

# **High-order methods and their implementation in Nektar++**

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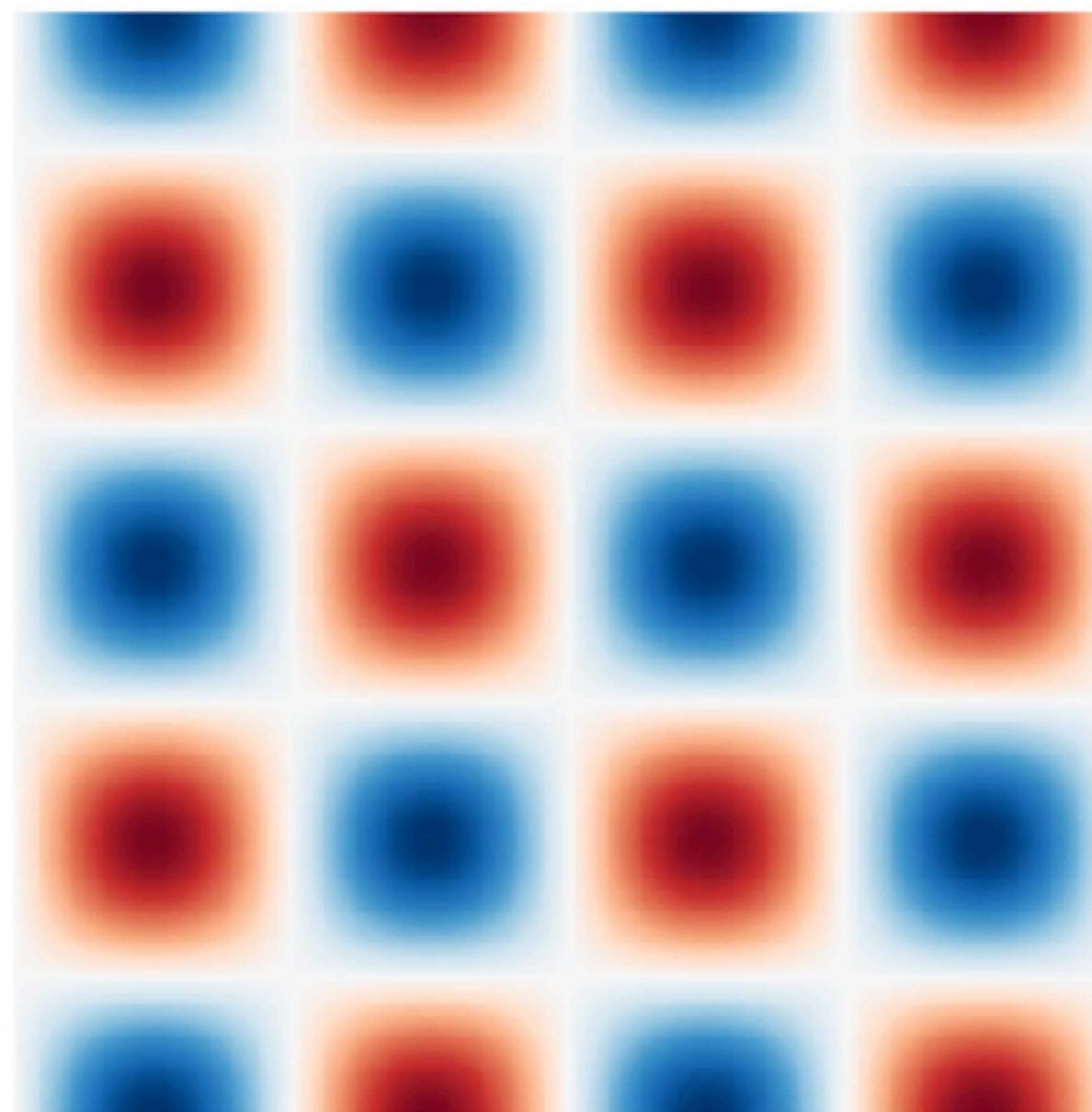
# Outline & agenda

- This morning (10am-12pm): this talk
  - Overview of high-order finite element methods.
  - Outline of their high-level implementation within Nektar++.
- Meant to be a dynamic presentation; please interrupt if you have questions!
- This afternoon:
  - 1:30pm - 3:30pm: NEPTUNE-specific talks (particles, review and overview of our proxyapps to date)
  - 3:30pm - 4:00pm: more hands-on demo from Bin Liu & Mashy Green: need to install docker if you don't have it
- Dinner this evening? Let Wayne/us know by lunchtime today...

# High-order methods

# How do we model a physical system?

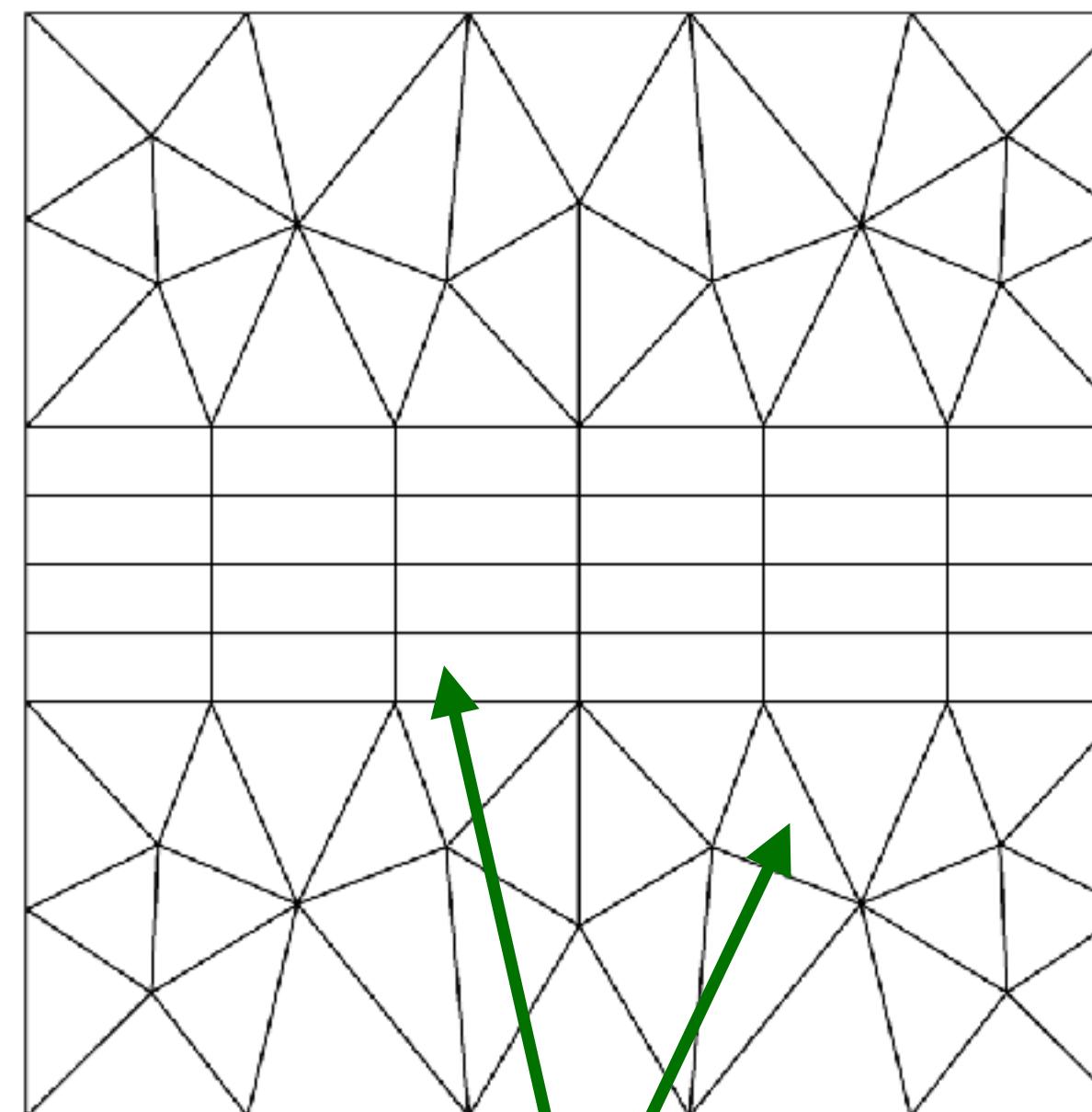
form underlying  
equations



advection velocity  $\mathbf{v}$

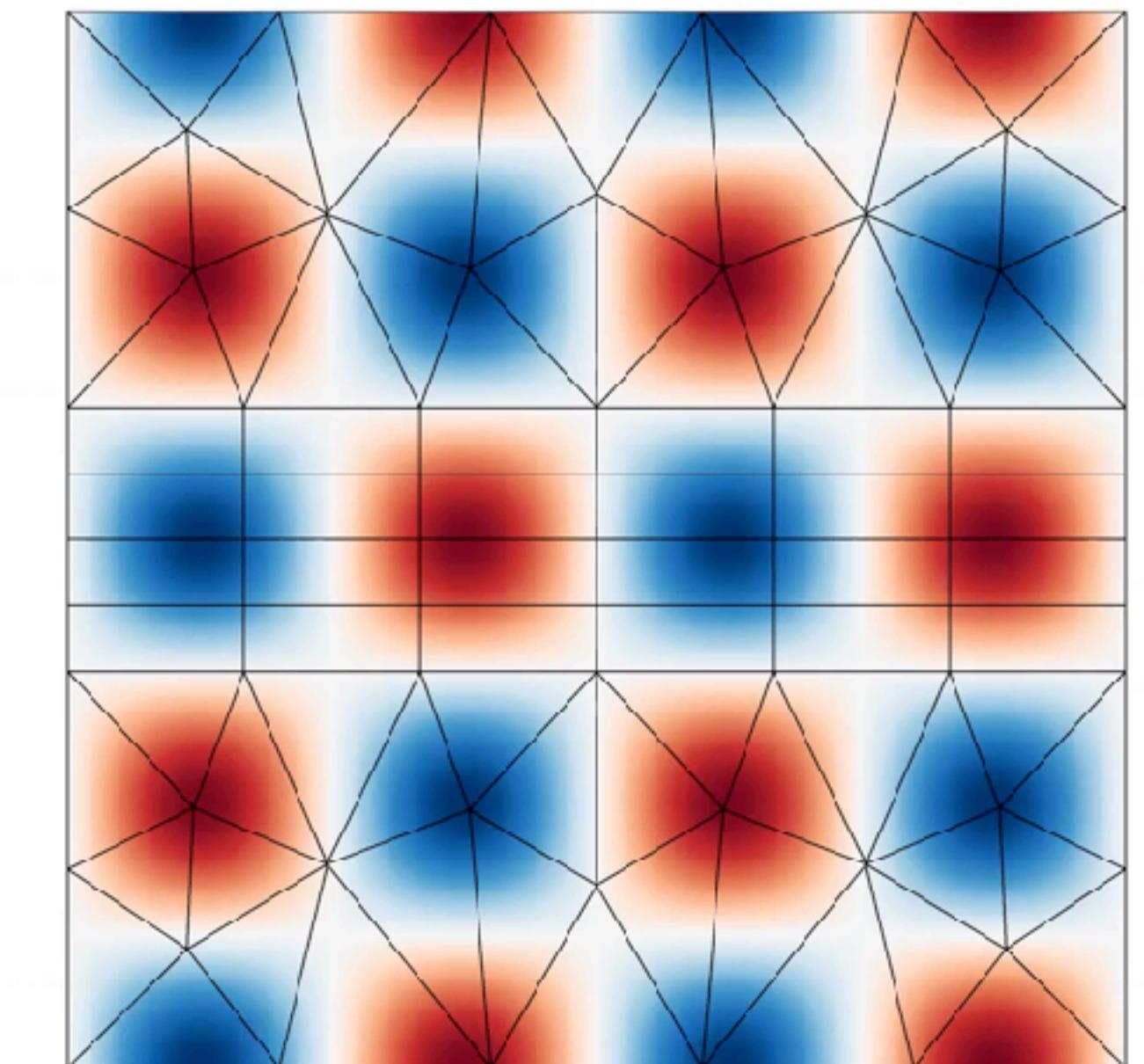
$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = 0$$

discretise a typically  
complex domain



elements on which  
the equations can be solved

solve resulting system



$$\mathbf{Ax} = \mathbf{b}$$

(+ timestepping)

# What is a spectral/hp element?

Consider an approximation to a function in terms of modes  $\phi_n$ .

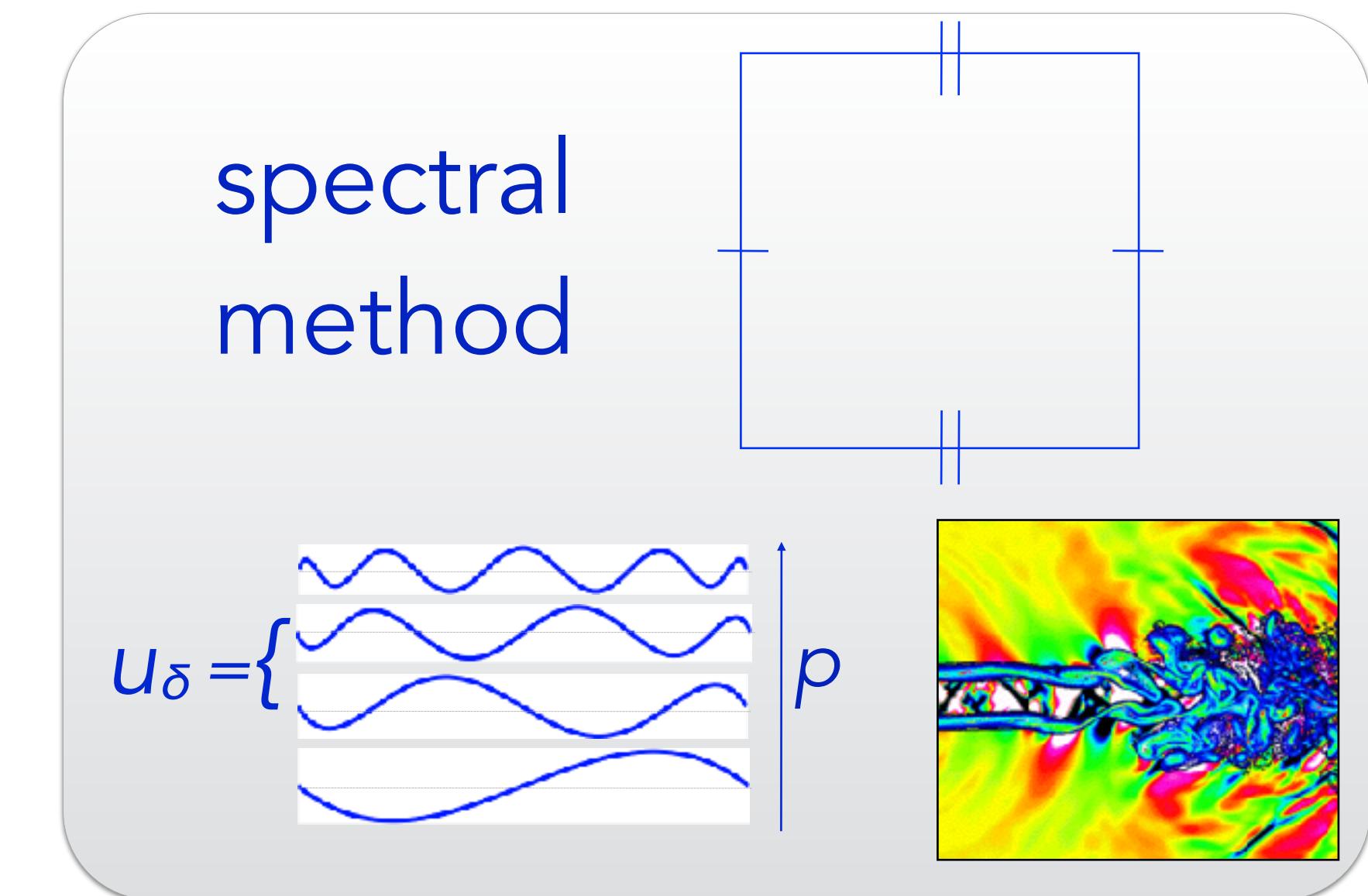
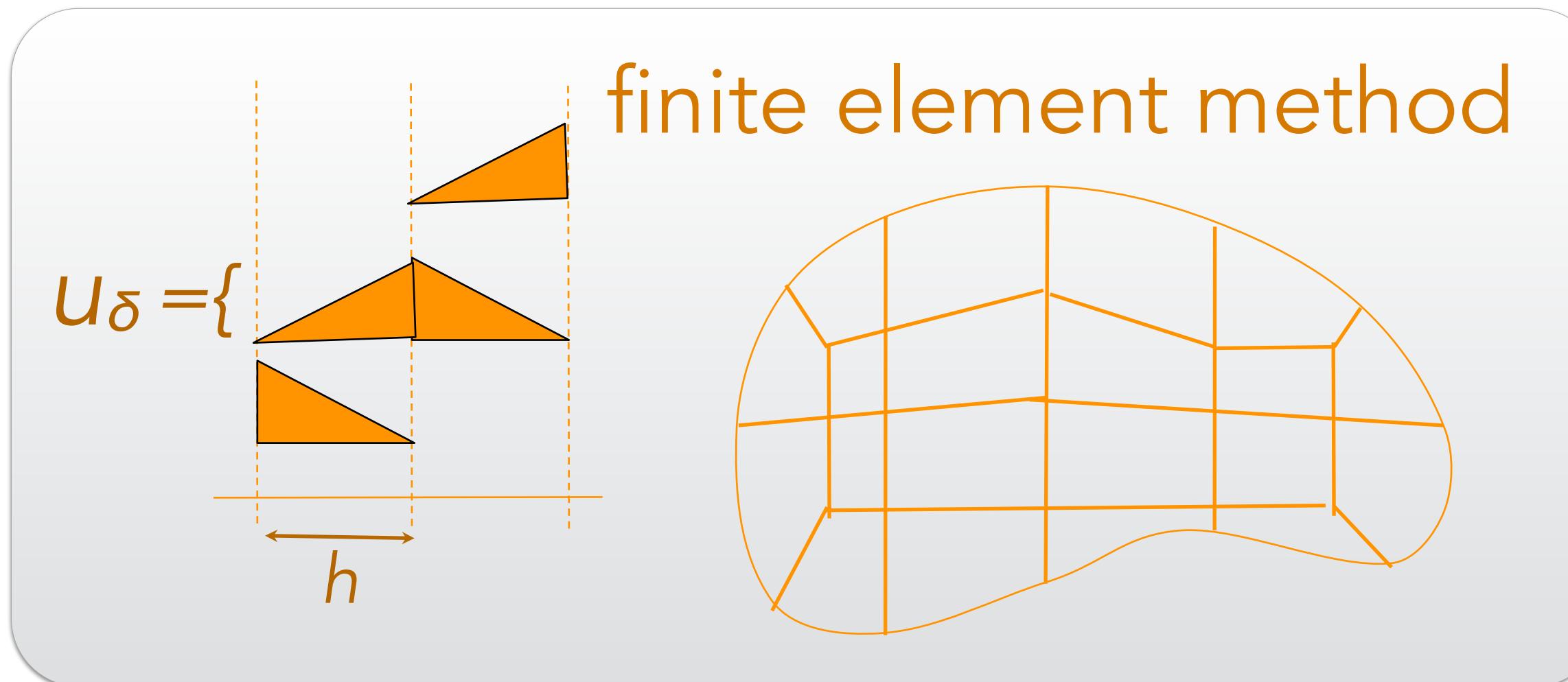
$$u^\delta(x) = \sum_{n=1}^N \hat{u}_n \phi_n(x)$$

