

# Course goals

- Learn the fundamentals of deal.II
  - Commonly used data structures, their interface
  - Structure of finite element problems
  - Good implementation practices
  - Navigate the documentation

# Course schedule

Time	Duration	Content	Speaker	Content	Speaker
<b>MONDAY 25.02.2019</b>				<b>TUESDAY 26.02.2019</b>	
09:30	1.25 hours	Introduction First steps	DD	Local refinement Hanging nodes - Part 1	DD
COFFEE / TEA					
11:15	1.25 hours	Introduction to FEM	LH	Exercises, Q&A	DD, LH
LUNCH					
14:00	1.25 hours	Solving Poisson's equation	DD	Local refinement Hanging nodes - Part 2	LH
COFFEE / TEA					
15:45	1.25 hours	Exercises, Q&A	DD, LH	Exercises, Q&A	DD, LH
<b>WEDNESDAY 27.02.2019</b>				<b>THURSDAY 28.02.2019</b>	
09:30	1.25 hours	Shared memory parallelisation	DD	MPI parallelisation: Part 1	DD
COFFEE / TEA					
11:15	1.25 hours	Exercises, Q&A	DD, LH	Exercises, Q&A	DD, LH
LUNCH					
14:00	1 hour	Denis' Talk (SISSA Main A-133)	DD	MPI parallelisation: Part 2	LH
COFFEE / TEA					
15:45	1.25 hours			Exercises, Q&A	DD, LH
<b>FRIDAY 01.03.2019</b>				Project	

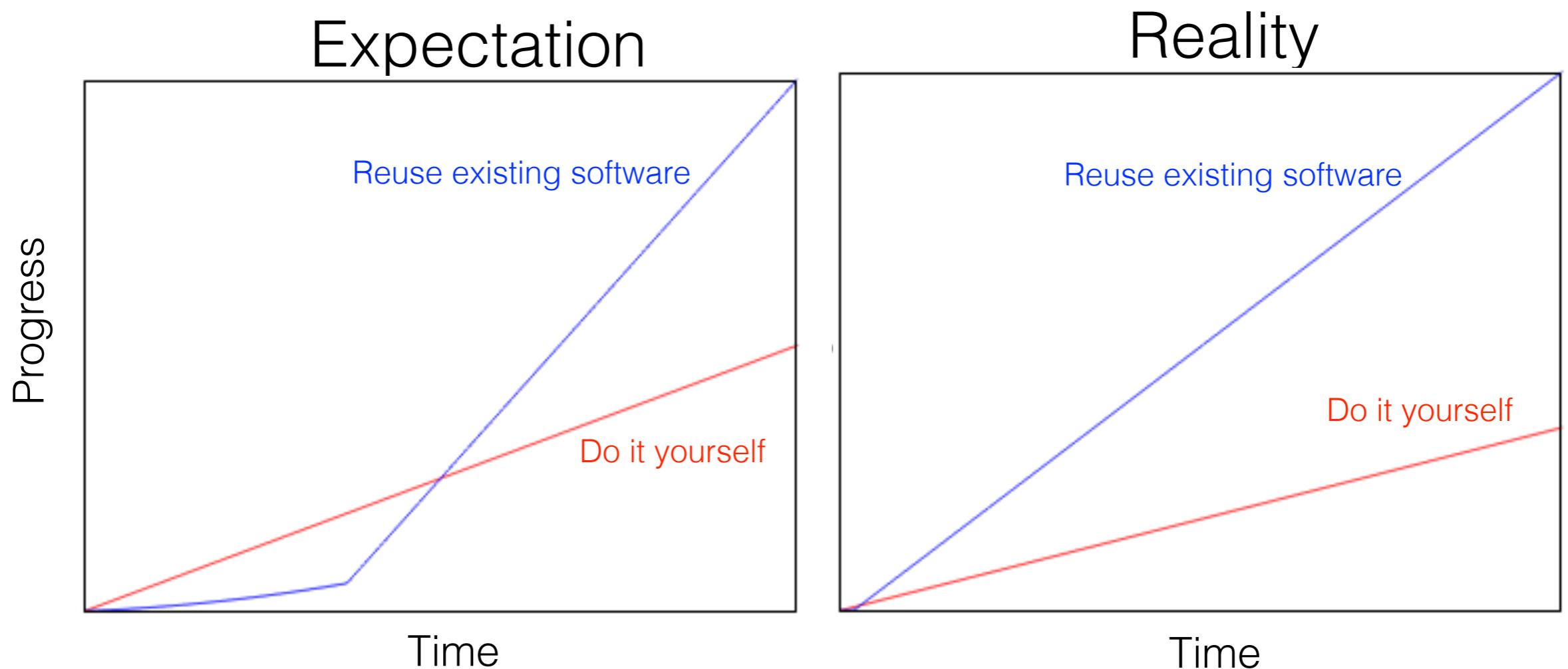
# How the course will be run

- Each module will have a lecture
  - Present salient information
  - Put what we'll learn into context
- Then we'll walk through aspects of the tutorials together
  - Discuss important functionality
    - What it does
    - How it works
    - Caveats and tips
- Remainder of the lecture will be spent doing some exercises
  - Suggestion: Work in groups of two/three
  - Continued at in the last session of the day

# Resources

- deal.II user manual
  - <https://www.dealii.org/developer/doxygen/deal.II/index.html>
  - <https://www.dealii.org/developer/doxygen/deal.II/modules.html>
  - <https://www.dealii.org/developer/doxygen/deal.II/DEALGlossary.html>
- deal.II tutorials and code gallery
  - <https://www.dealii.org/developer/doxygen/deal.II/Tutorial.html>
  - <https://www.dealii.org/developer/doxygen/deal.II/CodeGallery.html>
- Us :-)
  - Don't hesitate to ask questions

# Why use deal.II (or any other PDE toolbox)?

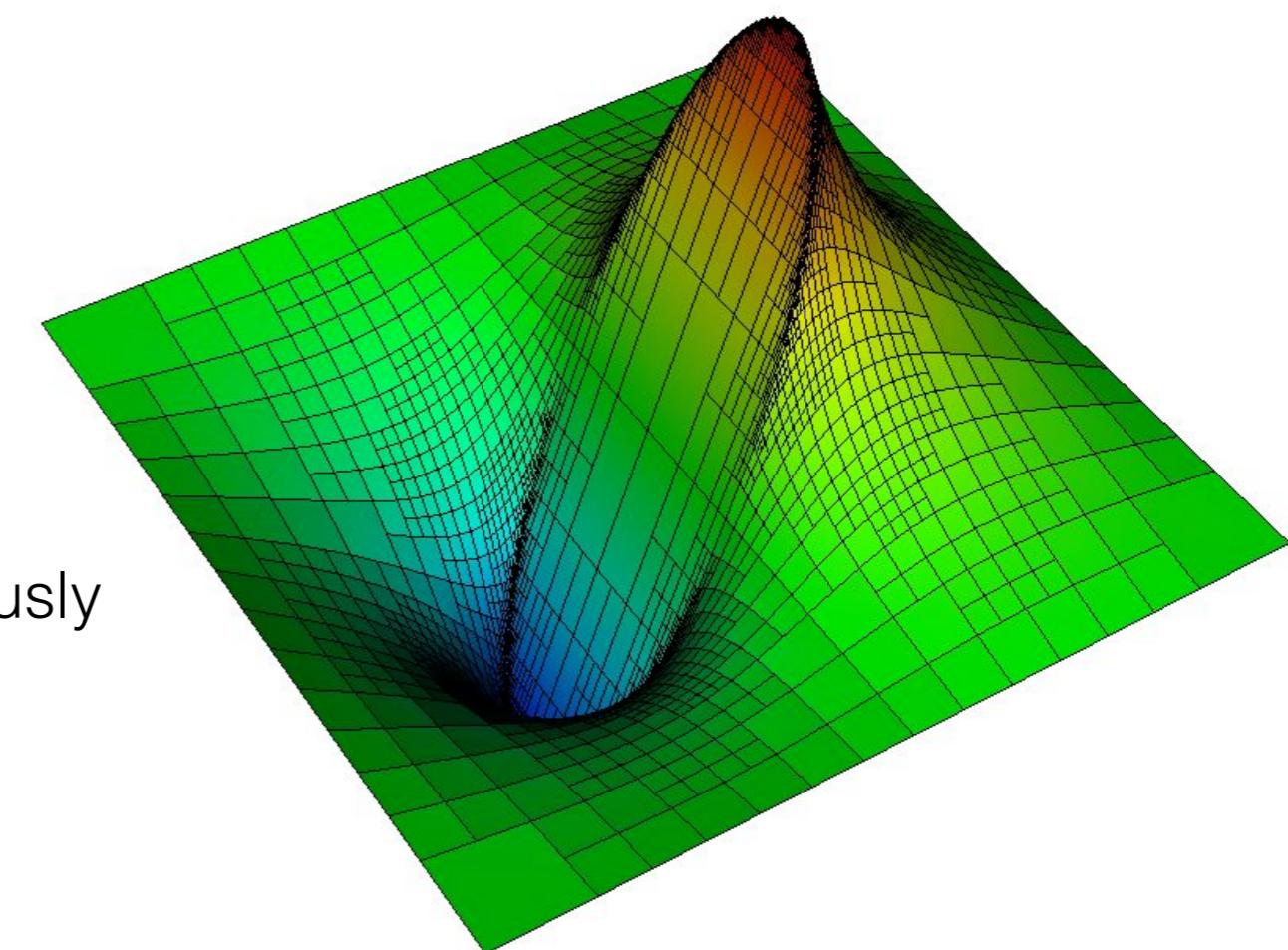


- Applies to:
  - Users
  - Developers
- “The secret to good scientific software is (re)using existing libraries”

# What is deal.II?

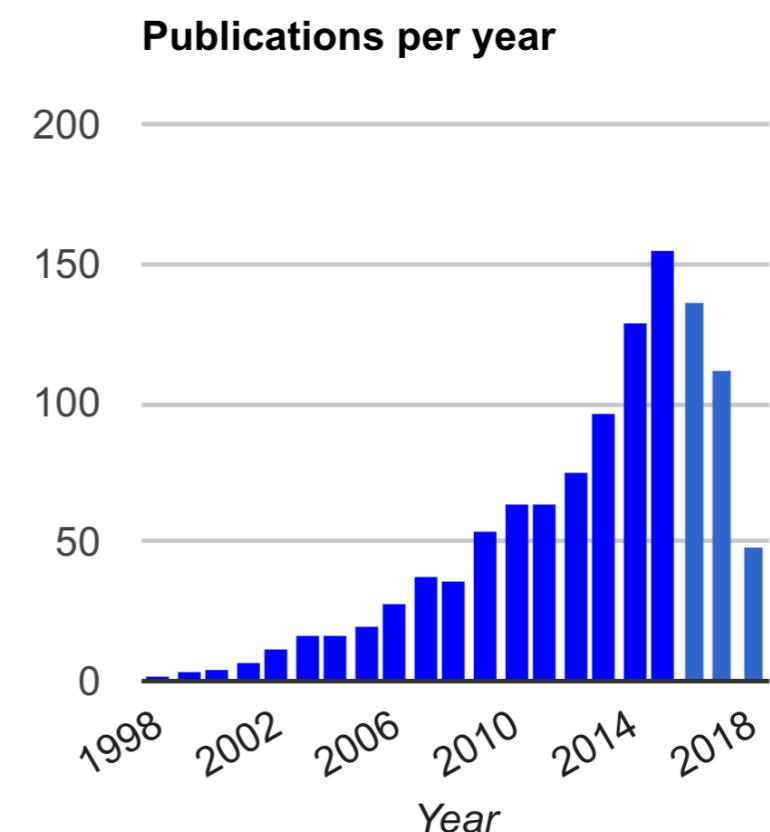
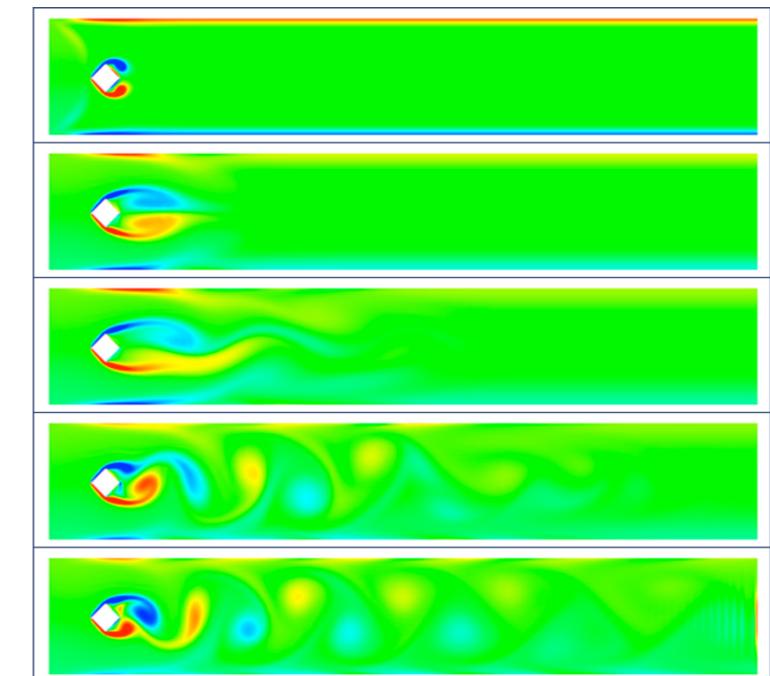
## Differential Equation Analysis Library

- Flexible open-source finite element toolkit
  - All the support functionality required to describe and solve a FE problem (PDEs)
  - Optimized for speed
  - Heavily tested
    - Many error checks (debug mode)
    - +10,000 regression tests run continuously
  - Part of SPEC CPU 2017 benchmark
- Templatized C++ library (Object Orientated)
  - Dimension independent programming
- Portable
  - OS, architecture, compiler



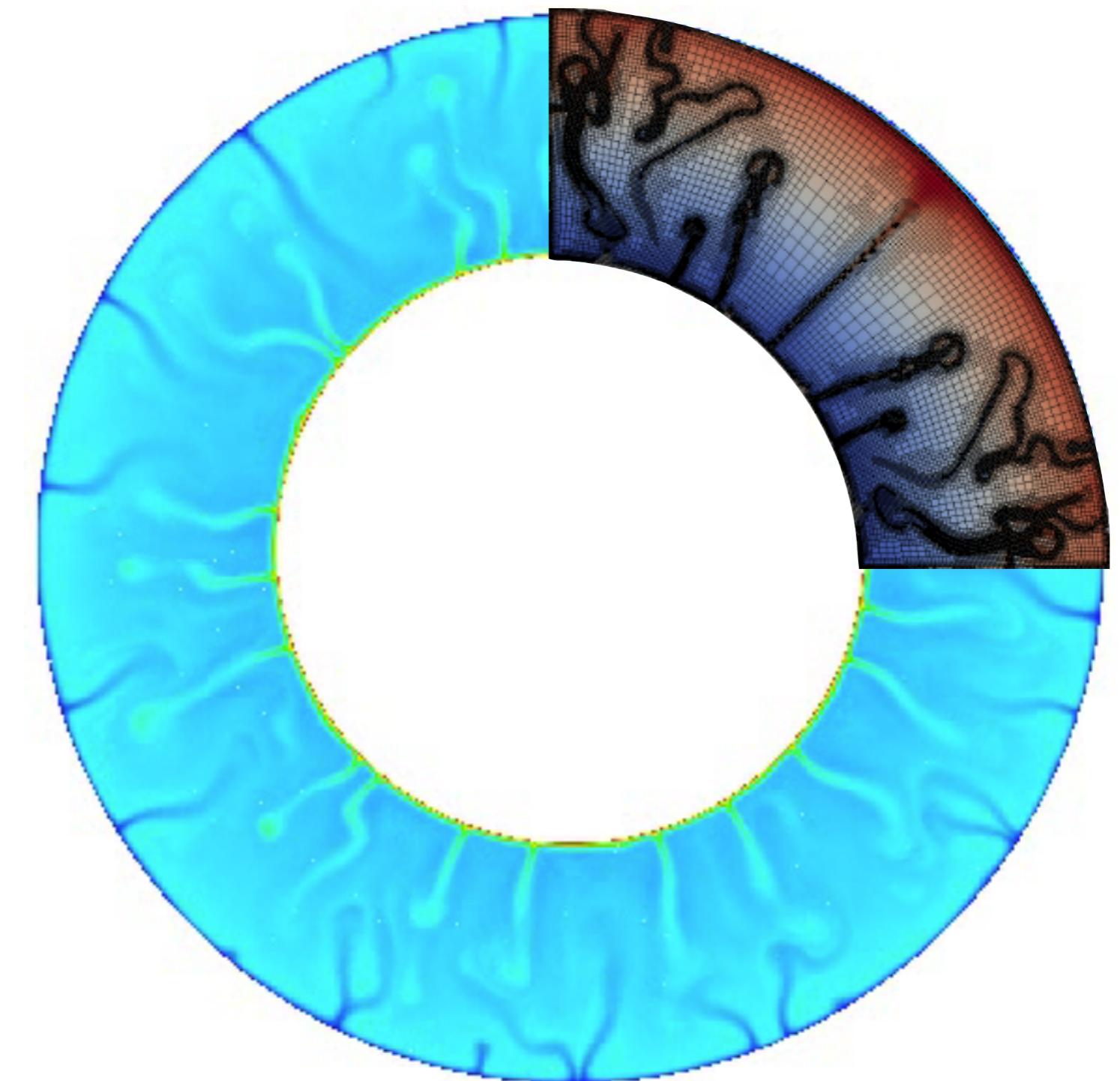
# What is deal.II?

