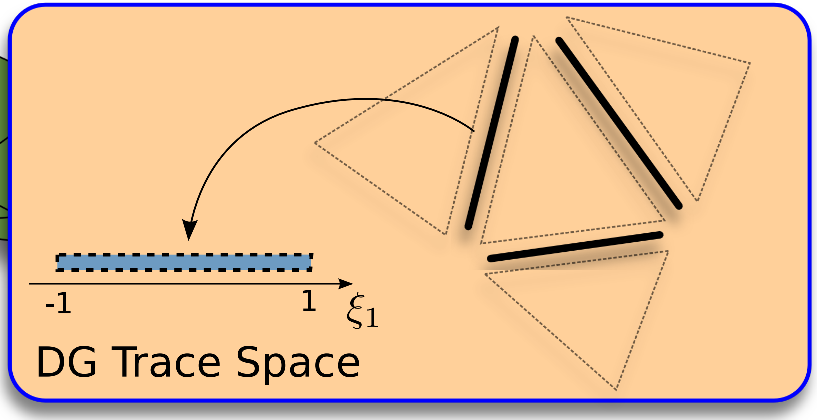
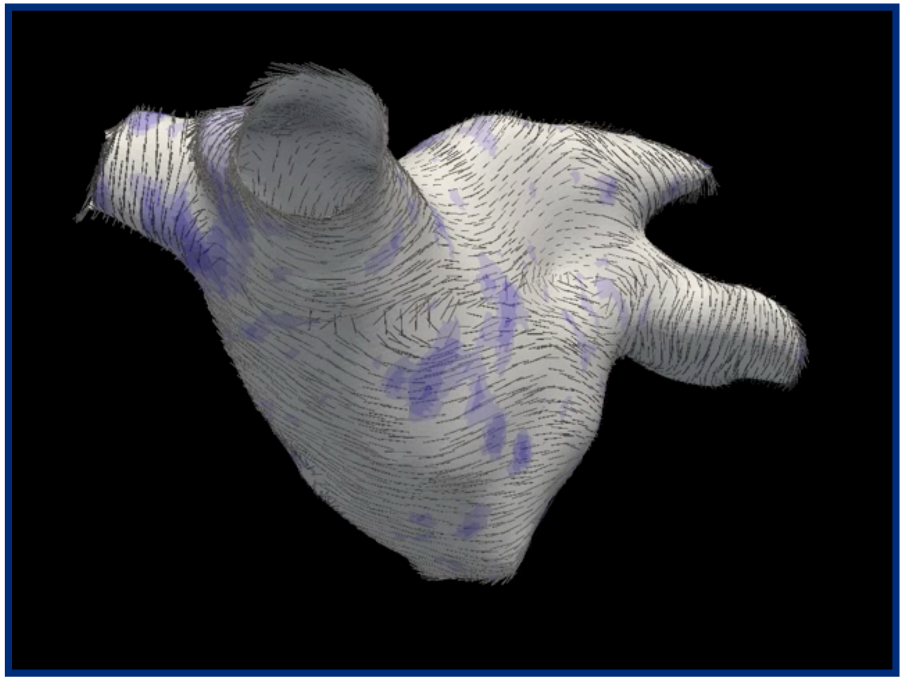


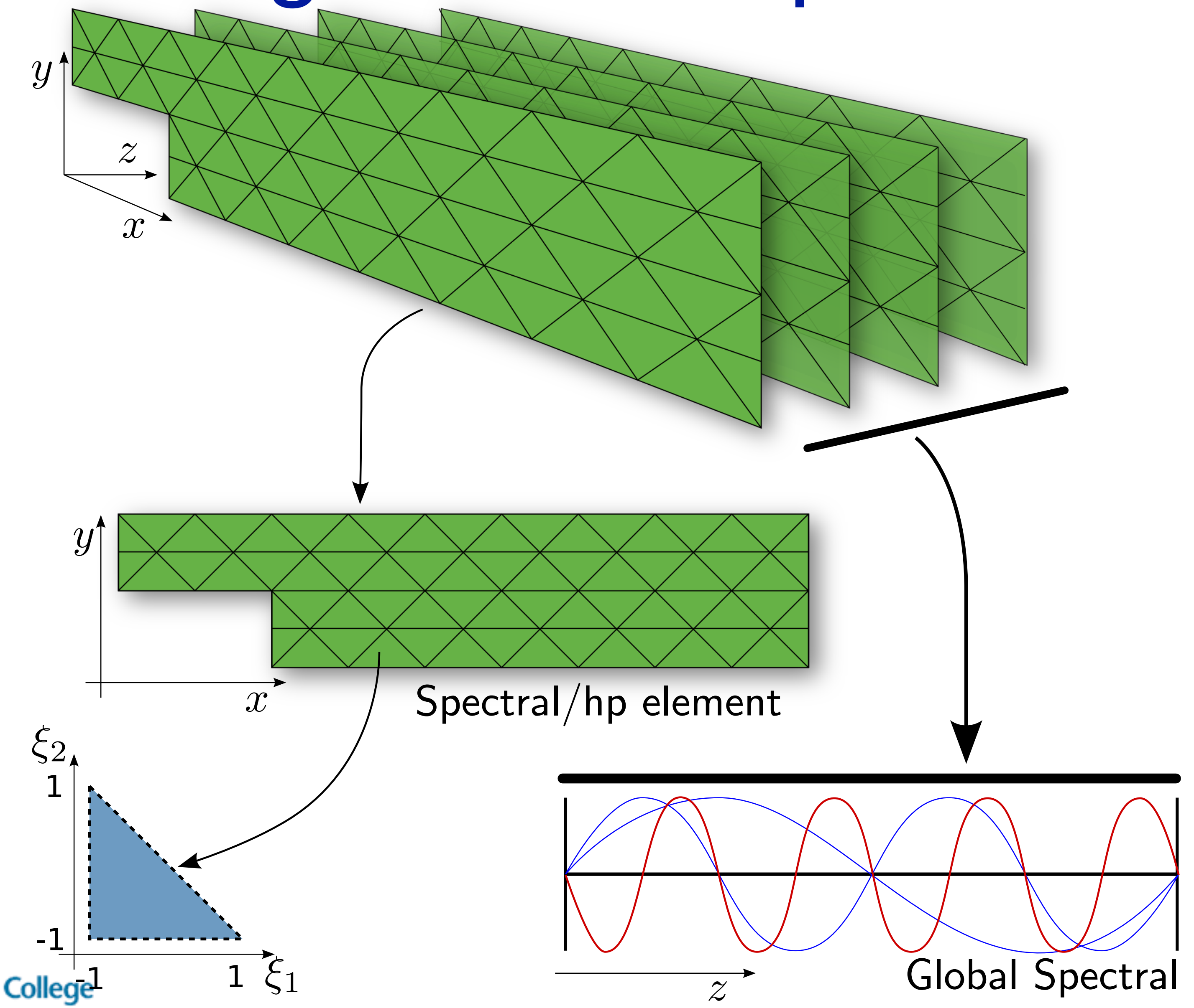

Examples



e.g. Laplace operator generalises to Laplace-Beltrami

# Homogeneous Expansions

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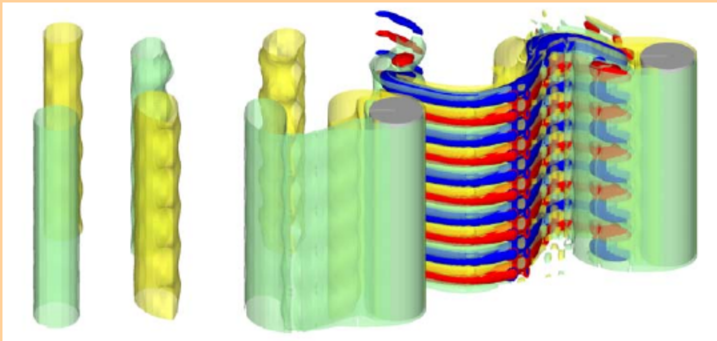
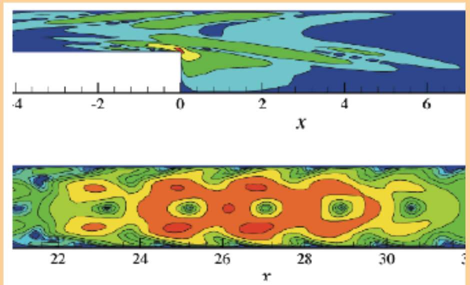
# Direct Stability Analysis



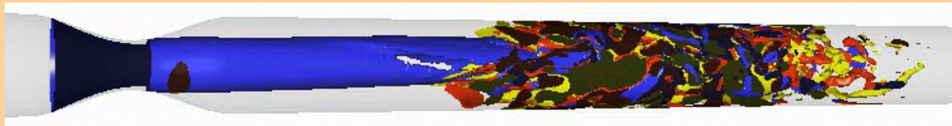
B. S. Carmo, S. J. Sherwin, P. W. Bearman, R. H. J. Willden
J. Fluid Mech. (2008), vol. 597, pp. 1–29.