**spatial flexibility ( $h$ )**

+

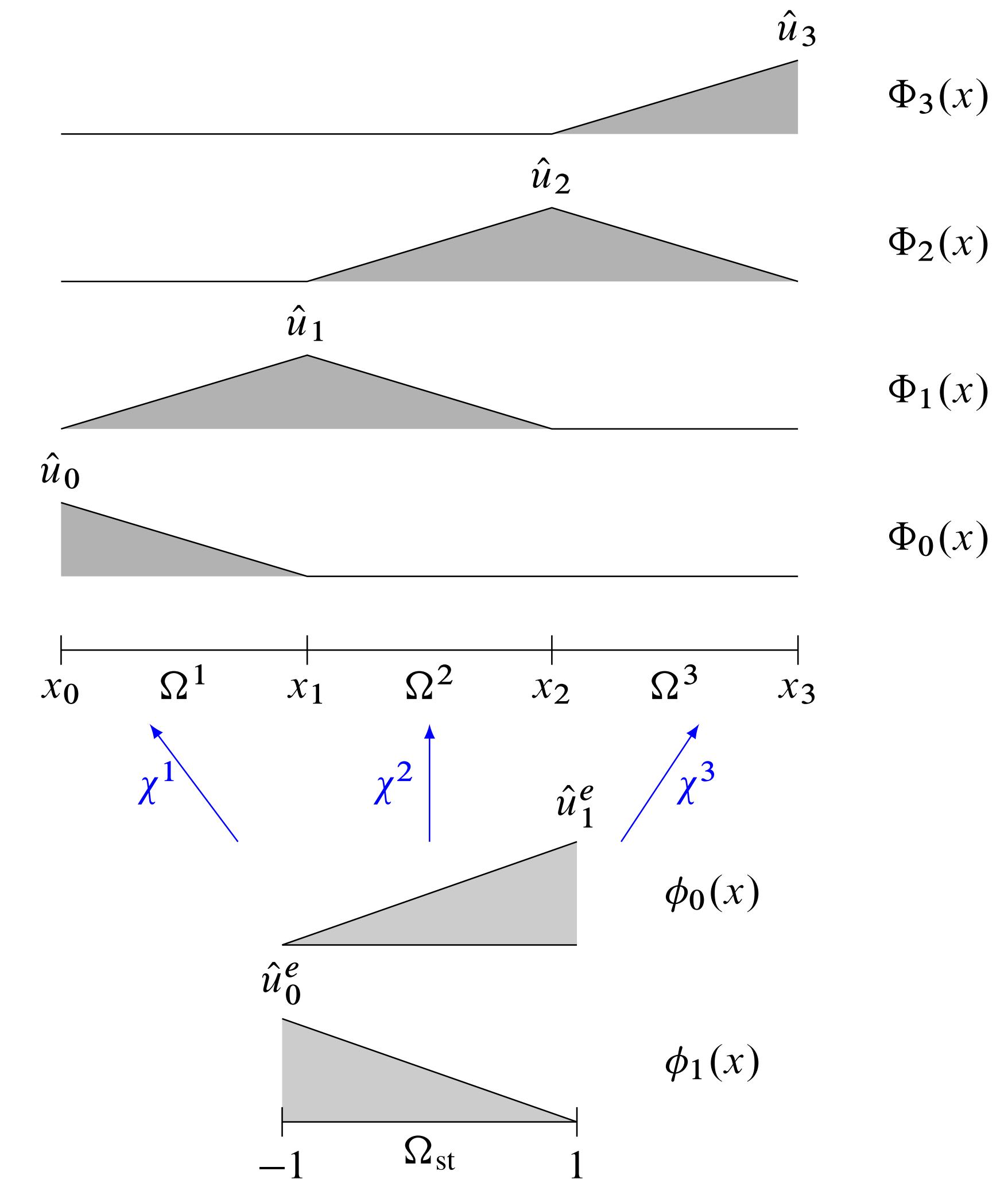
**accuracy ( $p$ )**

**spectral/hp element**

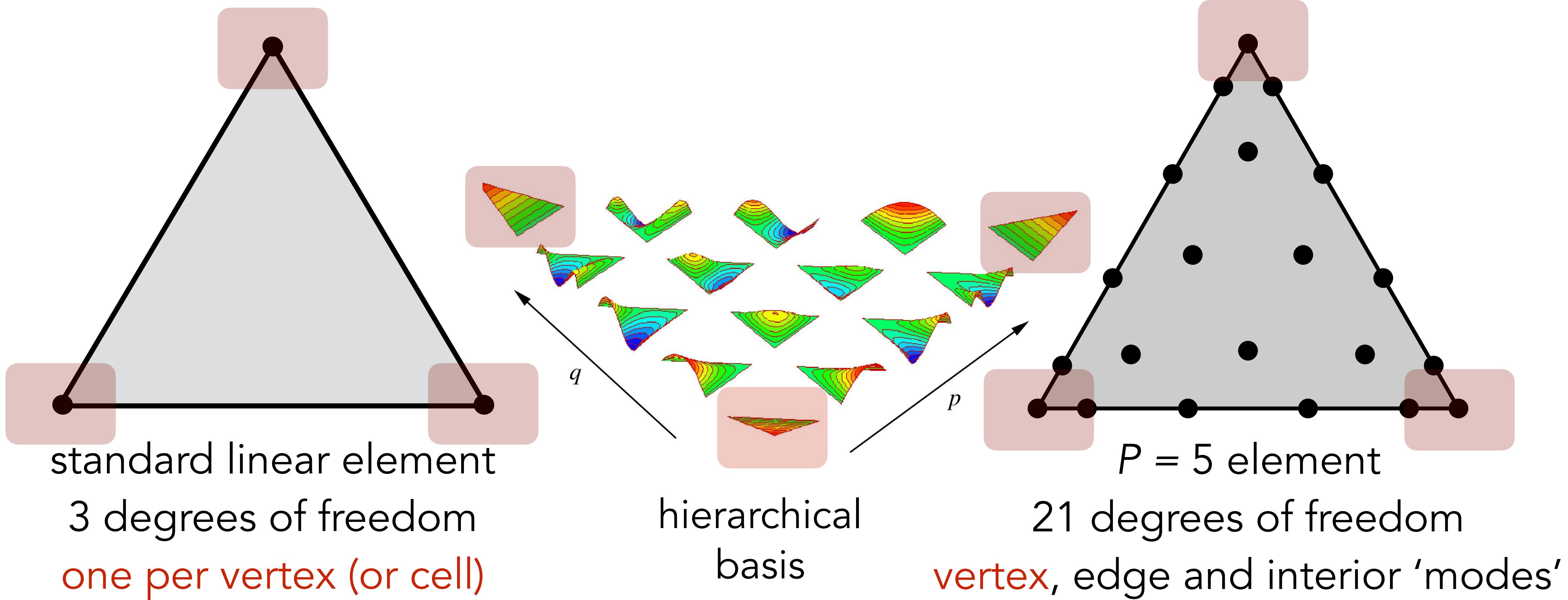


# Traditional finite elements

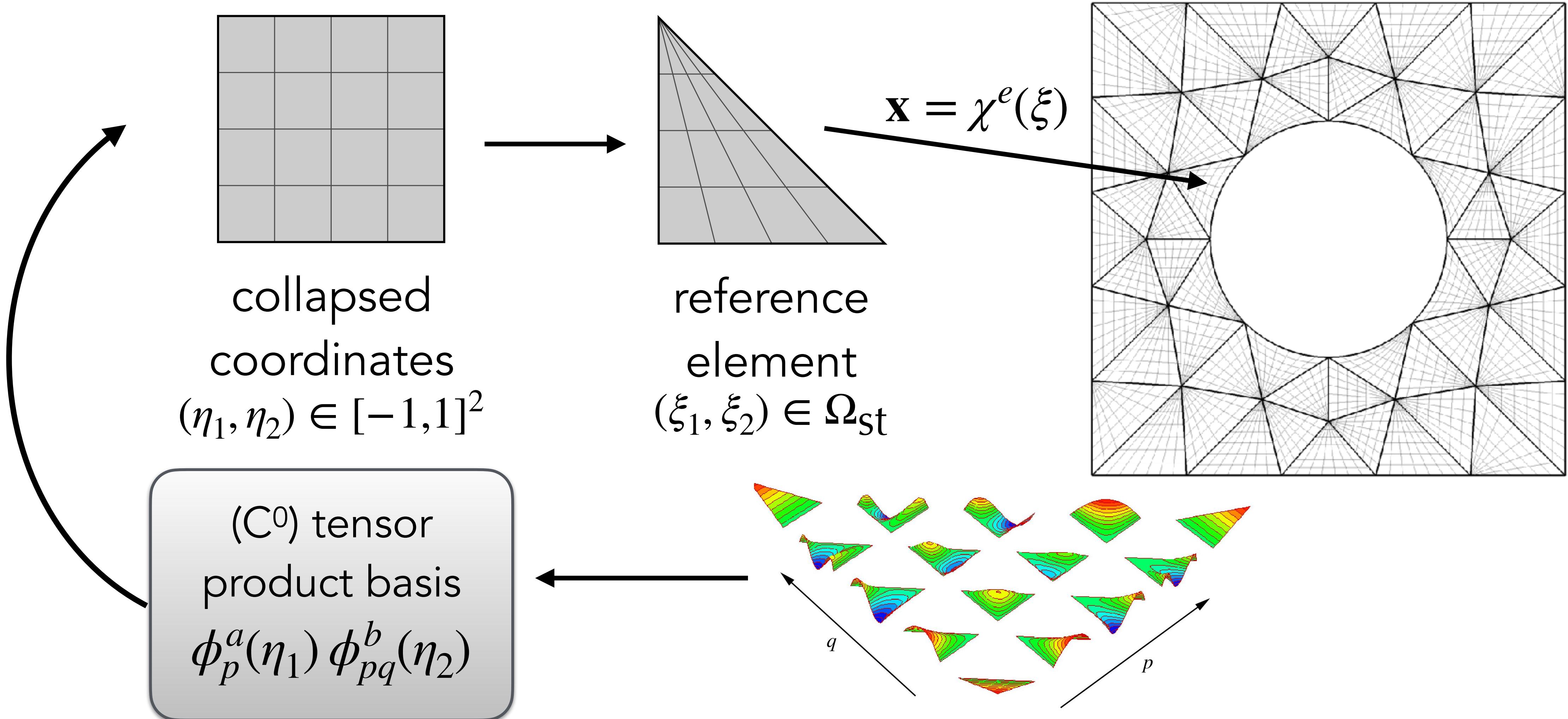
- In traditional linear FEM, the modes that represent functions are given by 'hat' functions.
- Linear interpolation then occurs between the vertices of each element.
- However to avoid need for modes in every element, we can define them instead inside of a standard element.
- Each element's modes are given by mapping  $\chi$  into world-space element.
- For a **high-order element**, we increase the order of the polynomial space that's being used.



# Anatomy of a spectral/ $hp$ element

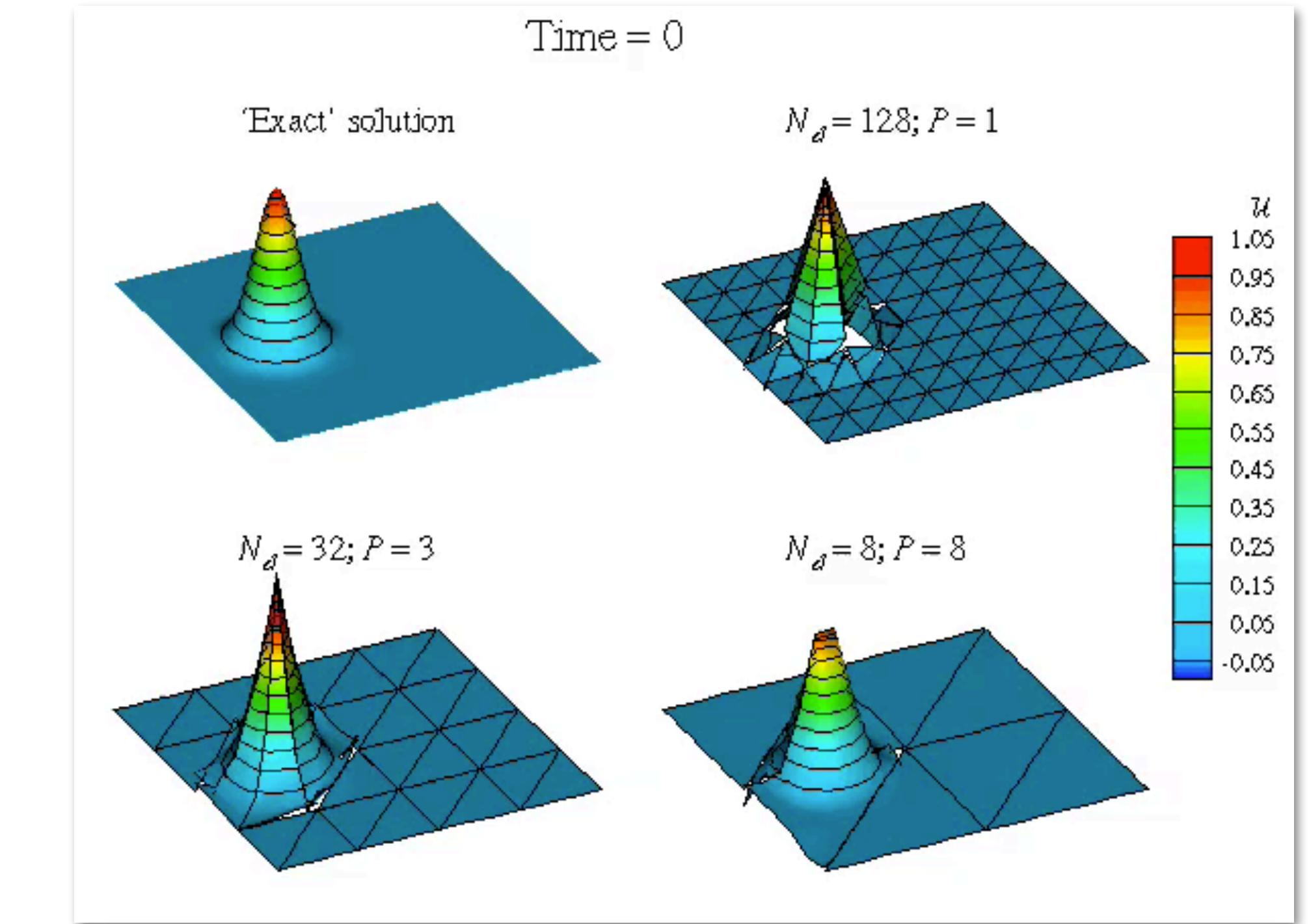
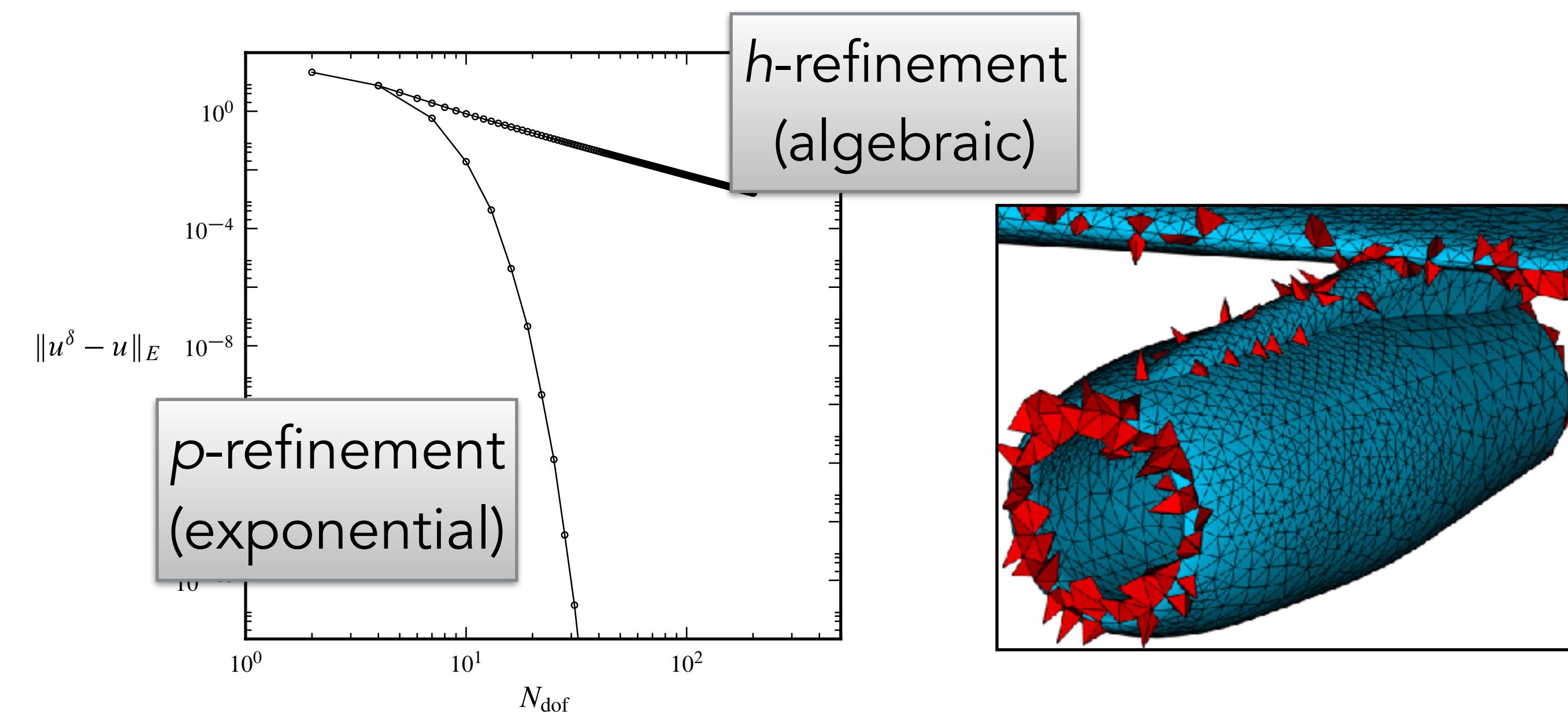


# Spectral/hp element methods

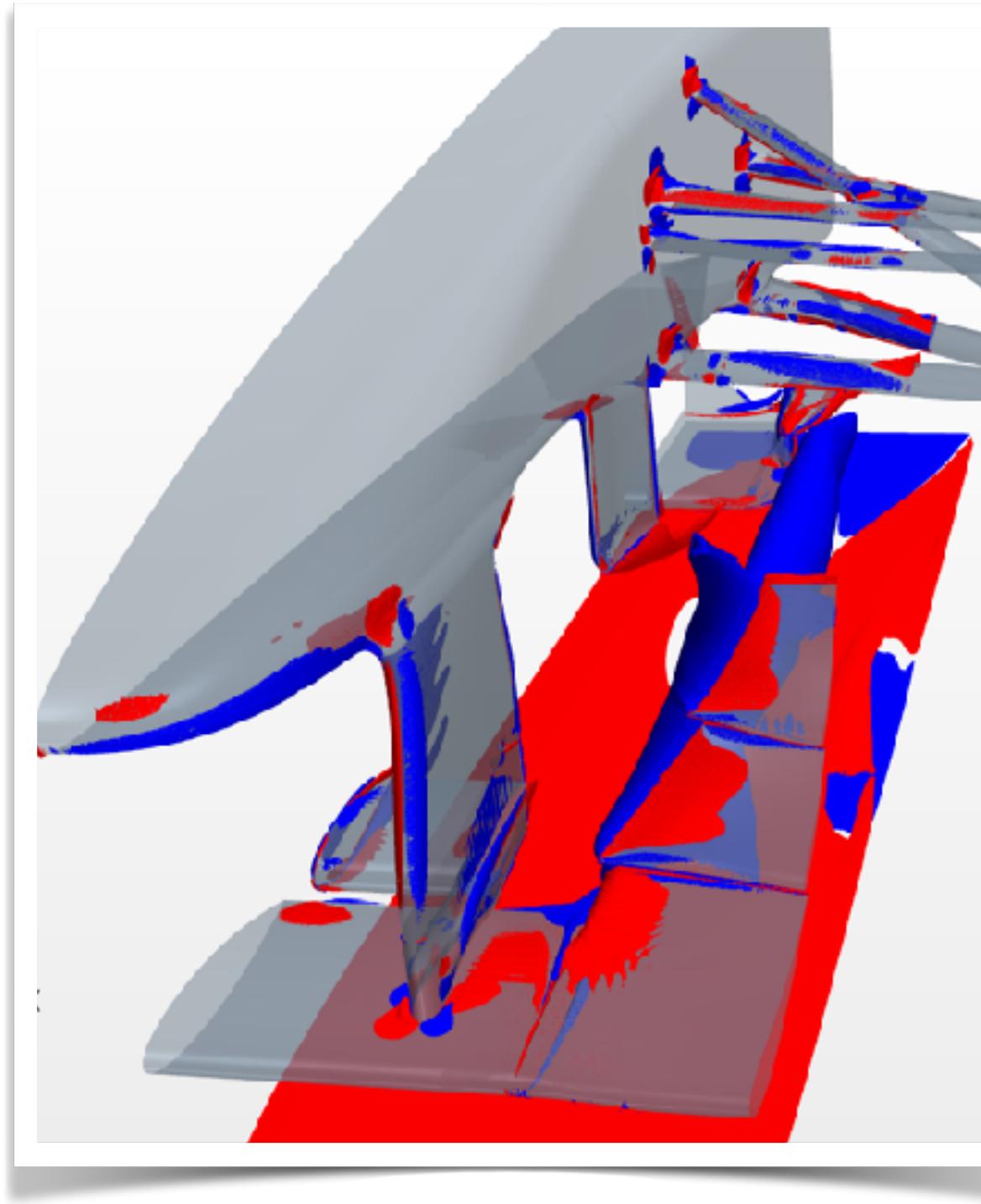


# Why use a high-order method?

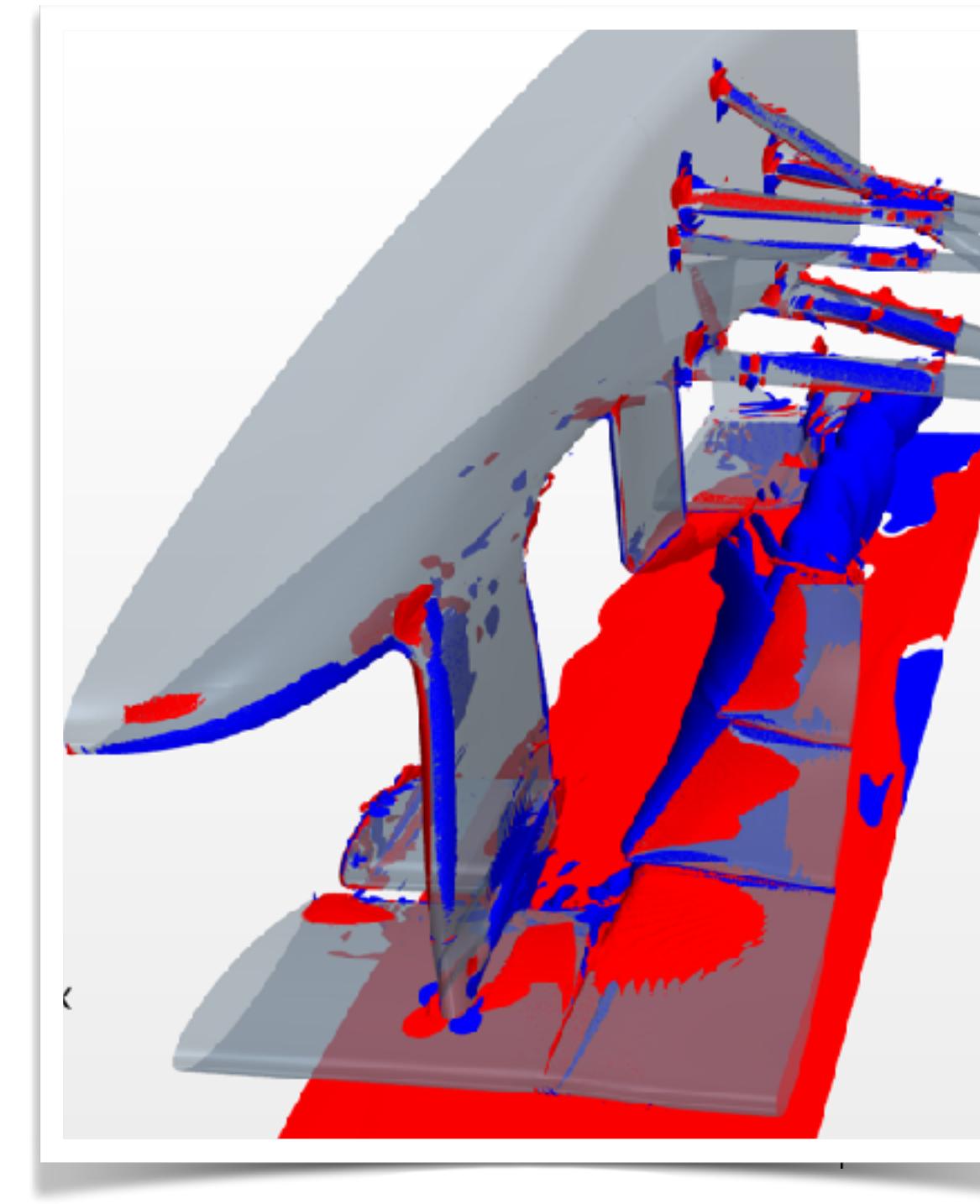
- ✓ error decays exponentially (smooth solutions);
- ✓ favorable diffusion & dispersion characteristics;
- ✓ model complex domains
- ✓ computational advantage: reduced memory bandwidth, better use of hardware.