- Heavily documented
  - Over 10000 pages of interface documentation
  - Numerous tutorials
    - Illustrate functionality
    - Present methods to solve problems
- Quite widely used, and growing
- Active community
  - Approachable developers
  - Helpful online forum



# Classes of problems solved using deal.II

- Geomechanics
- Fluid and gas dynamics
- Porous media
- Fluid-structure interaction
- Boundary element method
- Topology optimization
- Medical image reconstruction
- Structural mechanics
- Biomechanics
- Crystal growth
- Gradient and crystal plasticity
- Generalized continua
- Contact mechanics
- Atomistic-to-Continuum coupling
- Quantum mechanics
- Magneto- and electro-elasticity
- Thermo-plasticity

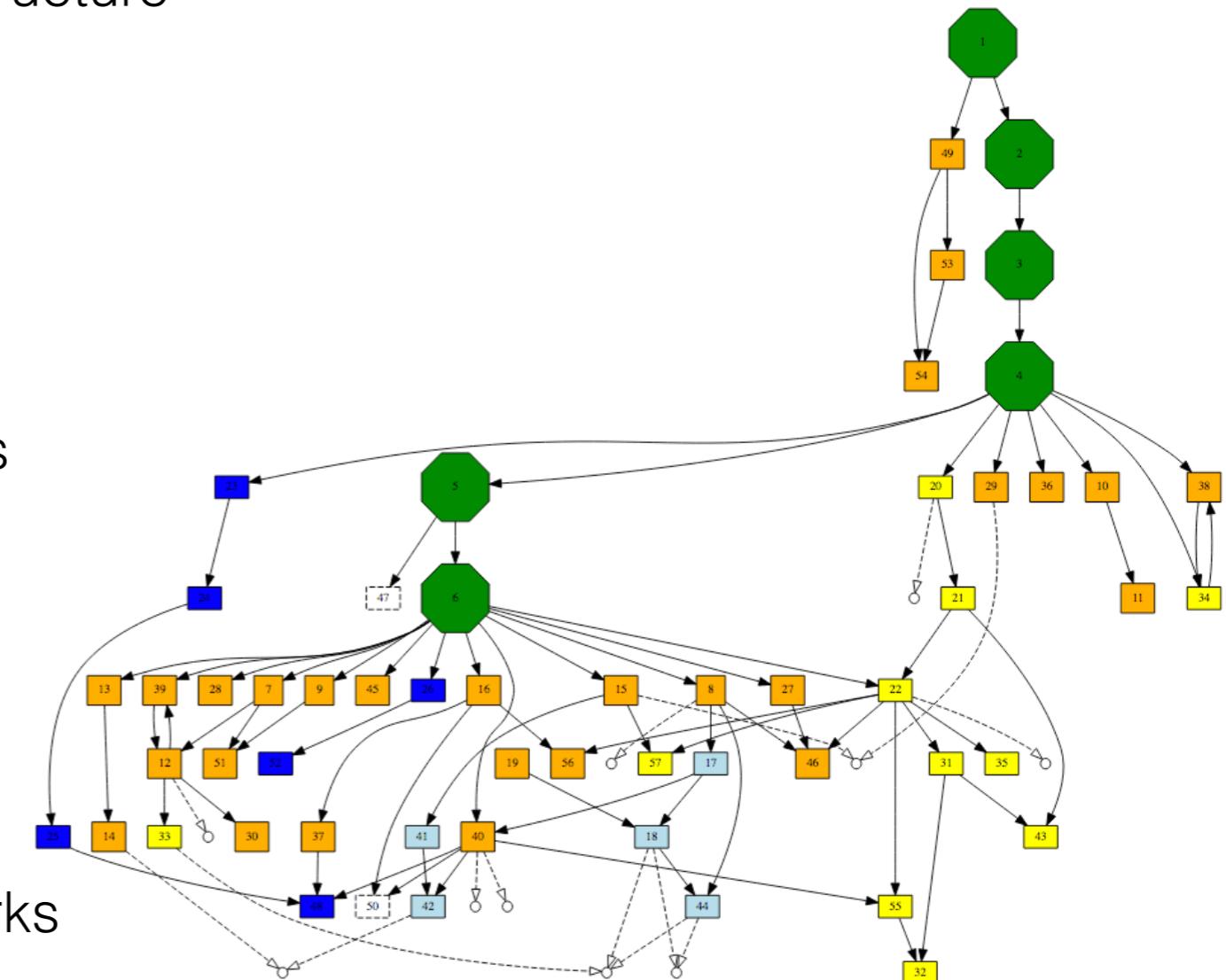


# What deal.II is not

- A black box
  - Can't throw any problem at it
  - Won't do anything more than you ask it to
- Knows little\* about
  - Numerical methods
  - Problem-specific details, i.e.
    - Preconditioners
    - Constitutive equations

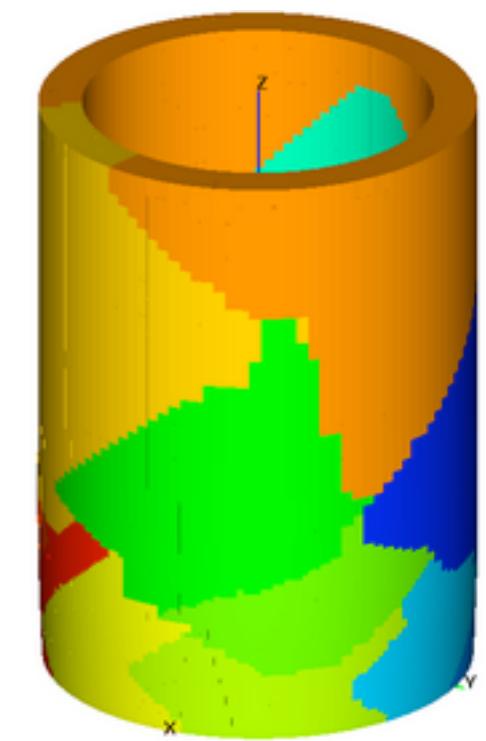
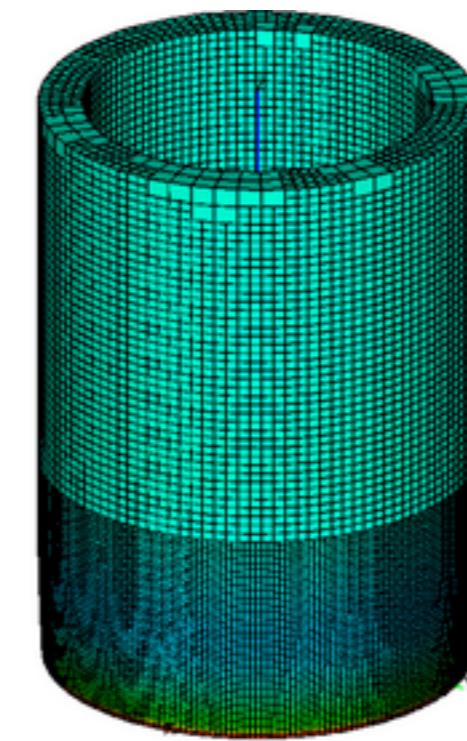
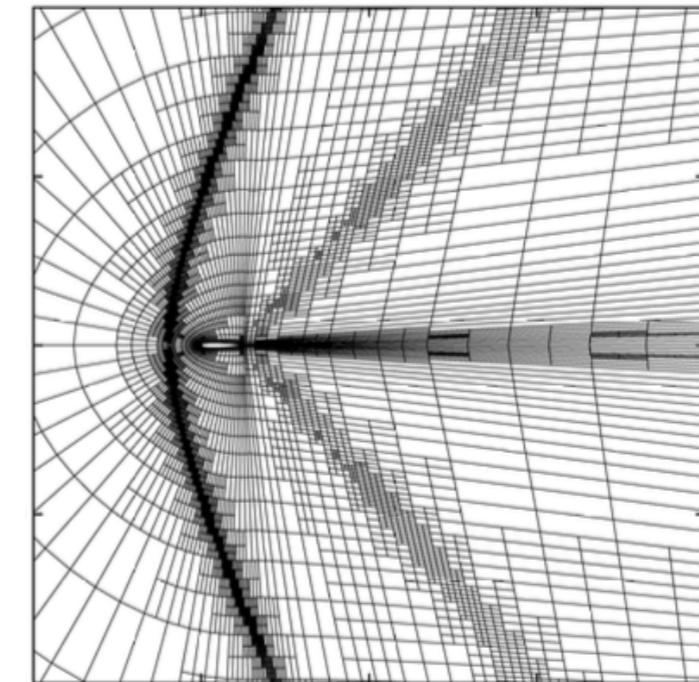
# How deal.II will help you

- Unified and well thought out data structure
  - Problem implementation
- Many tutorials
  - Baseline from which to build on
  - Demonstrate how to use features
- Comprehensive debugging support
  - Error messages everywhere!
- Some built in numerical tools
- Integration with advanced frameworks
  - Nonlinear solvers
  - Time integrators
  - Parallel sparse and dense linear algebra



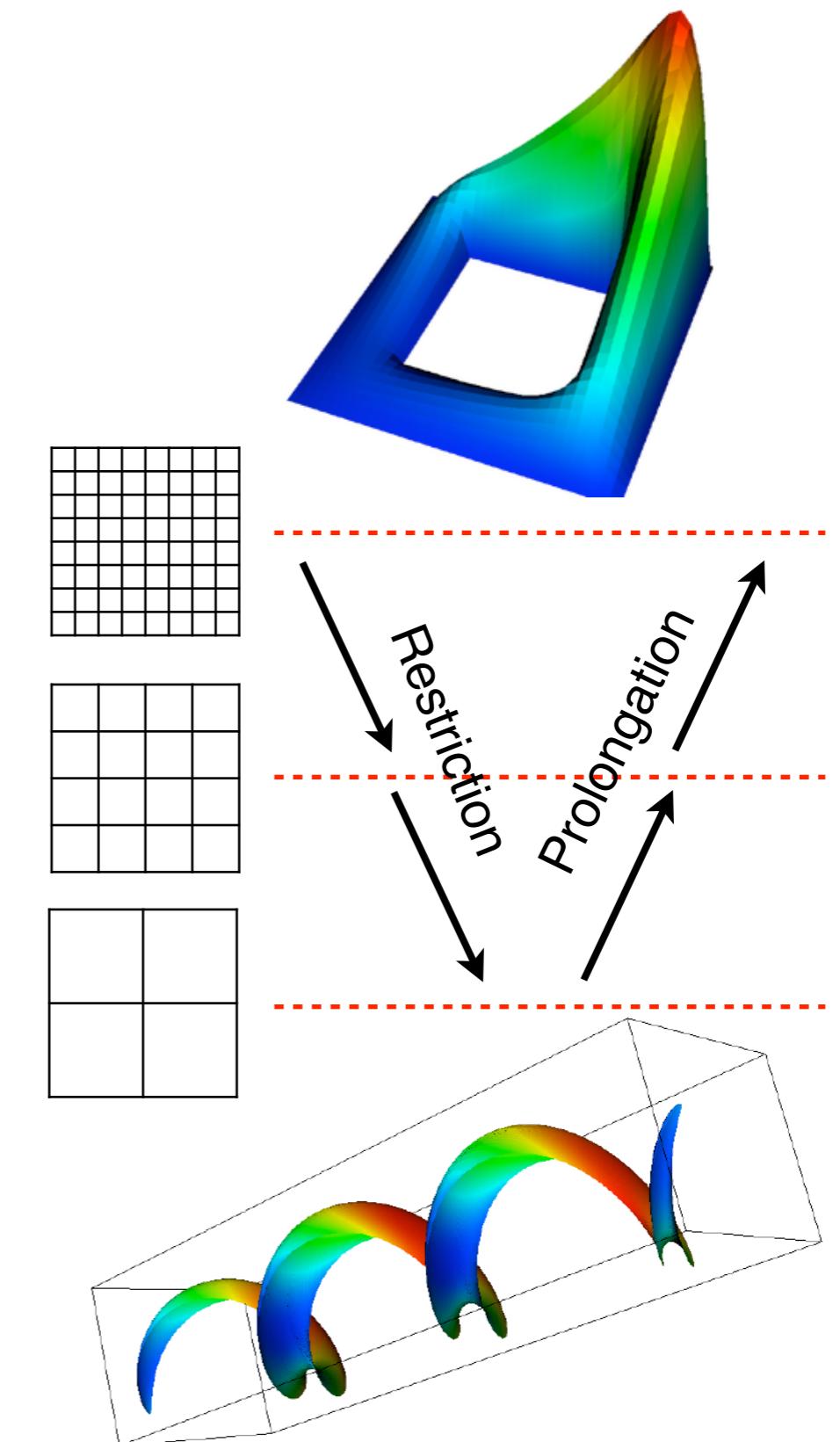
# Fundamental capabilities and frameworks

- Mesh adaptivity
- Dense and sparse linear algebra
  - Built in tensor, dense matrix/vector classes
  - BLAS and LAPACK integration; GSL
  - Built in linear solvers and preconditioners
  - Eigenvalue solvers
- Parallelization
  - MPI
    - Linear algebra libraries (PETSc, Trilinos)
    - Distributed meshes → Billion DoFs
  - Threading (Intel TBB)
  - Vectorized numbers (AVX extensions)
- Pre/post-processing



# Advanced capabilities and frameworks

- hp-finite element support
- Meshworker
  - Assembly assistance
  - Functions to perform assembly for specific problem classes
- Geometric multi-grid
  - Using coarse grid as preconditioner to solution for finer grid
- Matrix-free
  - No explicit storing of matrix elements
  - Exchange memory transfer for computations
- Charts and manifolds
  - Accurate description of topologically complex objects



# How deal.II is developed

- Open repository on GitHub
  - <https://github.com/dealii/dealii>
- Anyone can contribute!
  - We encourage all to participate

The screenshot shows the GitHub pull requests page for the deal.II repository. The repository name 'dealii / dealii' is at the top, along with statistics: 74 unwatched, 423 forks, and 338 stars. Below this are tabs for Code, Issues (310), Pull requests (26, highlighted in orange), Projects (11), Wiki, and Insights. A search bar filters for 'is:pr is:open'. There are buttons for Filters, Labels, Milestones, and New pull request. The main area lists 26 open pull requests, each with a title, number (#), author, and status. Some pull requests have green 'Reviewed and ready to merge' or 'ready to test' buttons. The last few pull requests show review counts (e.g., 7, 6, 8, 7, 5).

Author	Title	Status	Review Count
masterleinad	#7748 Restrict grid_tools_cache_04	Review required	0
masterleinad	#7747 Check SUNDIALS version when configuring	Reviewed and ready to merge	2
bangerth	#7746 More edits in the introduction of step-61.	Tutorials	0
davydden	#7744 add type traits to be used internally with FEEvaluation	Matrix-free	7
GivAlz	#7743 Using rtrees in GridTools::compute_point_locations_try_all for cell search	0	0
masterleinad	#7742 Avoid ambiguous function declaration/variable initialization	ready to test	6
tclevenger	#7738 Step-63	Review required	8
marcfehling	#7717 Added 'set_fe' functionality to DoFHandlers.	Changes requested	7
marcfehling	#7716 hp::DoFHandler: Moved containers with temporary content into a dedicated structure	Changes requested	5

# Aims for this module

- Gain familiarity with two core classes
  - Triangulation
  - DoFHandler
- Create and interrogate meshes
- Create and interrogate sparsity patterns

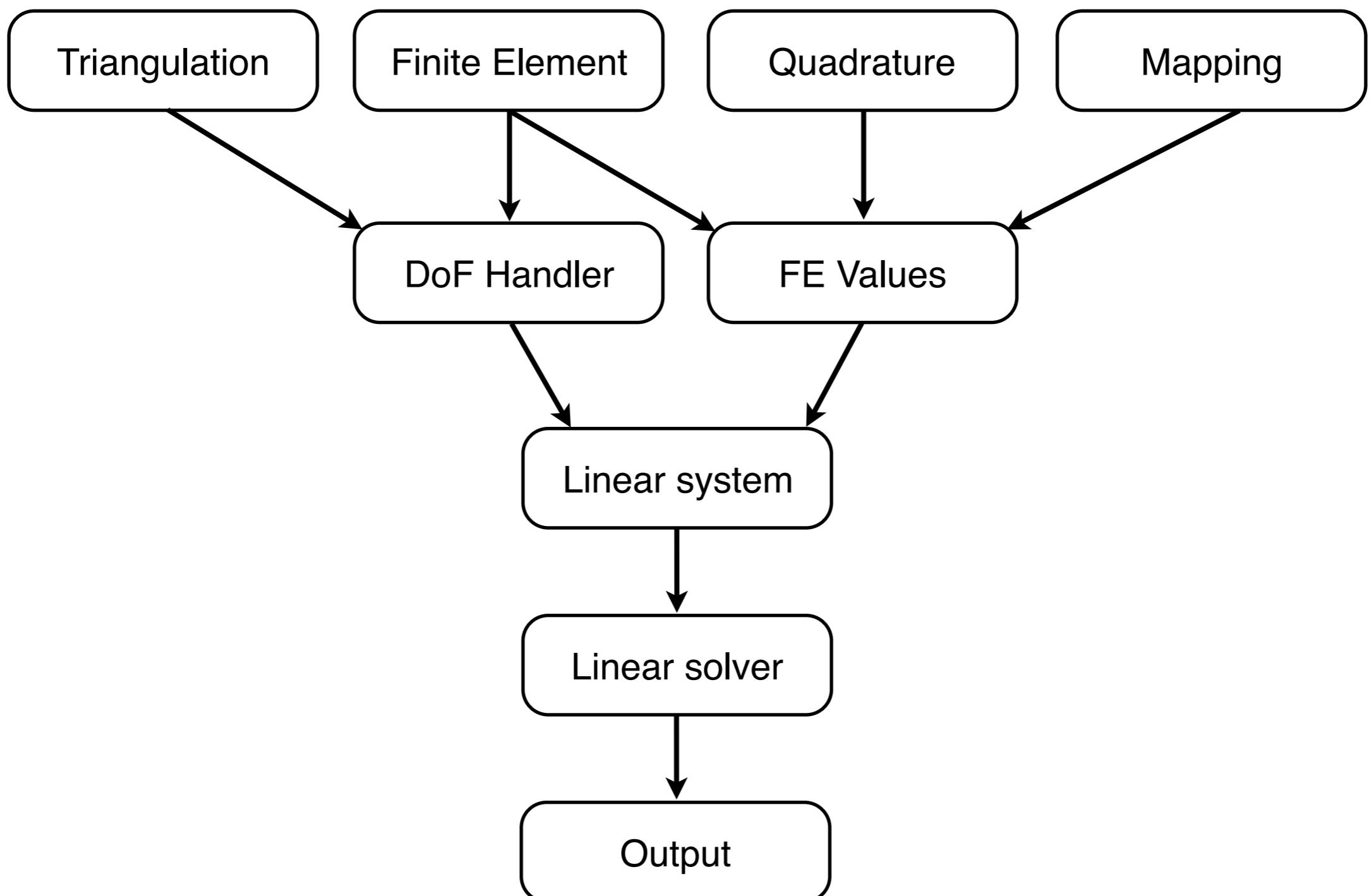
# Reference material

- Main page  
<https://dealii.org/9.0.0/doxygen/deal.II/index.html>
- Tutorials
  - Step-1  
[https://dealii.org/9.0.0/doxygen/deal.II/step\\_1.html](https://dealii.org/9.0.0/doxygen/deal.II/step_1.html)
  - Step-49  
[https://dealii.org/9.0.0/doxygen/deal.II/step\\_49.html](https://dealii.org/9.0.0/doxygen/deal.II/step_49.html)
  - Step-2  
[https://dealii.org/9.0.0/doxygen/deal.II/step\\_2.html](https://dealii.org/9.0.0/doxygen/deal.II/step_2.html)