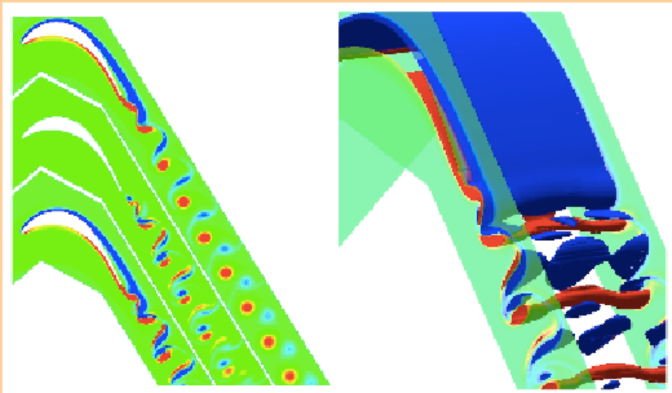

H. M. Blackburn, D. Barkley, S. J. Sherwin
J. Fluid Mech. (2008), vol. 603, pp. 271-304.

Stability of basic flows

Complex Geometry LNS & DNS



S. J. Sherwin, H. M. Blackburn
J. Fluid Mech. (2005), vol. 533, pp. 297–327.



A. S. Sharma, N. Abdessemed, S. J. Sherwin, V. Theofilis
Theor. Comput. Fluid Dyn. (2011) 25:19–30

Biomedical and Engineering applications

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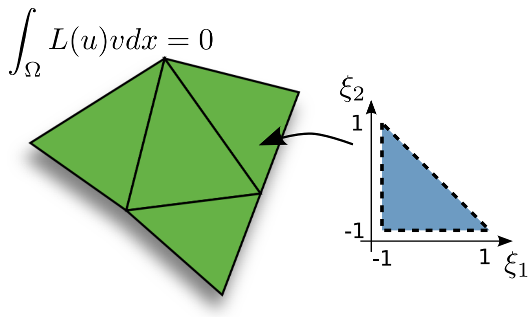


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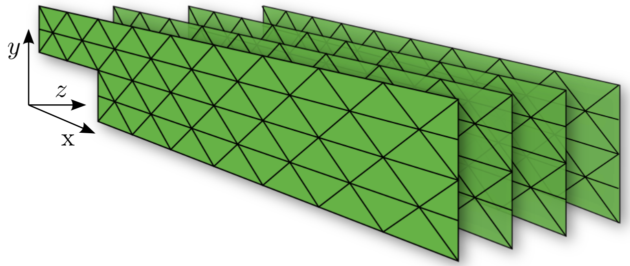
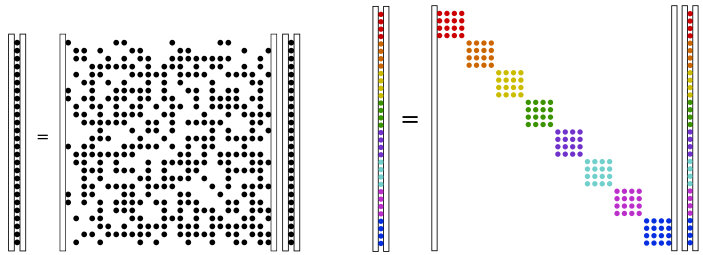



Retain and exploit domain symmetries and embeddings (homogeneous, cylindrical, manifold)

# Computational Implementation

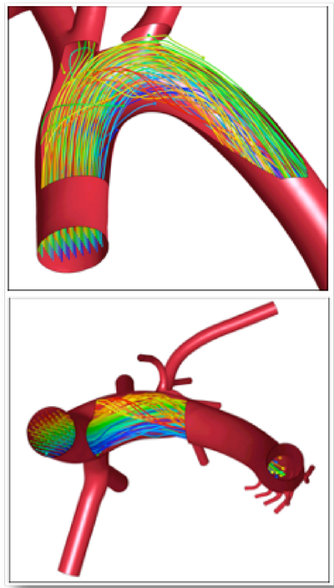
Challenge high-/low-order boundaries while maintaining efficiency.



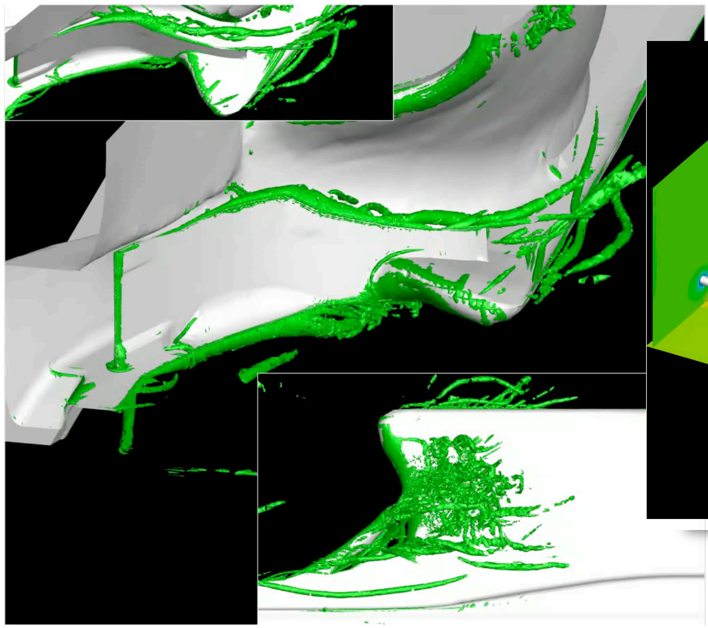
What do we understand by low and high order? When is each choice useful?

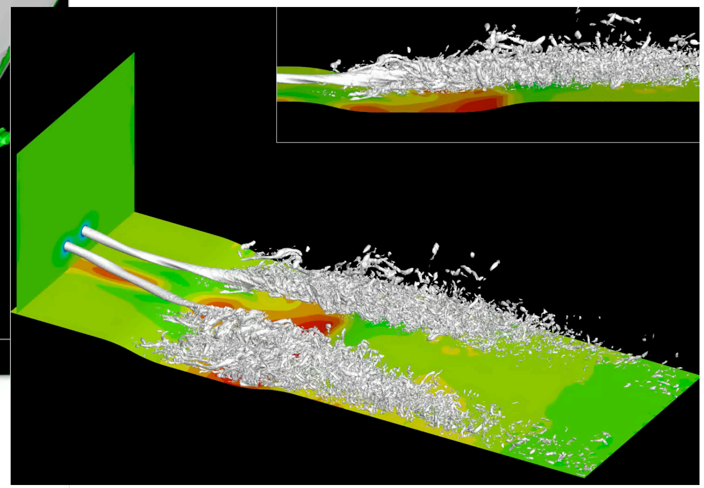
Low Order
$P = 1$

High Order
$P = 15$



P. E. Vincent, A. M. Plata, A. A. E. Hunt, P. D. Weinberg
J. R. Soc. Interface, 10.1098/rsif.2011.0116





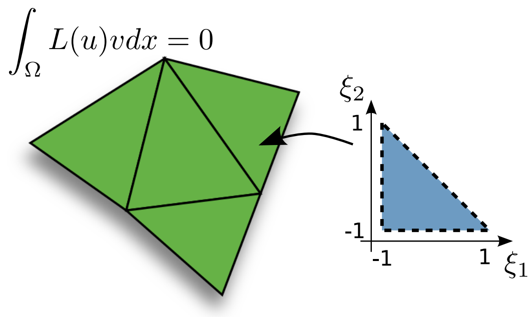
Julien Hoessler PhD Thesis 2012

High Reynolds number flows.

Low Reynolds number flows.

Complex geometry.

How do we implement low- and high-order techniques efficiently across current and future hardware?

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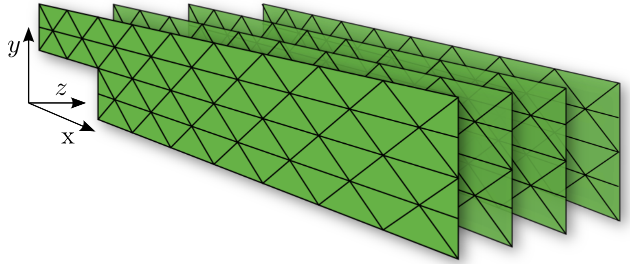


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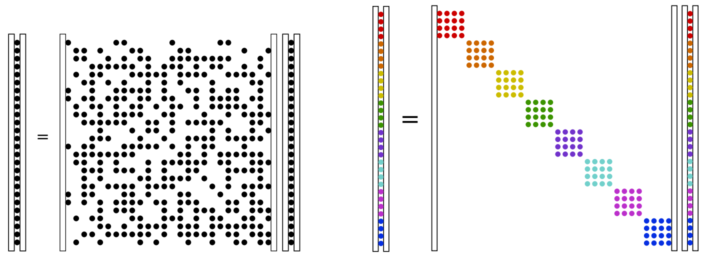
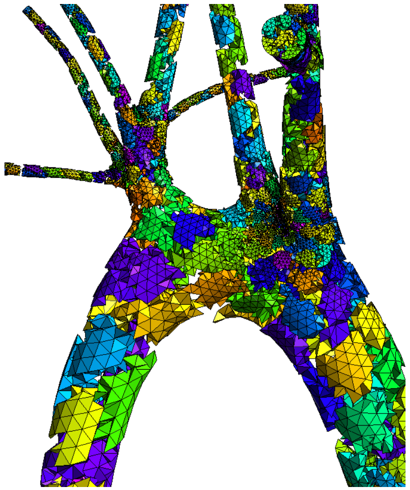
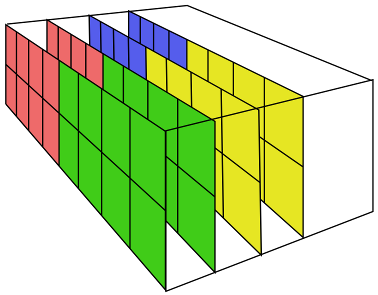


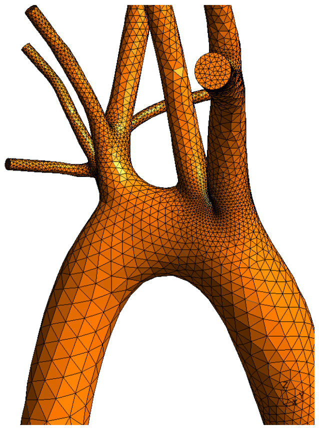



Bridge current and future hardware diversity through hybrid implementation strategies.