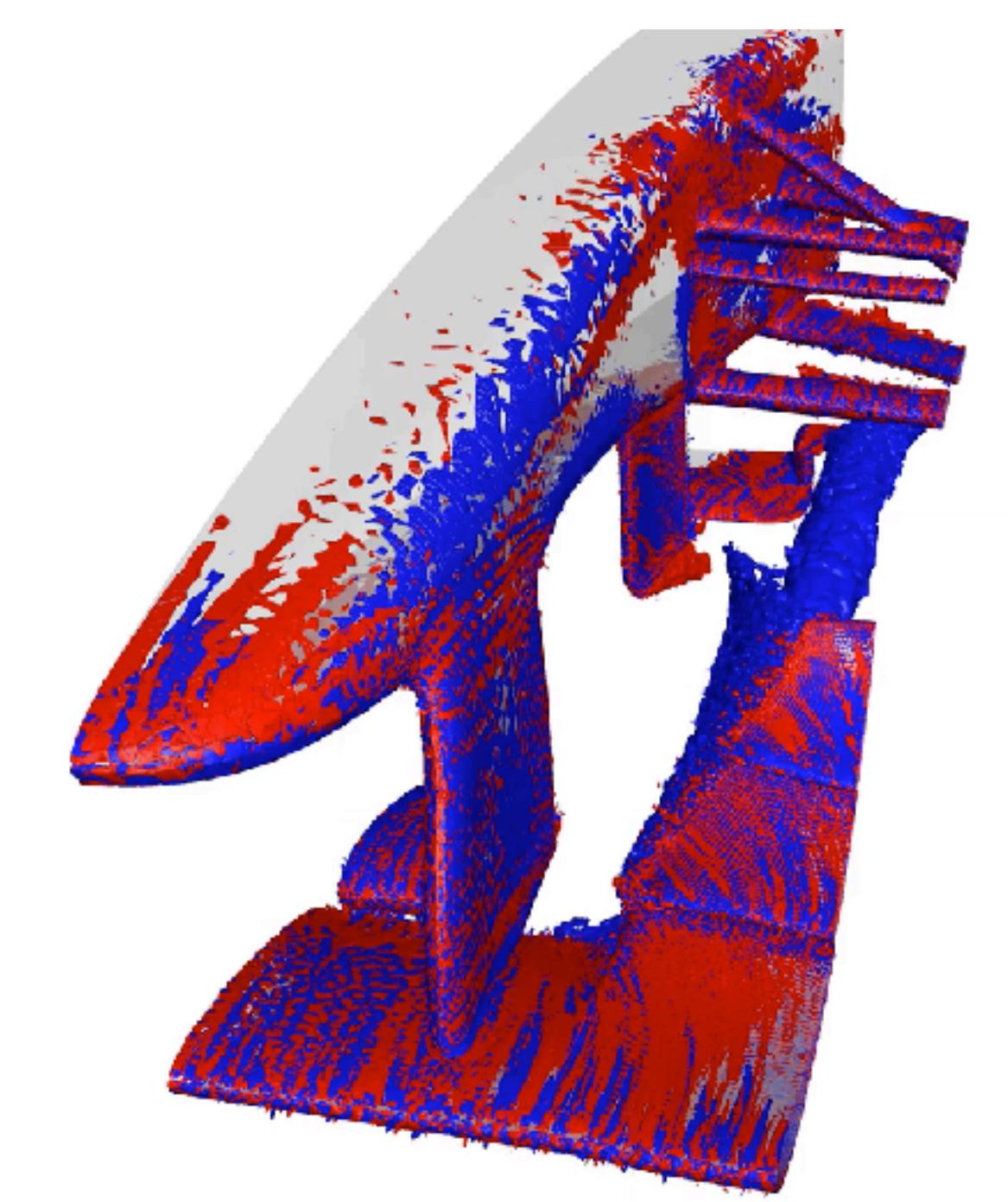
# Next generation modelling



Reynolds Averaged  
Navier-Stokes

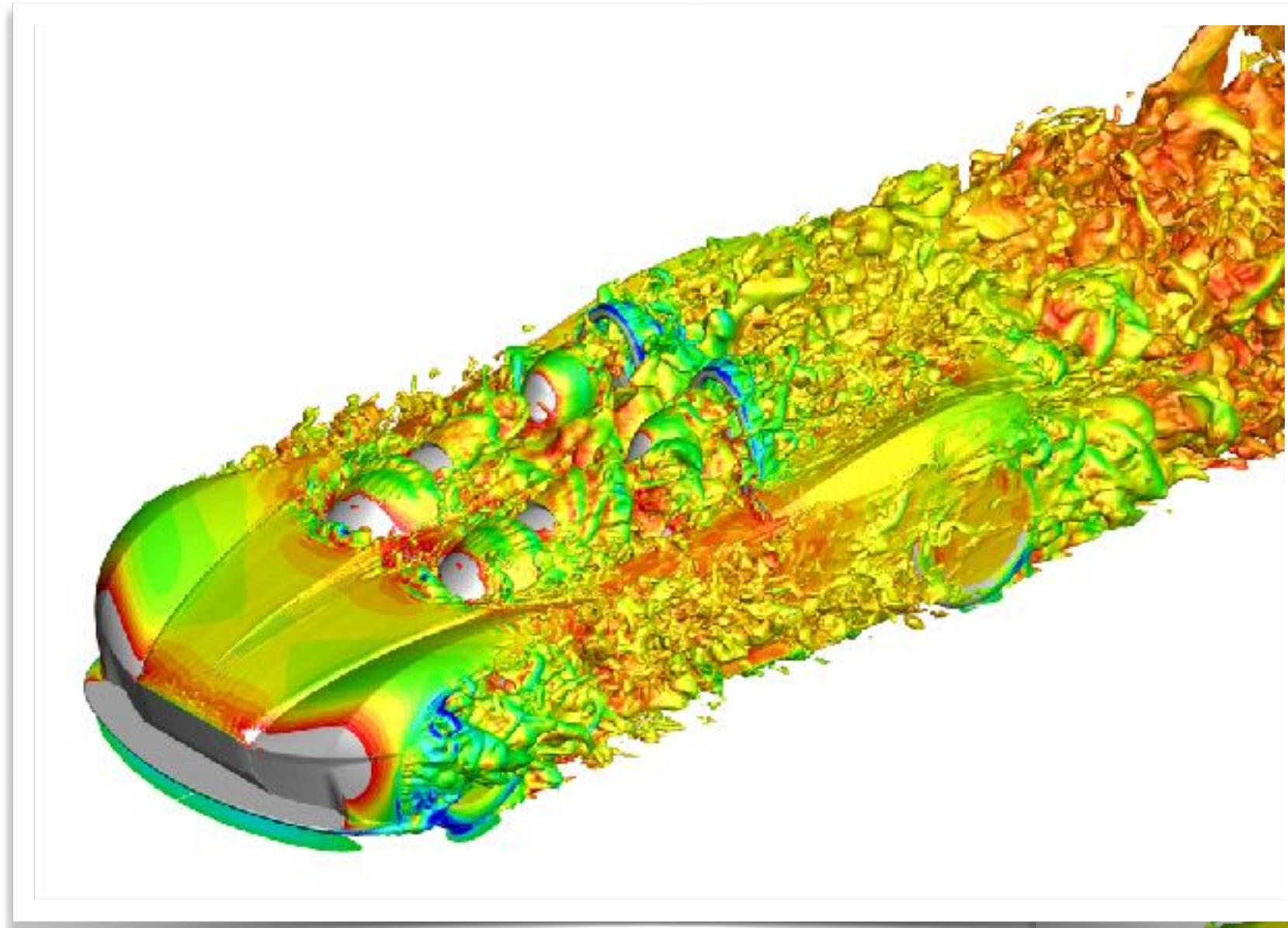


Detached Eddy  
Simulation

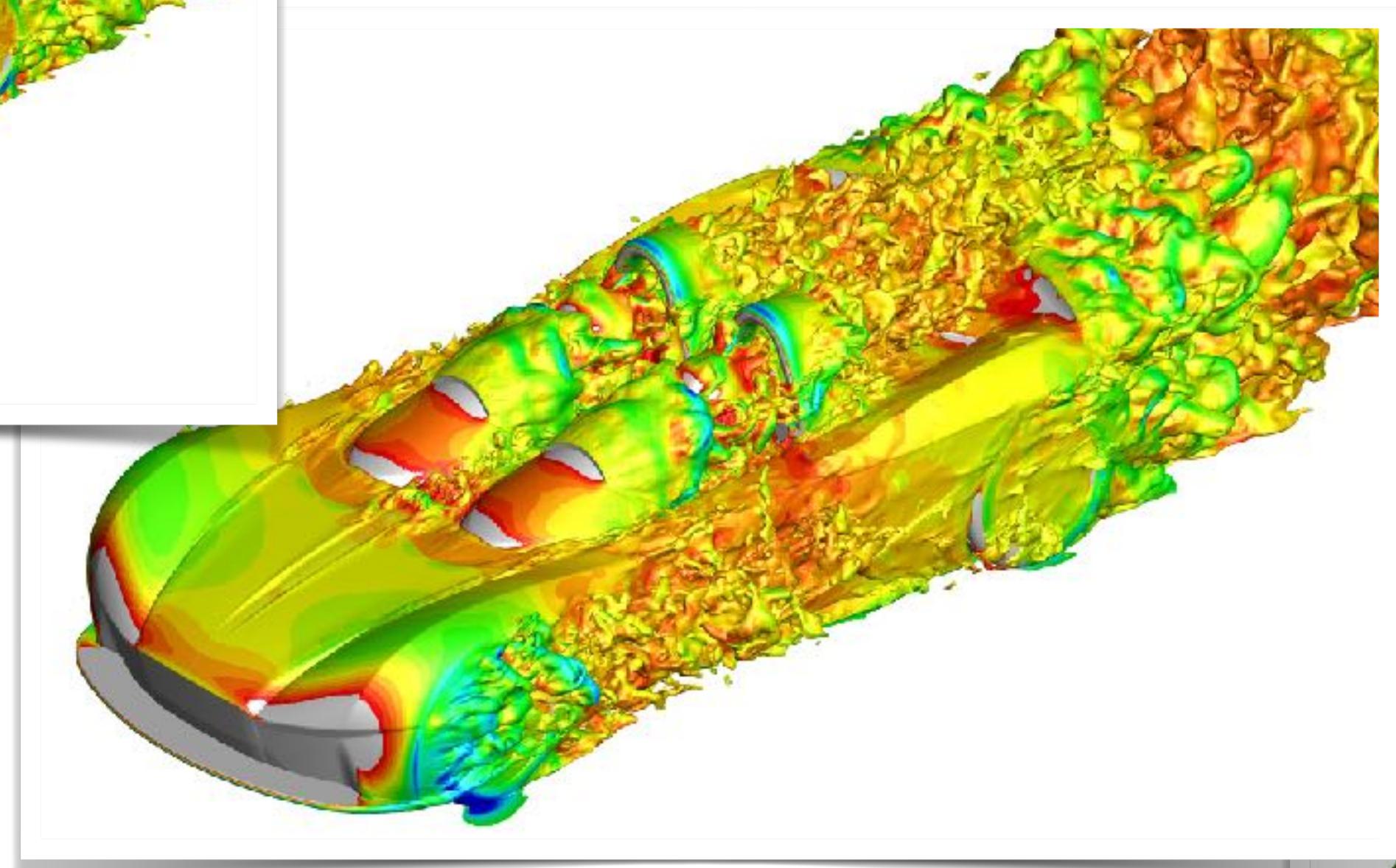


under-resolved  
Direct Numerical  
Simulation

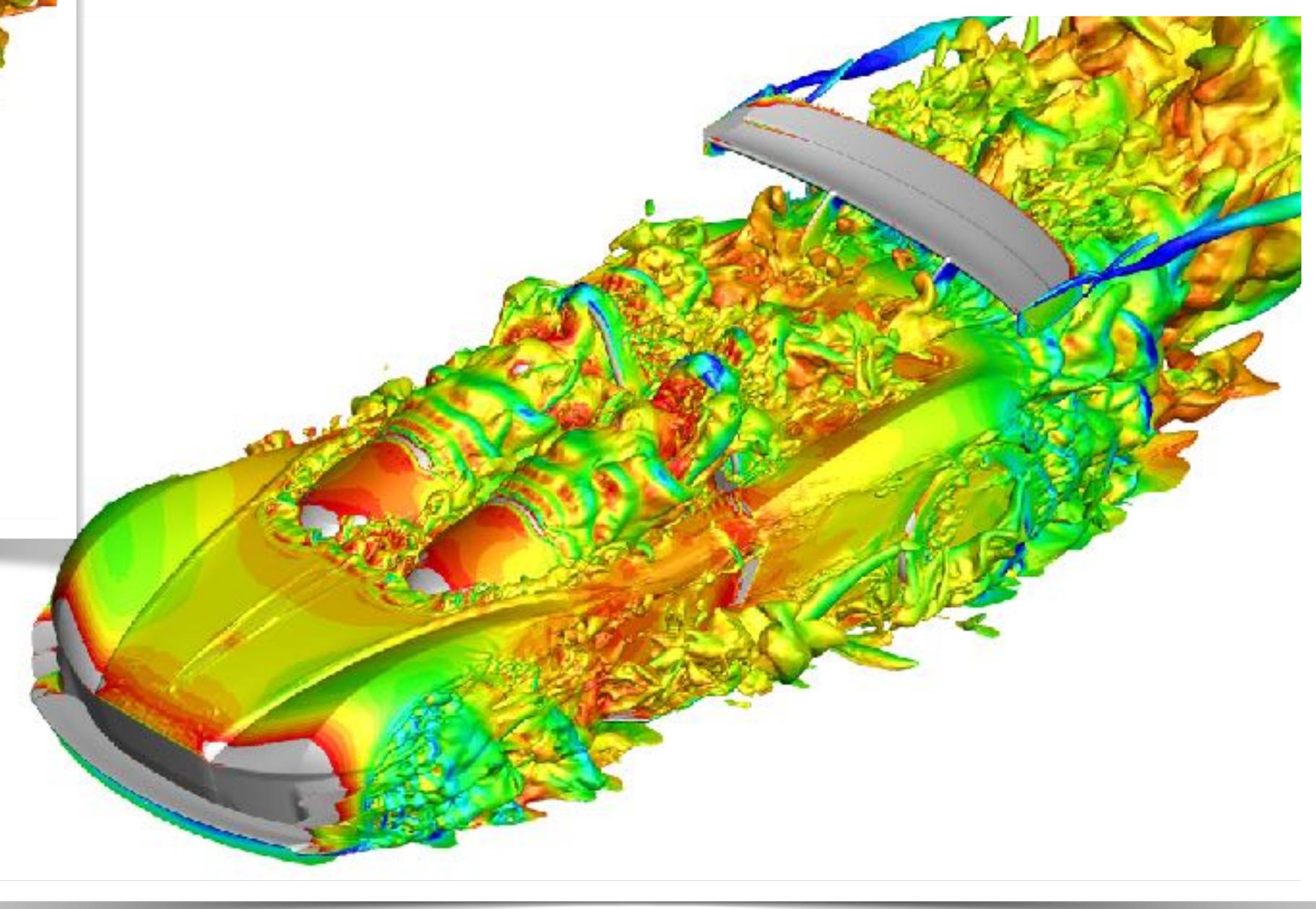
# Elemental road race car



5th order  
 $Re = 1m$



Design 2: +33% Downforce



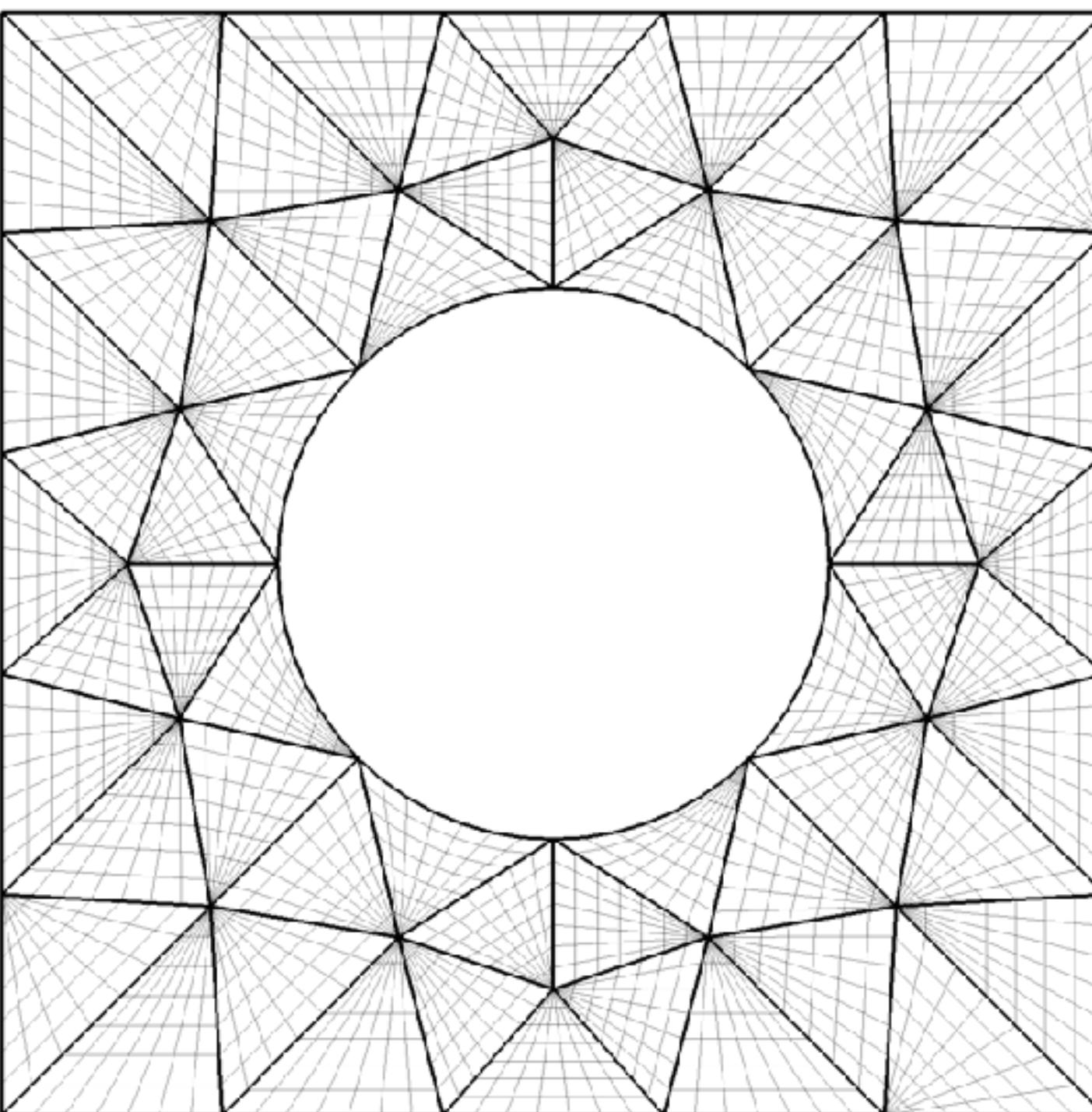
Design 3: +270% Downforce

# **Continuous formulations**

# The lingo of high-order elements

- Different high-order variants depending on which polynomial basis you're using, and how you bolt the elements together.
  - **spectral element**: typically uses Lagrange interpolants  $\ell_p(x)$
  - **hp-FEM**: automatic  $hp$  adaptivity, typically with quad/hex meshes and hanging node constraints; seems to be used more in structural mechanics applications.
  - **discontinuous Galerkin (DG)**: Galerkin approach where continuity between elements is removed; recovers finite volume methods at  $P = 0$ .
  - **flux reconstruction**: similar to DG, but uses correction functions to enforce continuity of fluxes between elements.
  - ...and many more!

# Classical $C^0$ finite elements



domain  $\Omega$

boundary  $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$

$$\nabla^2 u(x) - \lambda u(x) = -f(x)$$

**Boundary conditions**

$$u(x) = g_D(x) \quad \text{Dirichlet, } \partial\Omega_D$$

$$\frac{\partial u}{\partial n} = g_N(x) \quad \text{Neumann, } \partial\Omega_N$$

# Classical $C^0$ finite elements

$$\mathcal{U} = \{u \mid u|_{\Omega^e} \in \mathcal{P}_N(\Omega^e), u|_{\partial\Omega_D} = g_D\}$$

$$\mathcal{V} = \{v \mid v|_{\Omega^e} \in \mathcal{P}_N(\Omega^e), v|_{\partial\Omega_D} = 0\}$$

Choose test and trial spaces ( $C^0$ )

$$\int_{\Omega} v \nabla^2 u \, dx - \int_{\Omega} \lambda u \, dx = - \int_{\Omega} f v \, dx$$

Multiply by test function and integrate

$$\int_{\partial\Omega_N} v \frac{\partial u}{\partial n} \, ds - \int_{\Omega} \nabla u \nabla v \, dx$$

Apply the divergence theorem

$$u = u^D + u^H$$

Lift Dirichlet solution

$$\int_{\Omega} (\nabla u \nabla v + \lambda u) \, dx = \int_{\Omega} f v \, dx + \int_{\partial\Omega_N} v g_N \, ds$$

Arrive at the weak form

# Into matrix form

- In this form we can substitute expansions from the test and trial spaces to arrive at a matrix problem.

$$u^\delta(x) = \sum_{n=1}^N \hat{u}_n \phi_n(x) \xrightarrow{\text{substitute}} (\mathbf{L} + \lambda \mathbf{M}) \hat{\mathbf{u}} = \hat{\mathbf{f}}$$

$$\mathbf{M}_{ij} = \int \phi_i(x) \phi_j(x) dx \quad \mathbf{L}_{ij} = \int \nabla \phi_i(x) \nabla \phi_j(x) dx \quad \hat{\mathbf{f}}_i = \int f(x) \nabla \phi_i(x) dx$$

mass matrix      Laplacian matrix      forcing inner product

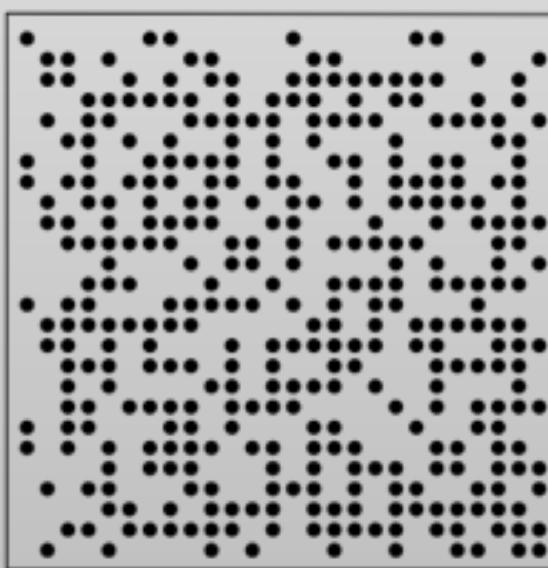
- To compute these matrices we split them up element by element, and then assemble across elements using a sparse assembly operator  $\mathcal{A}$ .
  - Also require sensible choice of quadrature.

# Solving the weak form

Solving the resulting matrices can be done in a number of ways, depending on the size of the mesh.

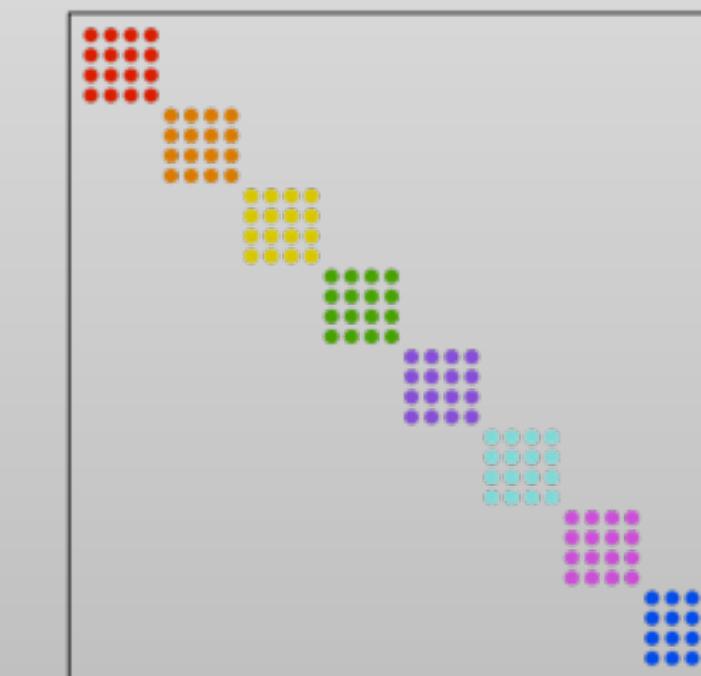
## Smaller problems

- Use a *direct* approach
- Form large SPD matrix
- Solve using e.g. LAPACK (Cholesky factorisation)
- Typically done in serial



## Larger problems

- Use an *iterative* approach
- No global matrix formed: only **local** matrices
- Symmetric problems solved using e.g. PCG
- Done in parallel



$\mathcal{A}$  +  
comms.

# Some numerical considerations

## Direct approach

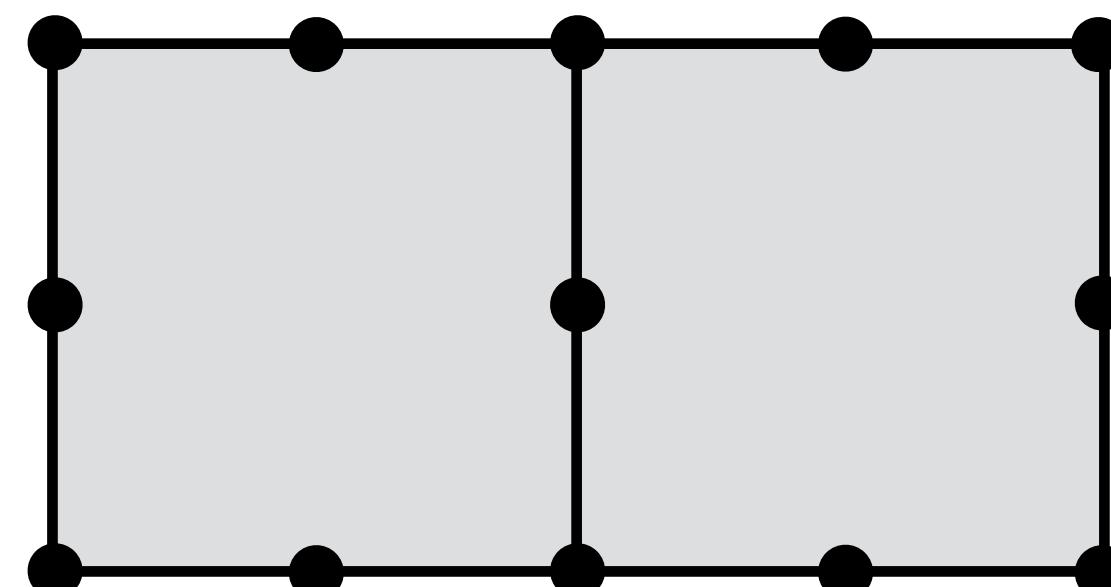
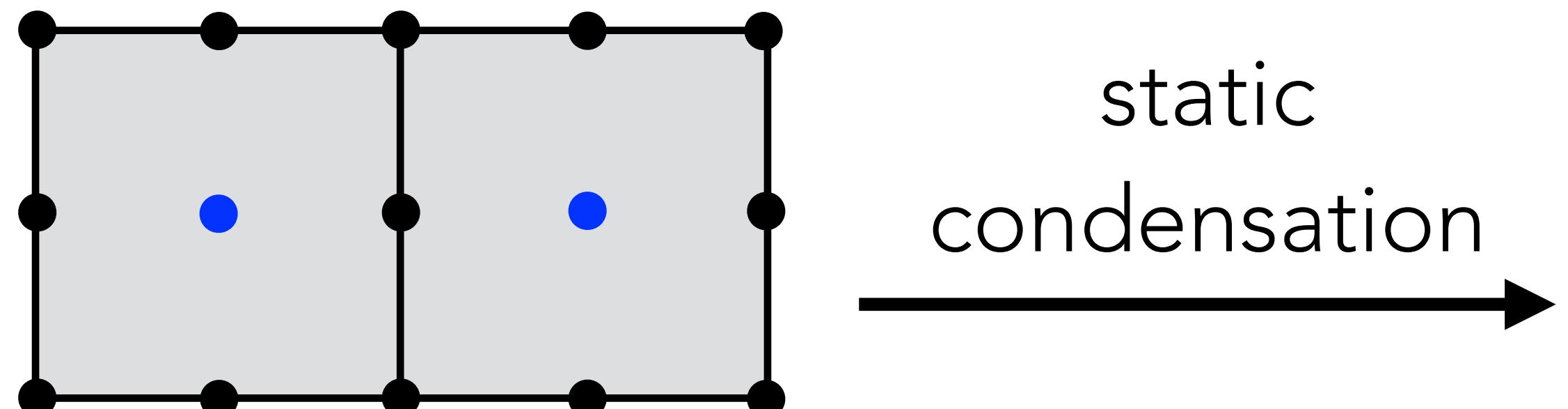
- Bandwidth of the system - use a reordering, e.g. reverse Cuthill-McKee
- Whether the problem is too big to fit in memory/be solved in a reasonable time
- Nearly all 3D problems are too large to solve this way

## Iterative approach

- Generally slower than using a direct solver
- Performance heavily governed by iteration count
- Needs effective preconditioning, particularly if  $\lambda = 0$
- Effective communication between elements needed in parallel

## Evaluation costs

- In iterative solvers, most cost comes from evaluation of finite element operator.
- In general, local matrix is rank  $O(P^{2d})$
- Two strategies to reduce this: **static condensation** and **matrix-free** evaluation.



$$H \rightarrow \begin{bmatrix} H_{bb} & H_{ib} \\ H_{bi} & H_{ii} \end{bmatrix}$$

Rank of  $H_{bb} = \mathcal{O}(P^{2(d-1)})$

# **Discontinuous formulations**

# Hyperbolic equations

- Consider the hyperbolic conservation law

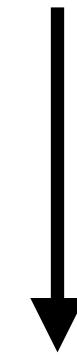
$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{u}) = \mathbf{0} \quad \mathbf{F}(\mathbf{u}) = [\mathbf{F}_1(\mathbf{u}), \mathbf{F}_2(\mathbf{u})] \text{ in 2D}$$

- This encapsulates a wide range of equations: e.g. compressible Euler or Navier-Stokes equations.
- Can apply  $C^0$  methods to this, but perhaps not the most natural method and some concerns around e.g. local conservation properties between elements.
- Discontinuous Galerkin methods very popular in this setting: have several advantages including favourable stability properties.