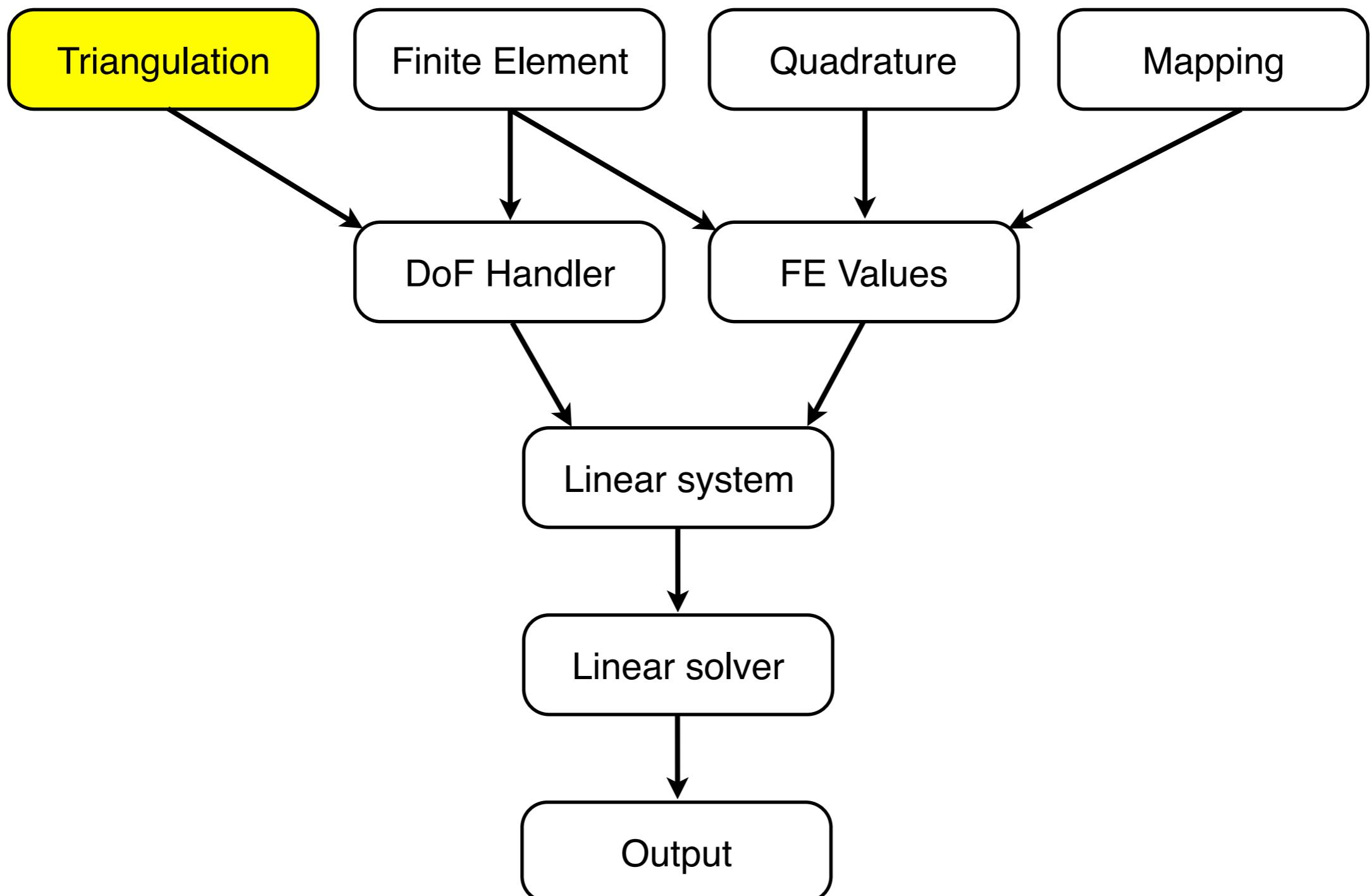
# First and biggest tip

- Program defensively
  - Program and test in debug mode
    - Additional compiler warnings
    - Add assertions
  - Perform studies in release mode

# Structure of a prototypical FE problem

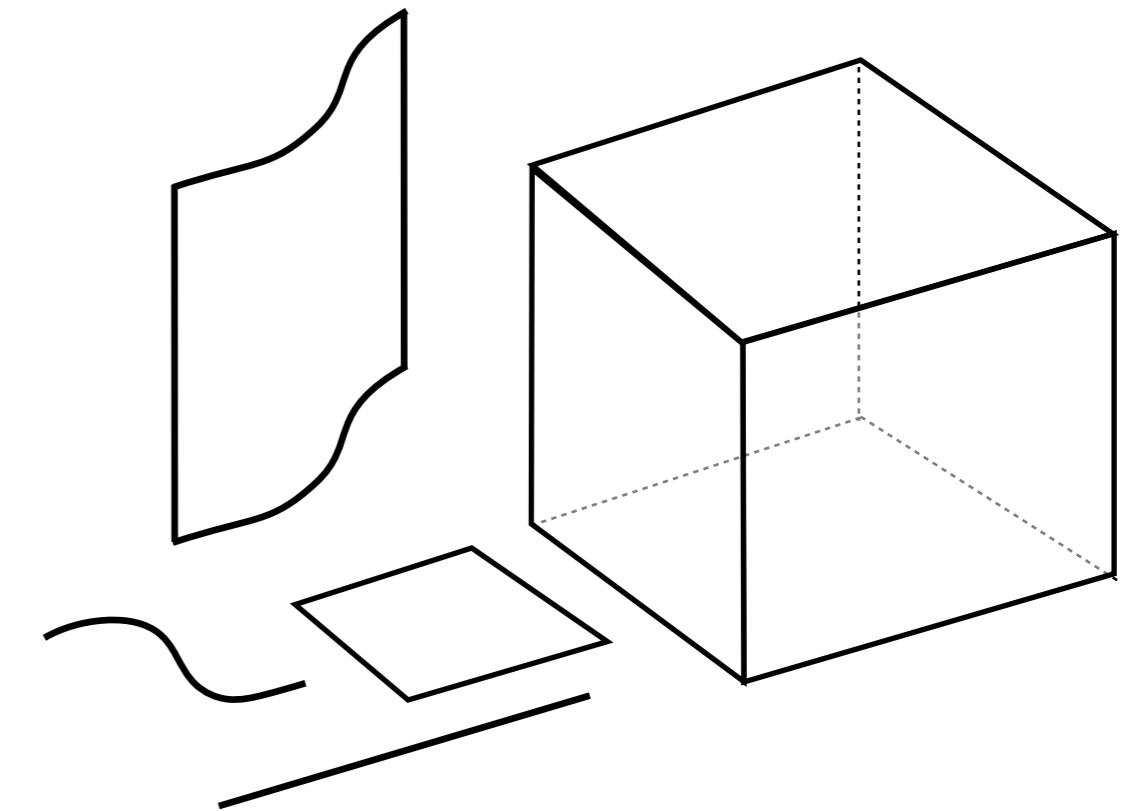


# Structure of a prototypical FE problem



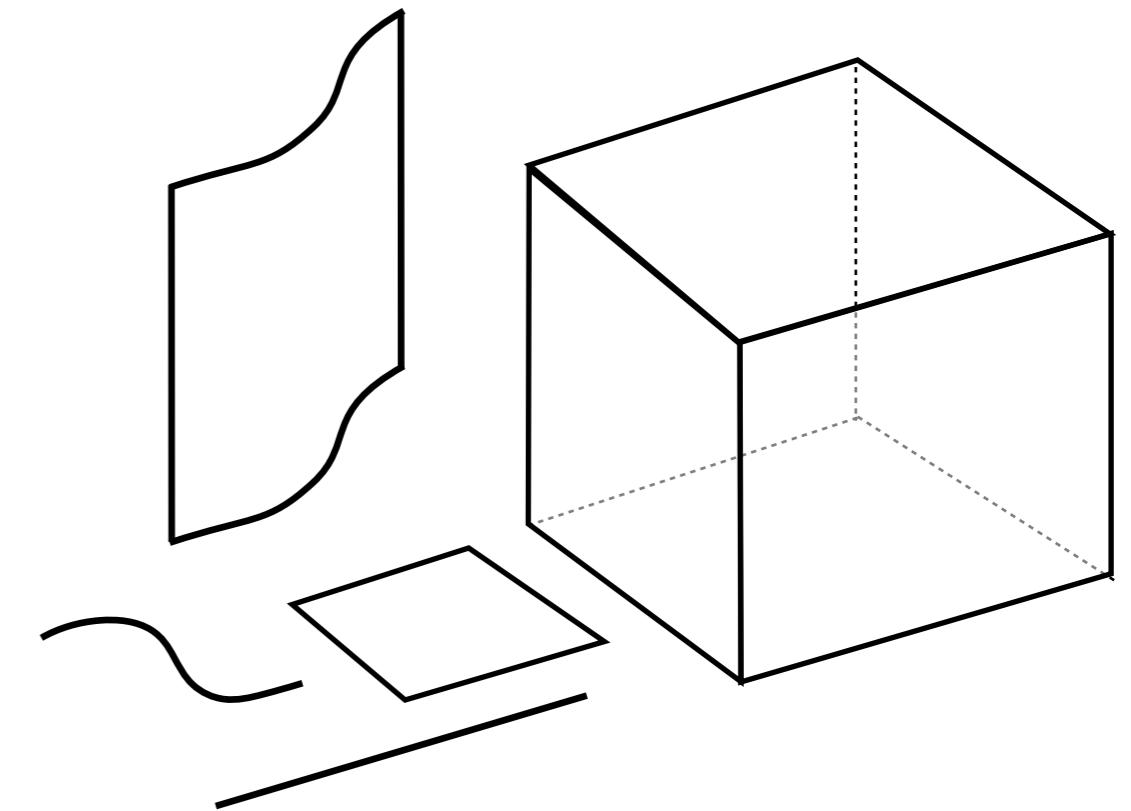
# Interaction with geometry: the Triangulation class

- Describes problem geometry
  - Support for lines, quad, hex elements
  - Conceptually even higher order!
  - Structured/unstructured meshes
  - Co-dimension 1 or 2 case
- Grid creation
  - Built-in basic grid generation and manipulation tools ([GridTools](#))
  - Can read in grids



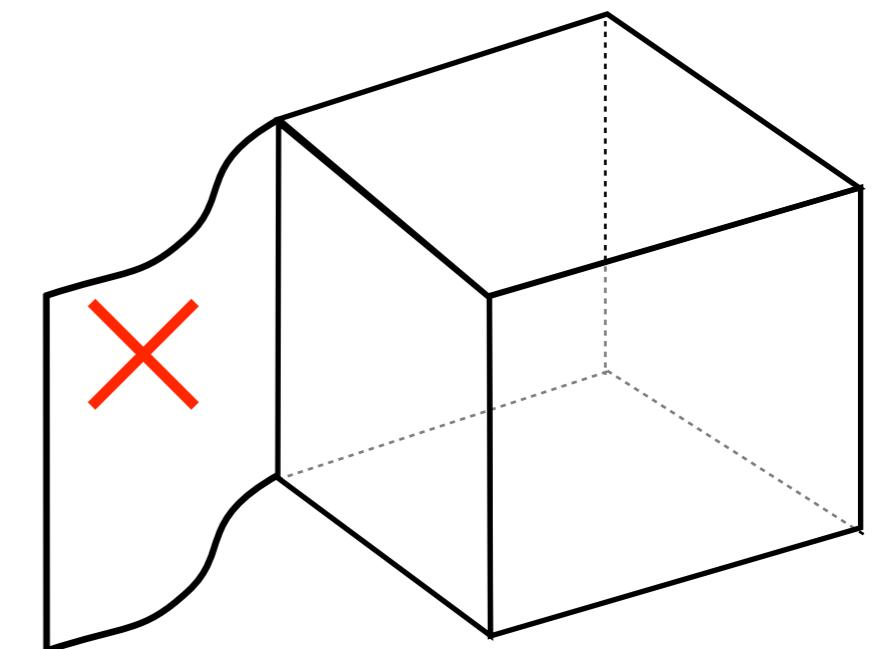
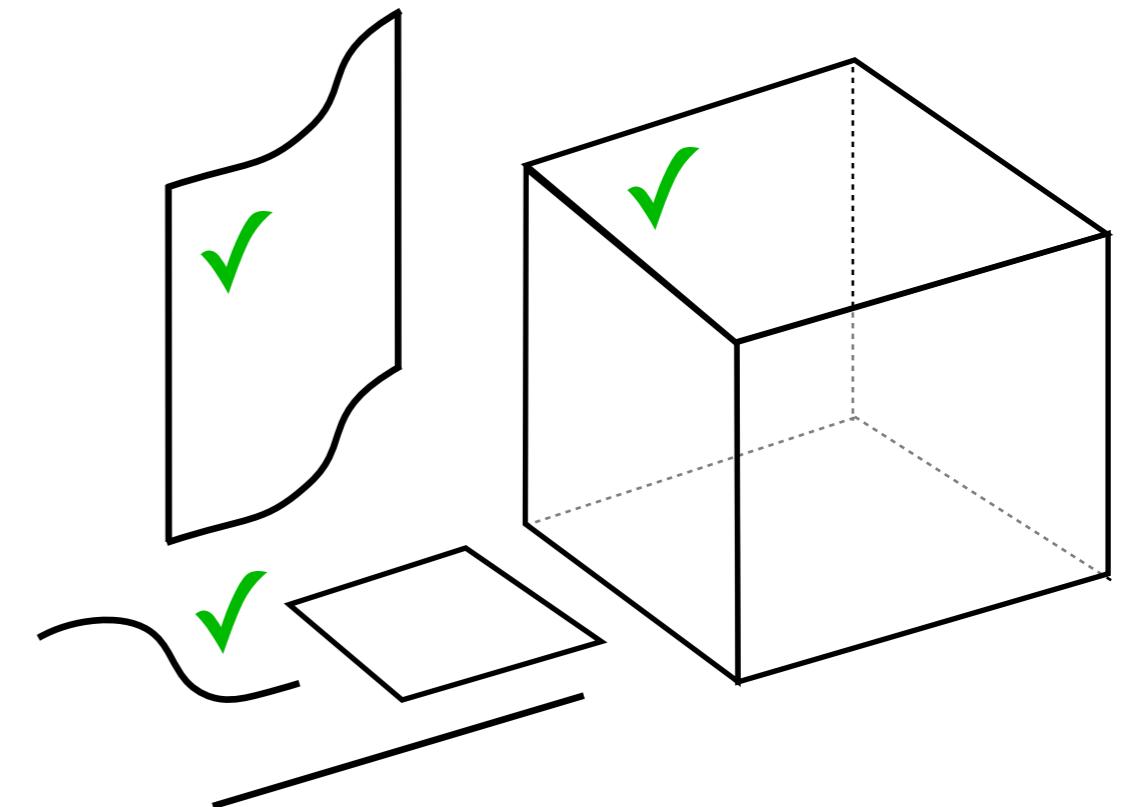
# Interaction with geometry: the Triangulation class

- Assign helper ID's
  - Materials
  - Boundaries
  - Manifolds
- Allows storage of custom data-structure attached to each cell/face
- Cells know about neighbor cells
  - Useful for DG methods



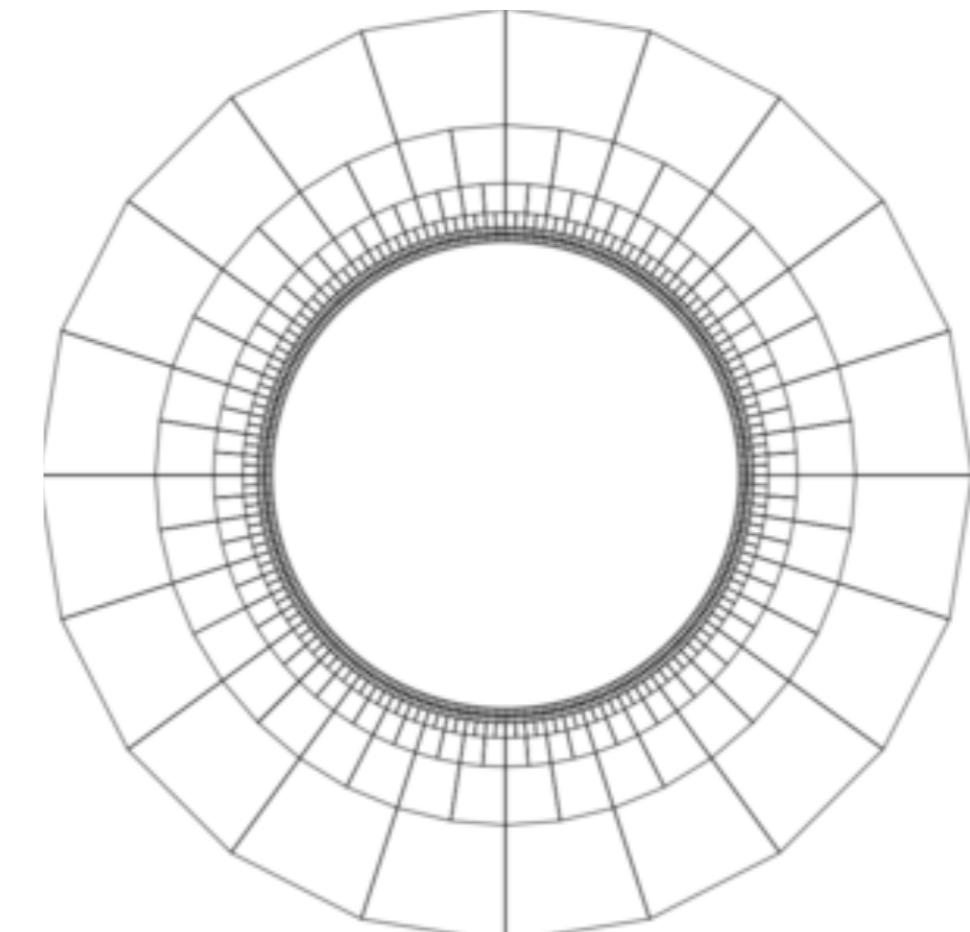
# Interaction with geometry: the Triangulation class

- Can enforce topologies
  - Manifolds on boundary
  - Internal manifolds
- Disadvantage
  - Cannot mix triangulation types
  - e.g. Volumetric body with extended manifold surface