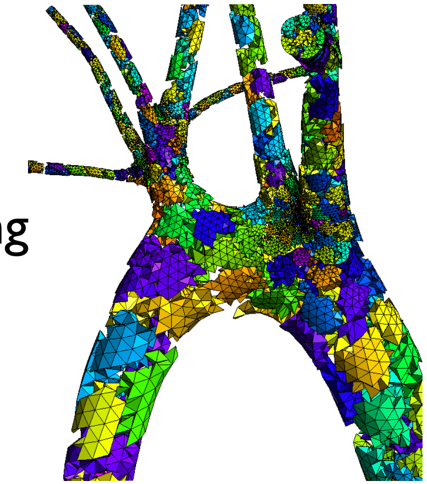


Achieve flexible HPC scalability and performance through mixed parallelism.

# Hybrid Numbering & Mixed Parallelisation

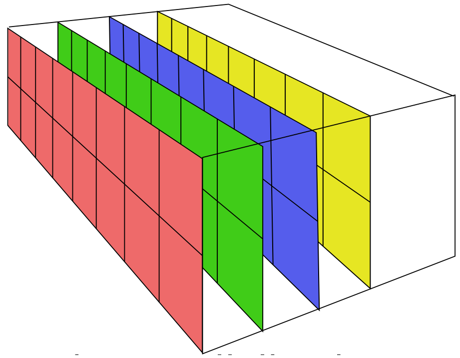


Global numbering

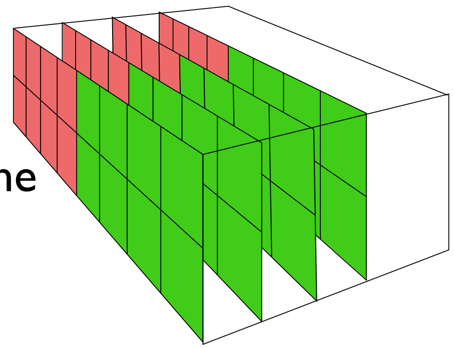


Hybrid numbering

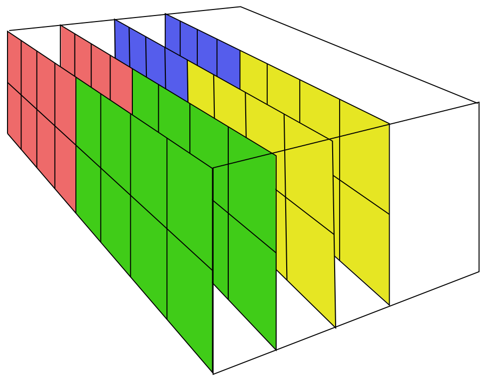
Local numbering



Fourier parallelisation



Spectral/hp plane parallelisation

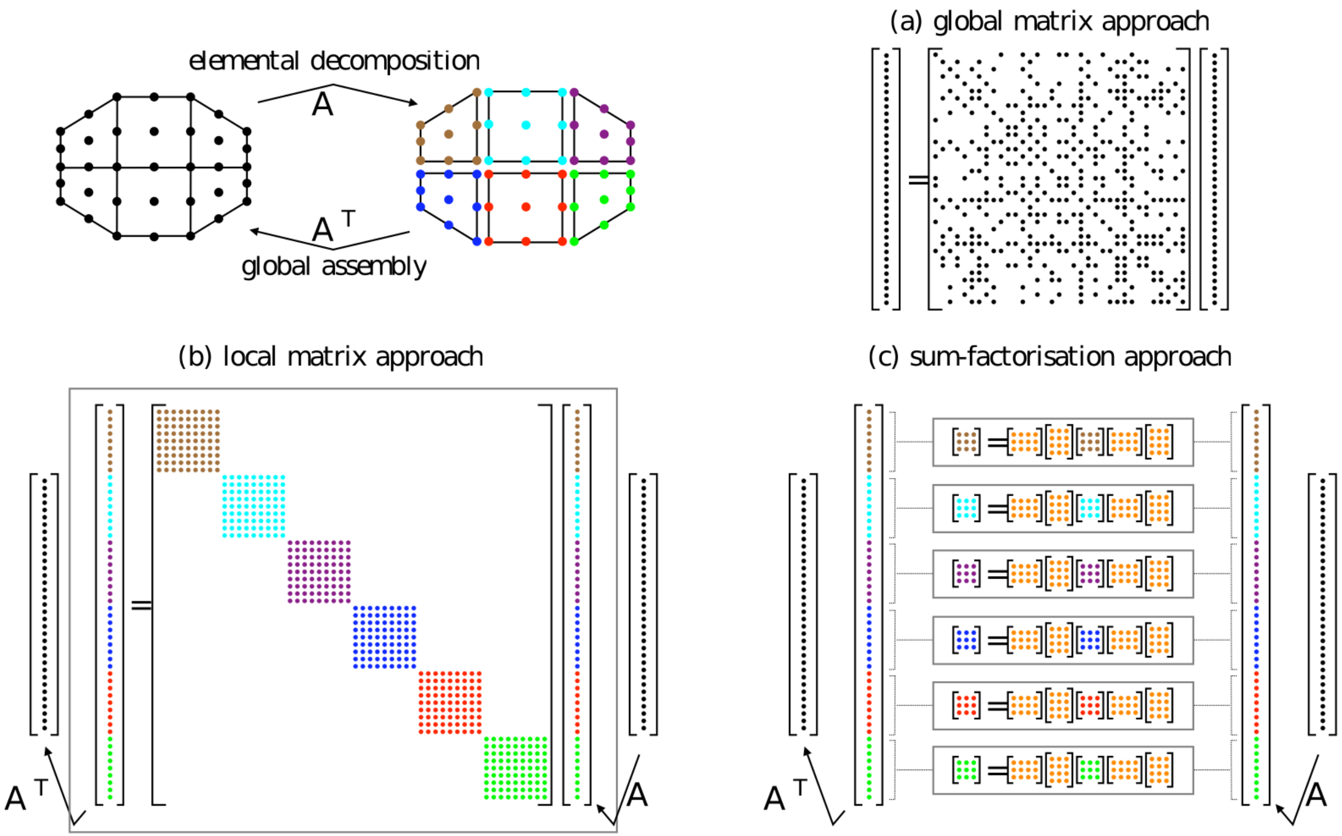


Mixed parallelisation

# Outline

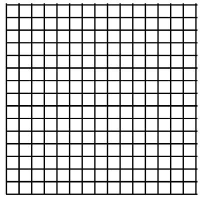
- What are we doing?
- Optimizing our implementations
  - From h to p efficiently
  - Variable p
  - Cloud Computing

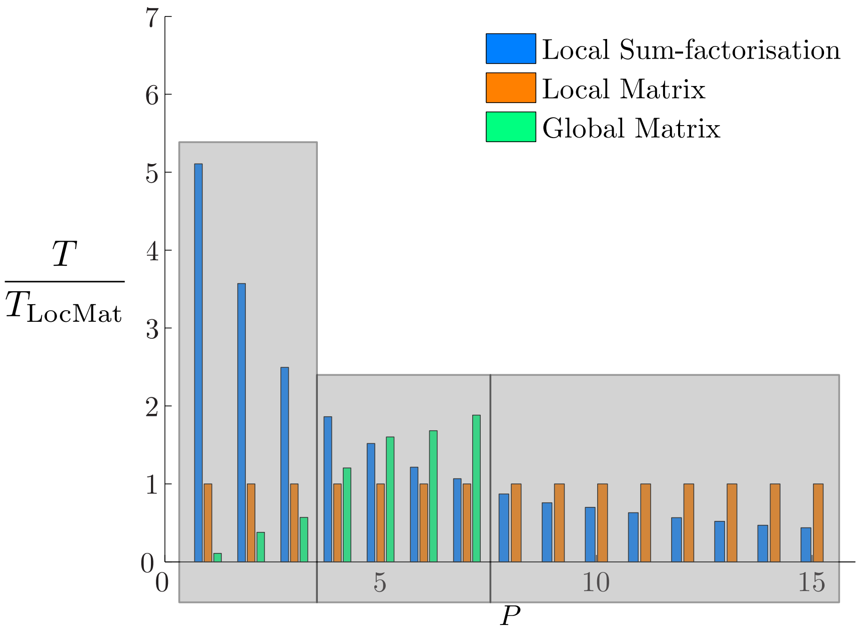
# Evaluation Strategies for iterative solvers

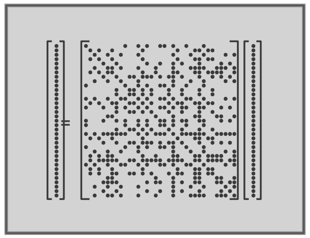


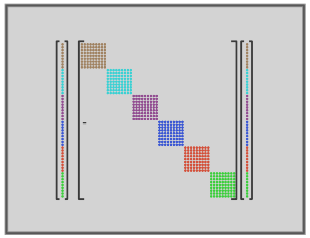
# Computational results

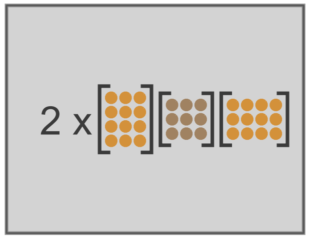
- mass matrix operator: $\hat{g}_i = \sum_j (\Phi_i, \Phi_j)_\Omega \hat{f}_j \quad \forall i$