# Discontinuous Galerkin method

Consider Galerkin approach on a single element, but remove the continuity of functions between elements. This leads to the formulation

$$\int_{\Omega^e} \mathbf{v} \frac{\partial \mathbf{u}}{\partial t} dx + \int_{\Omega^e} \mathbf{v} \nabla \cdot \mathbf{F}(\mathbf{u}) dx = 0$$



integration by parts

$$\int_{\Omega^e} \mathbf{v} \frac{\partial \mathbf{u}}{\partial t} dx - \int_{\Omega^e} \nabla \mathbf{v} \nabla \cdot \mathbf{F}(\mathbf{u}) dx + \oint_{\partial \Omega^e} \mathbf{v} \cdot \hat{\mathbf{F}}(\mathbf{u}^+, \mathbf{u}^-, \mathbf{n}) ds = 0$$

this numerical flux appears because  $u$  is discontinuous  
across element boundaries

# Discontinuous Galerkin method

- The discretisation gives the semi-discrete ODE system on each element:

$$\mathbf{M}^e \frac{d\hat{\mathbf{u}}^e}{dt} = \sum_{d=1}^D (\mathbf{D}_d^e \mathbf{B}^e)^\top \mathbf{W}^e F_d(u) - \mathbf{b}^e$$

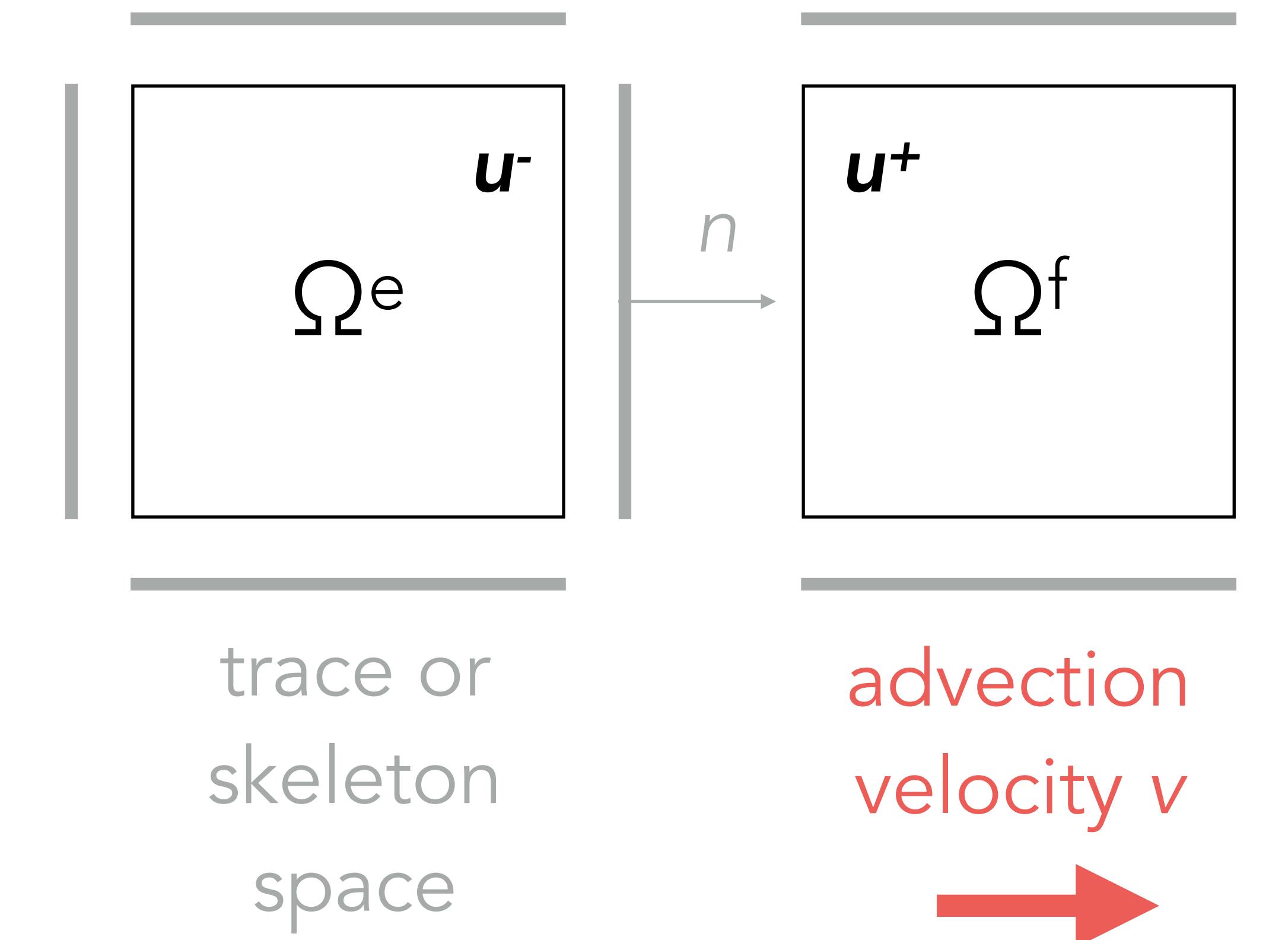
inner product w.r.t.  
derivative of basis

boundary flux  
contributions

- Note that elements aren't decoupled: boundary flux couples them together.
- Can now apply time-stepping schemes: e.g. forward Euler, Runge-Kutta, Adams-Bashforth, ...

# Discontinuous Galerkin method

- Need some consistent definition of which element is 'forward' and 'backward'
- Can then employ the usual machinery from finite volume methods:
  - ▶ e.g. for simple transport problems we can upwind based on forward and backward spaces
  - ▶ More complex Riemann solvers for nonlinear problems such as compressible N-S equations
- Other stabilisation techniques such as slope limiters also apply in this setting.



$$F(u^+, u^-, n) = \begin{cases} u^-, & v \cdot n \geq 0, \\ u^+, & v \cdot n < 0 \end{cases}$$

# Elliptic operators in DG

- Elliptic operators require careful consideration to ensure stability.
- For example in the Poisson equation  $-\nabla^2 u = f$ , we introduce an auxiliary variable  $\mathbf{q} = \nabla u$ , so that we instead solve the system

$$\begin{cases} -\nabla \cdot \mathbf{q} = f \\ \mathbf{q} = \nabla u \end{cases}$$

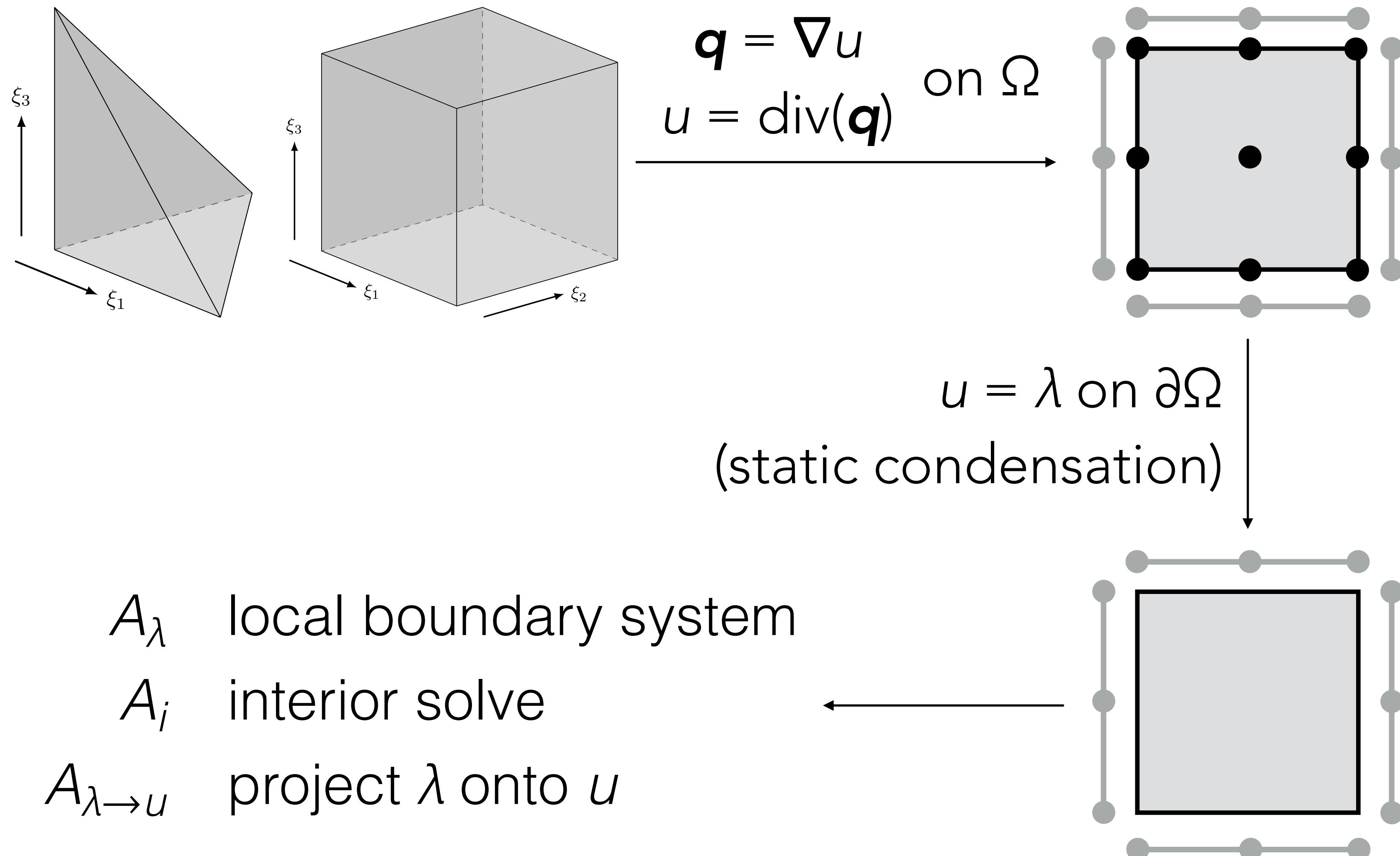
- Applying the DG formulation to the above equations leads to a weak form similar to that shown previously.
- A careful choice of fluxes for  $\mathbf{q}$  in particular (e.g. local discontinuous Galerkin, BR2) ensures convergence and stability.

# Hybridisable discontinuous Galerkin (HDG)

- An alternative is to consider static condensation in the formulation of DG.

- This leads to **HDG** where boundary matrices are formed for the trace space.

- Partially supported in Nektar++ but only for Helmholtz operator.



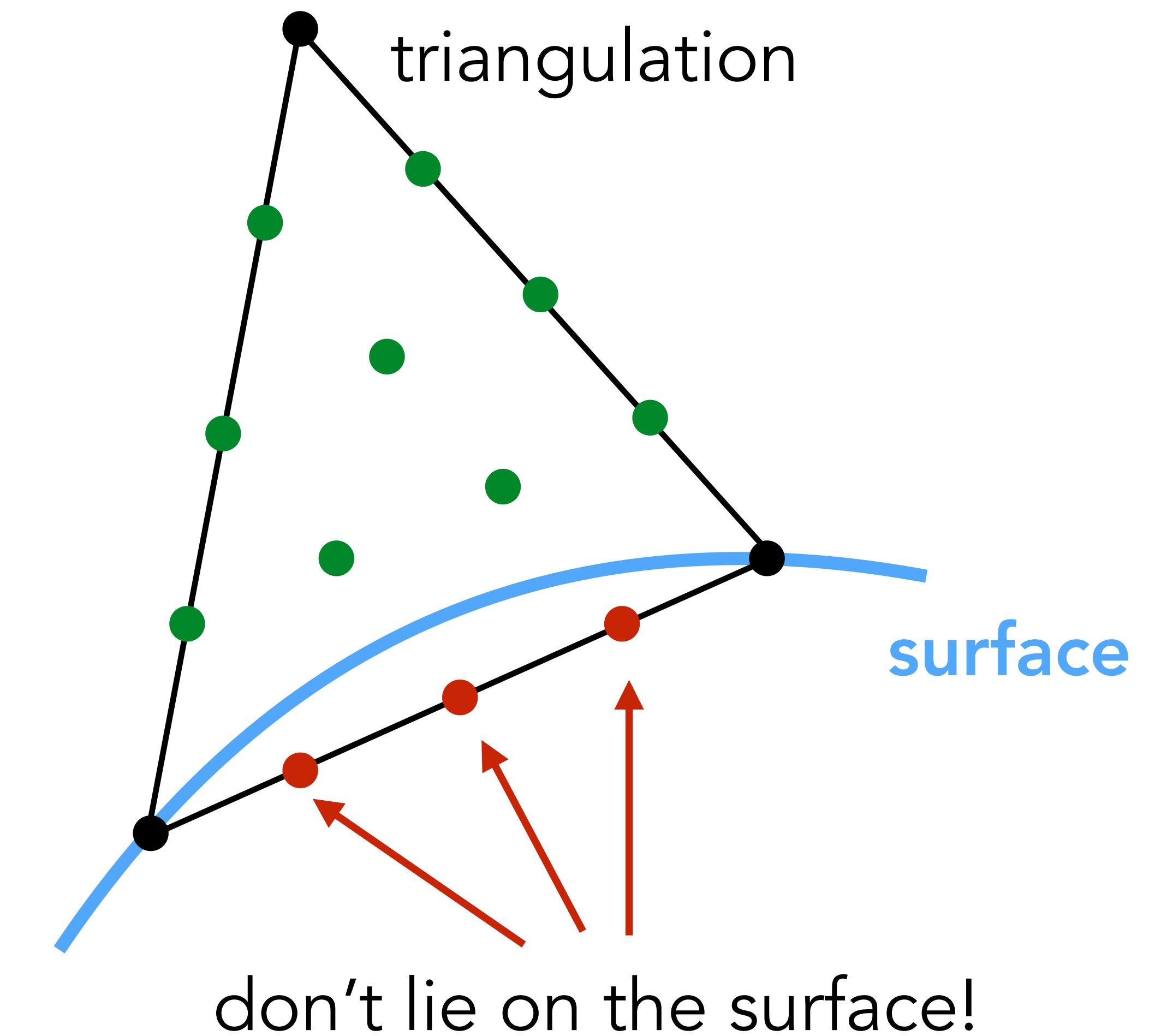
# Challenges

# The challenge of implementation

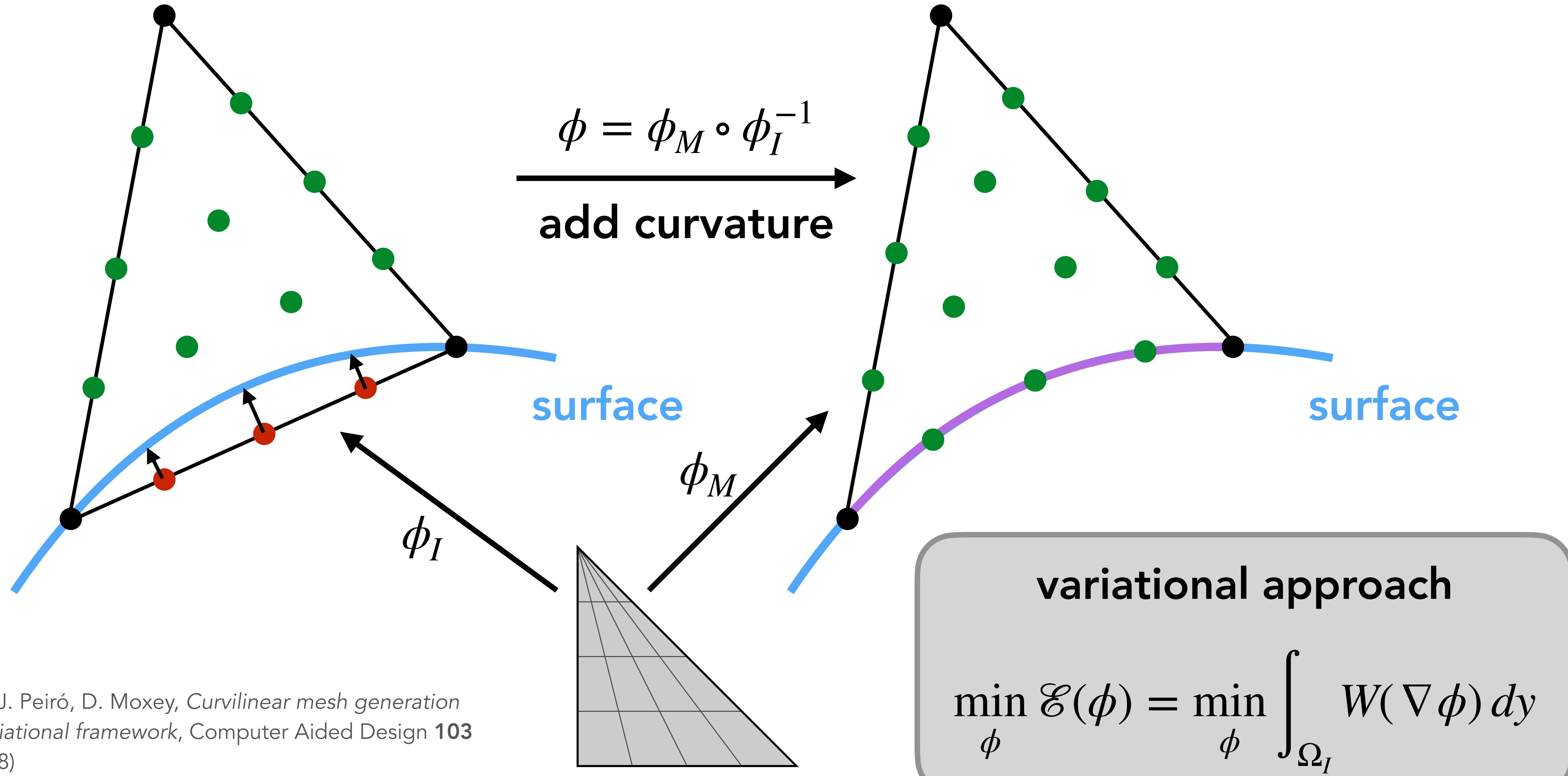
- High-order methods have potential to bring some nice numerical and computational benefits to bear on complex problems.
- Offer high(er) fidelity at equivalent or lower costs, as they have good implementation characteristics.
- However, one of the main barriers to using high-order methods is that they are **difficult to implement**.
- There are a number of other issues too including **stabilisation** and **mesh generation**.
- We'll touch on these briefly here.

# High-order mesh generation

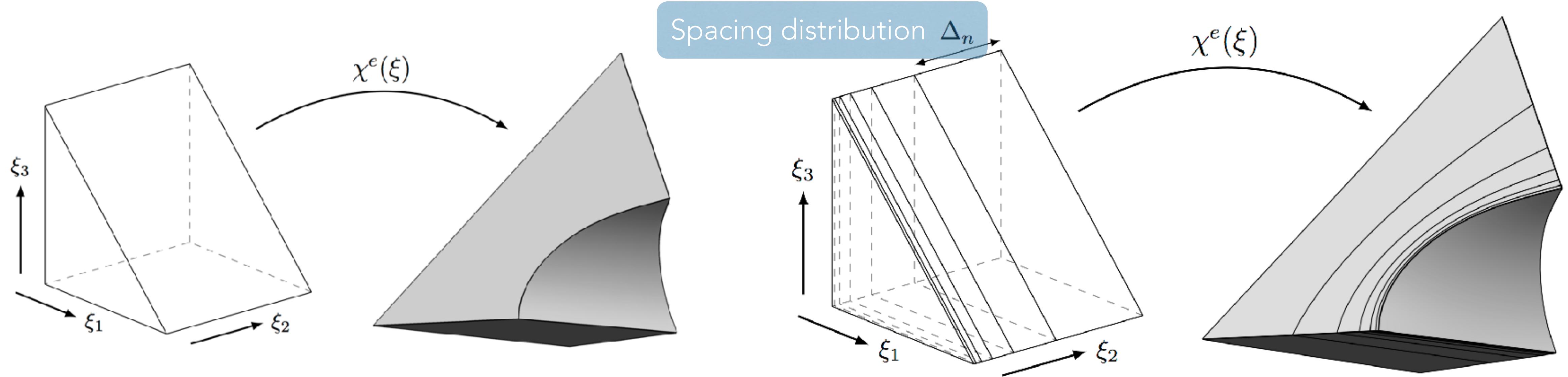
- Good quality meshes are **essential** to finite element and finite volume simulations.
- You can have a very fancy solver, but if you can't mesh your geometry then you **can't run your simulation!**
- At high orders we have an additional headache, as we must **curve the elements** to fit the geometry.
- This can easily cause self intersection, particularly when dealing with high-aspect ratio elements (e.g. in a fluid boundary layer).