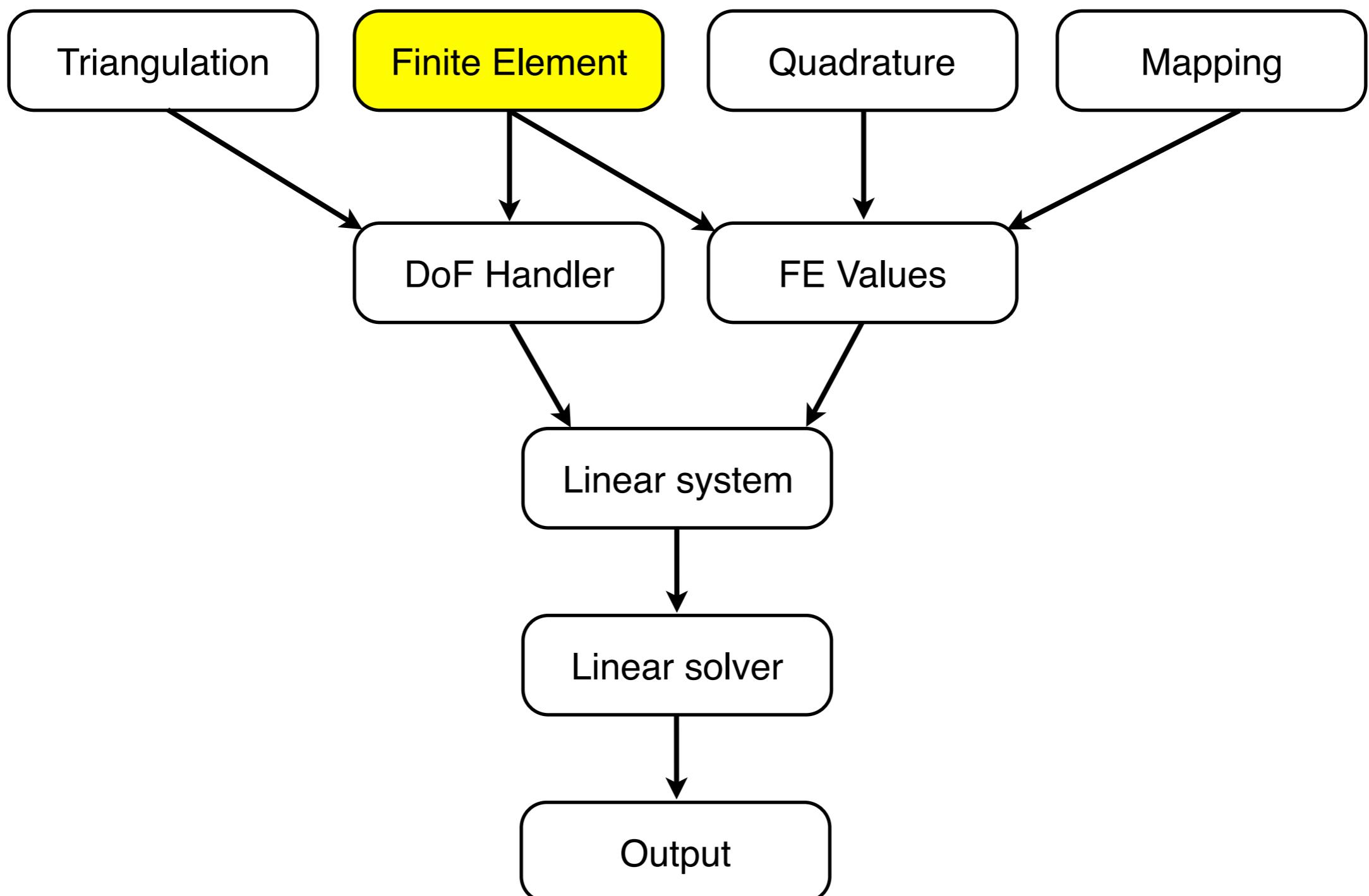


# Interaction with geometry: the Triangulation class

- Demonstration: [Step-1](#), [step-49](#),  
<http://www.math.colostate.edu/~bangerth/videos.676.5.html>  
<http://www.math.colostate.edu/~bangerth/videos.676.6.html>
- Key points
  - deal.II headers
  - Creating a triangulation
  - Boundary topology
  - Traversing a triangulation
  - Querying geometric information
  - Manipulating a triangulation
  - Aspects of grid refinement
  - Visualising a triangulation

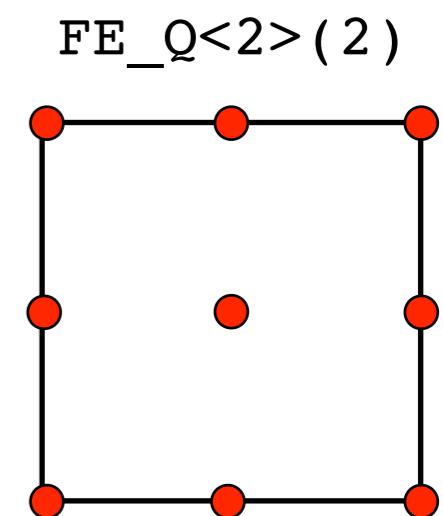
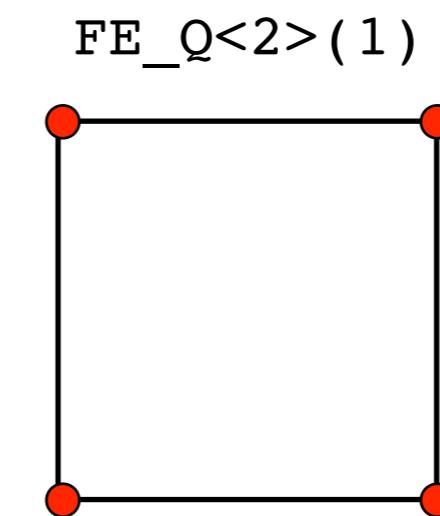


# Structure of a prototypical FE problem

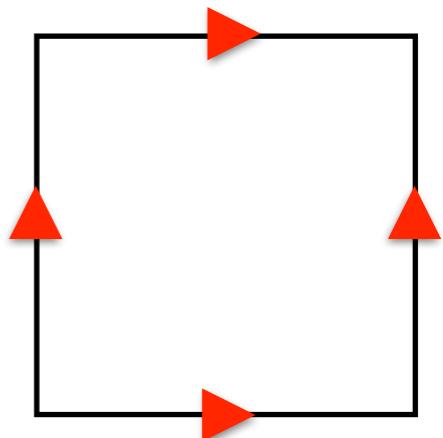
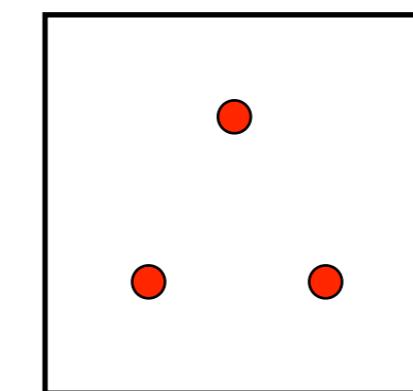


# Assigning degrees-of-freedom: the FiniteElement classes

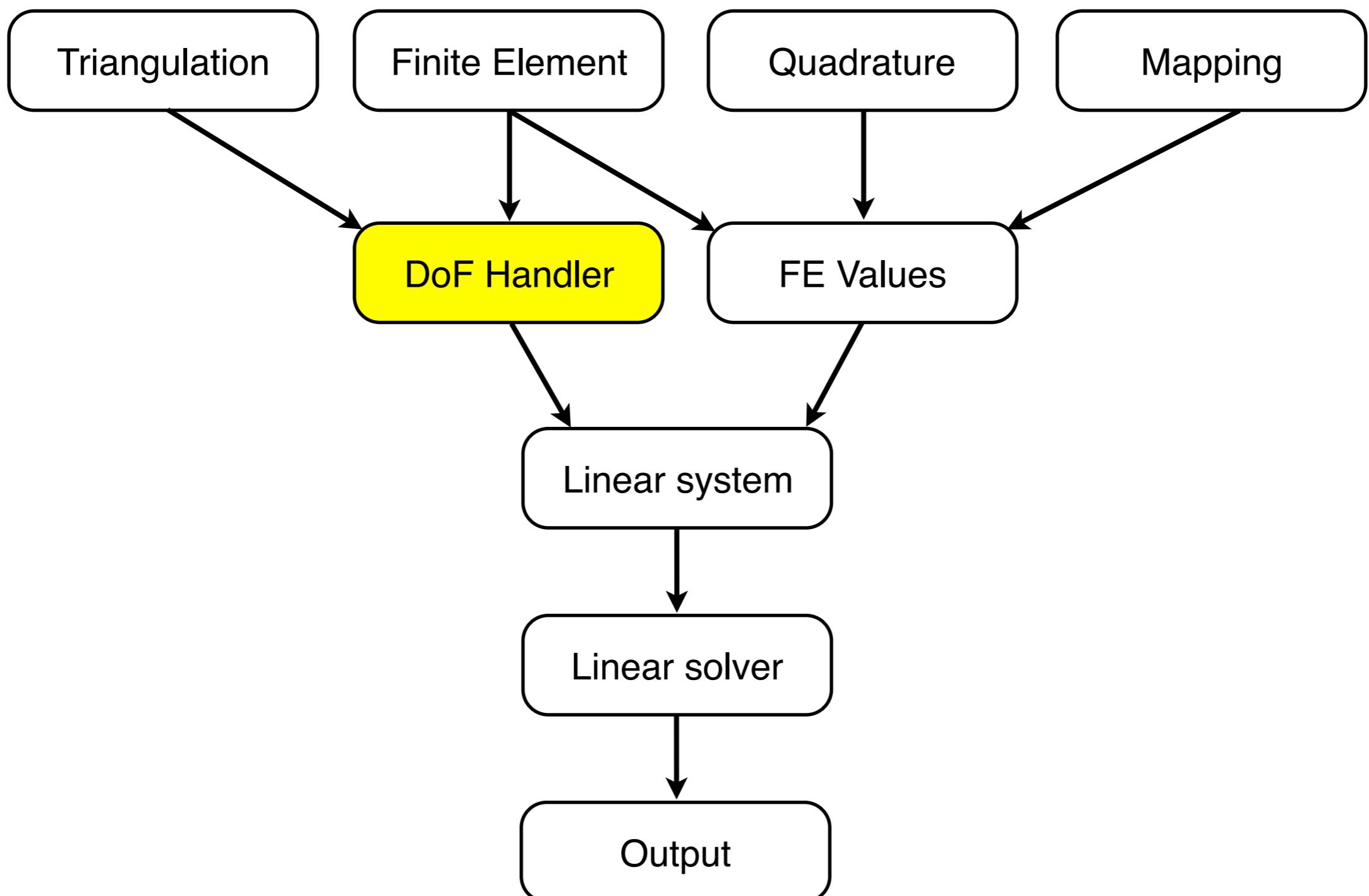
- Built in Finite Elements
  - Continuous
    - Piecewise Lagrange polynomials
  - Discontinuous
    - Monomials
    - Legendre polynomials
  - Vector-valued
    - Nedelec ( $H_{curl}$ )
    - Raviart-Thomas ( $H^{div}$ )
- Can develop finite elements from scratch
  - Specialization for FE's derived by polynomial expansions
  - Enhanced/bubble elements



`FE_DGPMonomial<2>(1)    FE_Nedelec<2>(0)`

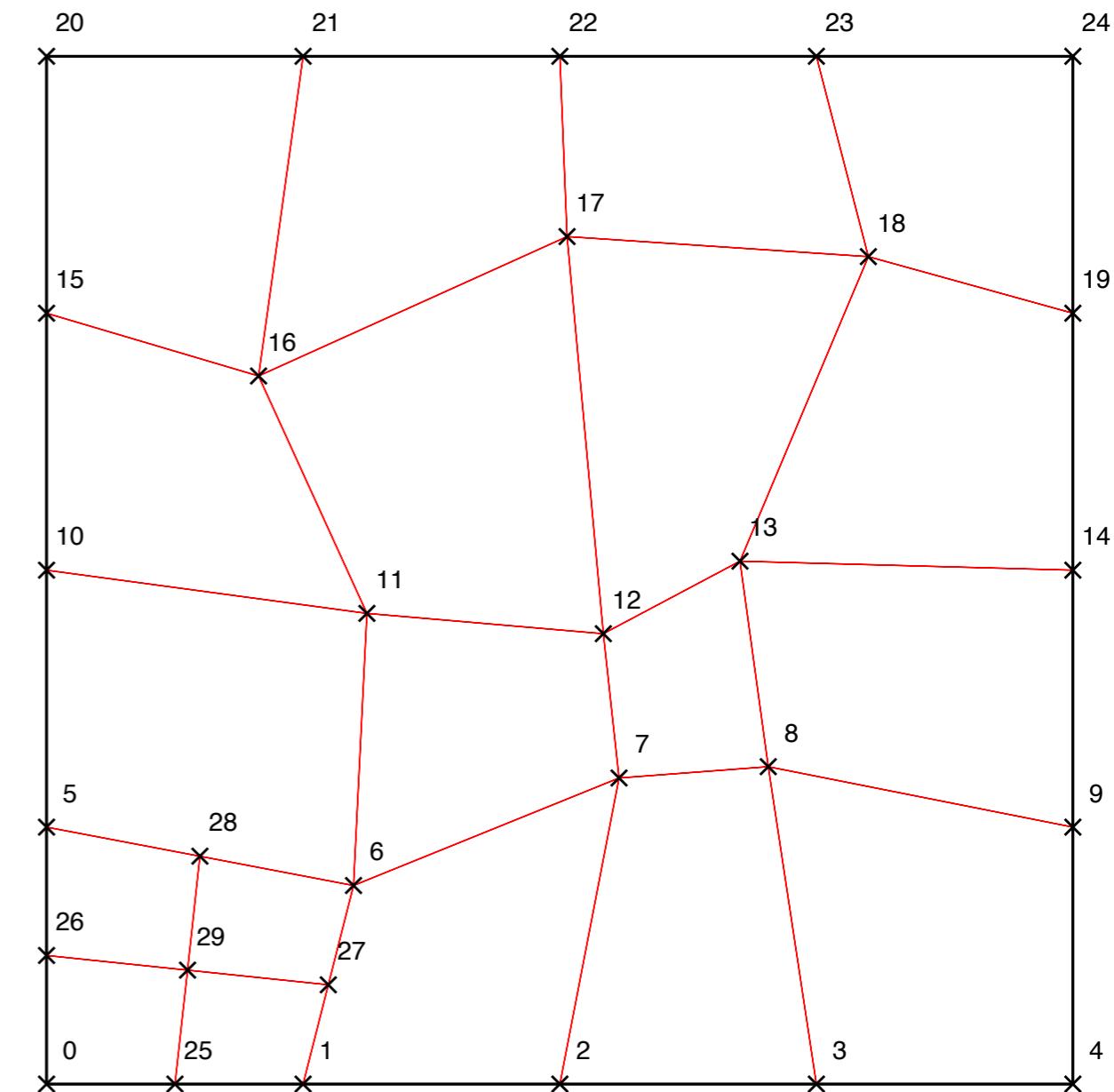


# Structure of a prototypical FE problem



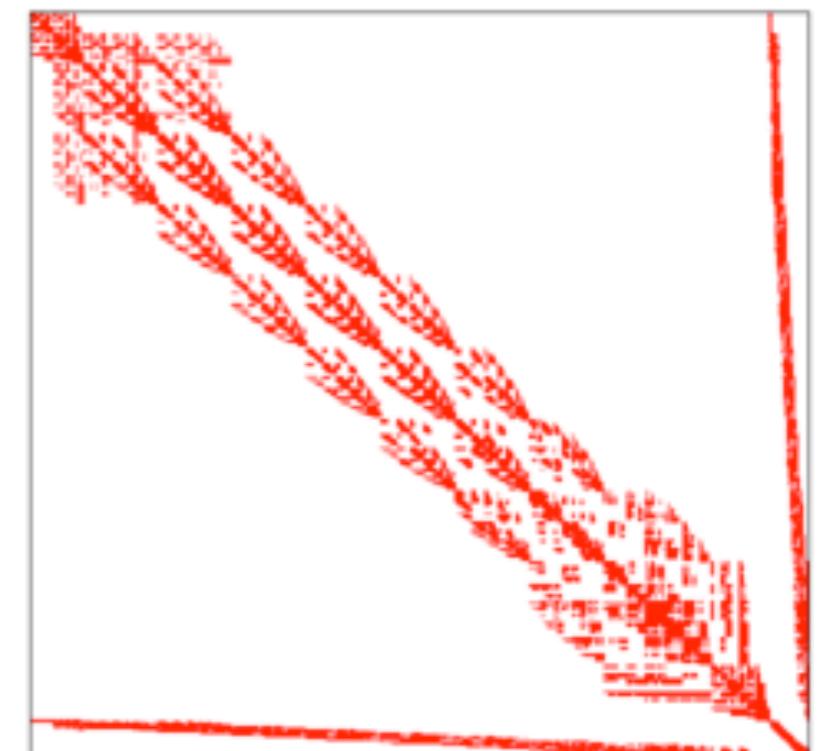
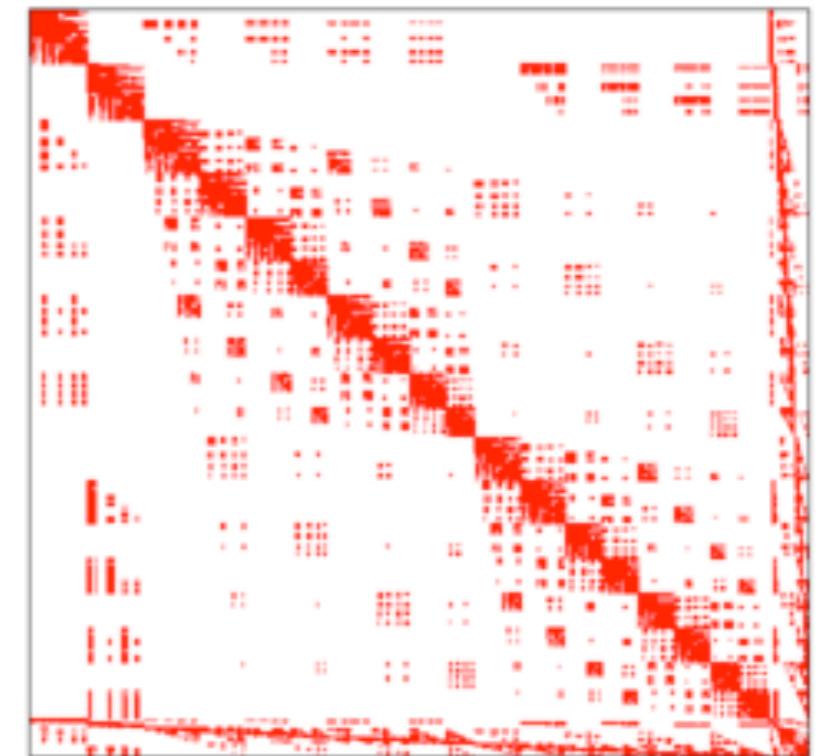
# Assigning degrees-of-freedom: the DoFHandler class

- DoFHandler assigns DoF's to grid
  - Important: separate to Triangulation!
- Unified way to access DoF's, regardless of FE used
  - e.g. Discontinuous elements: support points not necessarily at vertices
- Fast access and grid traversal
  - STL-type cell iterators
  - Access to faces and edges from cells
- Disadvantage
  - Not straight-forward (but possible) to ask location of nodes