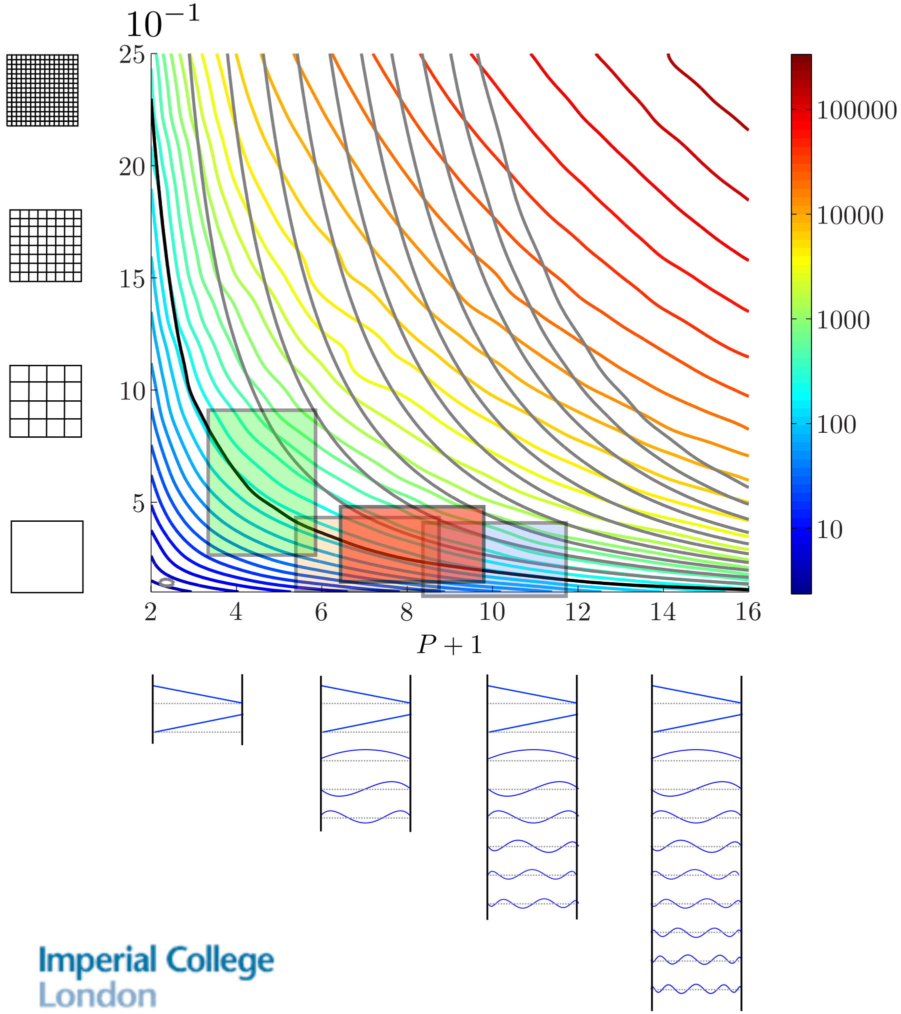


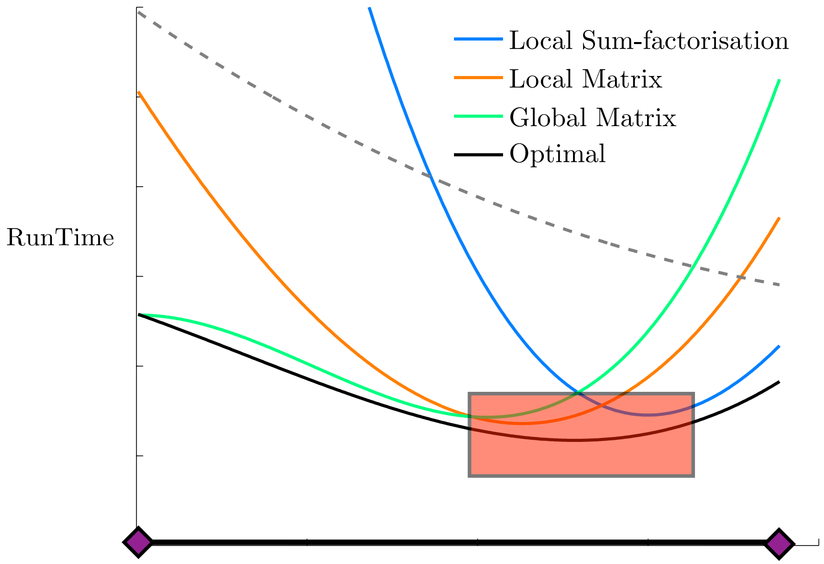



*Vos, Sherwin, Kirby, JCP, 2010*

# Error vs computational cost?

- minimal run-time




9 Elements, P=6

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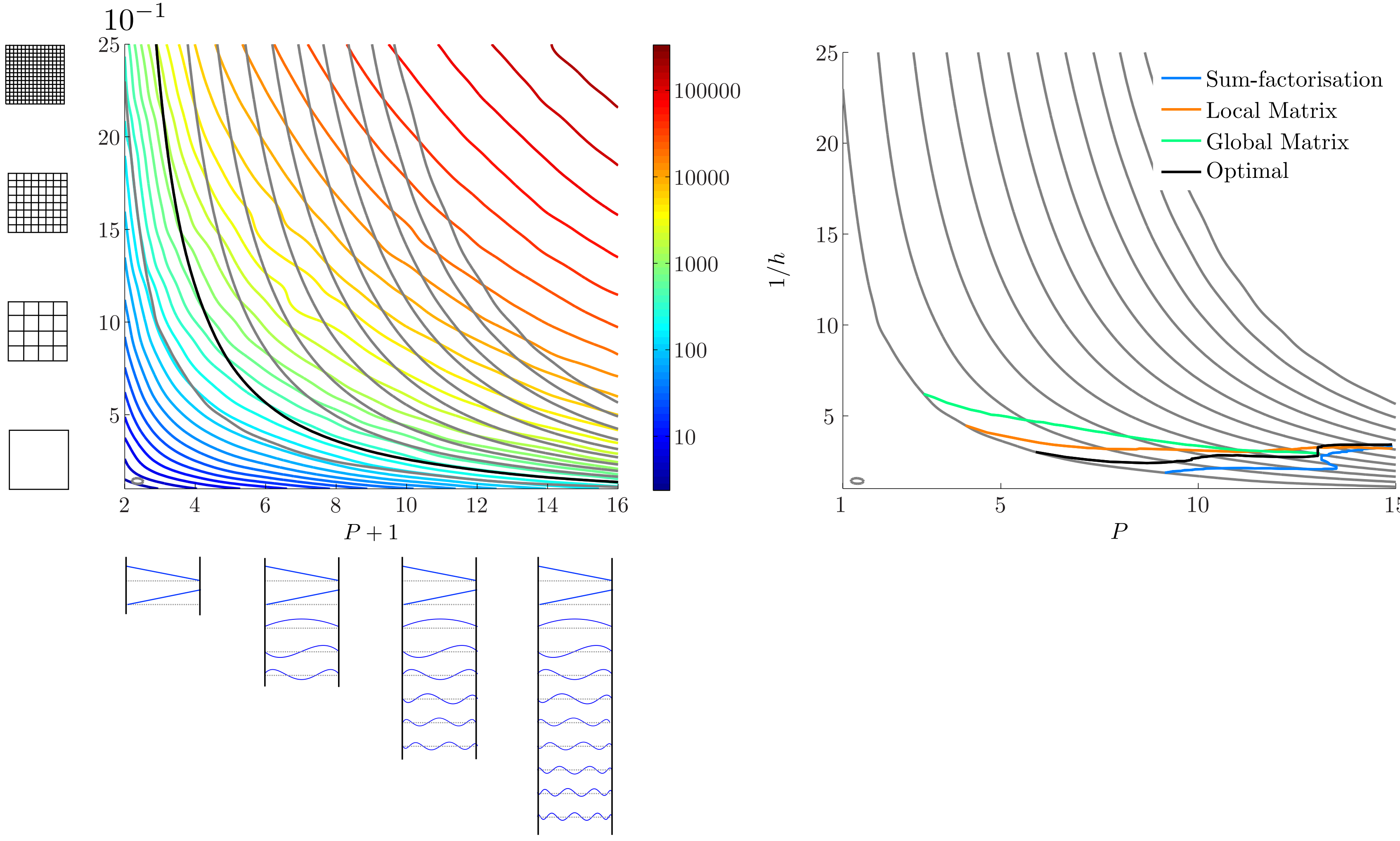
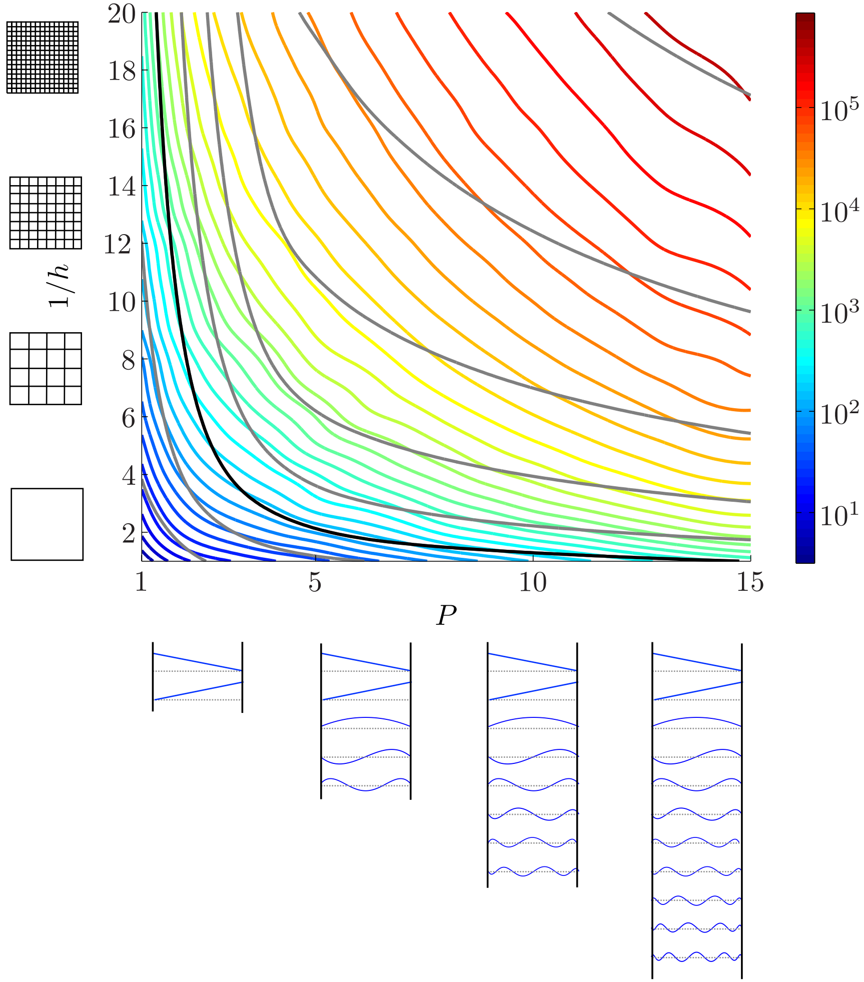
# Error vs computational cost?