# High-order mesh generation



# Boundary layer meshing



Shape function is a mapping from reference element (parametric coordinates) to mesh element (physical coordinates)

Subdivide the reference element in order to obtain a boundary layer mesh

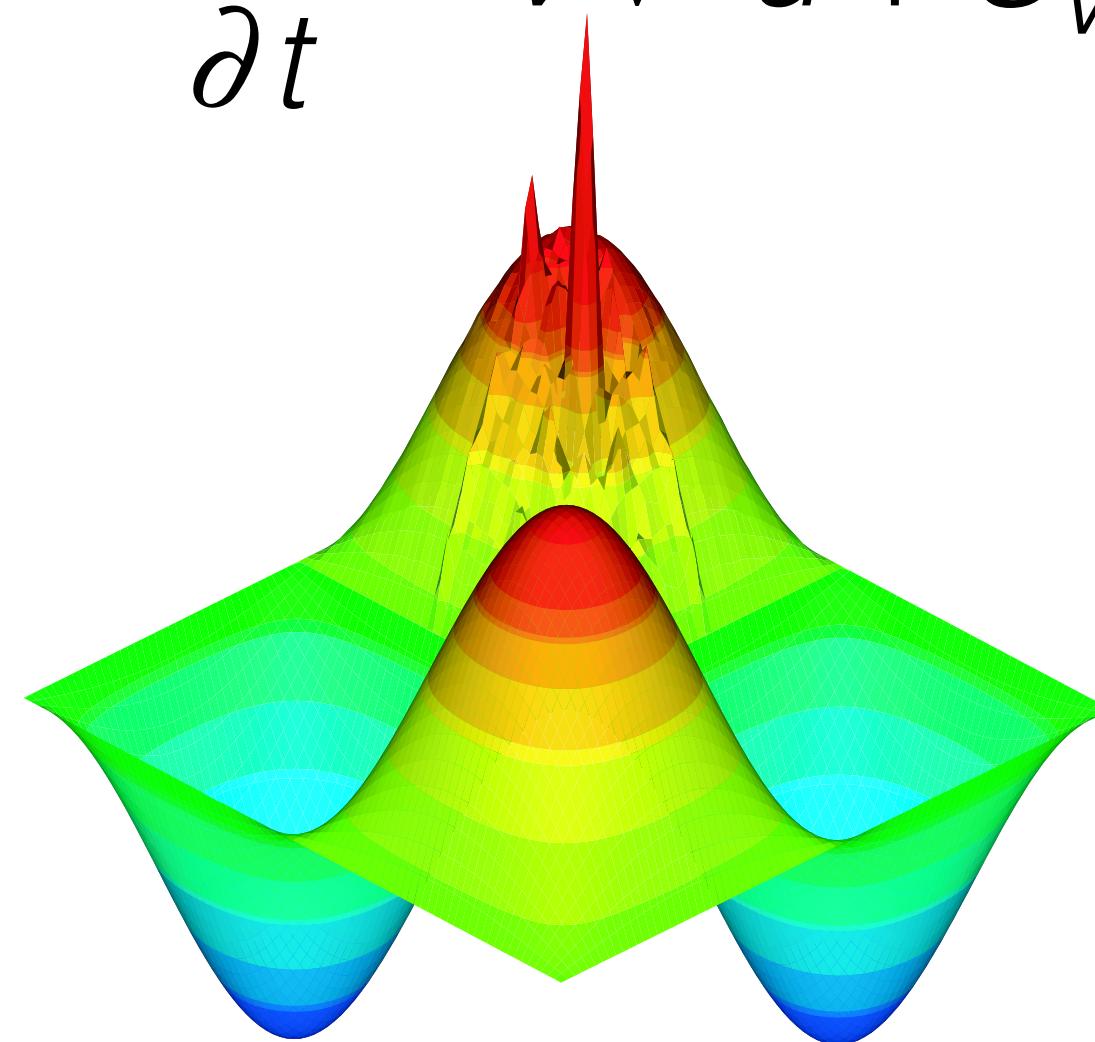
*An isoparametric approach to high-order curvilinear boundary-layer meshing*

D. Moxey, M. Hazan, S. J. Sherwin, J. Peiró, under review in Comp. Meth. Appl. Mech. Eng.

# Stabilisation

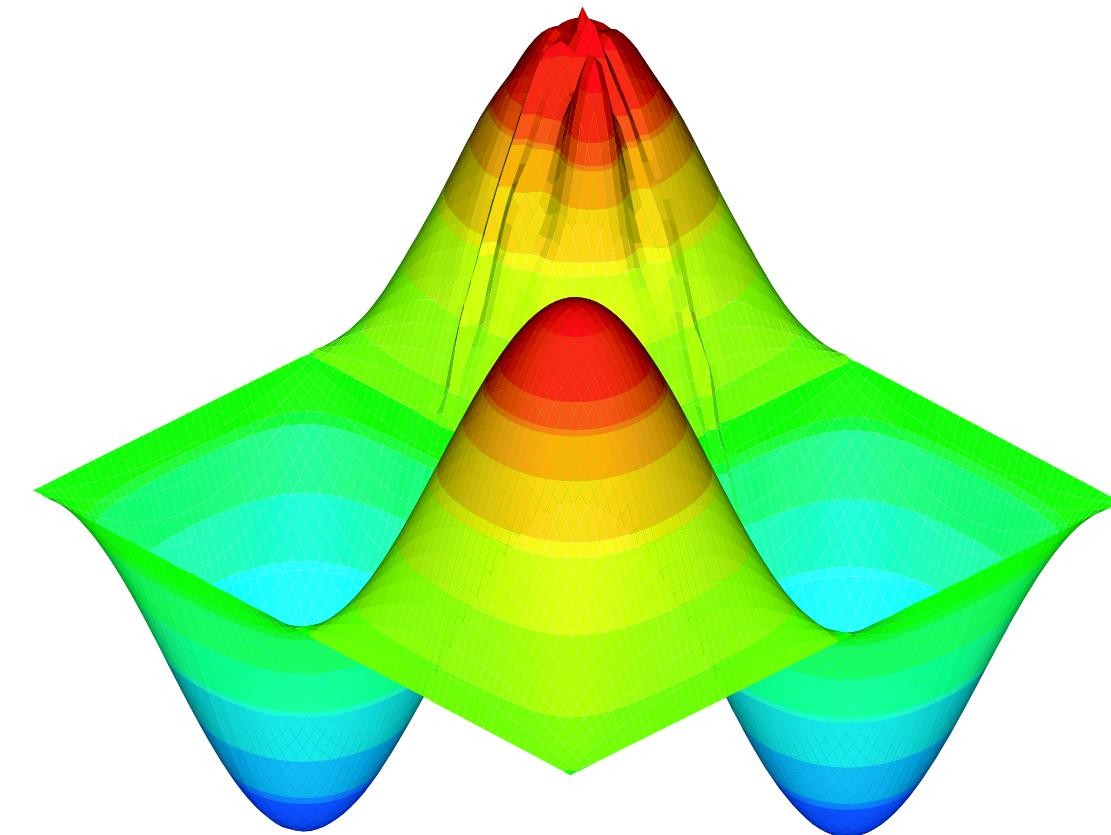
- Significant effort into stability analysis for under-resolved problems, much based around spectral vanishing viscosity (SVV):

$$\frac{\partial u}{\partial t} = \nu \nabla^2 u + S_{VV}(u),$$



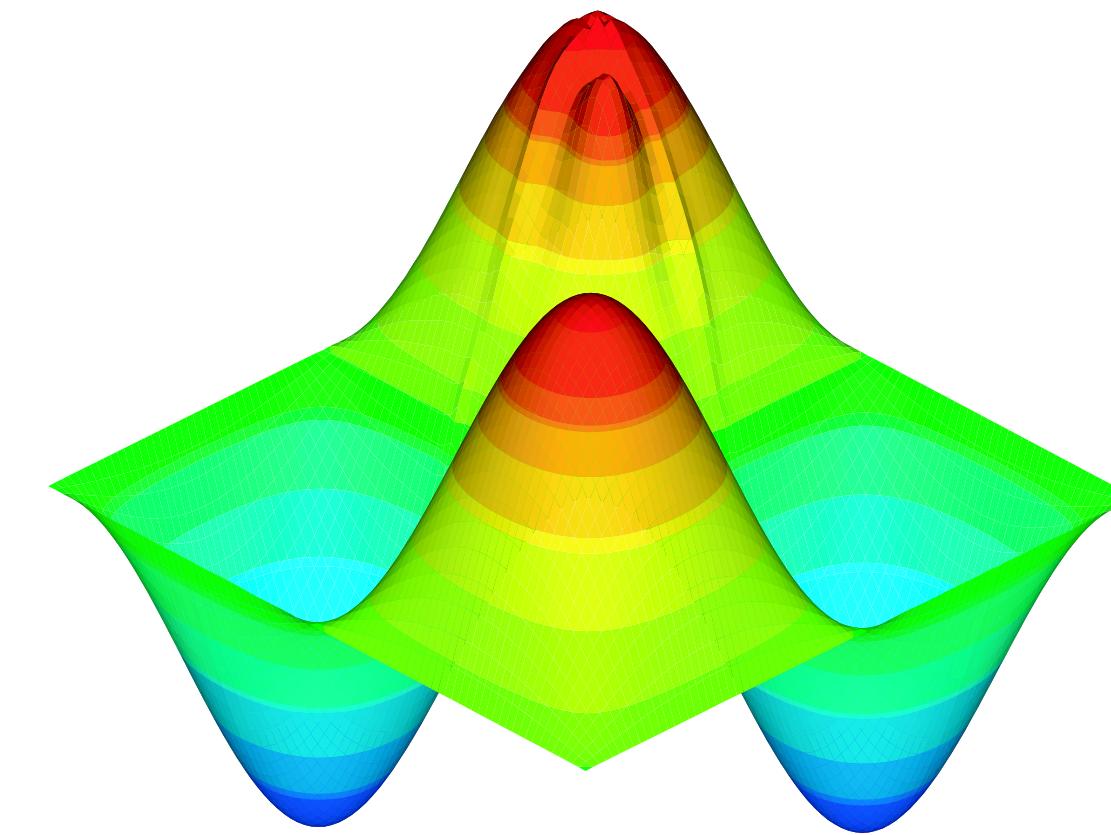
No SVV

$$S_{VV}(u) = \varepsilon \sum_{i=1}^{\text{dim}} \frac{\partial}{\partial x_i} \left[ Q_{\text{dim}} \star \frac{\partial u}{\partial x_i} \right]$$



$P_{cut} = 7,$

$\epsilon_{SVV} = 0.1$



$P_{cut} = 3,$

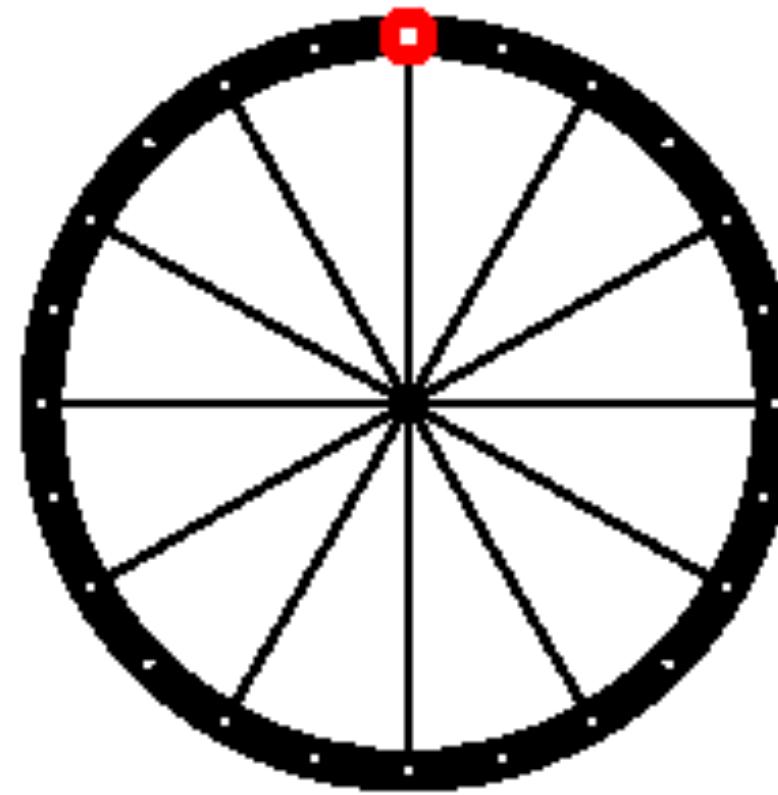
$\epsilon_{SVV} = 0.1$

# Stabilisation

- Large body of work more recently on emulating the stabilisation properties of DG for classical CG elliptic operators via eigenspectrum analysis.
- Naturally the DG method acts to dampen higher-order oscillations (and is one of the reasons that it is so popular for e.g. LES).
- See several references below!

- Mengaldo G, De Grazia D, Moura RC, Sherwin SJ, 2018, [Spatial eigensolution analysis of energy-stable flux reconstruction schemes and influence of the numerical flux on accuracy and robustness](#), Journal of Computational Physics, 358, 1-20
- Mengaldo G, Moura RC, Giralda B, Peiró J, Sherwin SJ 2017, [Spatial eigensolution analysis of discontinuous Galerkin schemes with practical insights for under-resolved computations and implicit LES](#), Computers and Fluids, 0045-7930
- Moura RC, Sherwin SJ, Peiro J, 2016, [Eigensolution analysis of spectral/hp continuous Galerkin approximations to advection-diffusion problems: Insights into spectral vanishing viscosity](#), Journal of Computational Physics, 307, 401-422
- Moura RC, Sherwin SJ, Peiro J, 2015, [Linear dispersion-diffusion analysis and its application to under-resolved turbulence simulations using discontinuous Galerkin spectral/hp methods](#), Journal of Computational Physics, 298, 695-710,

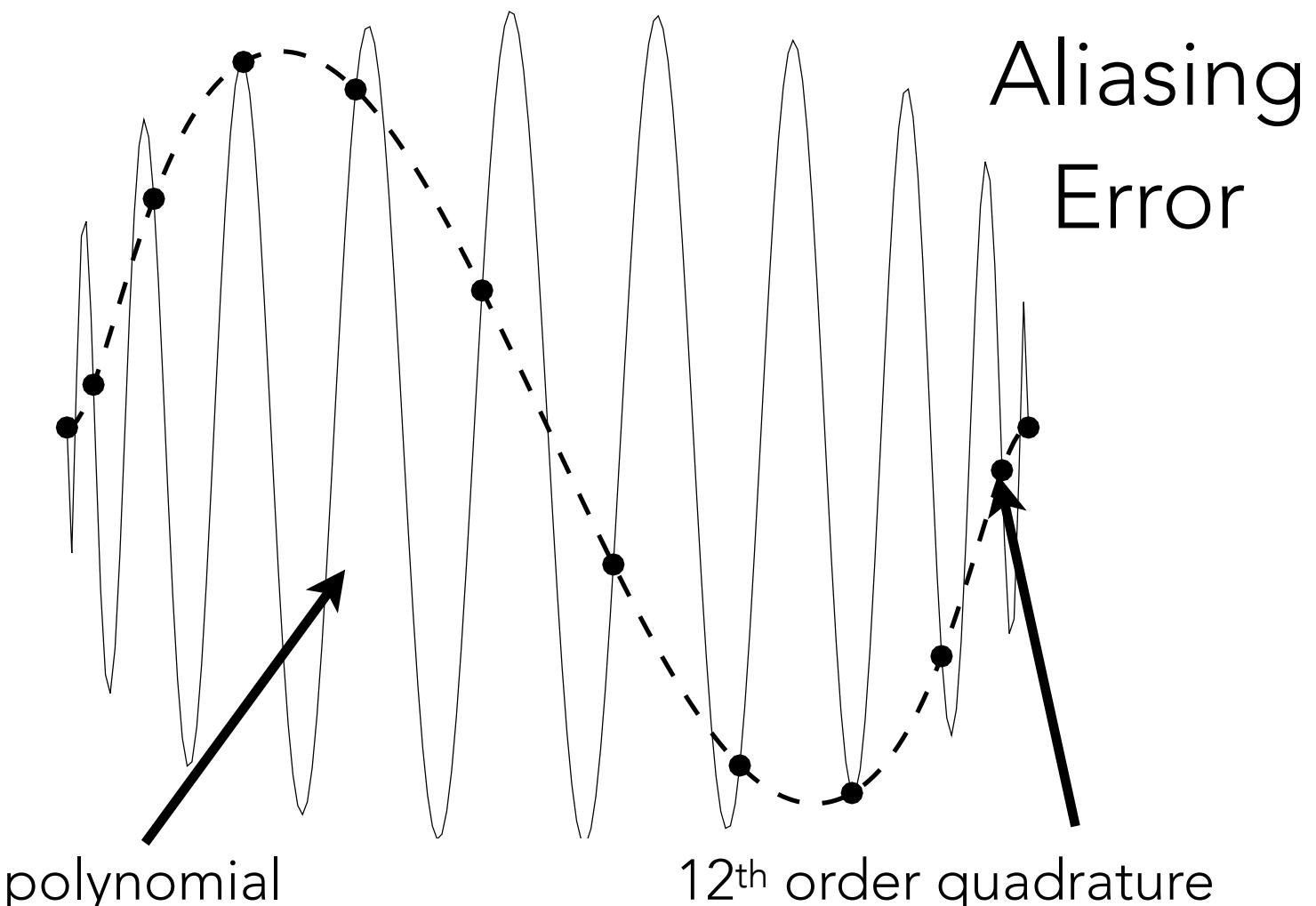
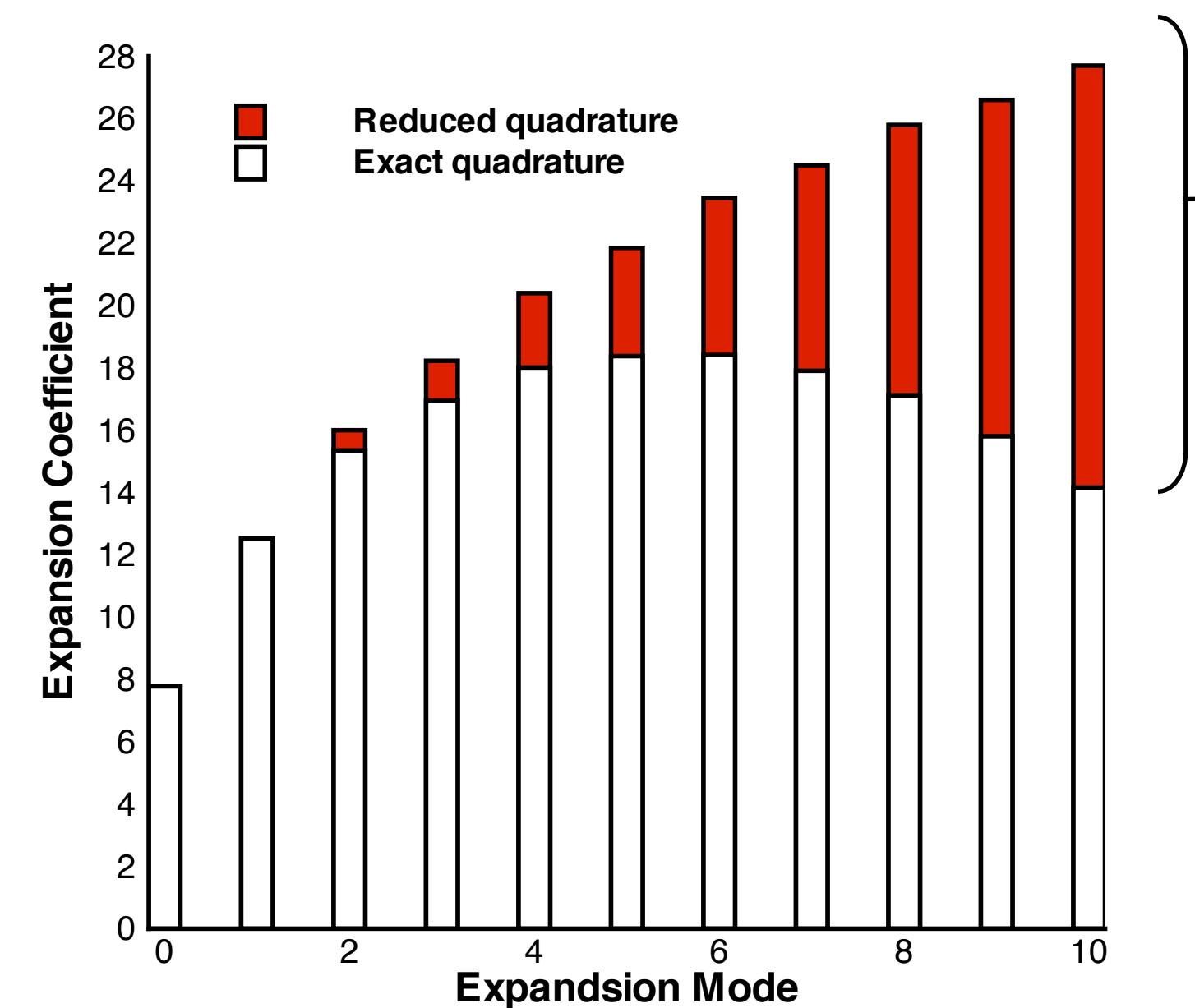
# Other considerations: aliasing



$$\text{Example: } u(\xi) = \sum_{i=0}^{10} \phi_i(\xi)$$

Galerkin projection of  $u^2$  using:

- $Q = 17$  – exact Quadrature
- $Q = 12$  – sufficient for integrating 20<sup>th</sup> degree polynomials

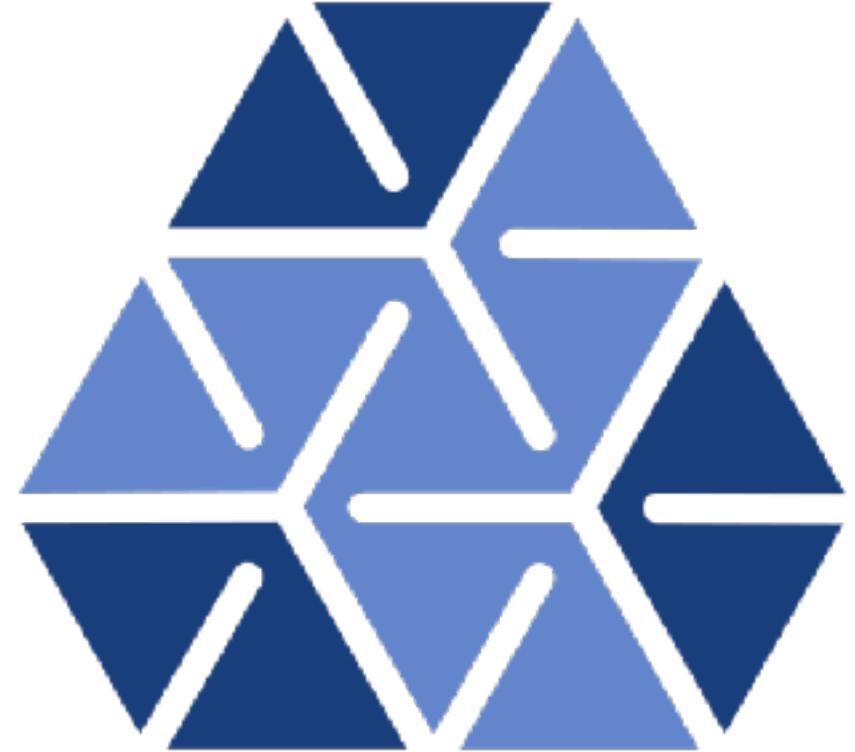




# Nektar++

*spectral/hp element framework*

High-fidelity numerical methods  
Highly parallel, designed for unsteady problems



# Nektar++

*spectral/hp element framework*

- Nektar++ is an **open source framework** for high-order methods.
- Although fluids is a key application area, we try to make it easier to use these methods in many areas, **not just fluids**.
- C++ API, with ambitions to bridge current and future hardware diversity (e.g. many-core processors, GPUs).
- Modern development practices with continuous integration, git, etc.