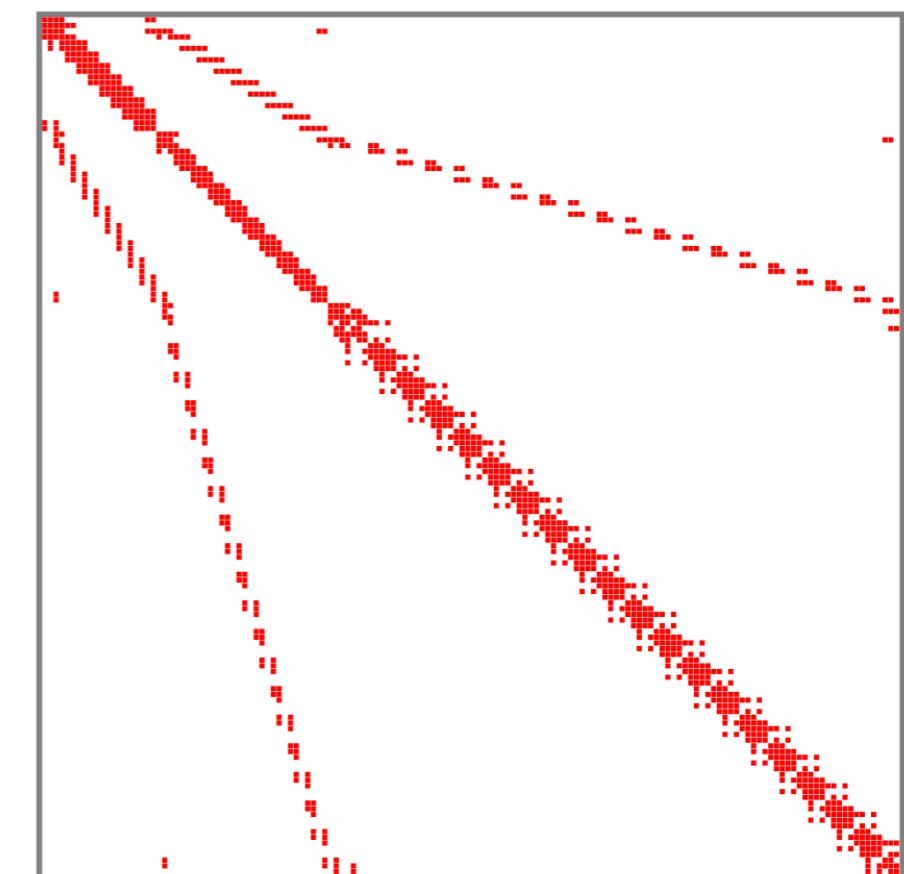
# Assigning degrees-of-freedom: the DoFRenumbering namespace

- Renumbering schemes
  - Cuthill McKee
  - King
  - Downwind
- Reduce bandwidth
- Collect like-components
- Induce block-structure
- Directional (fluid flow)
- MPI subdomain



# Assigning degrees-of-freedom: the FiniteElement and DoFHandler classes

- Demonstration: Step-2  
[https://www.dealii.org/9.0.0/doxygen/deal.II/step\\_2.html](https://www.dealii.org/9.0.0/doxygen/deal.II/step_2.html)  
<http://www.math.colostate.edu/~bangerth/videos.676.9.html>
- Key points
  - Choosing a Finite Element
  - Distributing degrees-of-freedom on a mesh
  - Renumbering degrees-of-freedom
  - Visualizing sparsity patterns



# Implementing the finite element method

**Brief re-hash of the FEM, using the Poisson equation:**

We start with the strong form:

$$\begin{aligned}-\Delta u &= f && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega\end{aligned}$$

# Implementing the finite element method

**Brief re-hash of the FEM, using the Poisson equation:**

We start with the strong form:

$$-\Delta u = f$$

...and transform this into the weak form by multiplying *from the left* with a test function:

$$(\nabla \varphi, \nabla u) = (\varphi, f) \quad \forall \varphi$$

The solution of this is a function  $u(x)$  from an infinite-dimensional function space.

# Implementing the finite element method

Since computers can't handle objects with infinitely many coefficients, we seek a finite dimensional function of the form

$$u_h = \sum_{j=1}^N U_j \varphi_j(x)$$

To determine the  $N$  coefficients, test with the  $N$  basis functions:

$$(\nabla \varphi_i, \nabla u_h) = (\varphi_i, f) \quad \forall i = 1 \dots N$$

If basis functions are linearly independent, this yields  $N$  equations for  $N$  coefficients.

This is called the *Galerkin* method.

# Implementing the finite element method

**Practical question 1:** How to define the basis functions?

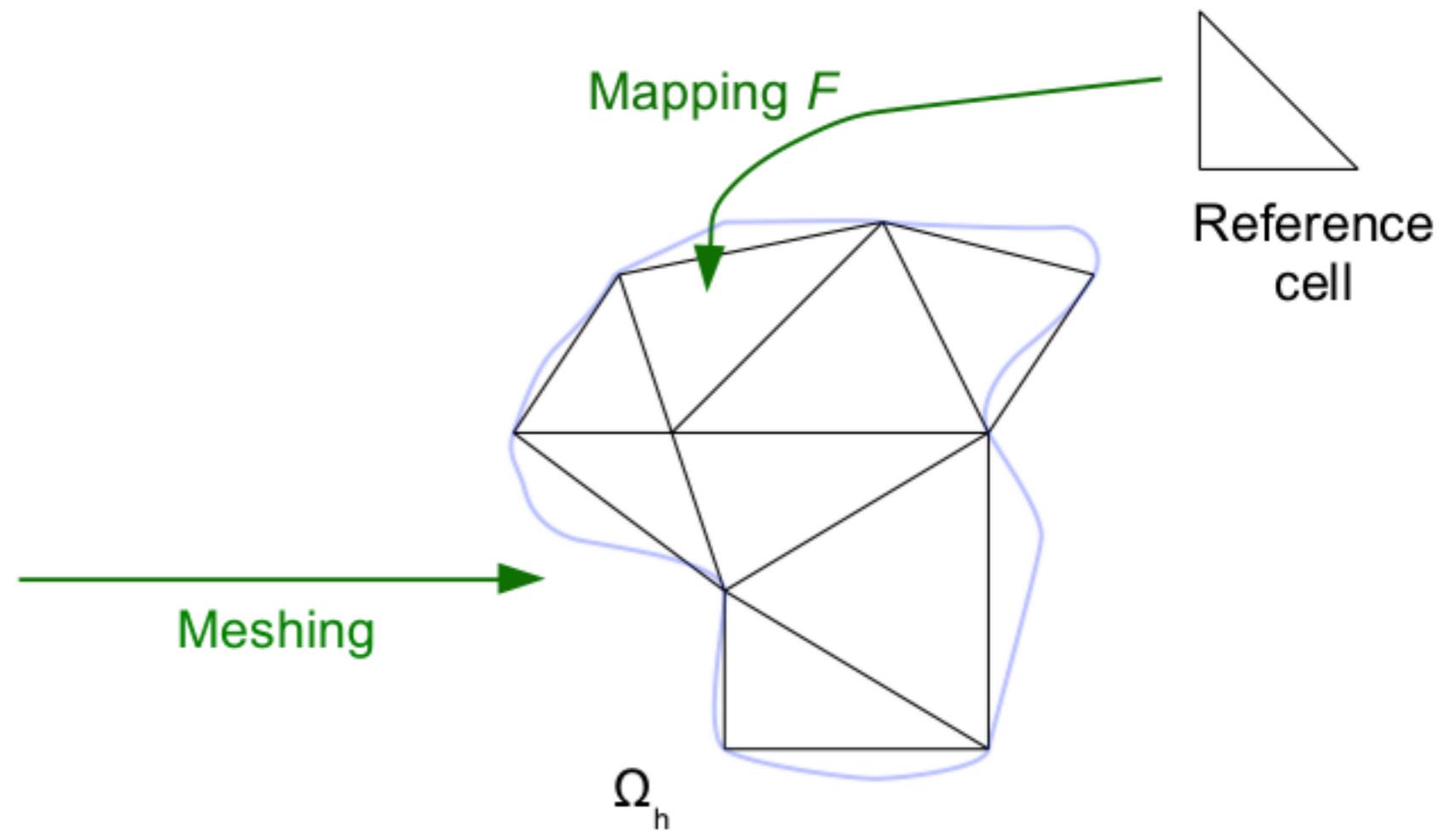
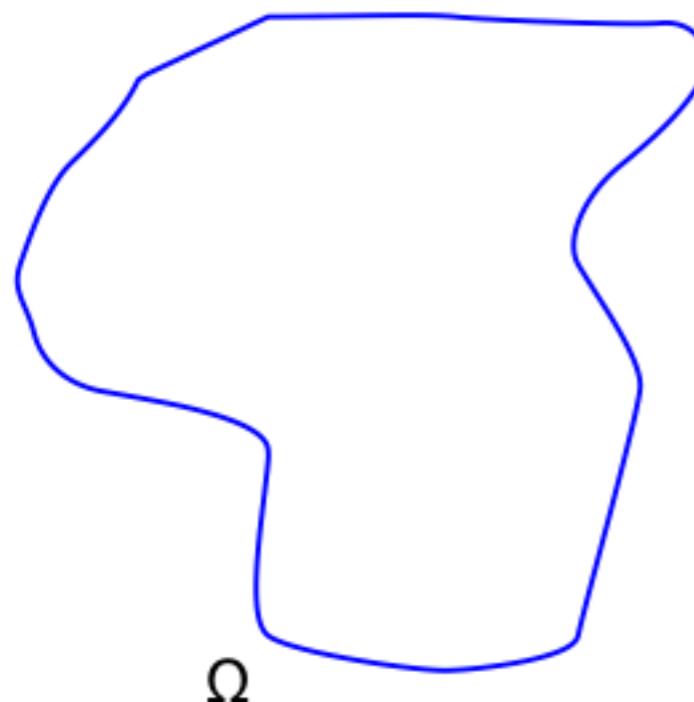
**Answer:** In the finite element method, this is done using the following concepts:

- Subdivision of the domain into a mesh
- Each cell of the mesh is a mapping of the reference cell
- Definition of basis functions on the reference cell
- Each shape function corresponds to a degree of freedom on the global mesh

# Implementing the finite element method

**Practical question 1:** How to define the basis functions?

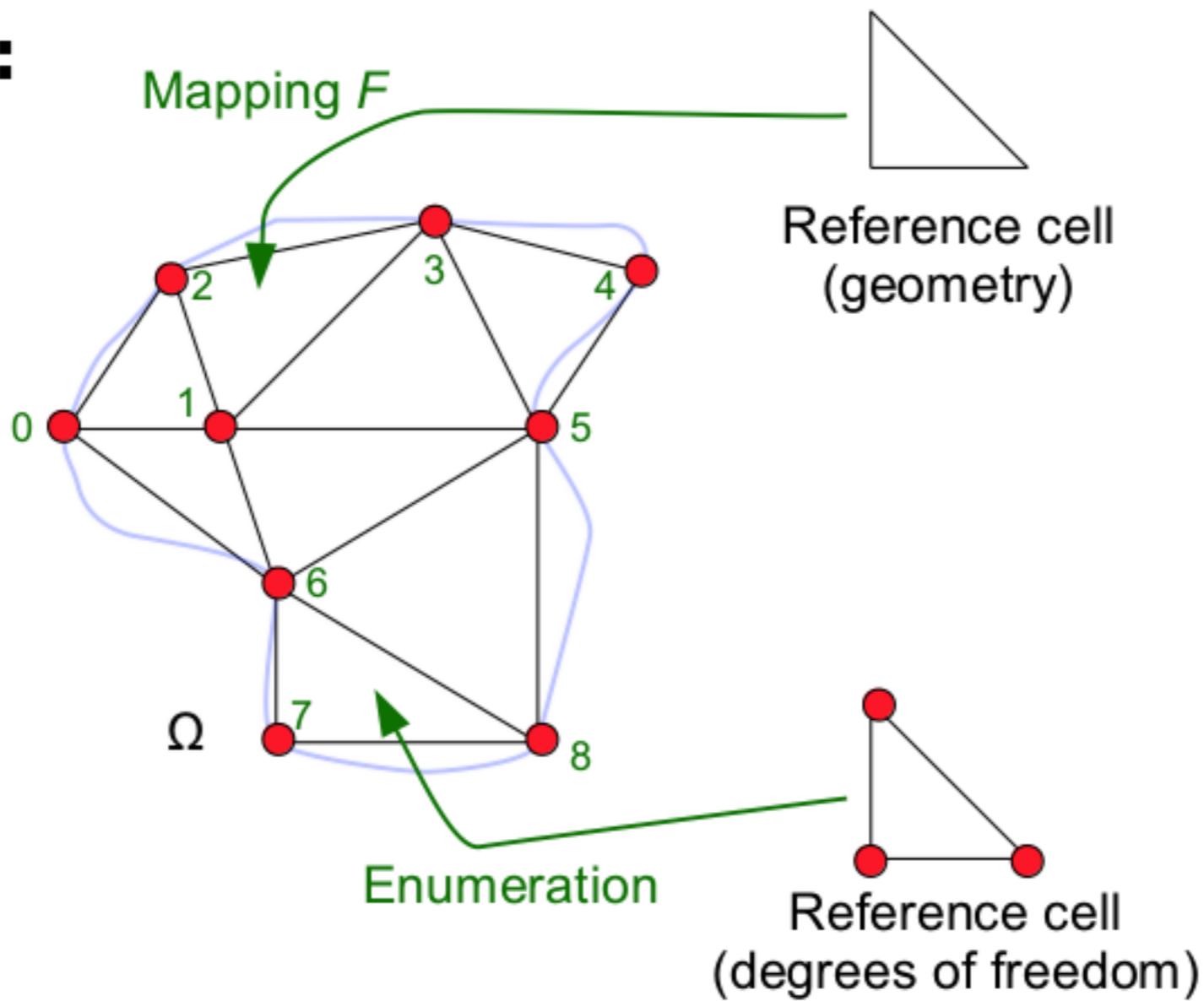
**Answer:**



# Implementing the finite element method

**Practical question 1:** How to define the basis functions?

**Answer:**



# Implementing the finite element method

**Practical question 1:** How to define the basis functions?

**Answer:** In the finite element method, this is done using the following concepts:

- Subdivision of the domain into a **mesh**
- Each cell of the mesh is a **mapping** of the **reference cell**
- Definition of **basis functions** on the reference cell
- Each shape function corresponds to a **degree of freedom** on the **global mesh**

Concepts in red will correspond to things we need to implement in software, explicitly or implicitly.

# Implementing the finite element method

Given the definition  $u_h = \sum_{j=1}^N U_j \varphi_j(x)$ , we can expand the bilinear form

$$(\nabla \varphi_i, \nabla u_h) = (\varphi_i, f) \quad \forall i = 1 \dots N$$

to obtain:

$$\sum_{j=1}^N (\nabla \varphi_i, \nabla \varphi_j) U_j = (\varphi_i, f) \quad \forall i = 1 \dots N$$

This is a linear system

$$A U = F$$

with

$$A_{ij} = (\nabla \varphi_i, \nabla \varphi_j) \qquad F_i = (\varphi_i, f)$$

# Implementing the finite element method

**Practical question 2:** How to compute

$$A_{ij} = (\nabla \varphi_i, \nabla \varphi_j) \quad F_i = (\varphi_i, f)$$

**Answer:** By **mapping** back to the reference cell...

$$\begin{aligned} A_{ij} &= (\nabla \varphi_i, \nabla \varphi_j) \\ &= \sum_K \int_K \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) \\ &= \sum_K \int_{\hat{K}} J_K^{-1}(\hat{x}) \hat{\nabla} \hat{\varphi}_i(\hat{x}) \cdot J_K^{-1}(\hat{x}) \hat{\nabla} \hat{\varphi}_j(\hat{x}) |\det J_K(\hat{x})| \end{aligned}$$

...and **quadrature**:

$$A_{ij} \approx \sum_K \sum_{q=1}^Q J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\varphi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\varphi}_j(\hat{x}_q) \underbrace{|\det J_K(\hat{x}_q)| w_q}_{=: JxW}$$

Similarly for the right hand side  $F$ .

# Implementing the finite element method

**Practical question 3:** How to store the matrix and vectors of the linear system

$$AU = F$$

## Answers:

- $A$  is sparse, so store it in **compressed row format**
- $U, F$  are just vectors, store them as **arrays**
- Implement efficient algorithms on them, e.g. **matrix-vector products, preconditioners**, etc.
- For large-scale computations, data structures and algorithms must be **parallel**

# Implementing the finite element method

**Practical question 4:** How to solve the linear system

$$AU = F$$

**Answers:** In practical computations, we need a variety of

- Direct solvers
- Iterative solvers
- Parallel solvers

# Implementing the finite element method

**Practical question 5:** What to do with the solution of the linear system

$$AU = F$$

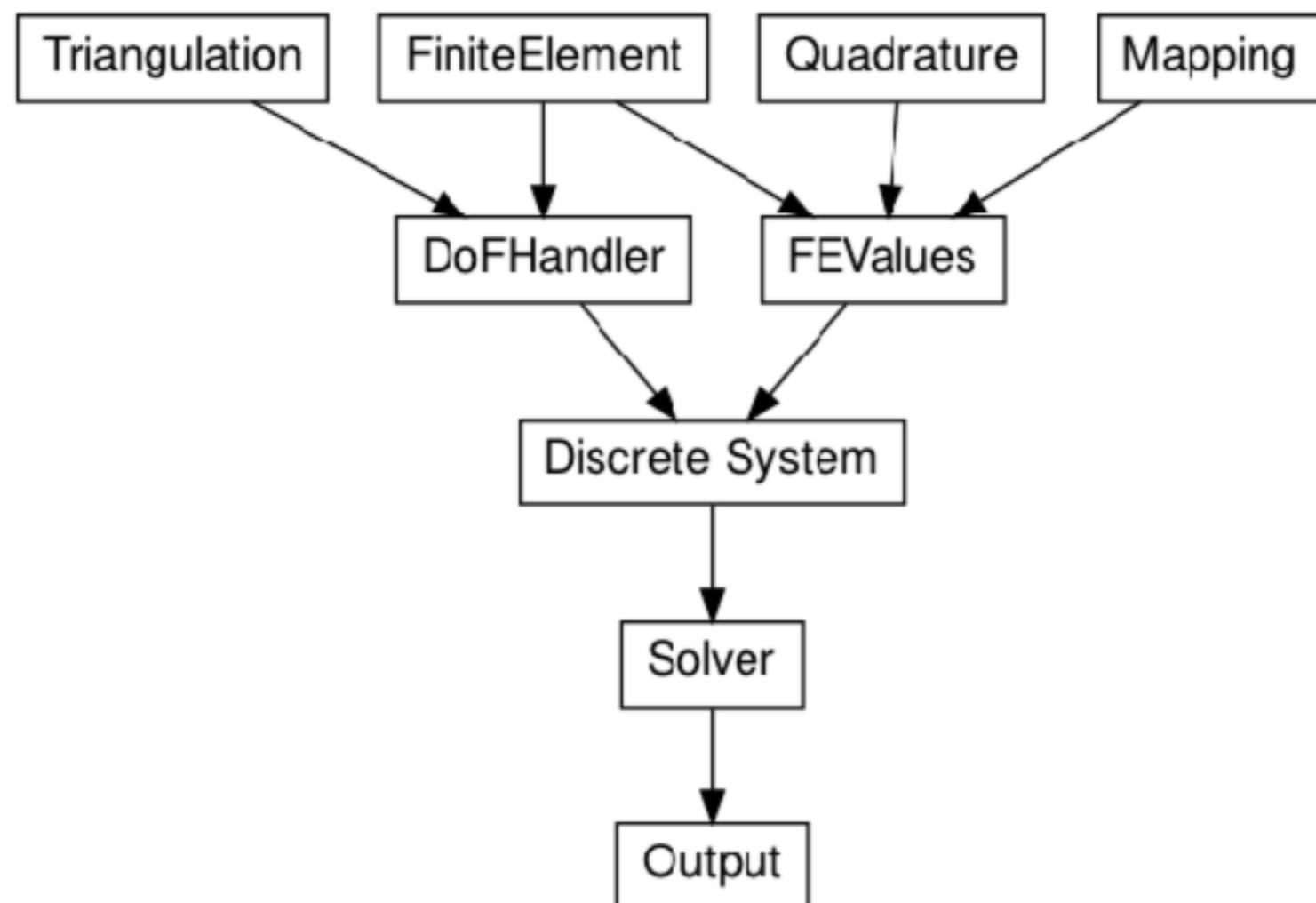
**Answers:** The goal is not to solve the linear system, but to do something with its solution:

- Visualize
- Evaluate for quantities of interest
- Estimate the error

These steps are often called *postprocessing the solution*.