- minimal run-time - *path of optimal discretisations*



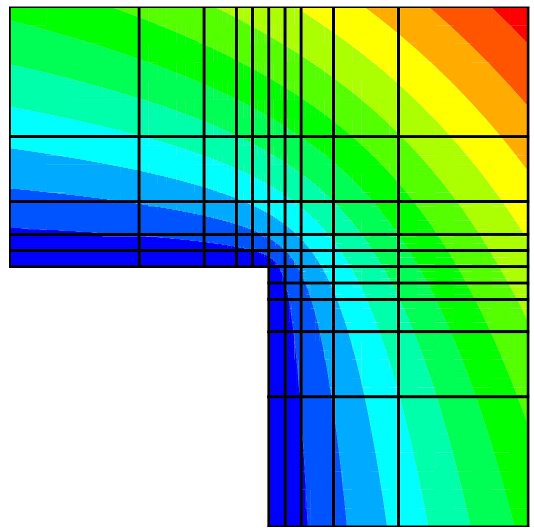
# Computational results: Non smooth solution

- minimal run-time - corner problem (error = $10^{-4}$)




Helmholtz equation

$$\nabla^2 u(\boldsymbol{x}) - \lambda u(\boldsymbol{x}) = f(\boldsymbol{x}) \qquad x_i = \left(\frac{i}{n_{el}}\right)^3$$



$$u(r,\theta) = r^{\frac{2}{3}} \sin(\frac{2}{3}\theta + \frac{\pi}{3})$$

irregular solution

# Computational results

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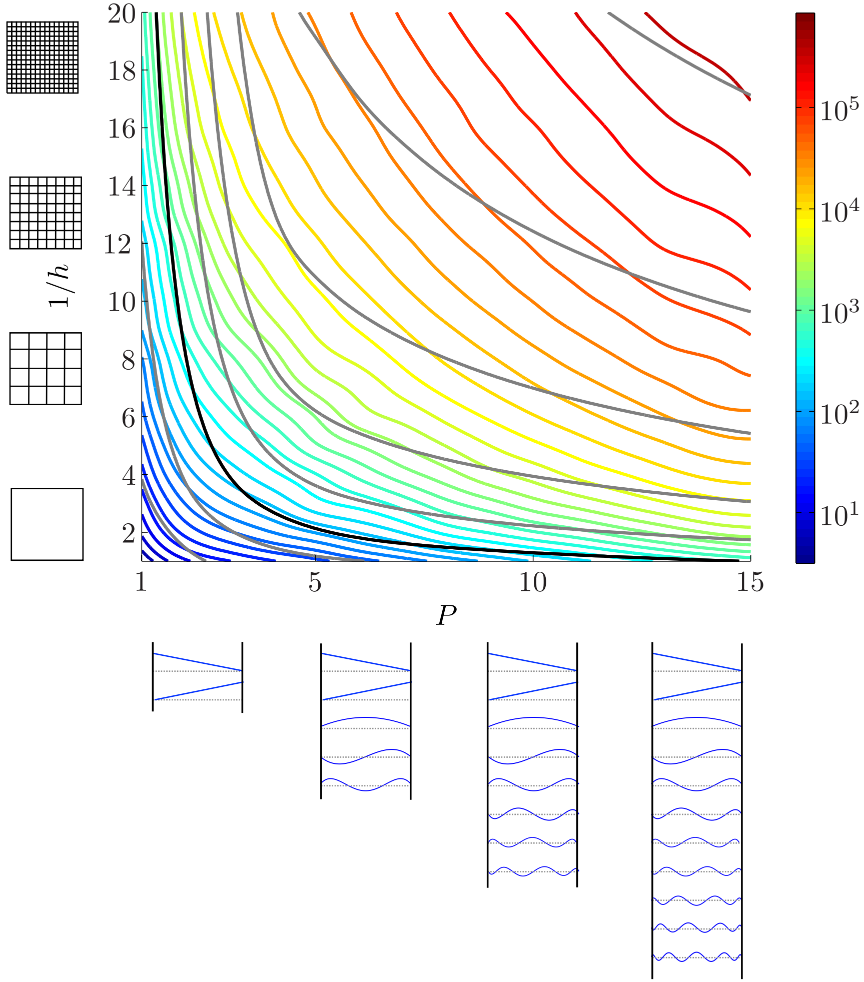
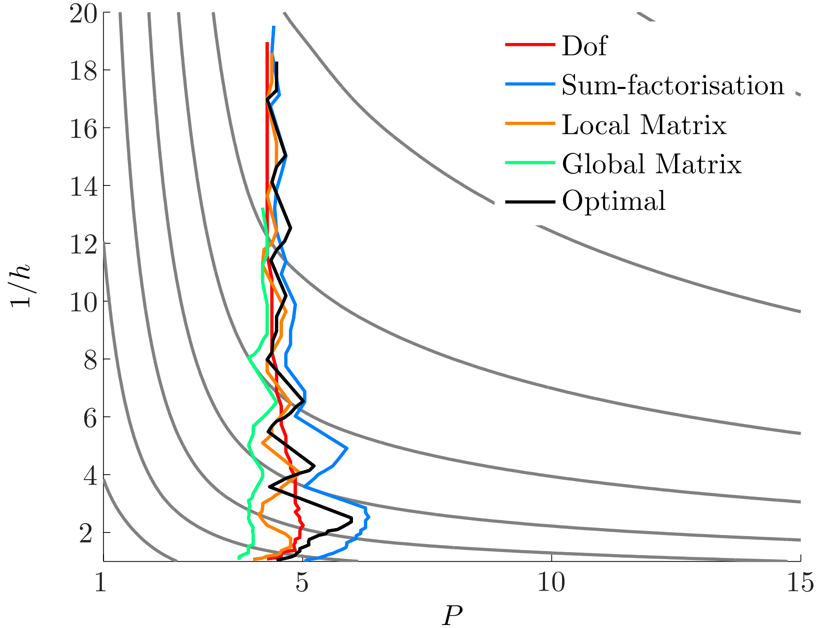
- minimal run-time - path of optimal discretisations