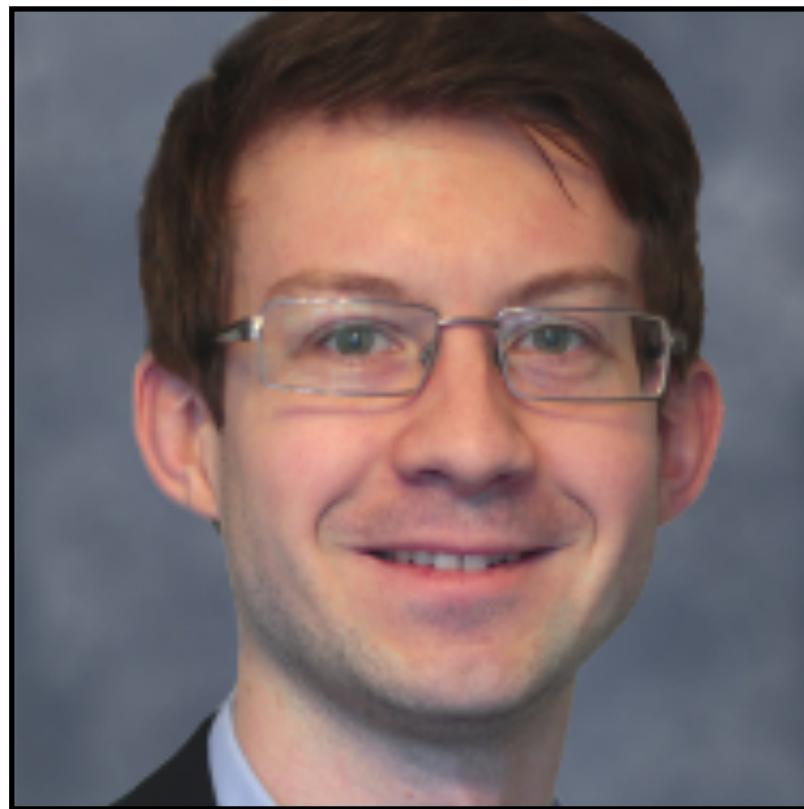
# Development team



Mike Kirby



Spencer Sherwin



Chris Cantwell



David Moxey

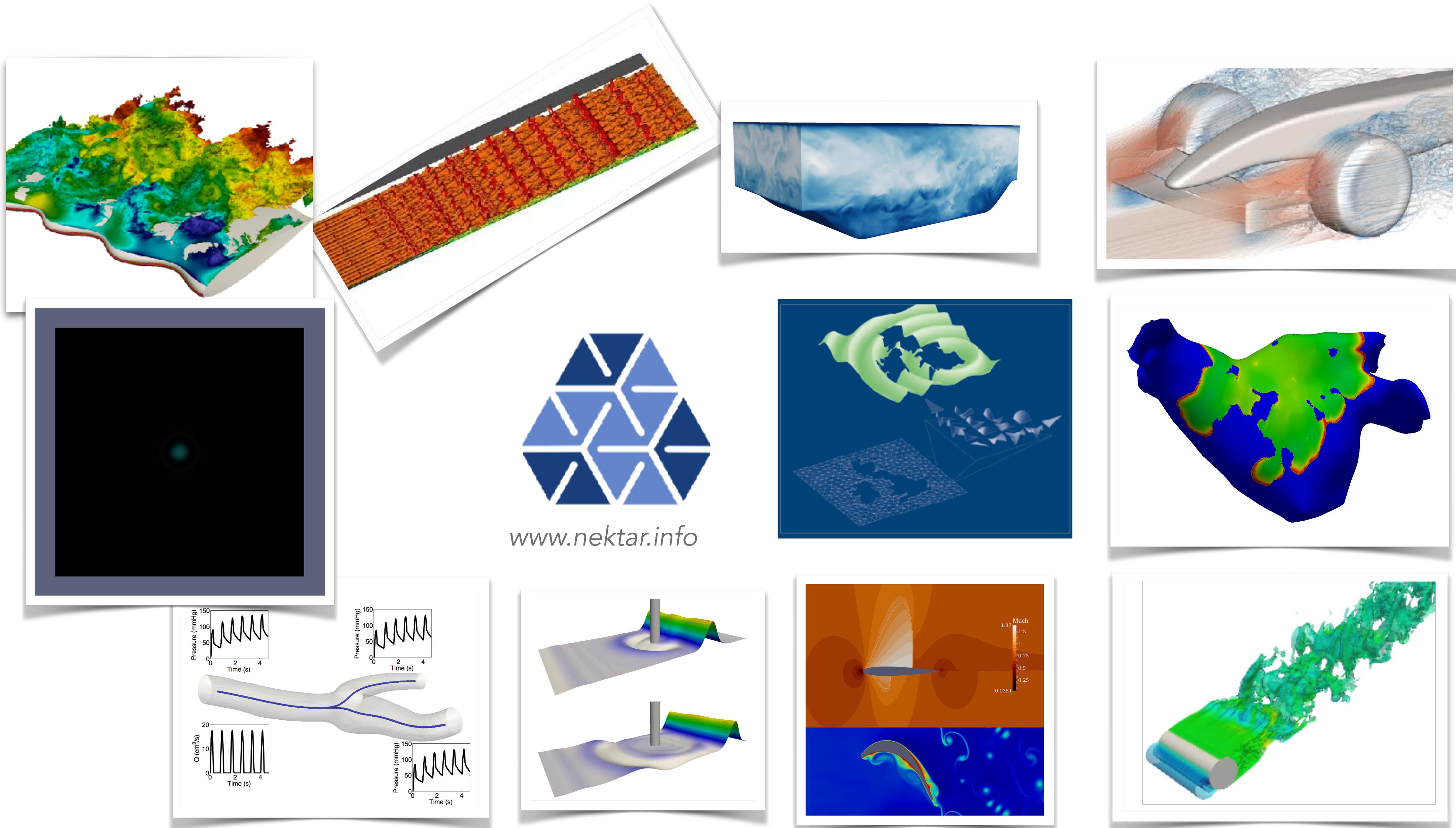


Imperial College  
London



- **Project coordinators:** Joaquim Peiró, Gianmarco Mengaldo
- **Senior developers:** Giacomo Castiglioni, Ankang Gao, Mohsen Lahooti, Zhengu Yan

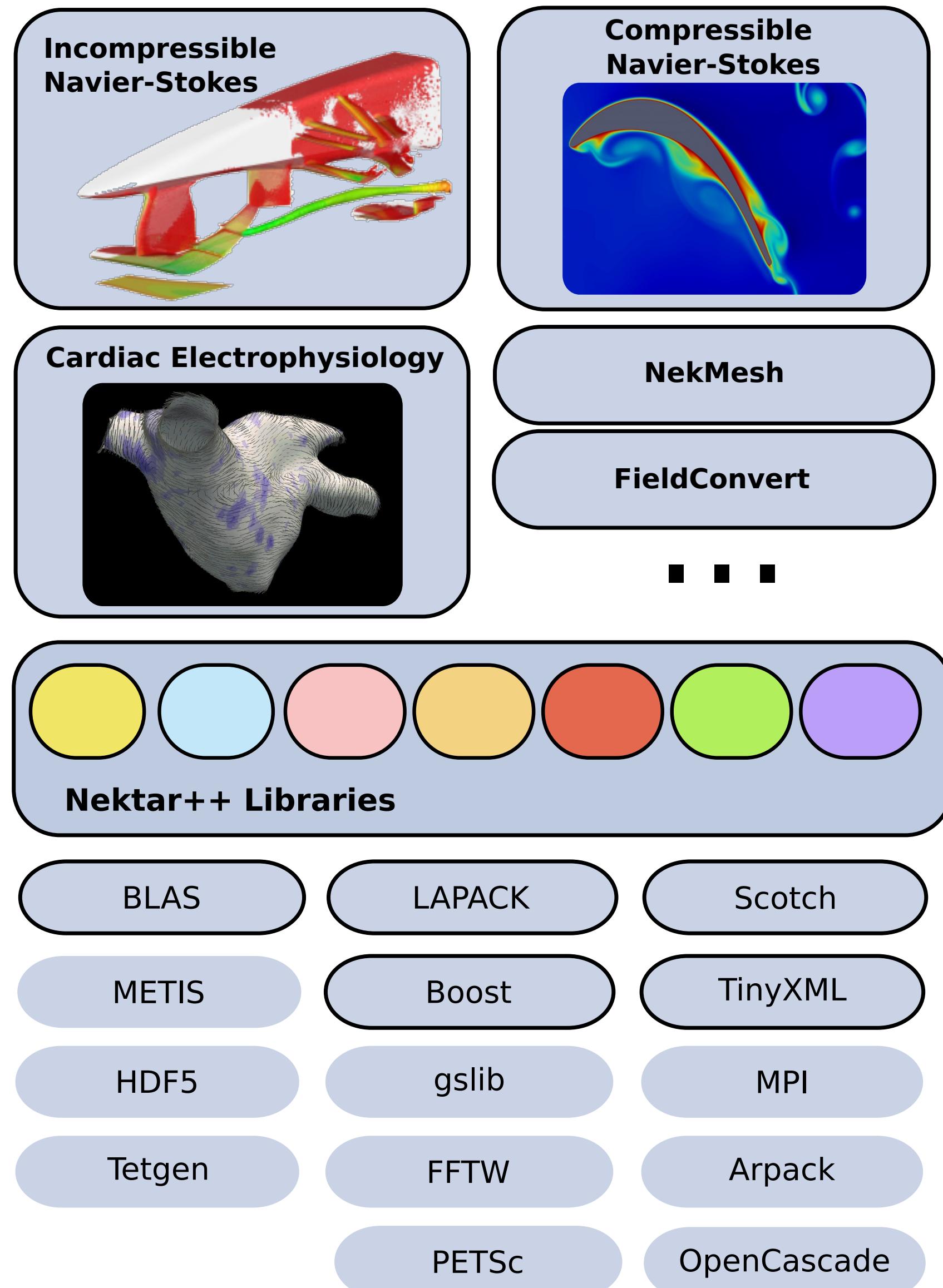
# Some application areas



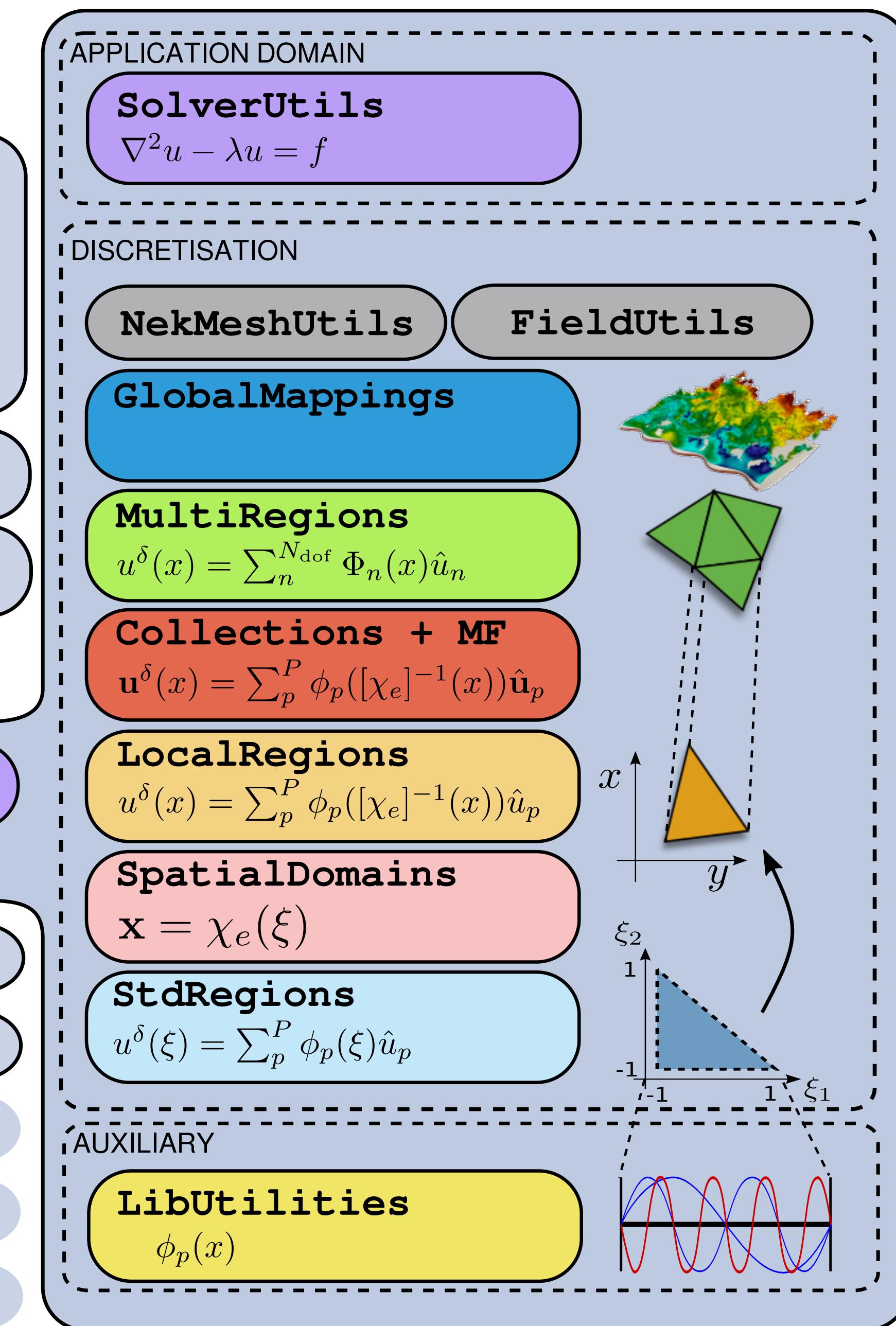
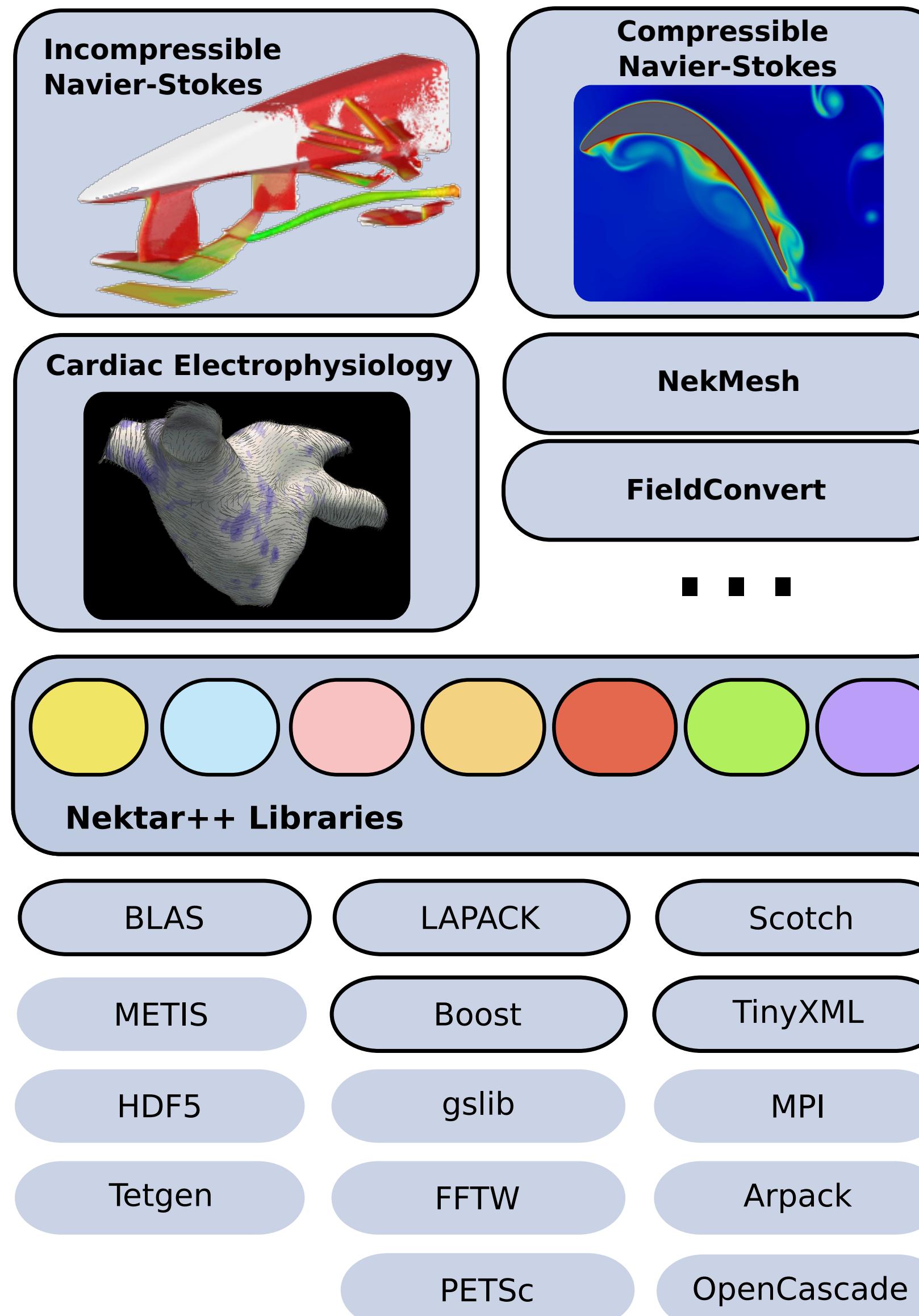
# Design Approach

- **Challenge:** Large software project, many developers.
  - Hide algorithmic complexity.
  - Tie implementation to mathematics wherever possible.
  - Compartmentalise features / algorithms / data structures.
  - Choice of abstraction - “*there is more than one way to skin a cat*”.
- Coding paradigms: template pattern, factory pattern
  - Switch algorithms transparently
  - Aids design of suitable interfaces between components
  - Decoupling of code - faster build times, more robust

# Library structure



# Library structure



# Operator Construction

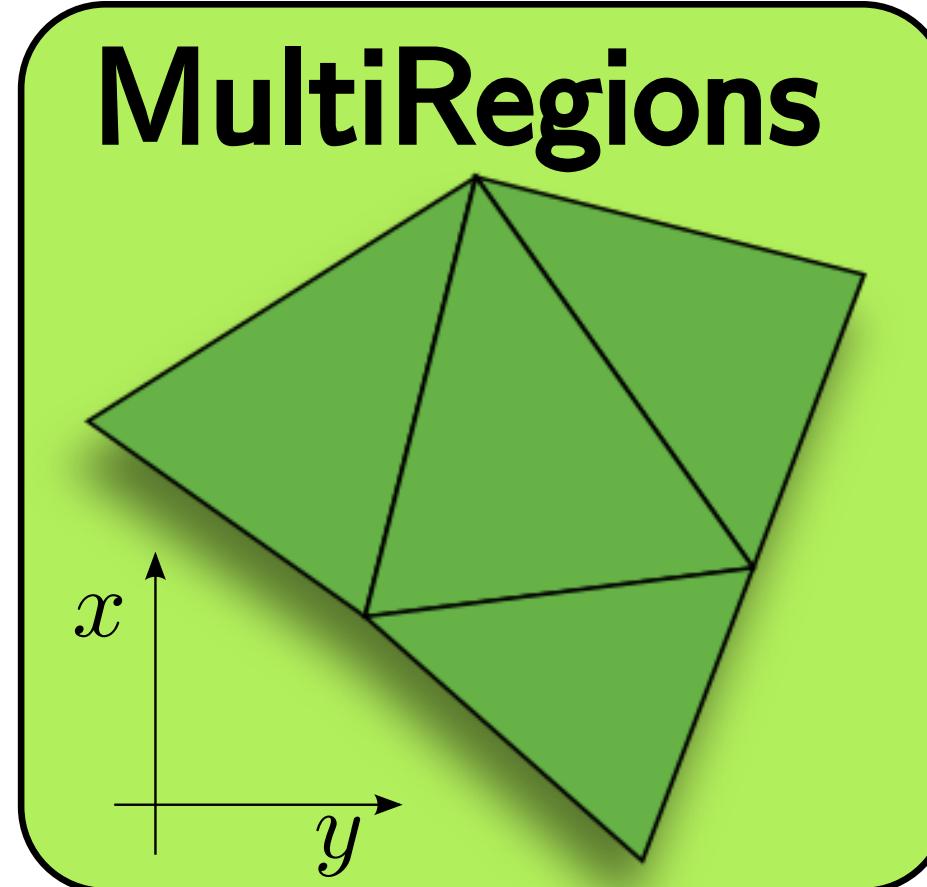
Helmholtz problem:

$$\nabla^2 u + \lambda u = f$$

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

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

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

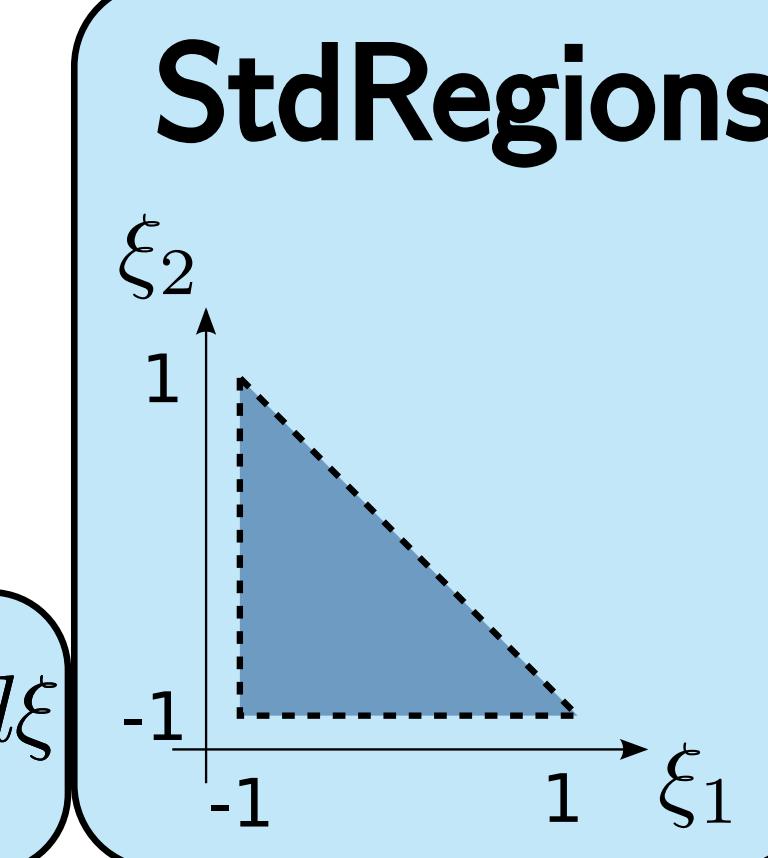
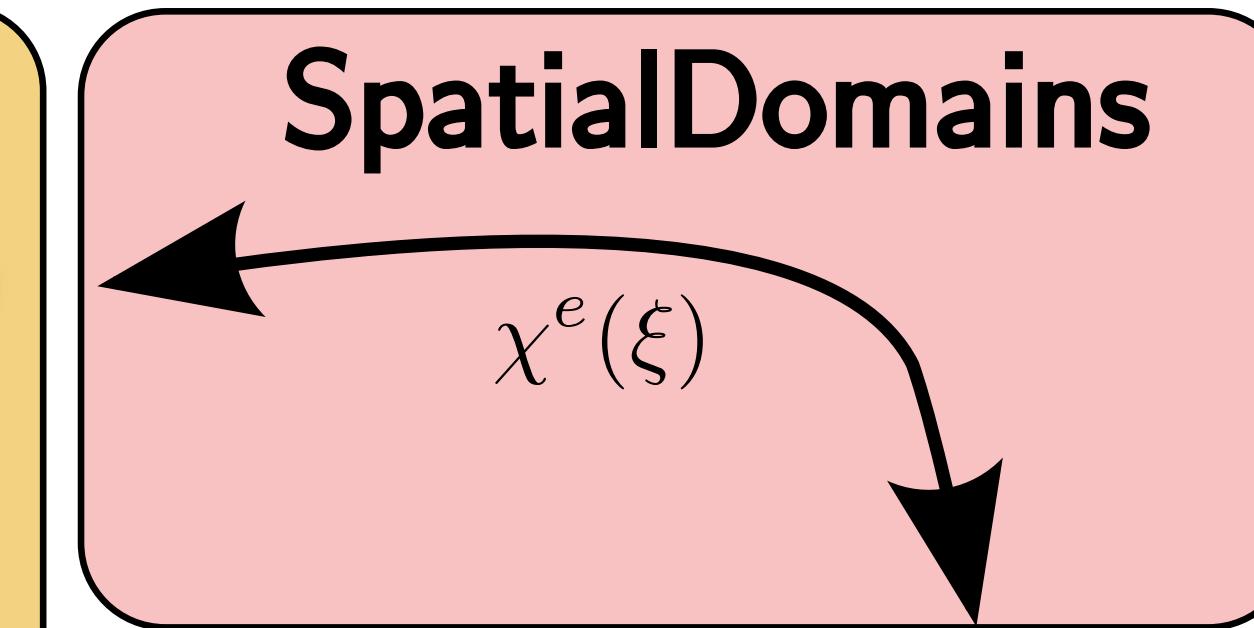