# Implementing the finite element method

Together, the concepts we have identified lead to the following components that all appear (explicitly or implicitly) in finite element codes:



# Implementing the finite element method

## Summary:

- By going through the mathematical description of the FEM, we have identified *concepts* that need to be represented by *software components*.
- Other components relate to what we *want to do* with numerical solutions of PDEs.
- The next few lectures will show the software realization of these concepts.

# On using state-of-the-art tools

**All of us have our favorite editor, often the first one we learned well:**

- vi/vim/gvim
- emacs
- ...

**But:** Just because we know them well, this doesn't mean:

- That they are well suited to the task
- That they are state of the art
- That they are the tools that let you be most productive.

**The rarest resource is *your time*, not CPU time etc.  
You *must* be willing to keep learning new tools!**

# IDEs

**All of us have our favorite editor, often the first one we learned well:**

- vi/vim/gvim
- emacs
- ...

**The problem with most of these:**

- They are (good) editors but not code exploration tools
- They are text-based, not graphical

**Excellent, modern tool are for example:**

- eclipse
- kdevelop
- Xcode, Microsoft Visual C/C++

# IDEs

## What an IDE can do for you:

IDEs “know” about your code base, i.e., they *parse all* of the files that belong to your project.

Thus, the IDE...

- Knows where a variable is declared (even if in a different file)
- Knows its type and can help you with *code completion*
- Can *rename* a variable everywhere
- Can keep declaration and definition in sync
- Can help you with function arguments
- Makes you *faster* and make *far fewer mistakes*.

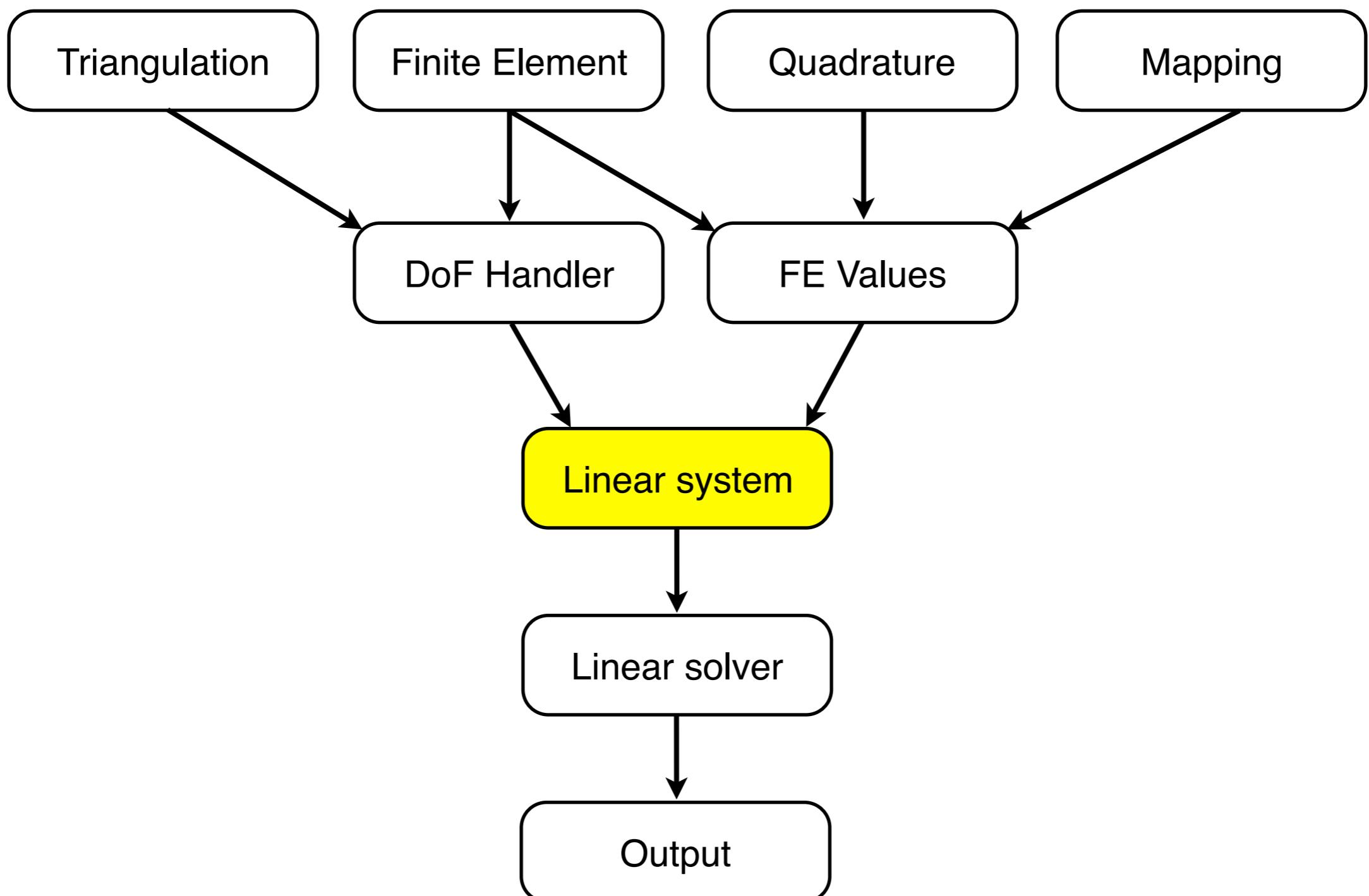
# Aims for this module

- First introduction into assembly of sparse linear systems
  - Translation of weak form to assembly loops
  - Applying boundary conditions
- Using linear solvers
- Post-processing and visualization

# Reference material

- Tutorials
  - Step-3  
[https://dealii.org/9.0.0/doxygen/deal.II/step\\_3.html](https://dealii.org/9.0.0/doxygen/deal.II/step_3.html)
- Documentation
  - [https://www.dealii.org/9.0.0/doxygen/deal.II/group\\_FE\\_vs\\_Mapping\\_vs\\_FEValues.html](https://www.dealii.org/9.0.0/doxygen/deal.II/group_FE_vs_Mapping_vs_FEValues.html)
  - [https://www.dealii.org/9.0.0/doxygen/deal.II/group\\_UpdateFlags.html](https://www.dealii.org/9.0.0/doxygen/deal.II/group_UpdateFlags.html)

# Structure of a prototypical FE problem



# Sparse linear systems

- Minimize data storage
  - Evaluate grid connectivity
- Functions to help set up
  - Sparsity pattern
  - Constraints
- Minimal access times
  - Direct manipulation of (non-zero) entries
  - Matrix-vector operations (skip over zero-entries)
- Types
  - Unity (monolithic, contiguous)
  - Block sparse structures
- Sub-organisation (e.g. component-wise)

$$[K] \{d\} = \{F\}$$

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \end{Bmatrix} = \begin{Bmatrix} F_1 \\ F_2 \end{Bmatrix}$$

$$(K_{11} - K_{12}K_{22}^{-1}K_{21}) d_1$$

$$= F_1 - K_{12}K_{22}^{-1}F_2$$

$$d_2 = K_{22}^{-1} (F_2 - K_{21}d_1)$$

# Constraints on sparse linear systems

- Strong Dirichlet boundary conditions
  - Apply user-defined spatially-dependent functions to specific boundaries
  - Can restrict to components of a multi-dimensional field
  - Limited to interpolatory FEM
- Neumann boundary conditions
  - Implementation dependent
- Other constraints need special consideration
  - Periodic boundary conditions
  - Refinement with hanging nodes
  - Some time-dependent formulations

$$[K] \{d\} = \{F\}$$

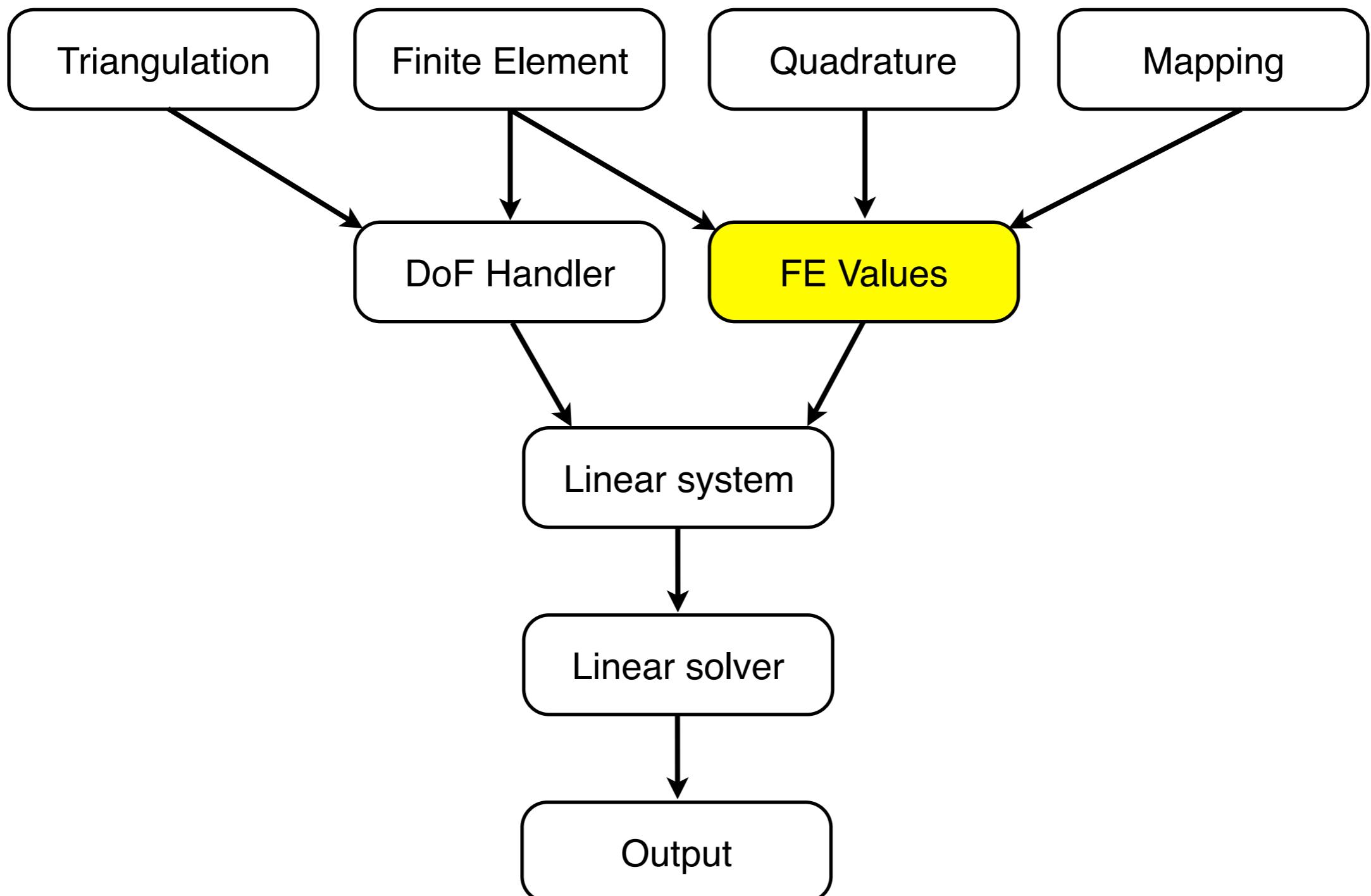
$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \end{Bmatrix} = \begin{Bmatrix} F_1 \\ F_2 \end{Bmatrix}$$

$$(K_{11} - K_{12}K_{22}^{-1}K_{21}) d_1$$

$$= F_1 - K_{12}K_{22}^{-1}F_2$$

$$d_2 = K_{22}^{-1} (F_2 - K_{21}d_1)$$

# Structure of a prototypical FE problem



# Integration on a cell: the FEValues class

$$K = \int_{\Omega} \nabla \delta\phi(\mathbf{x}) \cdot k \nabla \phi(\mathbf{x}) dV$$

$$\approx \delta\phi^I \sum_K \left( \int_{\Omega_K^h} \nabla N^I(\mathbf{x}) \cdot k \nabla N^J(\mathbf{x}) dV^h \right) \phi^J$$

$$\approx \delta\phi^I \underbrace{\sum_K \left( \sum_q \nabla N^I(\mathbf{x}_q) \cdot k_q \nabla N^J(\mathbf{x}_q) w_q \right)}_{K_{IJ} = (\nabla N^I, k \nabla N^J)} \phi^J$$

$$\approx \delta\phi^I \underbrace{\sum_K \left( \sum_q J_K^{-1}(\hat{\mathbf{x}}_q) \hat{\nabla} \hat{N}^I(\hat{\mathbf{x}}_q) \cdot k_q J_K^{-1}(\hat{\mathbf{x}}_q) \hat{\nabla} \hat{N}^J(\hat{\mathbf{x}}_q) |\det J_K(\hat{\mathbf{x}}_q)| w_q \right)}_{K_{IJ}} \phi^J$$

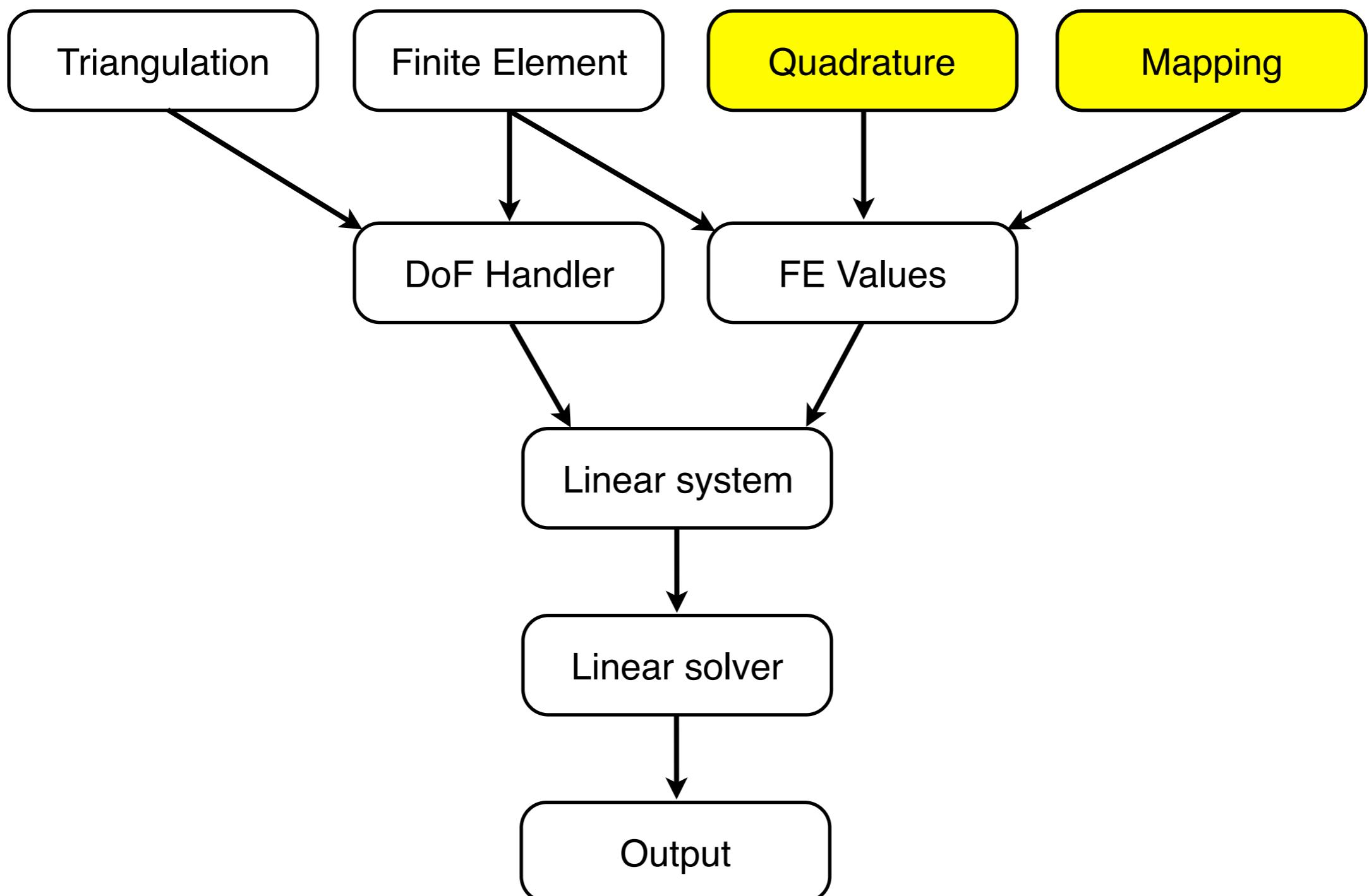
# Integration on a cell: the FEValues class