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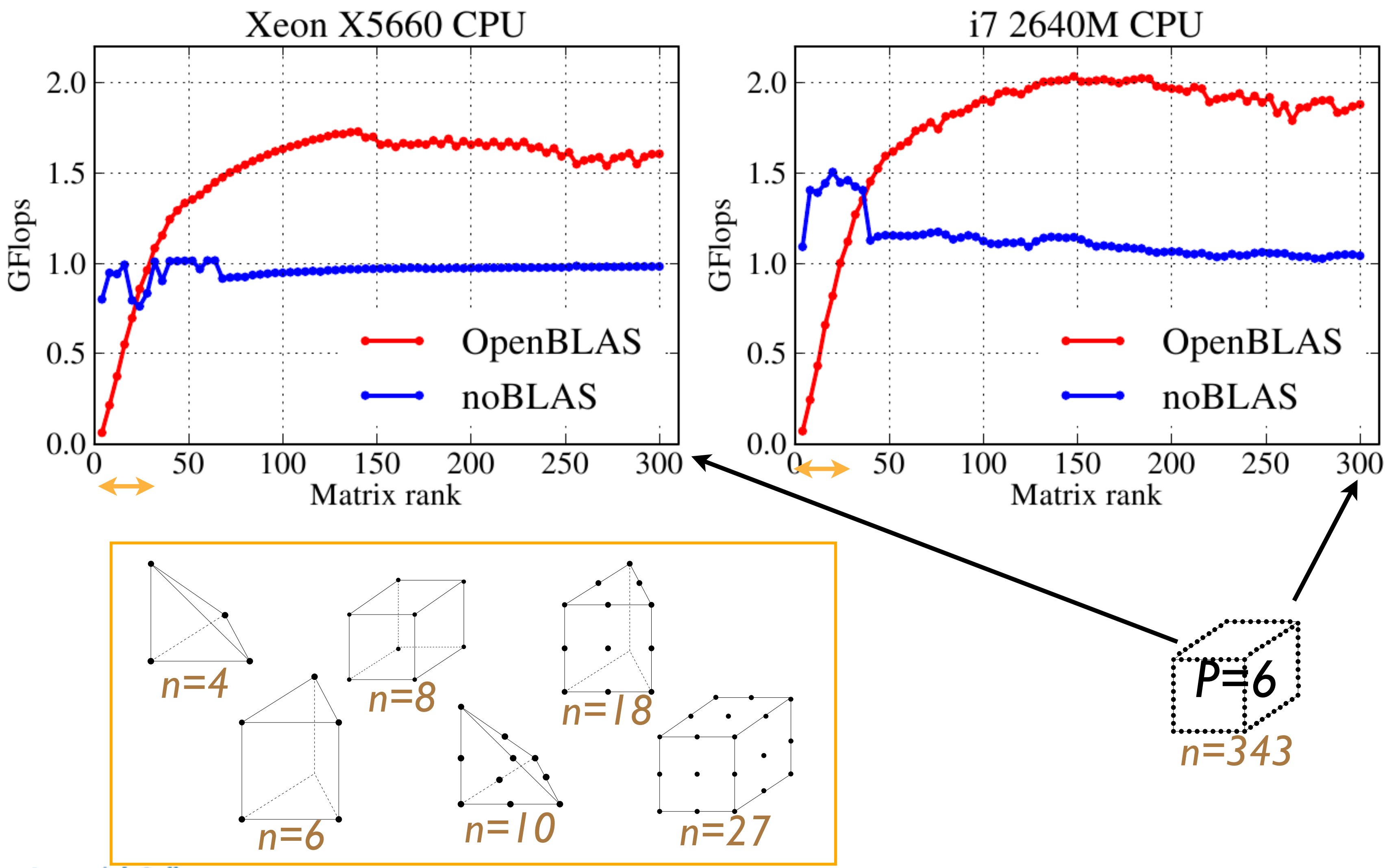
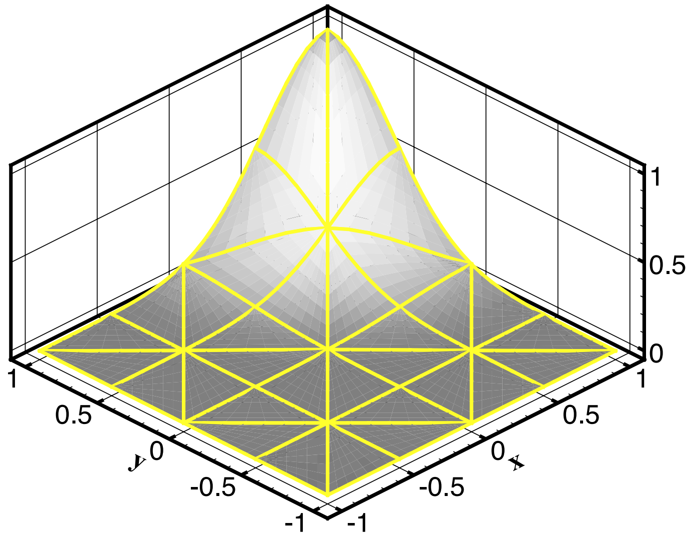
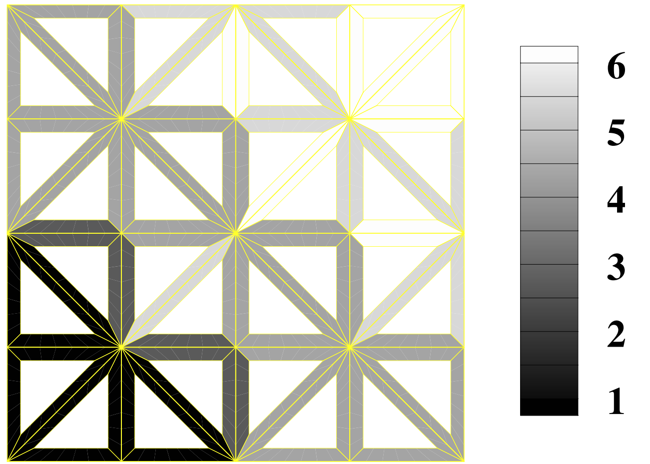
# Local Matrix: Hardware diversity



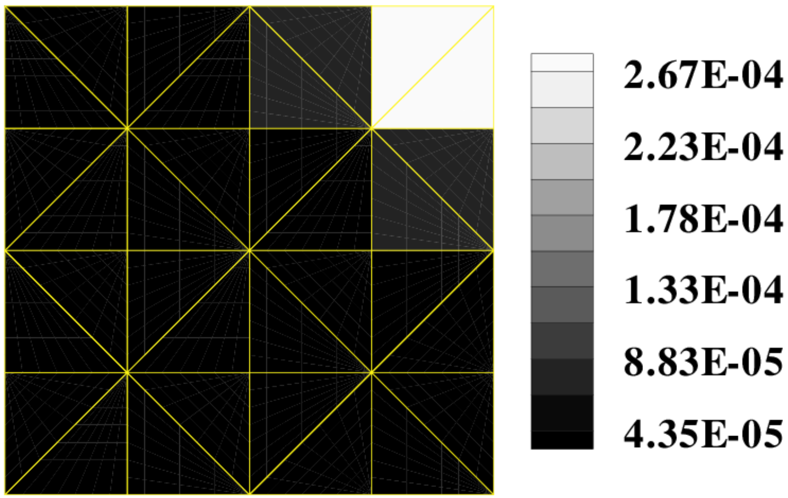
# Variable matrix size due to variable p



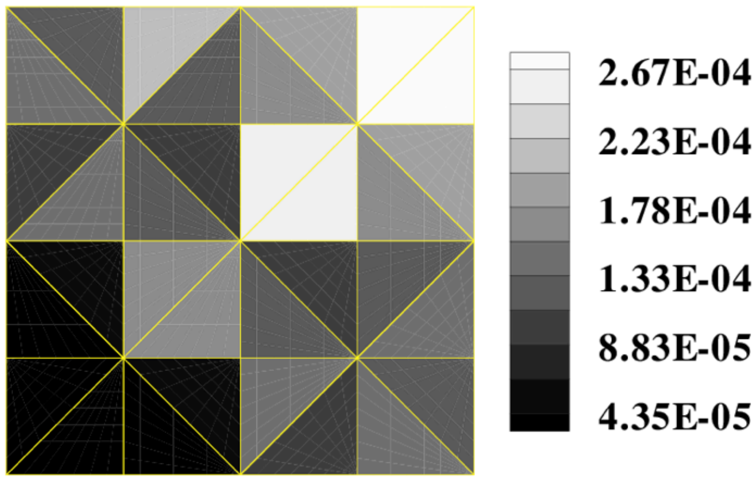

Solution




Variable P




Fixed P error




Variable P Error

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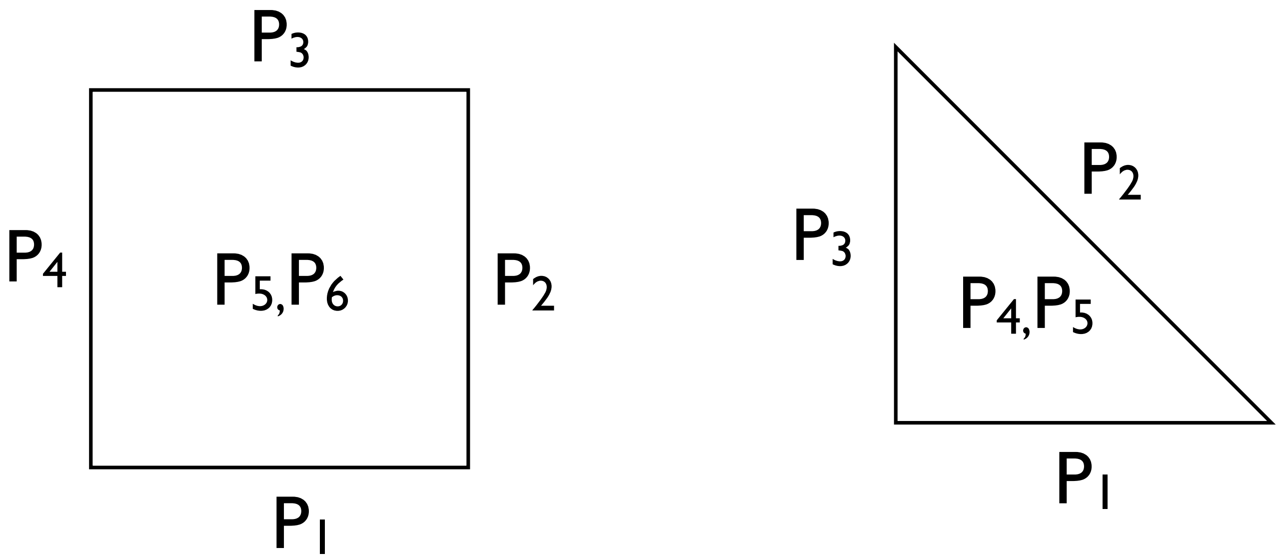
# How many parameters?