$$\mathbf{f}[i] = \int_{\Omega} \Phi_i(x) f(x) dx$$



$$= \sum_e^{N^{el}} \sum_p \int_{\Omega^e} \phi_p(x) f(x) dx$$

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



# Operator Construction

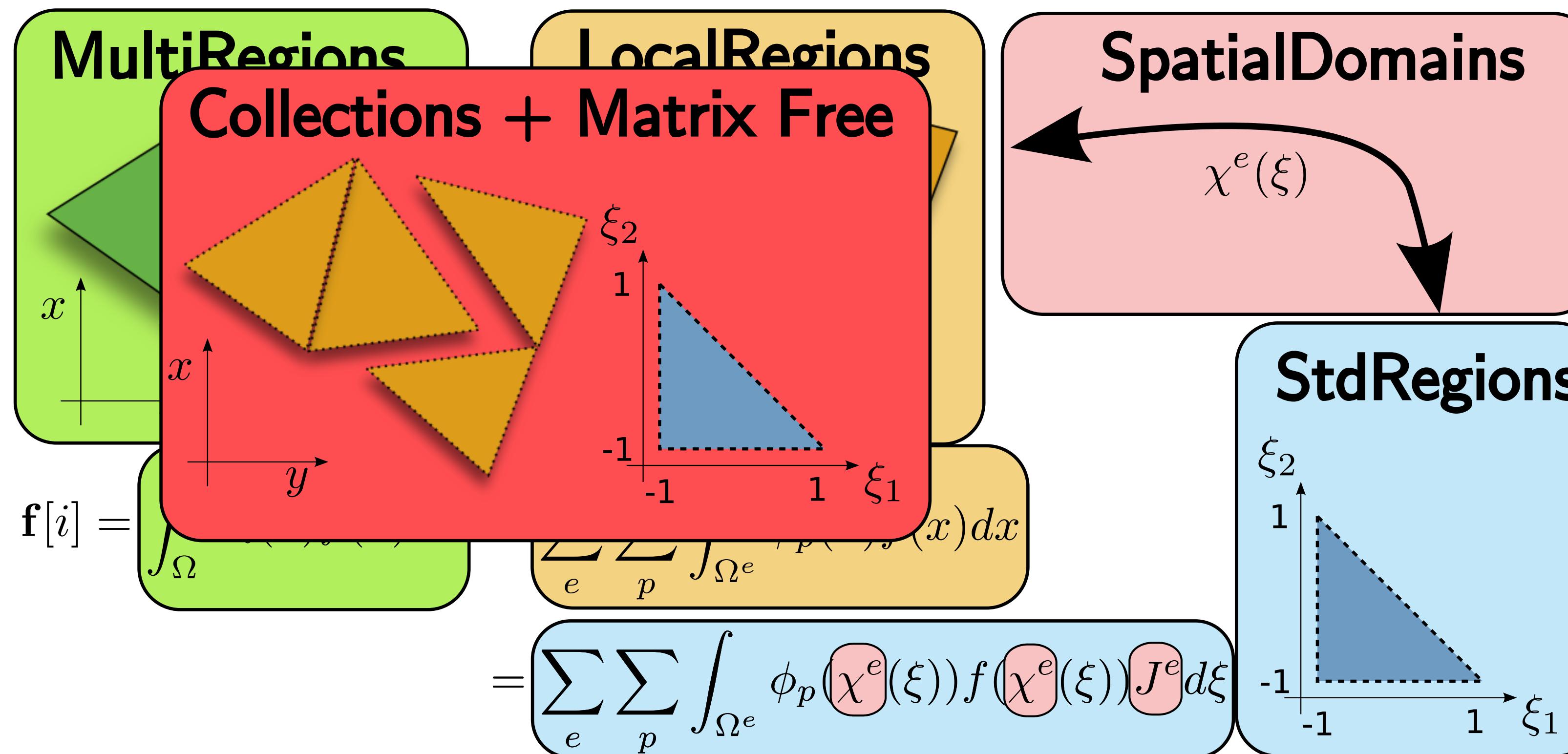
Helmholtz problem:

$$\nabla^2 u + \lambda u = f$$

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

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

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



# Diffusion solver

- Quick example: solve the diffusion equation with backward Euler:

$$\frac{\partial u}{\partial t} = \varepsilon \nabla^2 u \longrightarrow \frac{u^{n+1} - u^n}{\Delta t} = \varepsilon \nabla^2 u^{n+1} \longrightarrow \nabla^2 u^{n+1} - \frac{u^{n+1}}{\varepsilon \Delta t} = - \frac{u^n}{\varepsilon \Delta t}$$

- Involves the solution of a **Helmholtz equation**.
- We'll use basic routines to highlight how you might solve this using fundamentals of the library.
- In Nektar++, see solvers/DiffusionSolver for full source code.

# Diffusion solver

Create session

```
session = LibUtilities::SessionReader::CreateInstance(argc, argv);
```

Set up a mesh

```
string var = session->GetVariable(0);
auto mesh = SpatialDomains::MeshGraph::Read(session);
auto field = MemoryManager<MultiRegions::ContField2D>
    ::AllocateSharedPtr(session, mesh, var);
```

Initial conditions

```
int nq = field->GetNpoints();
Array<OneD, double> x0(nq), x1(nq), x2(nq);
field->GetCoords(x0, x1, x2);
icond->Evaluate(x0, x1, x2, 0.0, field->UpdatePhys());
```

Parameters

```
double epsilon = session->GetParameter("epsilon");
double delta_t = session->GetParameter("delta_t");
```

# Diffusion solver

Time integrate

```
for (int n = 0; n < nSteps; ++n)
{
    Vmath::Smul(nq, -1.0/delta_t/epsilon,
                field->GetPhys(), 1,
                field->UpdatePhys(), 1);

    field->HelmSolve(field->GetPhys(),
                      field->UpdateCoeffs(),
                      NullFlagList,
                      factors);

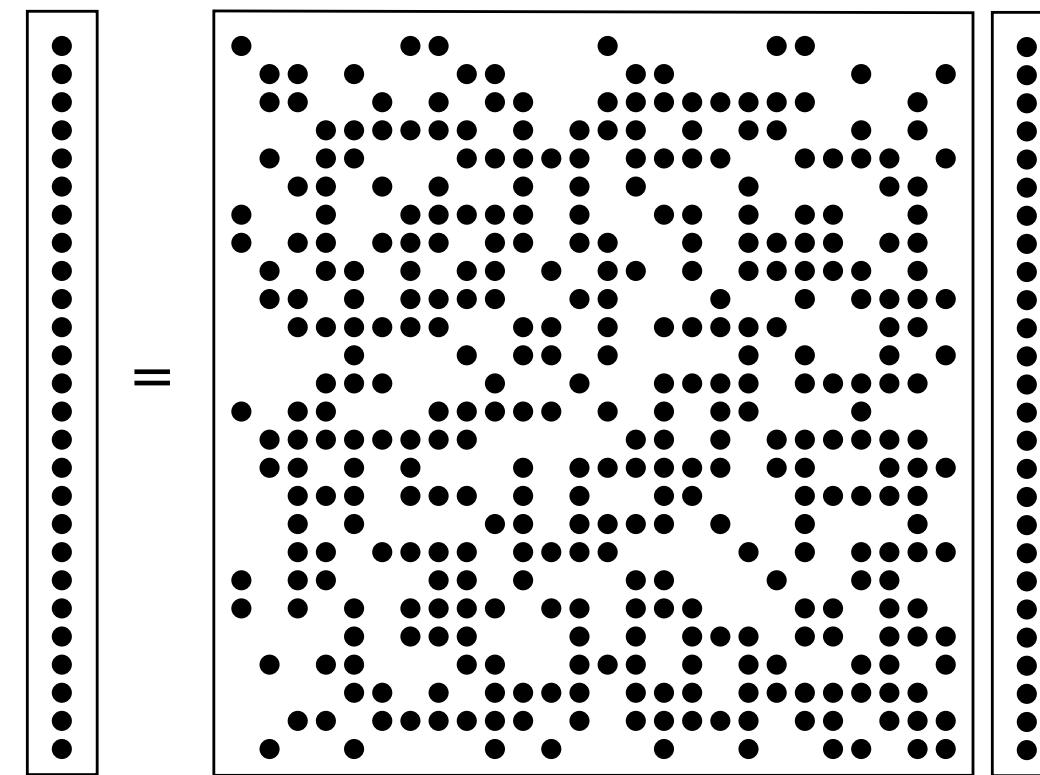
    field->BwdTrans (field->GetCoeffs(),
                     field->UpdatePhys());
}
```

Output

```
fldIO->Write(outFile, FieldDef, FieldData);
```

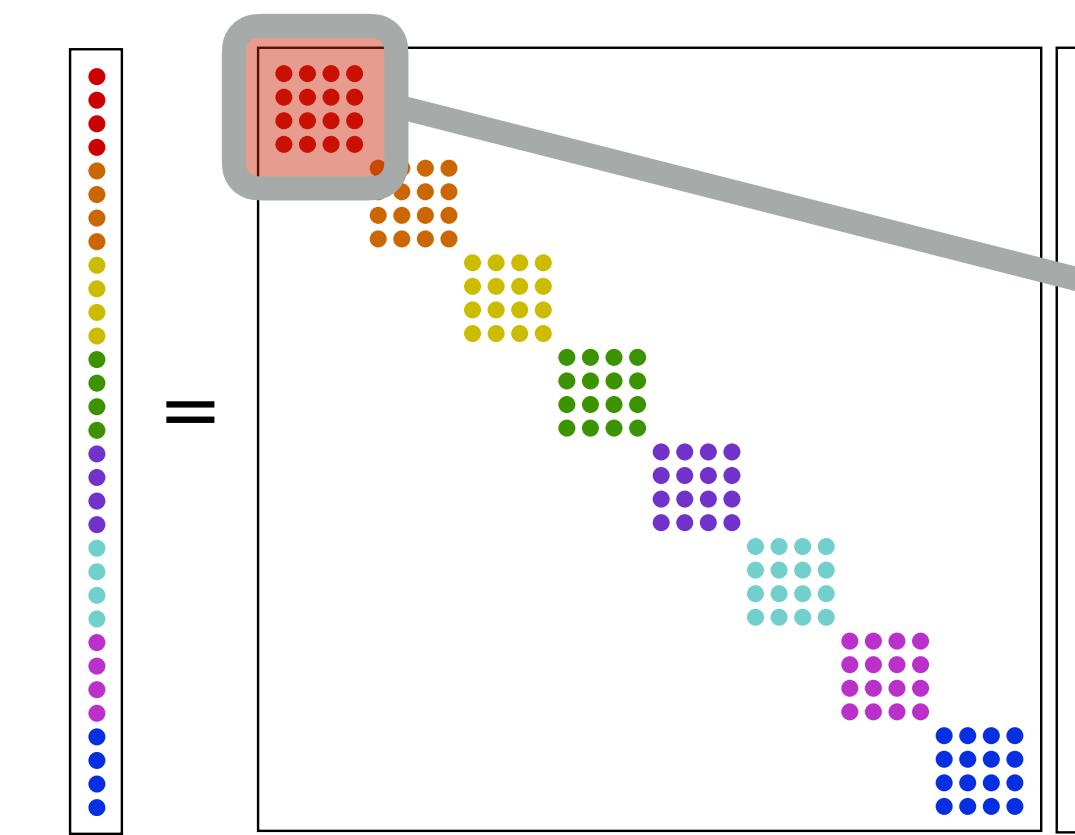
# Implementation choices

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



**Global matrix**

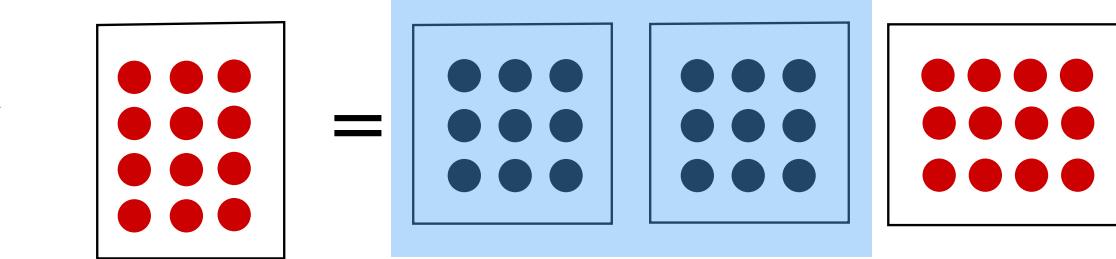
assemble a sparse matrix



**Local evaluation**

create elemental dense  
matrices + assembly map

**1D basis functions**



**Matrix free**

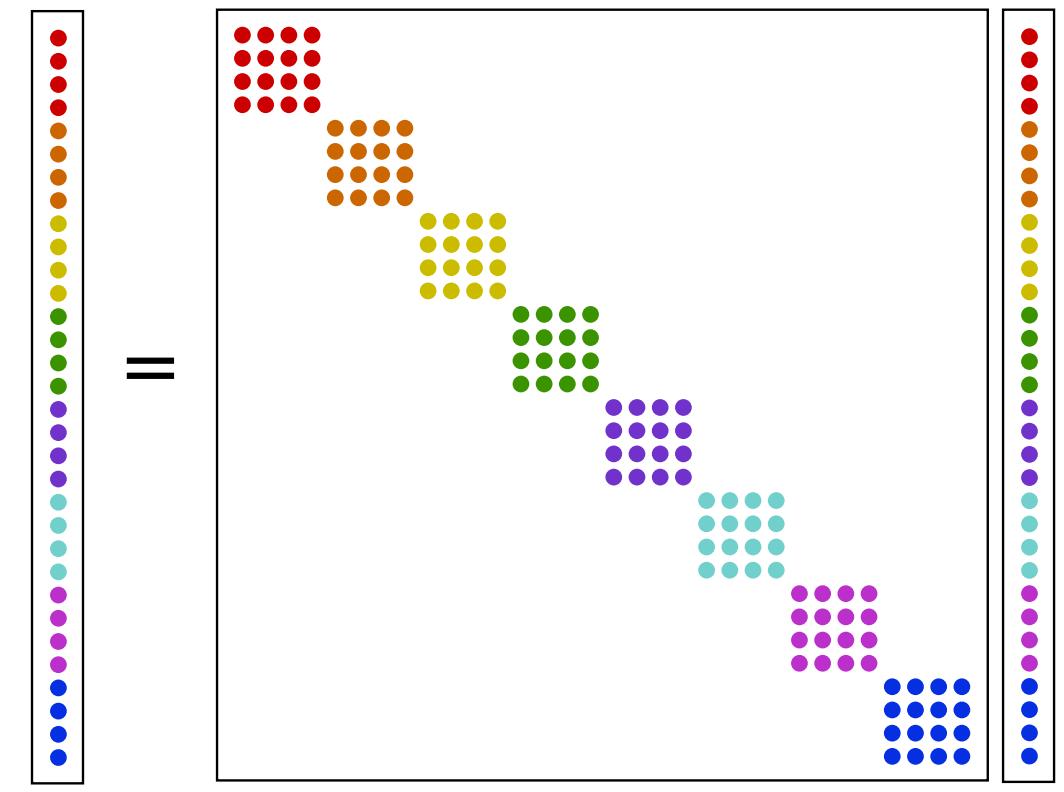
no local matrices at all  
**sum factorisation** speedup



increasing arithmetic intensity

# Collections

## Local Matrix



## StdMat

1. Apply Jacobian (L1)

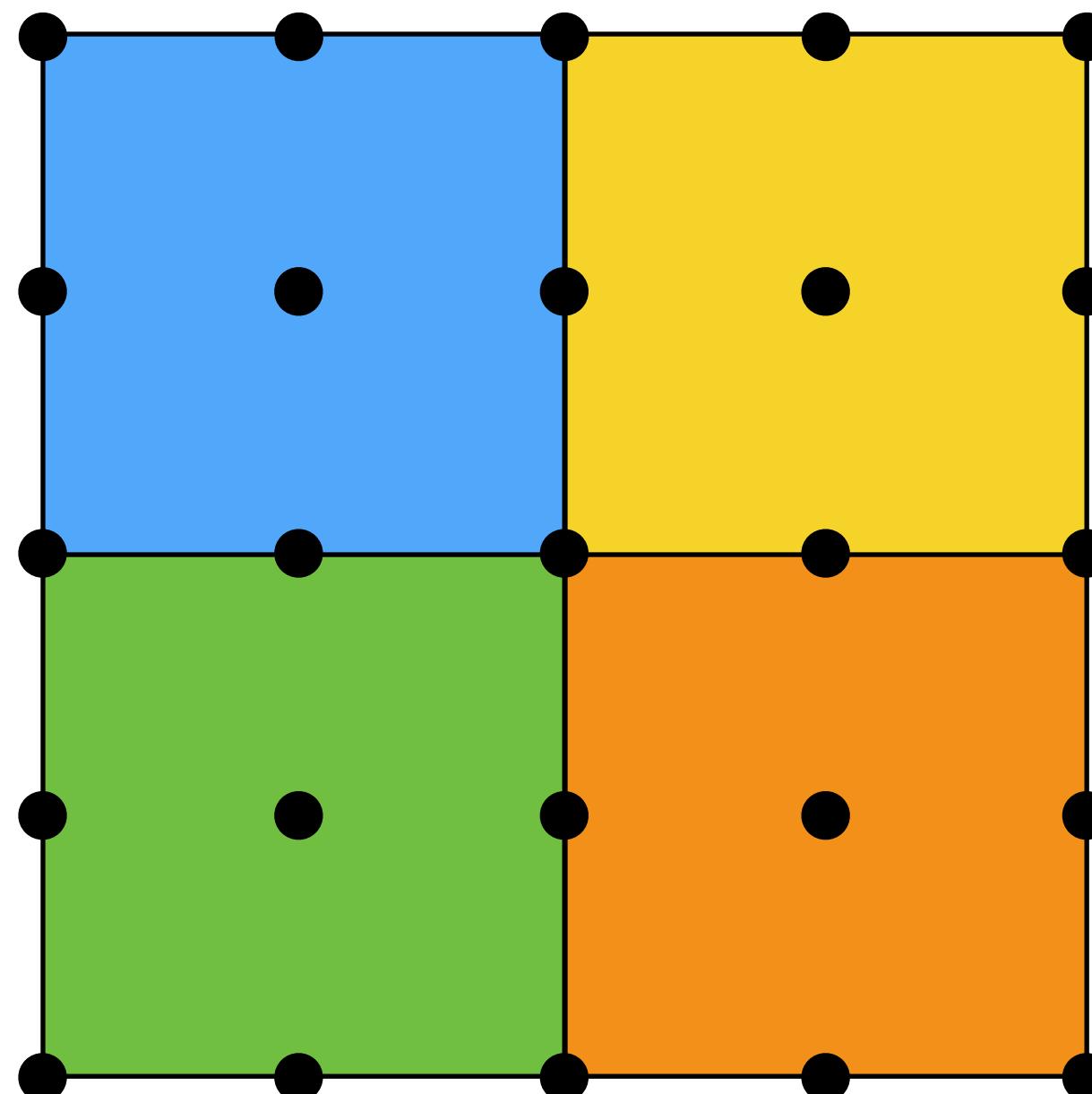
A diagram showing the application of the Jacobian (L1). It consists of three parts: a colored matrix, an equals sign, a multiplication symbol (a circle with a dot), and another colored matrix. The matrices have the same color scheme as the Local Matrix.

2. L3 Multiply by ref. matrix

A diagram showing the multiplication of the colored matrix from the previous step by a reference matrix. It consists of three parts: a colored matrix, an equals sign, and two matrices. The first matrix is black and has a 3x3 block pattern. The second matrix is colored and has the same structure as the others.

# Data layout

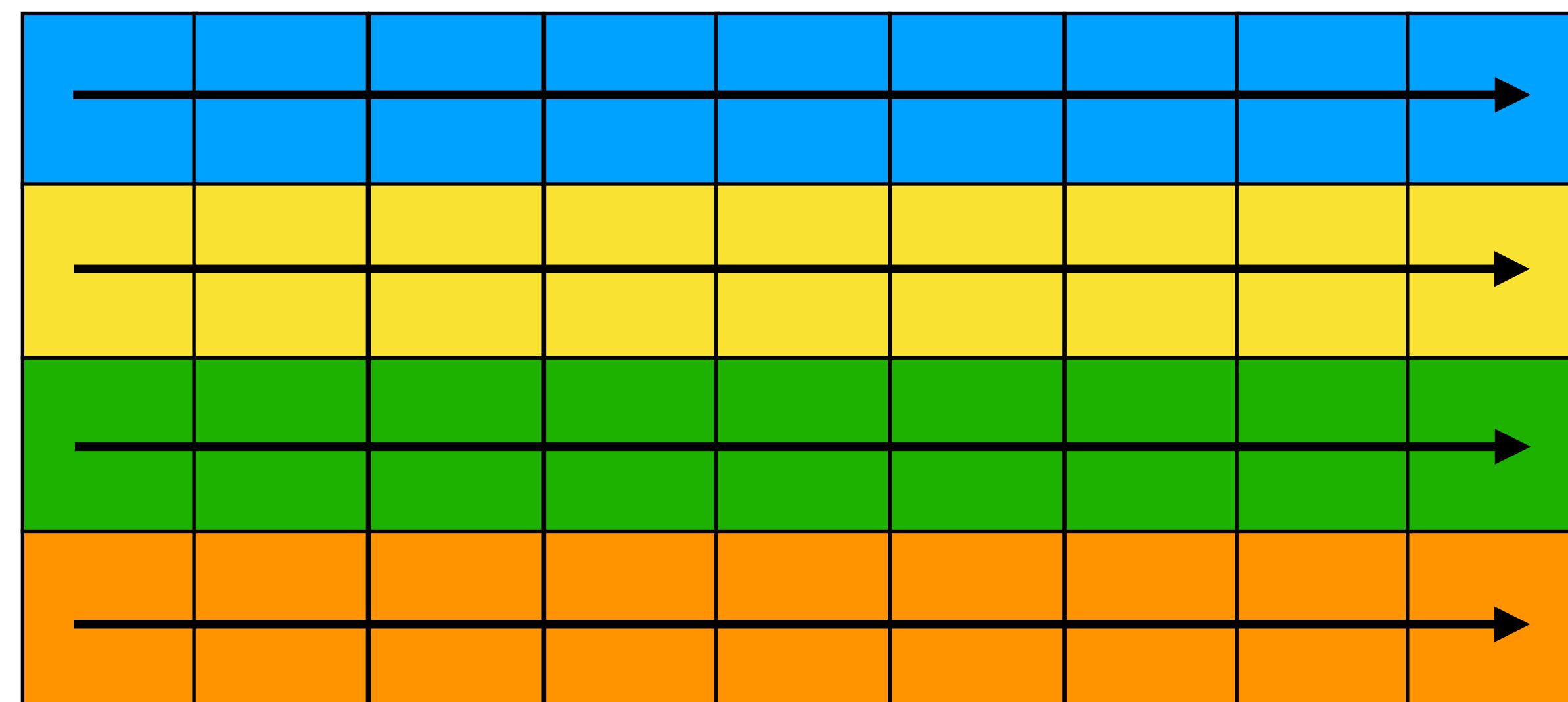
Natural to consider data laid out element by element