- Object that helps perform integration
- Combines information of:
  - Cell geometry
  - Finite-element system
  - Quadrature rule
  - Mappings
- Can provide:
  - Shape function data
  - Quadrature weights and mapping jacobian at a point
  - Normal on face surface
  - Covariant/contravariant basis vectors
- More ways it can help:
  - Object to extract shape function data for individual fields
  - Natural expressions when coding
- Low level optimizations

$$K_{IJ} = \sum_K \left( \sum_q J_K^{-1}(\hat{\mathbf{x}}_q) \hat{\nabla} \hat{N}^I(\hat{\mathbf{x}}_q) \cdot J_K^{-1}(\hat{\mathbf{x}}_q) \hat{\nabla} \hat{N}^J(\hat{\mathbf{x}}_q) |\det J_K(\hat{\mathbf{x}}_q)| w_q \right)$$

```
cell_matrix(I,J) += k
  * fe_values.shape_grad (I, q_point)
  * fe_values.shape_grad (J, q_point)
  * fe_values.JxW (q_point);
```

# Structure of a prototypical FE problem



# Matrix form

$$\mathbf{K} \cdot \mathbf{u} = \mathbf{F}$$

$$K_{ij} := a(N_i, N_j) \quad i, j \in \mathcal{N}_U$$

$$F_i := (N_i, f) + (N_i, h)_{\partial\Omega} - \sum_{j \in \mathcal{N}_D} a(N_i, N_j) q(\mathbf{x}_j)$$

$$(S) = (W) \approx (W^h) = (D)$$

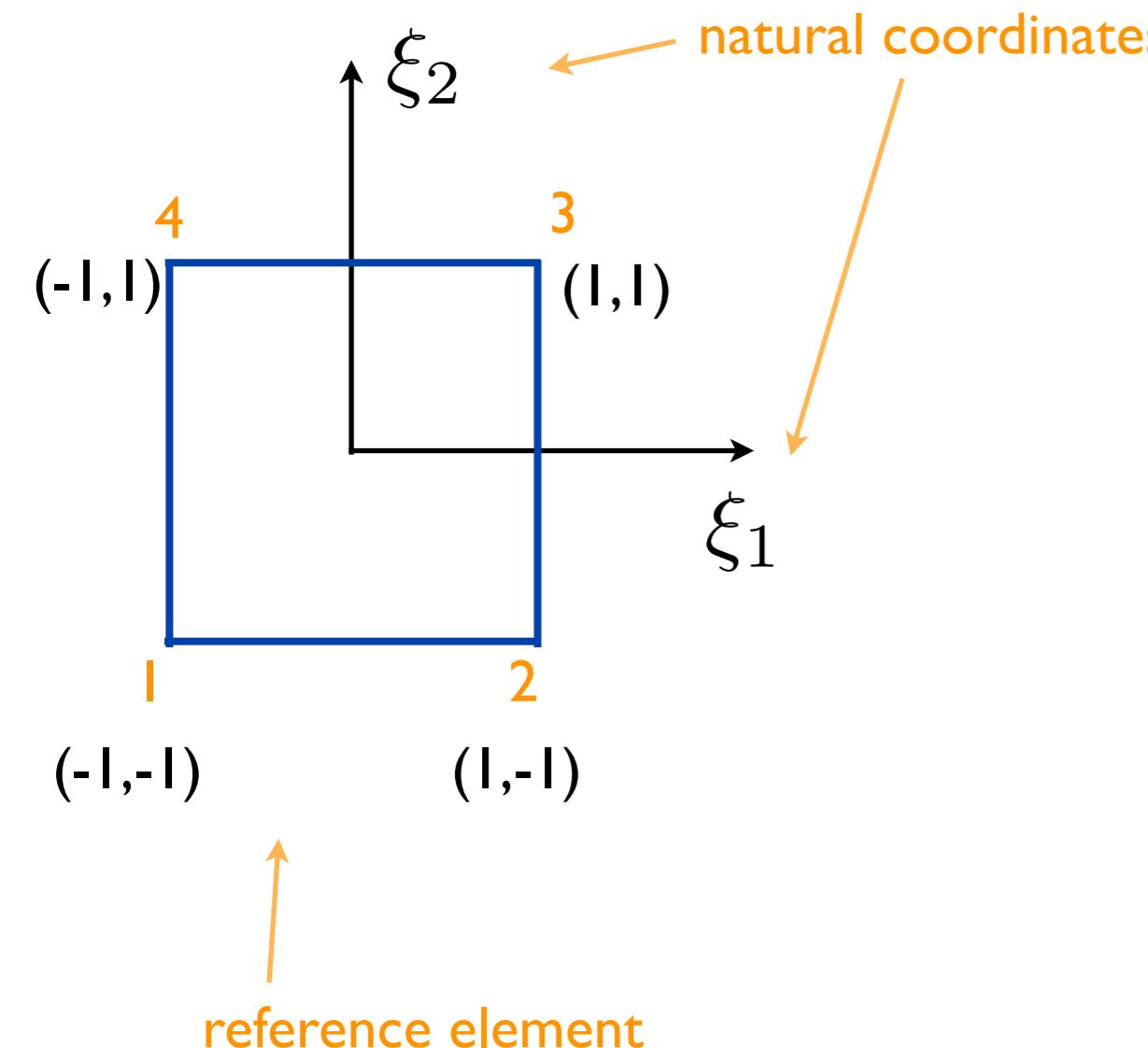
need to evaluate  
integrals numerically

$$a(N_i, N_j) := \sum_K \int_{\Omega_K} \nabla N_i \cdot \mathbf{k} \cdot \nabla N_j d\mathbf{v}$$

$$(N_i, f) := \sum_K \int_{\Omega_K} N_i f(\mathbf{x}) d\mathbf{v}$$

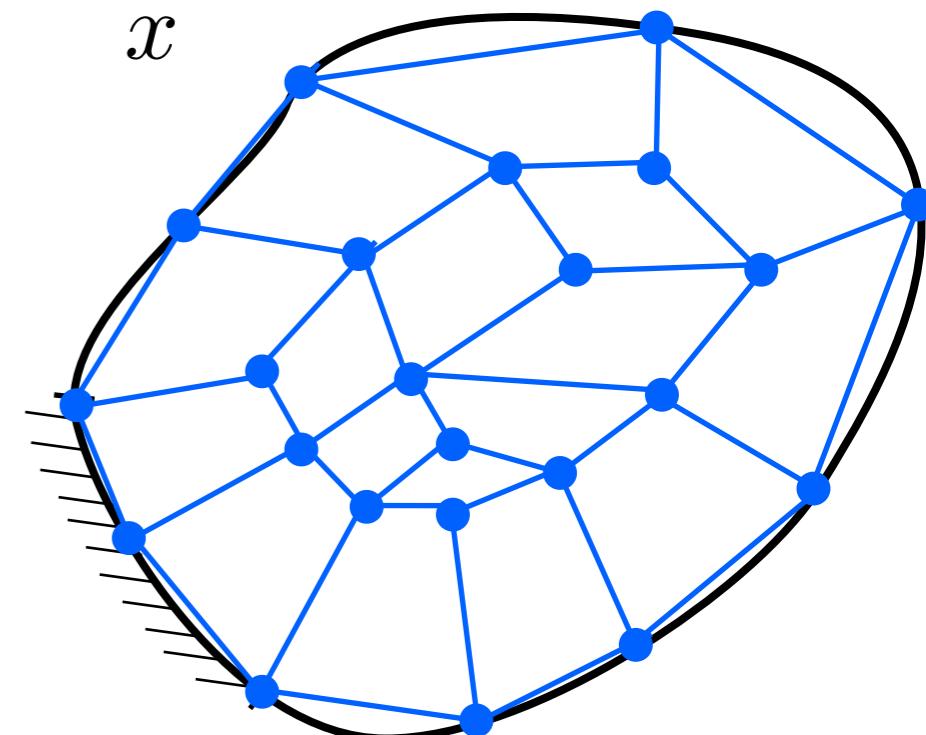
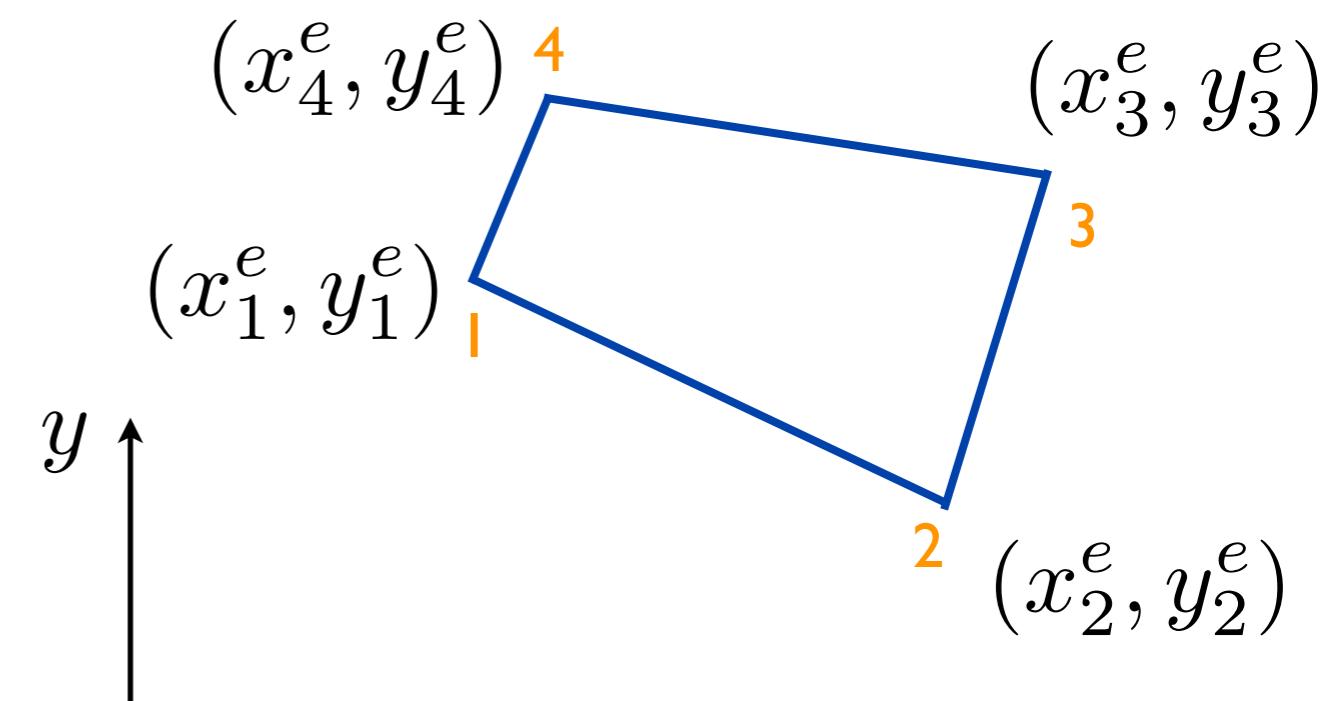
$$(w, h)_{\partial\Omega} := \sum_K \int_{\partial\Omega_K^N} w h ds$$

# Q1 mapping



we can construct the mapping  
between the two elements

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{\xi})$$



# Bilinear Quadrilateral Element

Bilinear expansion

$$x(\xi_1, \xi_2) =: \alpha_0 + \alpha_1 \xi_1 + \alpha_2 \xi_2 + \alpha_3 \xi_1 \xi_2$$

$$y(\xi_1, \xi_2) =: \beta_0 + \beta_1 \xi_1 + \beta_2 \xi_2 + \beta_3 \xi_1 \xi_2$$

+

$$x(\xi_1^a, \xi_2^a) = x_a^e \quad a = \overline{1, 4}$$

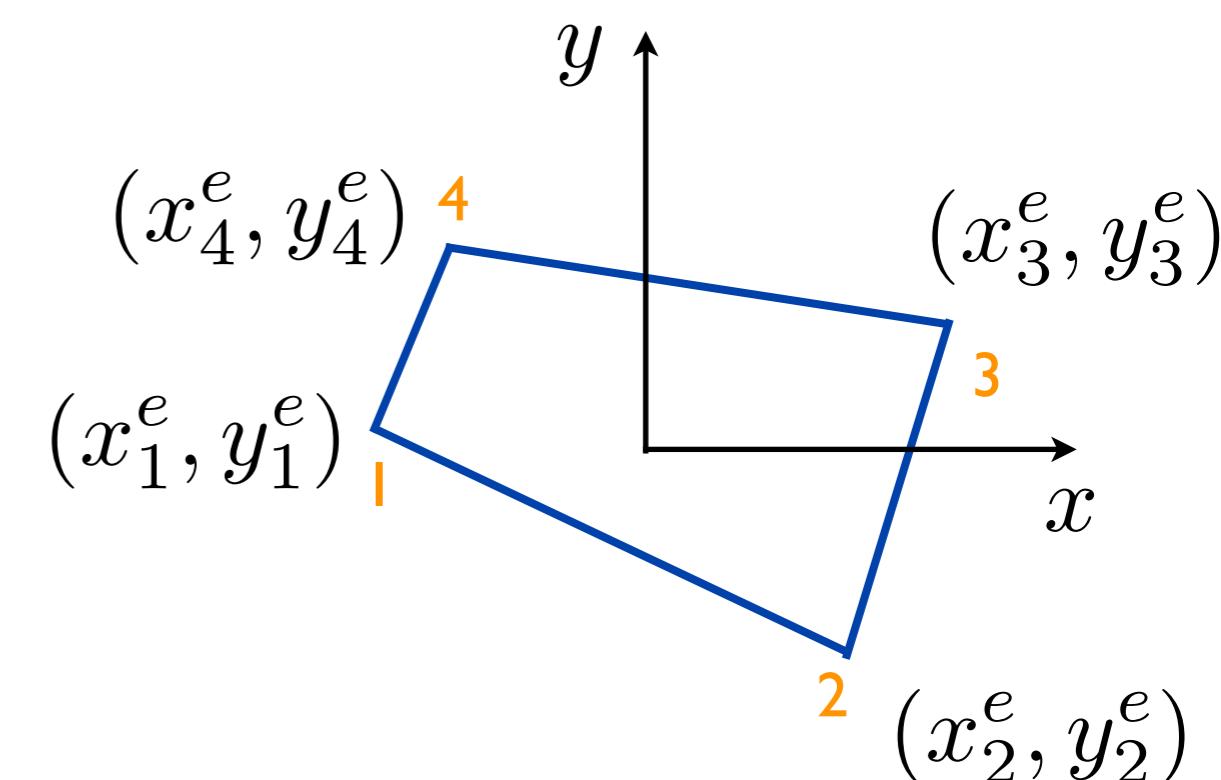
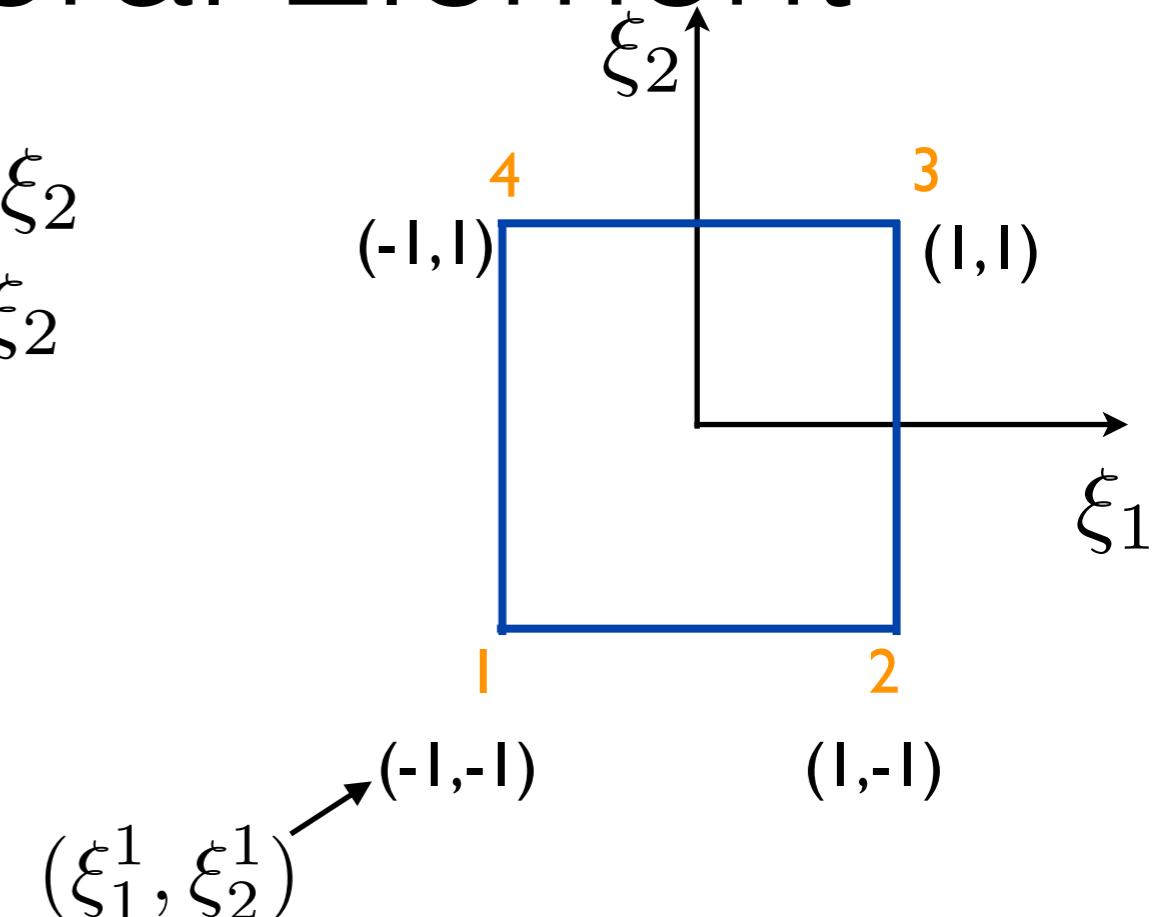
$$y(\xi_1^a, \xi_2^a) = y_a^e$$

=

$$\boldsymbol{x}(\xi) = \sum_{a=1}^4 N_a(\xi) \boldsymbol{x}_a^e$$

maps any point  
in the reference  
element to the  
actual element

$$N_a(\xi) = \frac{1}{4} [1 + \xi_1^a \xi_1][1 + \xi_2^a \xi_2]$$



# Mapping to the reference element:

$$\mathbf{J} := \frac{\partial \mathbf{x}}{\partial \xi}$$

$$\nabla = \frac{\partial}{\partial x_i} \mathbf{e}_i$$

$$\text{grad}(\bullet) = (\bullet) \nabla = \frac{\partial(\bullet)}{\partial x_i} \mathbf{e}_i = \frac{\partial(\bullet)}{\partial \xi_j} \frac{\partial \xi_j}{\partial x_i} \mathbf{e}_i = \widehat{\text{grad}}(\bullet) \cdot \mathbf{J}_K^{-1}$$