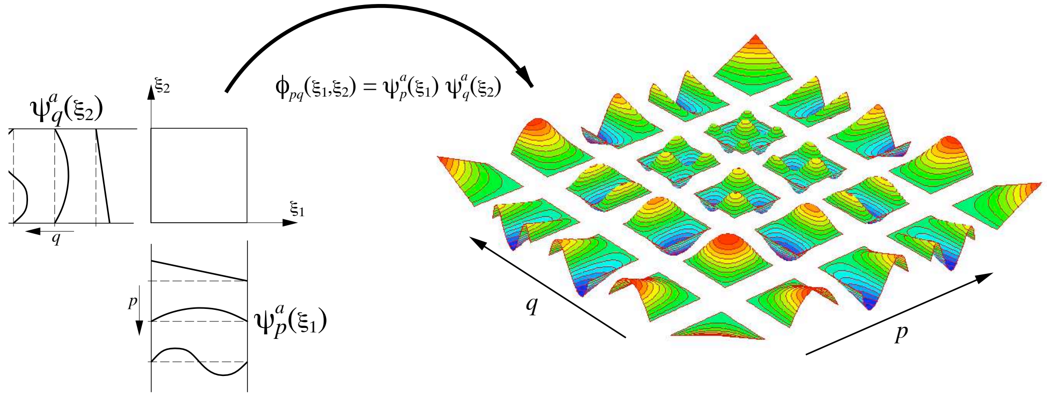

6 parameters

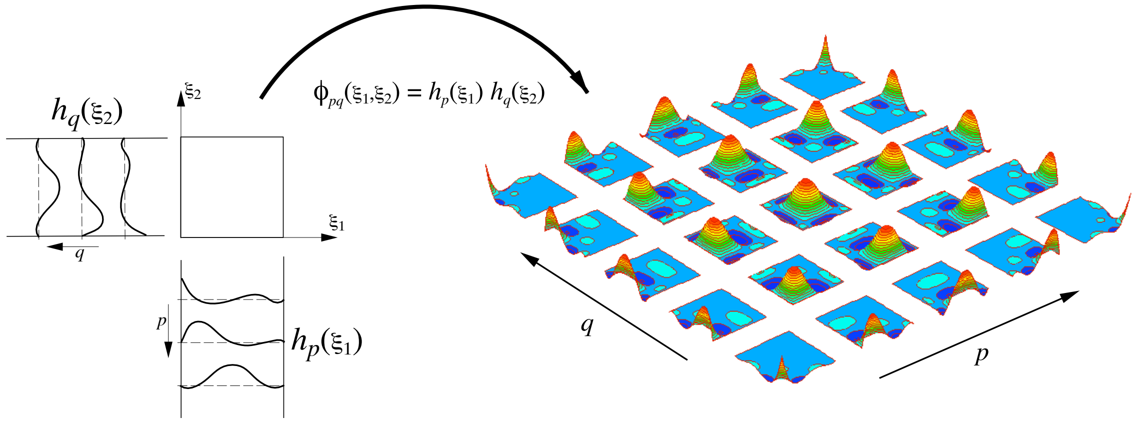
5 parameters

Hexahedral: 12 edges, 8 faces, 1 interior = 31 parameters

Tetrahedral: 6 edges, 4 faces, 1 interior = 17 parameters

# Tensor product design

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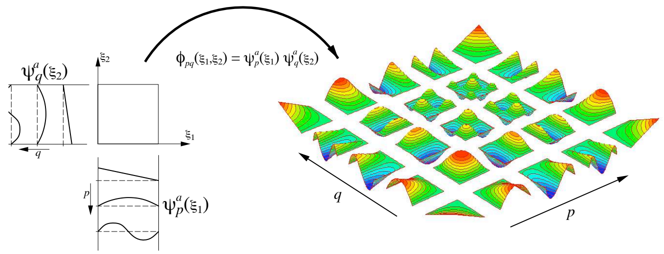
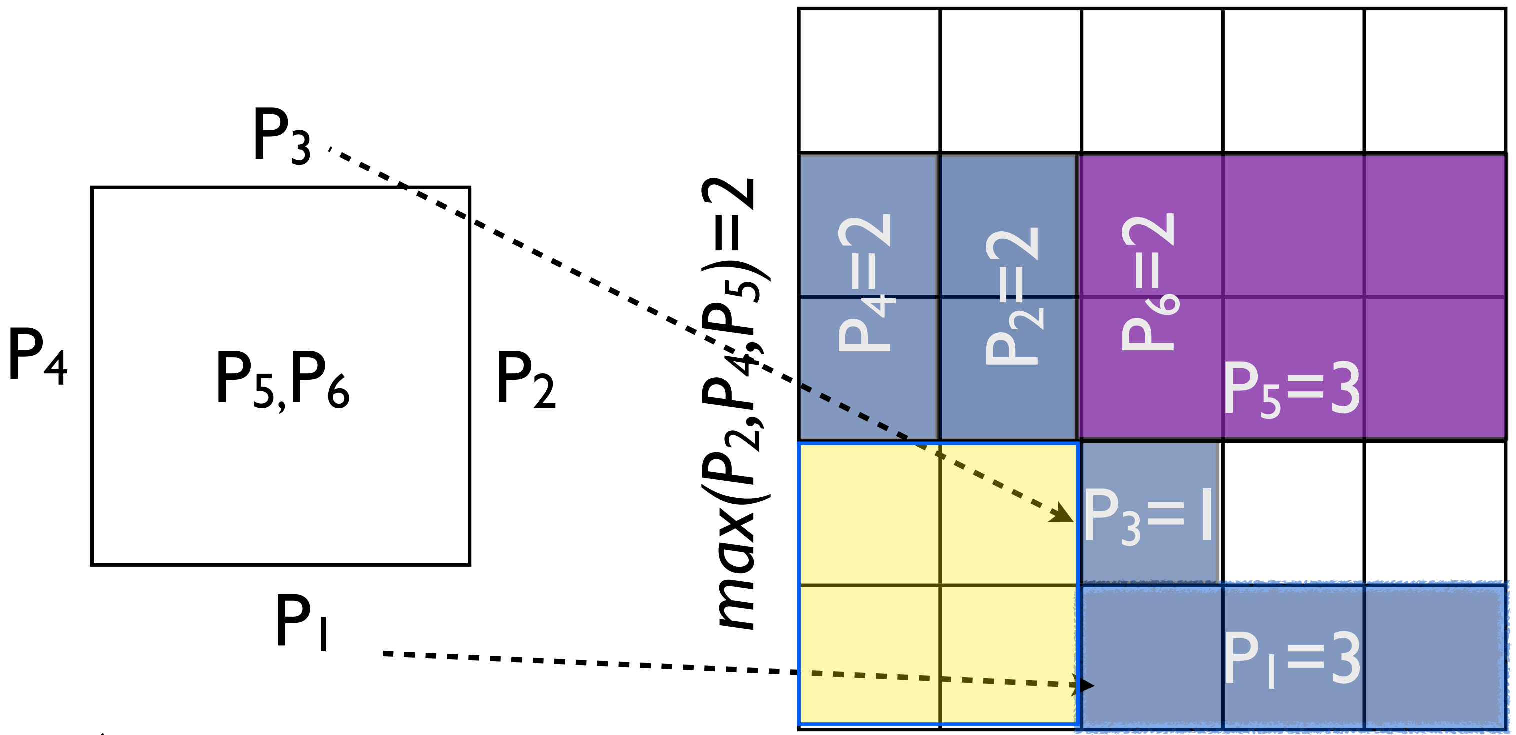
# Zero packing