elements

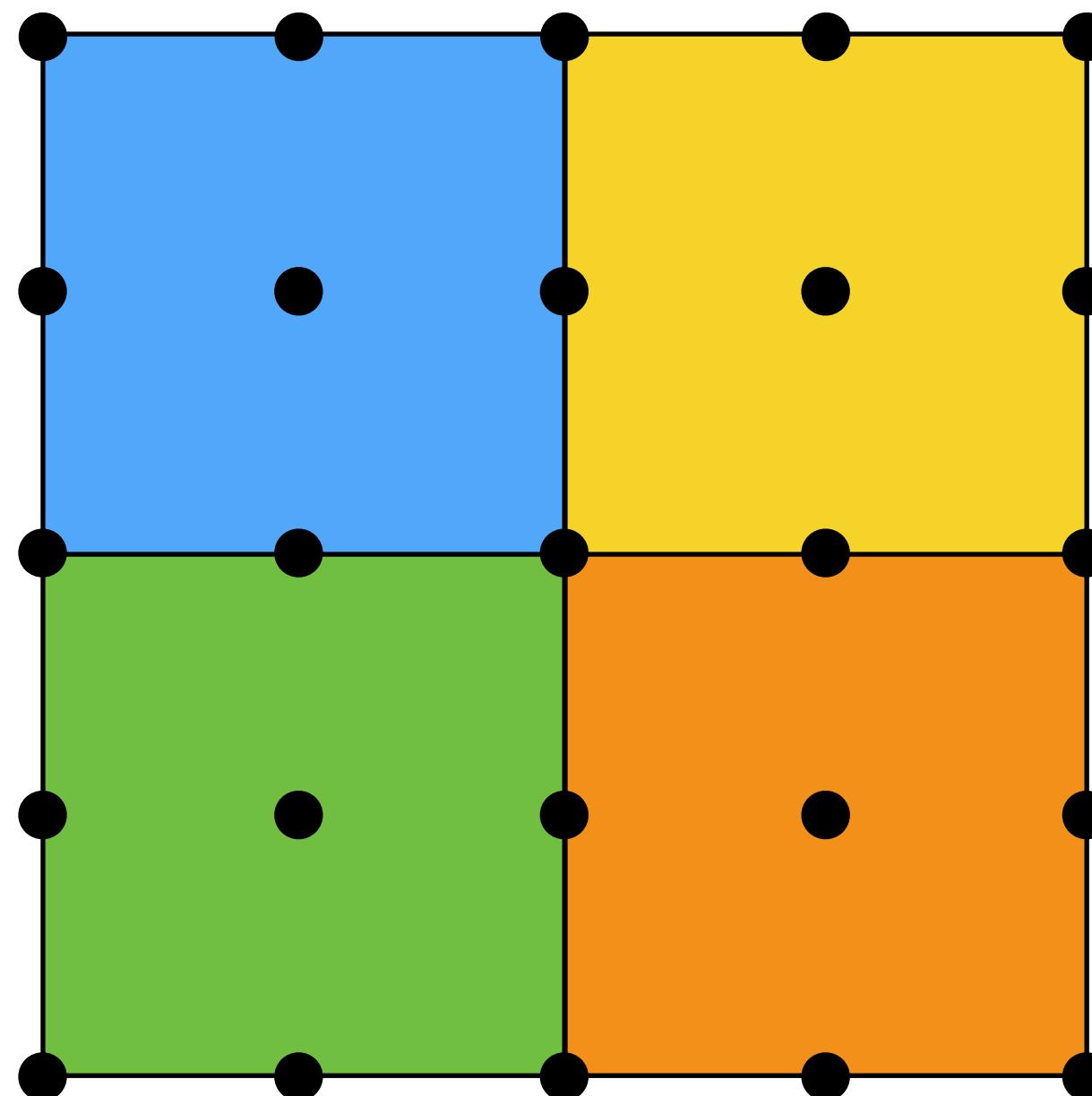


degrees of freedom



# Data layout

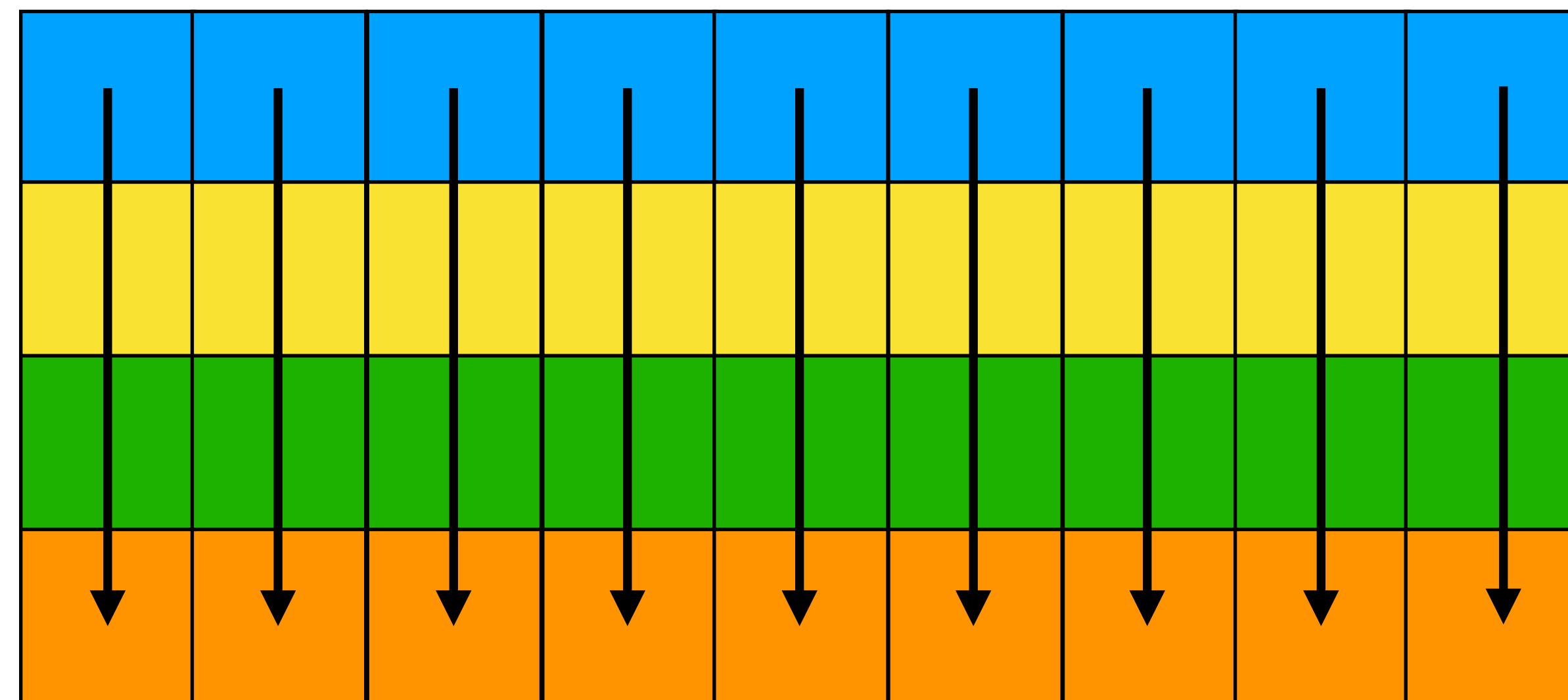
Exploit vectorisation by grouping DoFs by vector width



elements

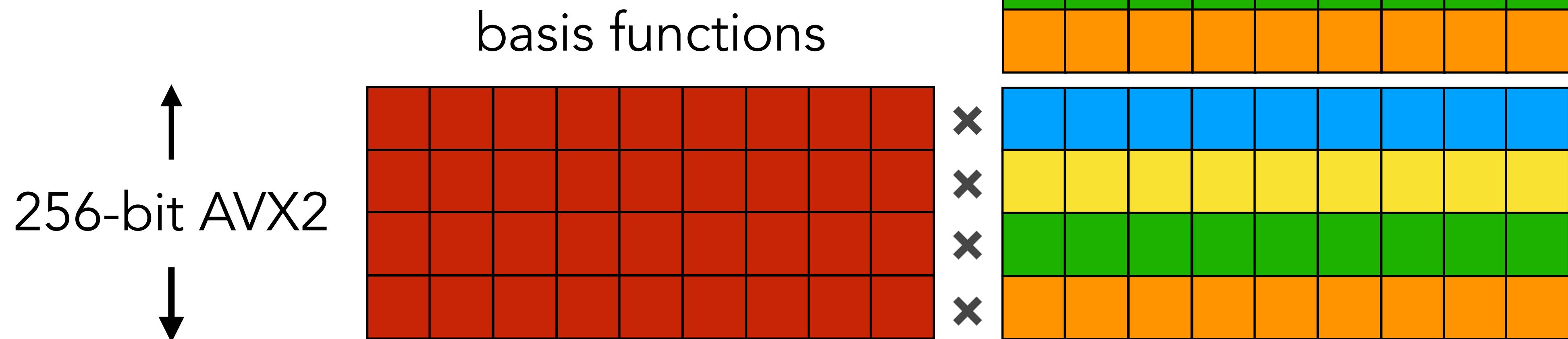


degrees of freedom →



# Use of vectorisation

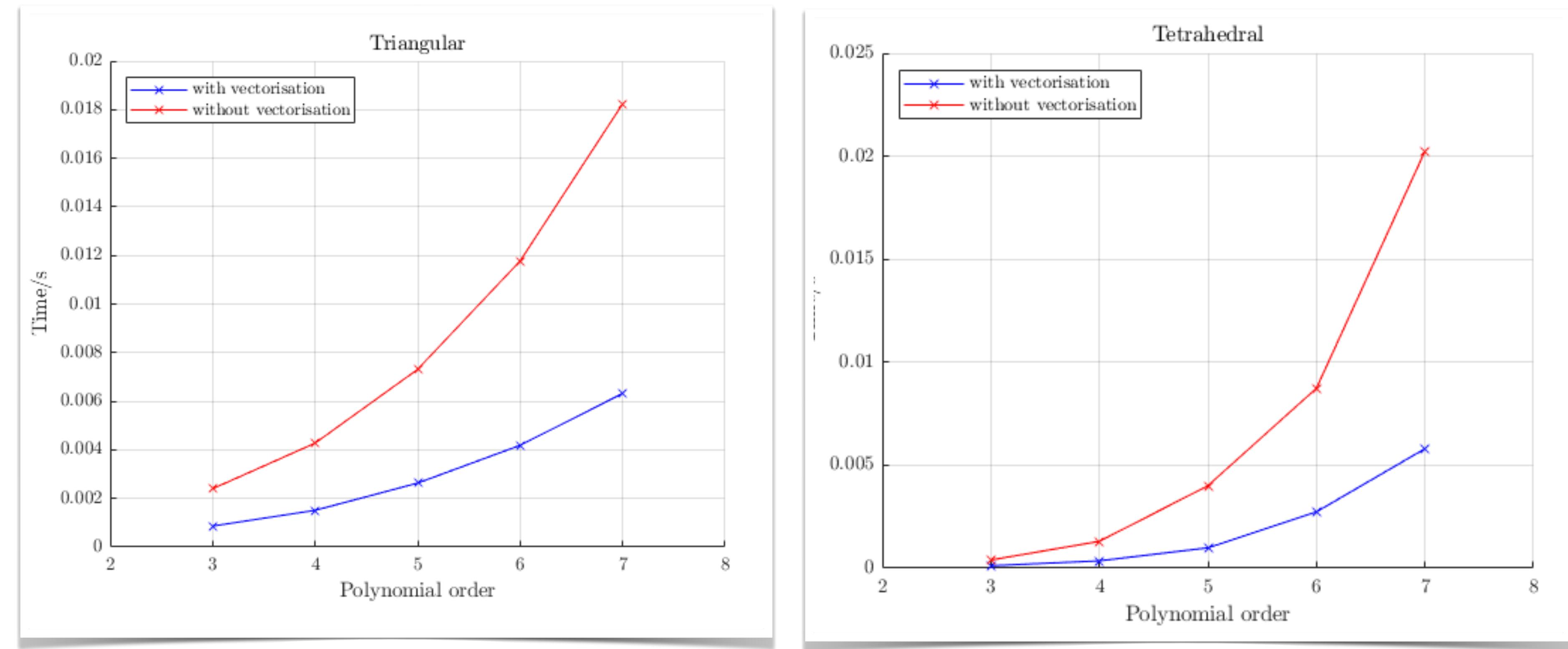
- Operations occur over groups of elements of size of vector width
- Use C++ data type that encodes vector operations vs. compiler intrinsics.
- Templating used to allow compiler to unroll as much as possible.



# Software implementation

$$\mathcal{L}(u) = \nabla [D \cdot \nabla u]$$

$d \times d$  spatially-constant  
diffusion tensor

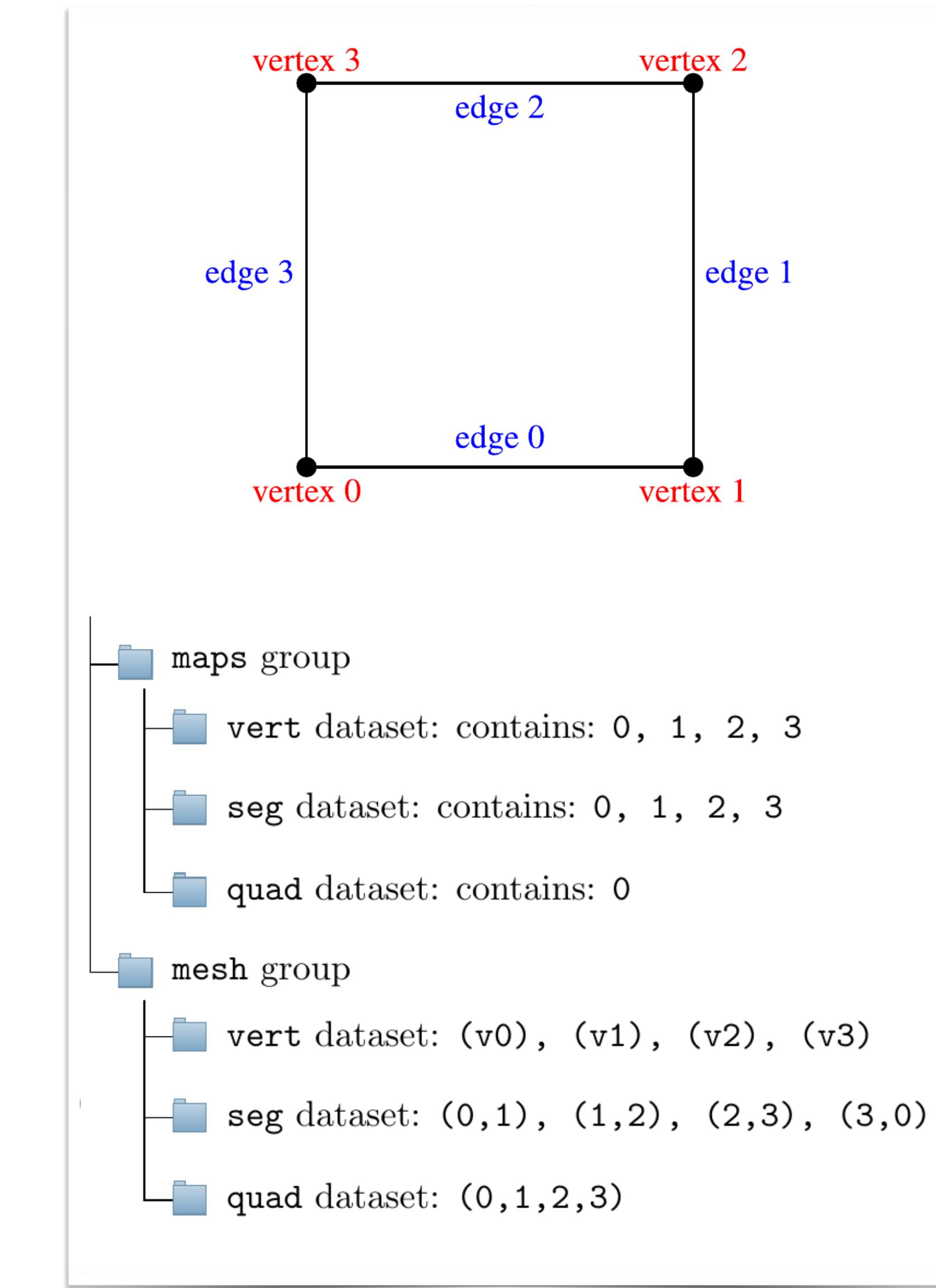


Good speedups observed over non-vectorised versions of  
this operator for both 2D & 3D elements

# Parallel I/O



- **Hierarchical Data Format**
  - ▶ Scalable and high-performance
  - ▶ Used for both input and output
  - ▶ Read/write in parallel
- **Usage**
  - ▶ Distribute reading of elements
  - ▶ Parallel partition: PTScotch
  - ▶ Top-down reading of mesh
  - ▶ Bottom-up object construction
  - ▶ Read ancillary data (composites).

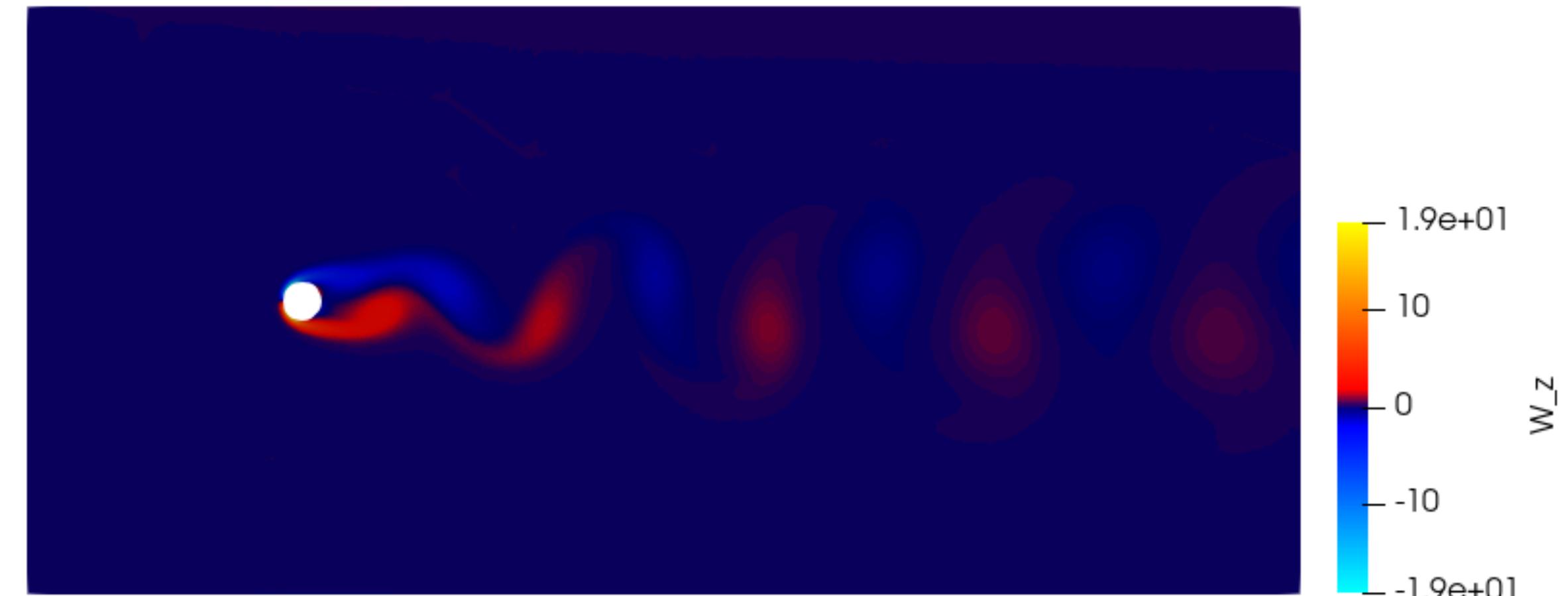


Mesh structure & its layout within a HDF5  
mesh file.

# In-situ processing

- Post-processing poses storage/memory challenges.
- In-situ filter for using existing post-processing algorithms.
- Enables efficient calculation of derived quantities during run.
- Modules specified in XML session file.

```
1 <FILTER TYPE="FieldConvert">
2   <PARAM NAME="OutputFile"> vorticity.vtu </PARAM>
3   <PARAM NAME="OutputFrequency"> 100 </PARAM>
4   <PARAM NAME="Modules">
5     vorticity
6     removefield:fieldname=u,v,p
7   </PARAM>
8 </FILTER>
```



Computation of vorticity performed every 100 timesteps using the FieldConvert filter.

# Python interface

- Bindings for key libraries.
- Simplify usage for new users and for teaching.
- Access from other software packages.
- Leverages Boost.Python.
- Interoperability with NumPy: explicit memory sharing between Nektar++ arrays.

```
import NekPy.LibUtilities as LibUtil
import NekPy.StdRegions as StdReg
import numpy as np

# Set P = 8 modes and Q = P + 1 quadrature points.
nModes = 8
nPts   = nModes + 1

# Create GLL-distributed quadrature points.
pType  = LibUtil.PointsType.GaussLobattoLegendre
pKey   = LibUtil.PointsKey(nPts, pType)

# Create modified C^0 basis on these points.
bType  = LibUtil.BasisType.Modified_A
bKey   = LibUtil.BasisKey(bType, nModes, pKey)

# Create quadrilateral expansion using this basis
# in each coordinate direction (tensor product).
quad   = StdReg.StdQuadExp(bKey, bKey)

# L^2 projection of f(x,y) = cos(x)*cos(y) onto the
# quadrilateral element. Note x,y are numpy ndarrays
# and evaluation of cos() is performed using numpy.
x, y   = quad.GetCoords()
fx      = np.cos(x) * np.cos(y)
proj    = quad.FwdTrans(fx)

# Integrate function over the element.
print("Integral = {:.4f}".format(quad.Integral(fx)))
```

Simple example of integration within a quadrilateral region.

# **Summary**

# Summary

- Hopefully a useful overview of high-order methods and some of our implementation within Nektar++.
- We see high-order methods as an enabling technology for many of these challenging physics problems.
- Some areas for us to work on (some discussion on this later):
  - Mesh generation continues to be a focus and typically quite a challenge for new users.
  - Performance portability across architectures and multi-architecture support.

# Nektar++ workshop

- We're holding our 6th annual(ish) workshop for Nektar++.
- Good opportunity to see (or contribute!) some talks around recent developments in Nektar++ and application areas around it.
- Also good opportunity to connect with the various developers around Nektar++.
- Will be held **13-16th September 2022** at Imperial College London.
- Registration free!

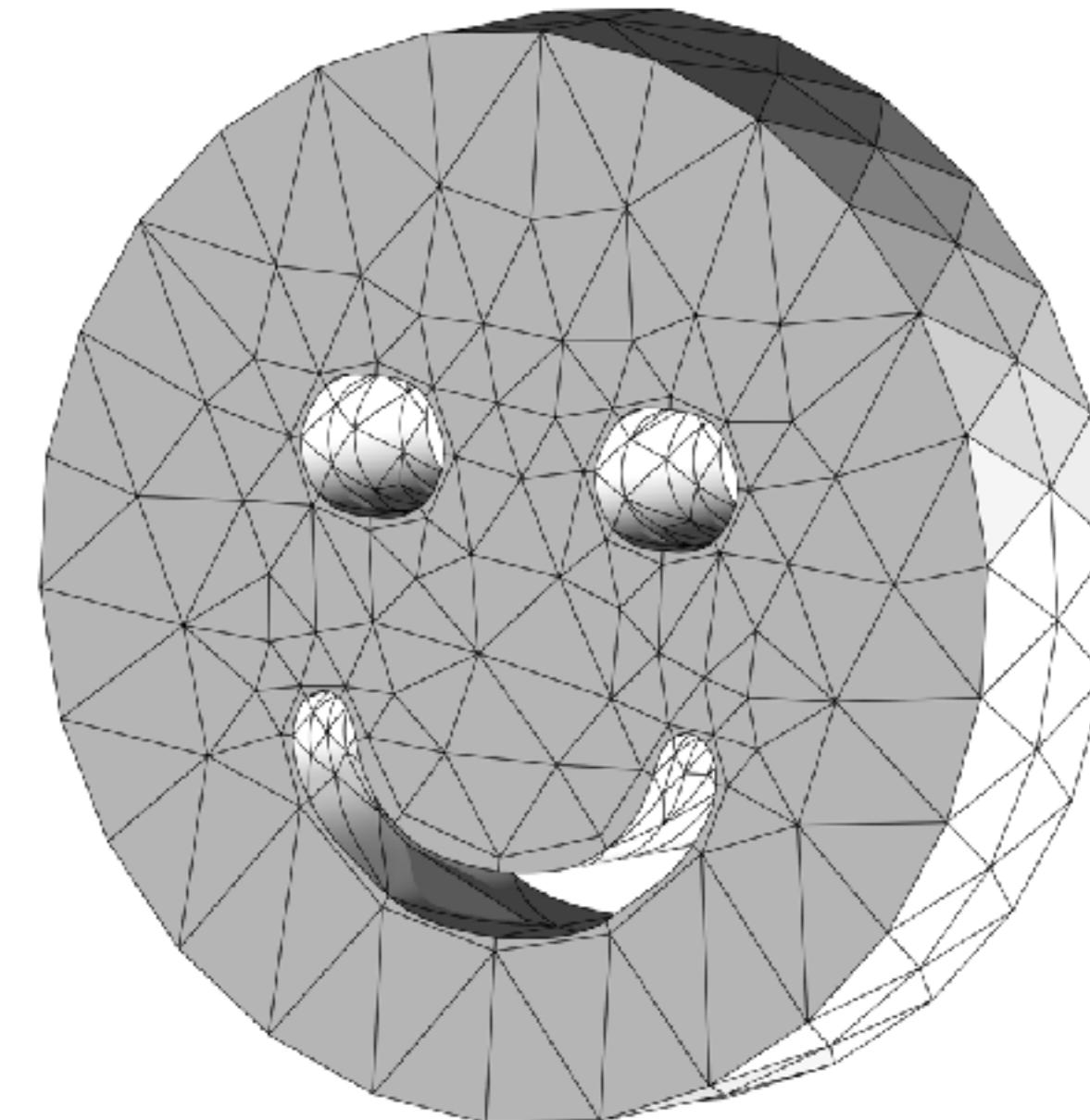
<https://www.nektar.info/community/workshops/nektar-workshop-2022/>

Thanks for listening! Questions?



[www.nektar.info](http://www.nektar.info)

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