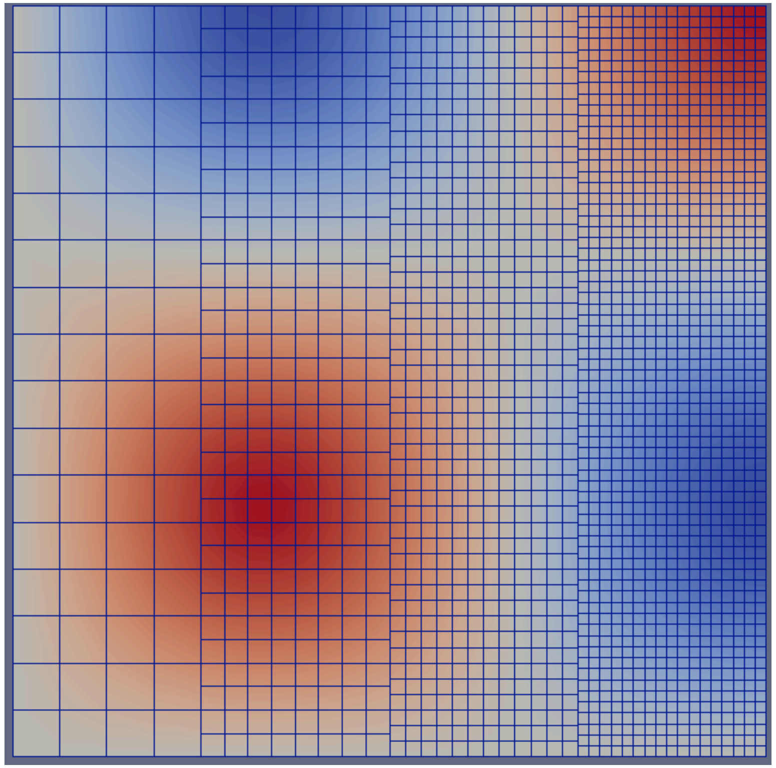




6 parameters

$max(P_1,P_3,P_5)=3$

2 parameters

# Helmholtz example

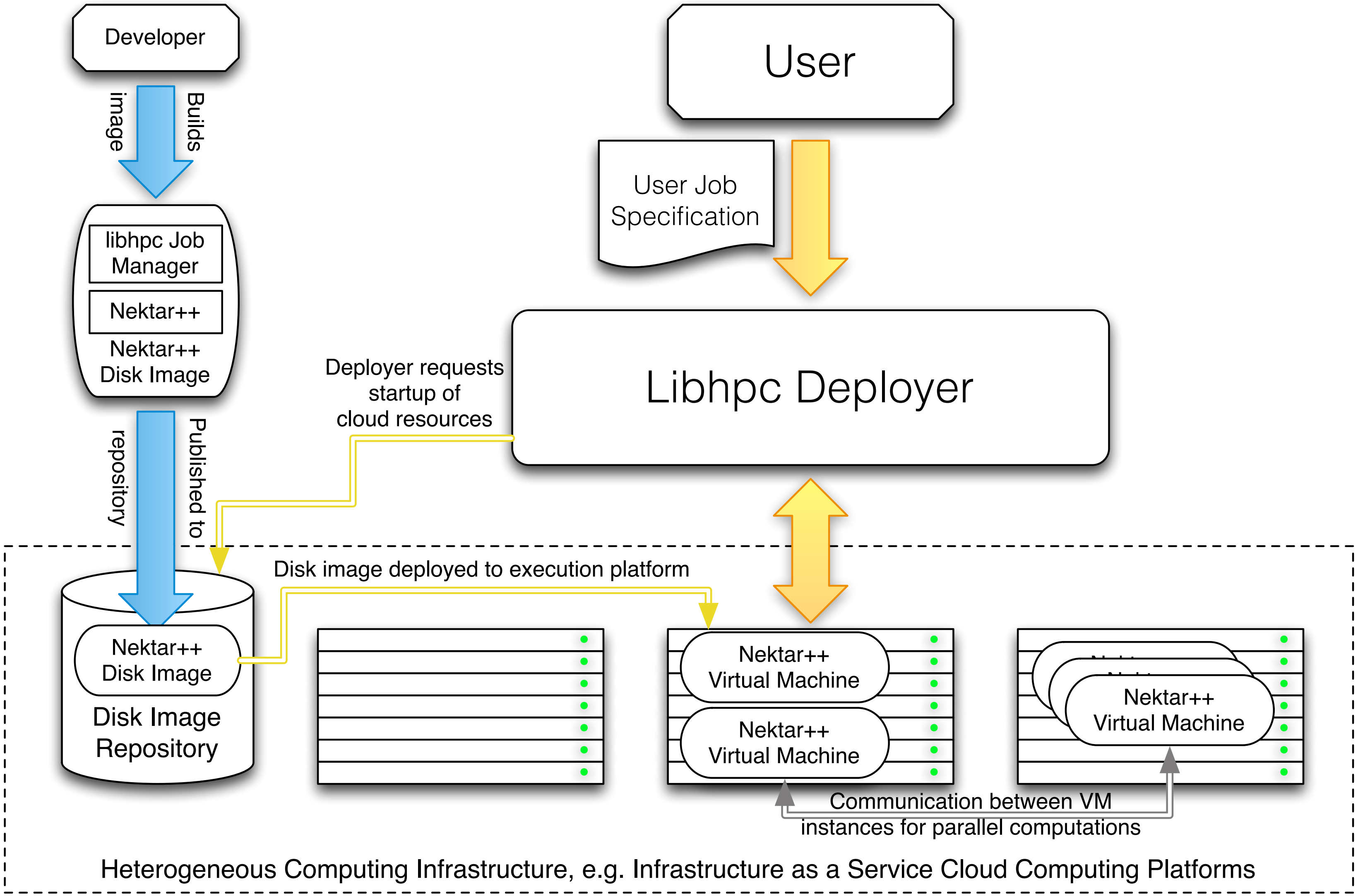


P=4 P=8 P=12 P=17

# LibHPC

*J. Cohen, P. Burovskiy, J. Darlington*

- Target software on multi-core, distributed & hetrogeneous platforms
- Run on Infrastructure-as-a-service (IaaS) clouds
- Why?
  - Intermittent running makes access to HPC difficult
  - Scale resource beyond local capacity

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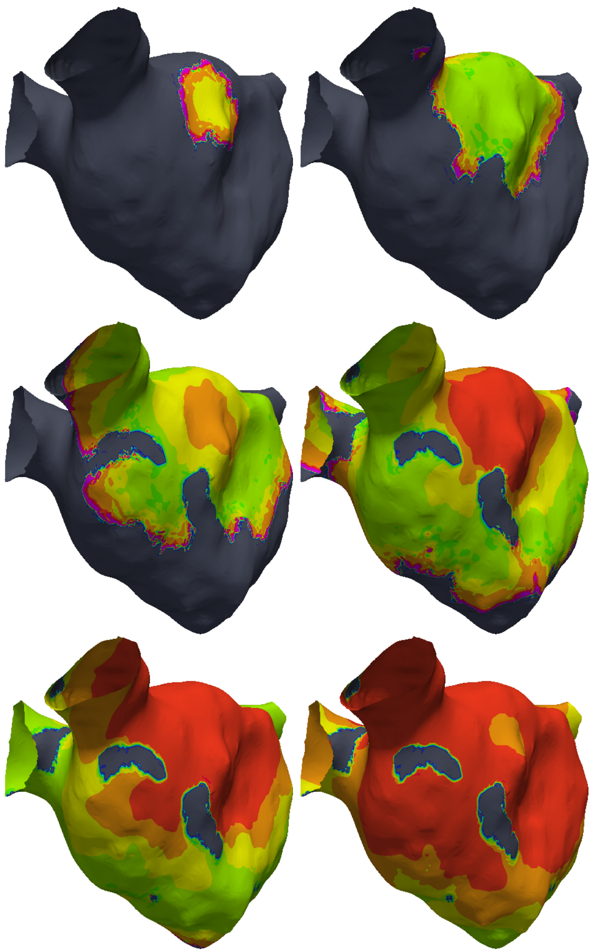

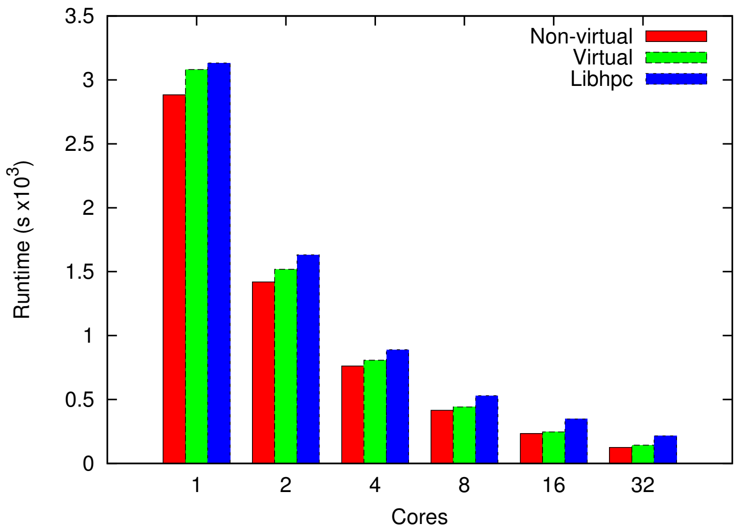


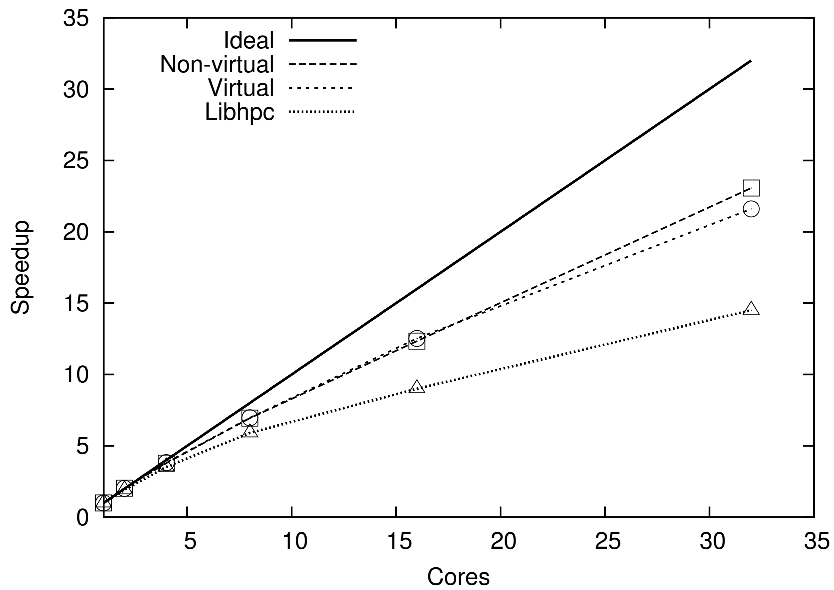


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# Summary

- Presented implementation optimisations to blend high and low order polynomial order
  - Mixed implementation of basic operators
  - Mixed Fourier discretisations.
- Does cloud computing offer possibilities?

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