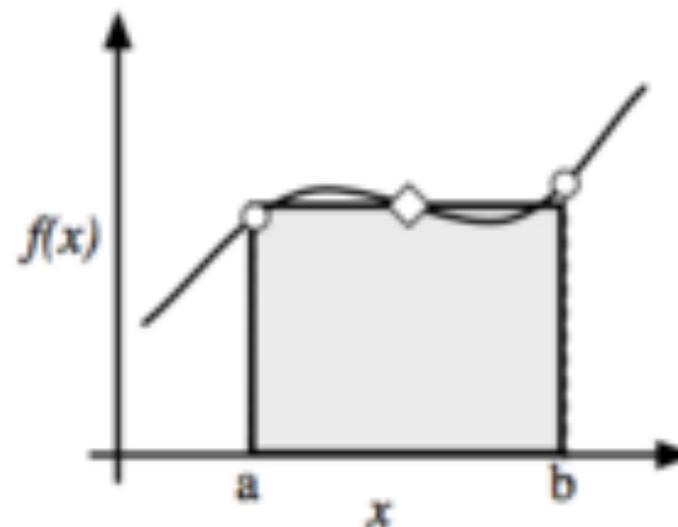
$$(S) = (W) \approx (W^h) = (D) \approx (D^q)$$

$$\begin{aligned}
 a(N_i, N_j) &= \sum_K \int_{\Omega_K} \text{grad } N_i(\mathbf{x}) \cdot \text{grad } N_j(\mathbf{x}) dv \\
 &= \sum_K \int_{\hat{\Omega}_K} [\widehat{\text{grad }} \widehat{N}_i(\xi) \cdot \mathbf{J}_K^{-1}(\xi)] \cdot [\widehat{\text{grad }} \widehat{N}_j(\xi) \cdot \mathbf{J}_K^{-1}(\xi)] \det(\mathbf{J}_K(\xi)) d\hat{v} \\
 &\approx \sum_K \sum_q [\widehat{\text{grad }} \widehat{N}_i(\xi_q) \cdot \mathbf{J}_K^{-1}(\xi_q)] \cdot [\widehat{\text{grad }} \widehat{N}_j(\xi_q) \cdot \mathbf{J}_K^{-1}(\xi_q)] \det(\mathbf{J}_K(\xi_q)) w_q
 \end{aligned}$$

do not depend on a particular cell
 

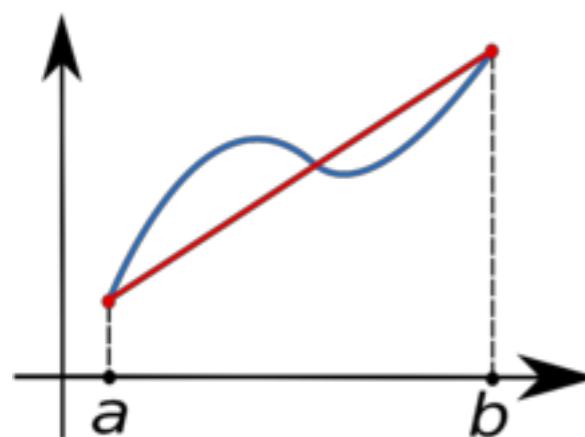
# Integration rules:

## 1. midpoint



$$\int_a^b f(x)dx \approx f\left(\frac{a+b}{2}\right) [b-a]$$

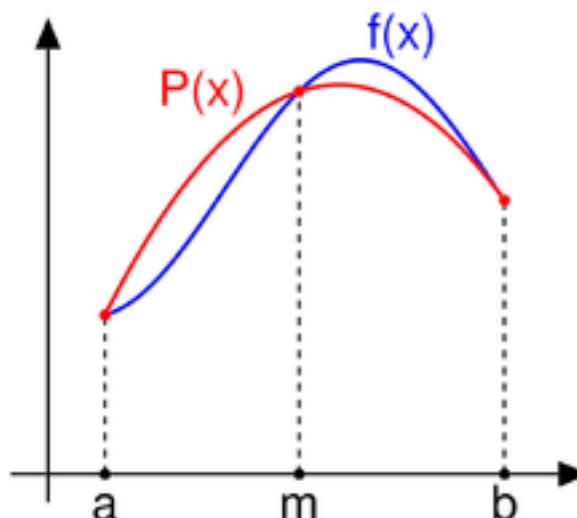
## 2. trapezoidal



$$\int_a^b f(x)dx \approx \left[ \frac{f(a) + f(b)}{2} \right] [b-a]$$

# Integration rules:

## 3. Simpson



$$\int_a^b f(x)dx \approx \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \frac{b-a}{6}$$

## 4. Gauss quadrature rule

Constructed to be exact for polynomials of degree  $2n-1$

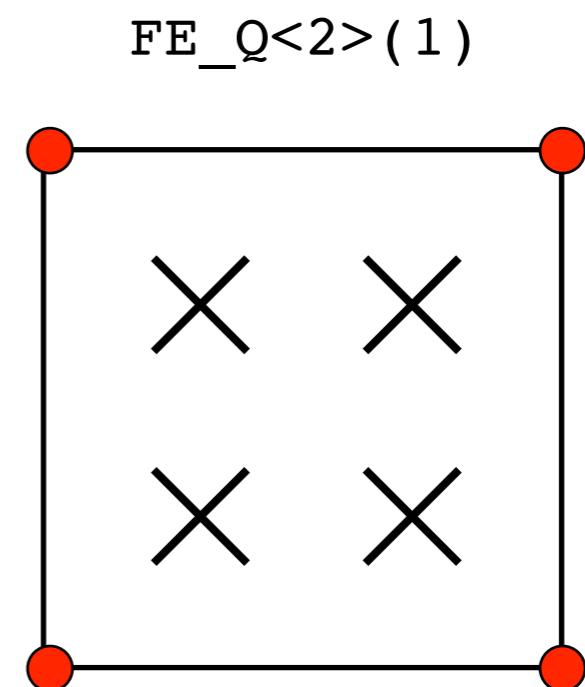
$$\int_{-1}^1 f(x)dx \approx \sum_q f(x_q)w_q$$

$n_q$	$x_1$	$x_2$	$x_3$	$w_1$	$w_2$	$w_3$
1	0			2		
2	$-1/\sqrt{3}$	$1/\sqrt{3}$		1	1	
3	$-\sqrt{3/5}$	0	$\sqrt{3/5}$	$5/9$	$8/9$	$5/9$

there are other integration rules: Monte Carlo, Newton-Cotes, Runge-Kutta,...

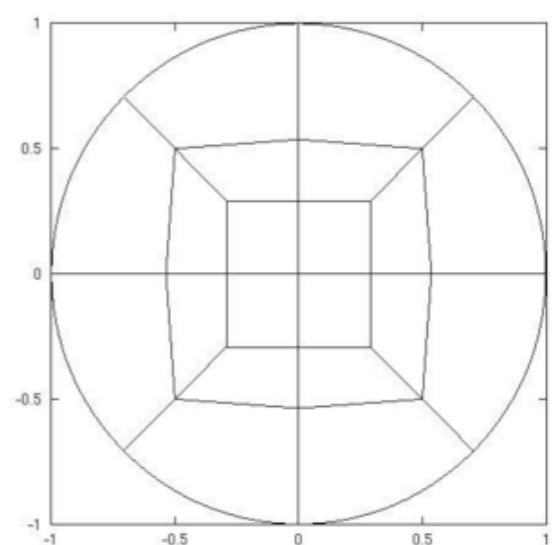
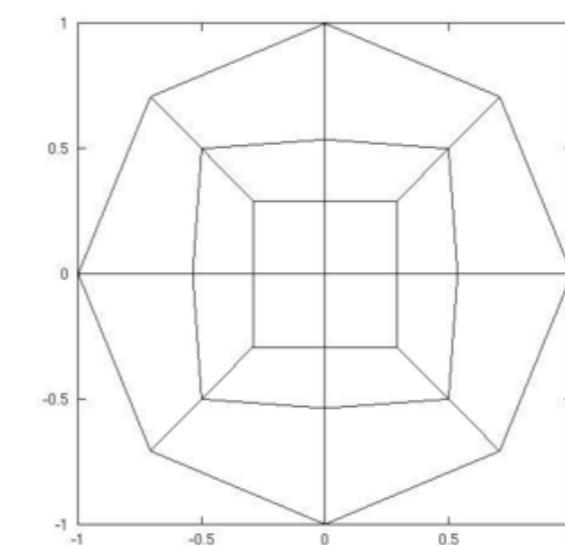
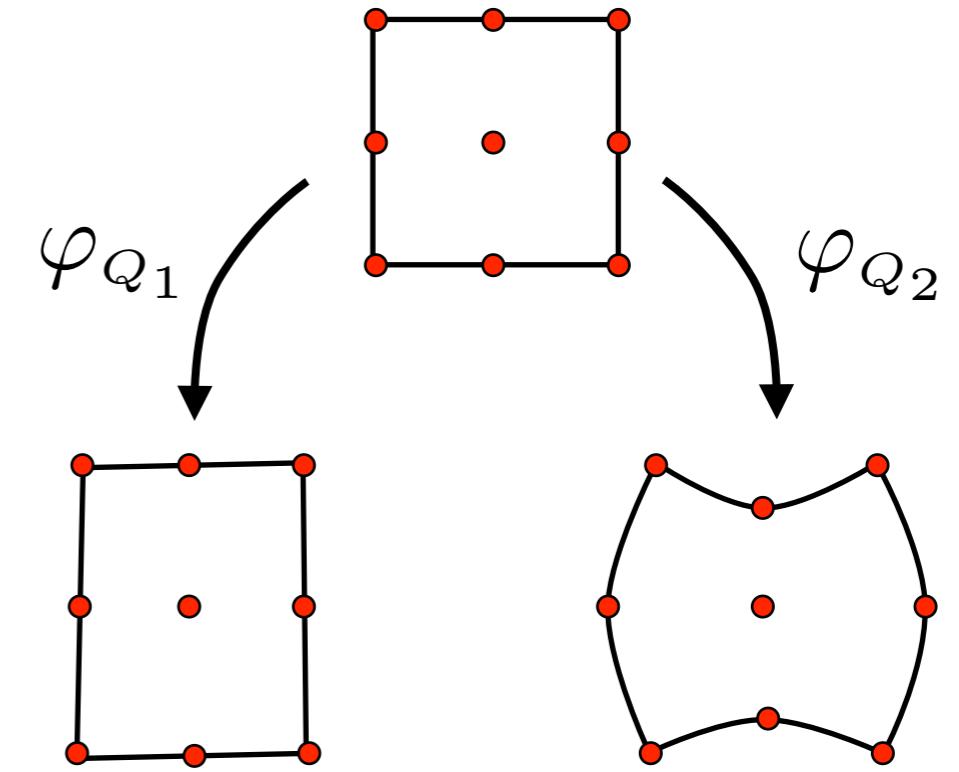
# Integration on a cell: the Quadrature classes

- QGauss<dim> n-Order Gauss quadrature
- Other rules
  - QGaussLobattom<dim> Gauss Lobatto
  - QSimpson<dim> Simpson
  - QTrapez<dim> Trapezoidal
  - QMidpoint Midpoint
  - ...

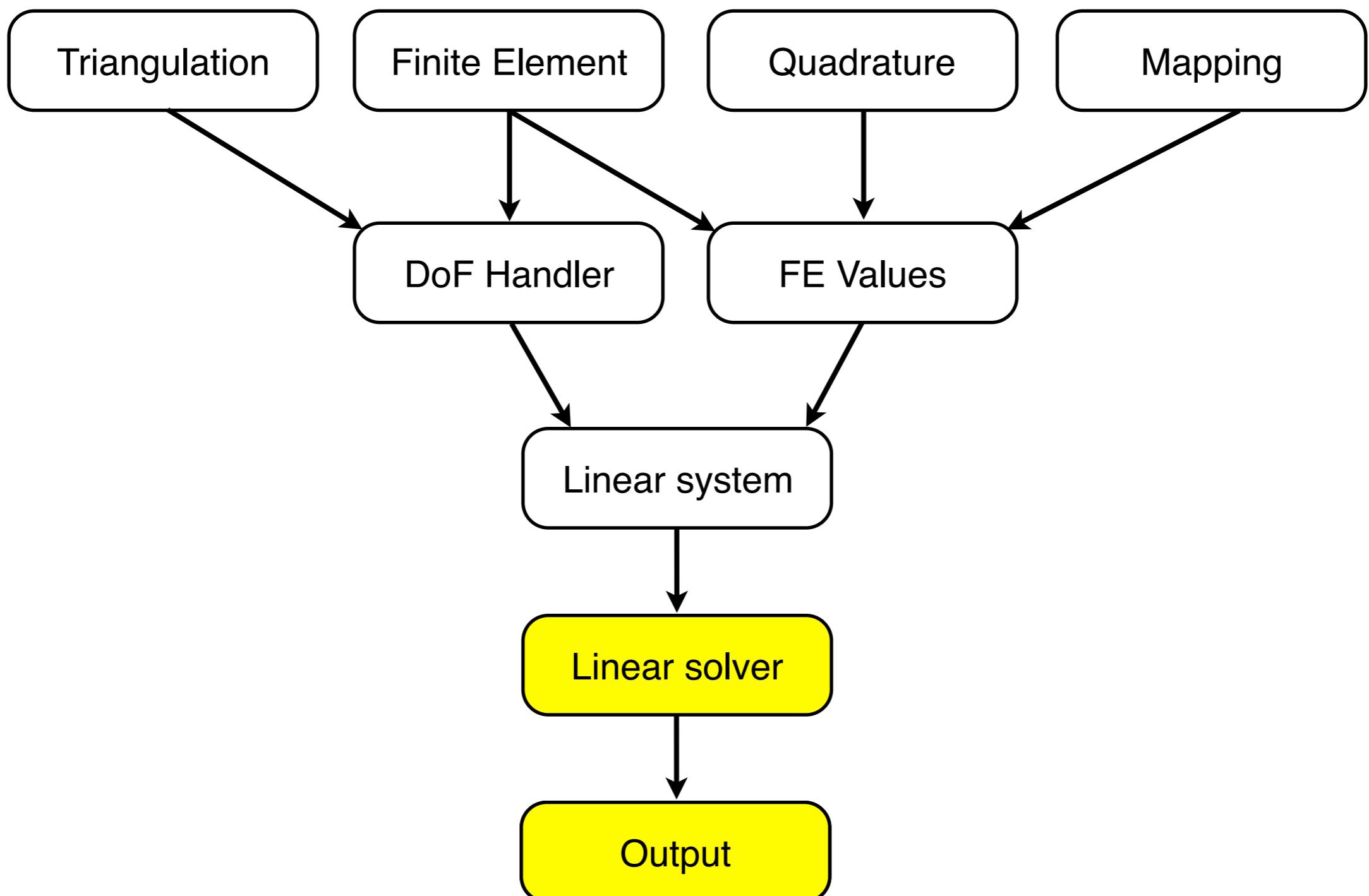


# Integration on a cell: the Mapping classes

- n-order mappings
  - Increase accuracy of:
    - Integration schemes
    - Surface basis vectors
- Lagrangian / Eulerian
  - Latter useful for fluid and contact problems, data visualization
- Boundary and interior manifolds

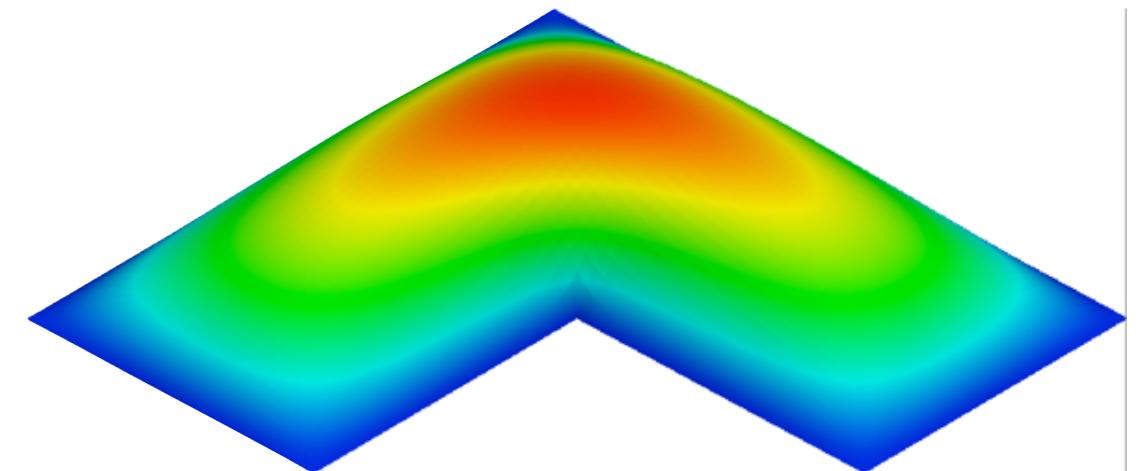


# Structure of a prototypical FE problem



# Solving Poisson's equation

- Demonstration: Step-3  
[https://www.dealii.org/9.0.0/doxygen/deal.II/step\\_3.html](https://www.dealii.org/9.0.0/doxygen/deal.II/step_3.html)  
<http://www.math.colostate.edu/~bangerth/videos.676.10.html>
- Key points
  - Local assembly + quadrature rules
  - Distribution of local contributions to the global linear system
  - Application of boundary conditions
  - Solving a linear system
  - Output for visualisation





# Shared memory parallelization

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# Aims for this module

- Identify parts / blocks of code that are (easily) parallelizable
- Learn how to parallelize using
  - ThreadGroup (Posix threads)
  - Workstream (Threaded building blocks)

# Reference material

- Tutorials
  - [https://dealii.org/9.0.0/doxygen/deal.II/step\\_9.html](https://dealii.org/9.0.0/doxygen/deal.II/step_9.html)
  - [https://dealii.org/9.0.0/doxygen/deal.II/step\\_13.html](https://dealii.org/9.0.0/doxygen/deal.II/step_13.html)
  - <http://www.math.colostate.edu/~bangerth/videos.676.39.html>
  - <http://www.math.colostate.edu/~bangerth/videos.676.40.html>
- Documentation:
  - [https://dealii.org/9.0.0/doxygen/deal.II/group\\_threads.html](https://dealii.org/9.0.0/doxygen/deal.II/group_threads.html)
  - <https://www.dealii.org/9.0.0/doxygen/deal.II/namespaceWorkStream.html>
  - <https://dealii.org/9.0.0/doxygen/deal.II/namespaceparallel.html>

# Identifying parallelizable code

- Consider this example:

```
template <int dim>
void MyProblem<dim>::setup_system () {
    dof_handler.distribute_dofs();
    DoFTools::make_hanging_node_constraints (...);      // 1
    DoFTools::make_sparsity_pattern (...);              // 2
    VectorTools::interpolate_boundary_values (...);     // 3
...
}
```

- Operations (1,2,3) are independent of one another
  - Could be reordered without consequence

# Identifying parallelizable code

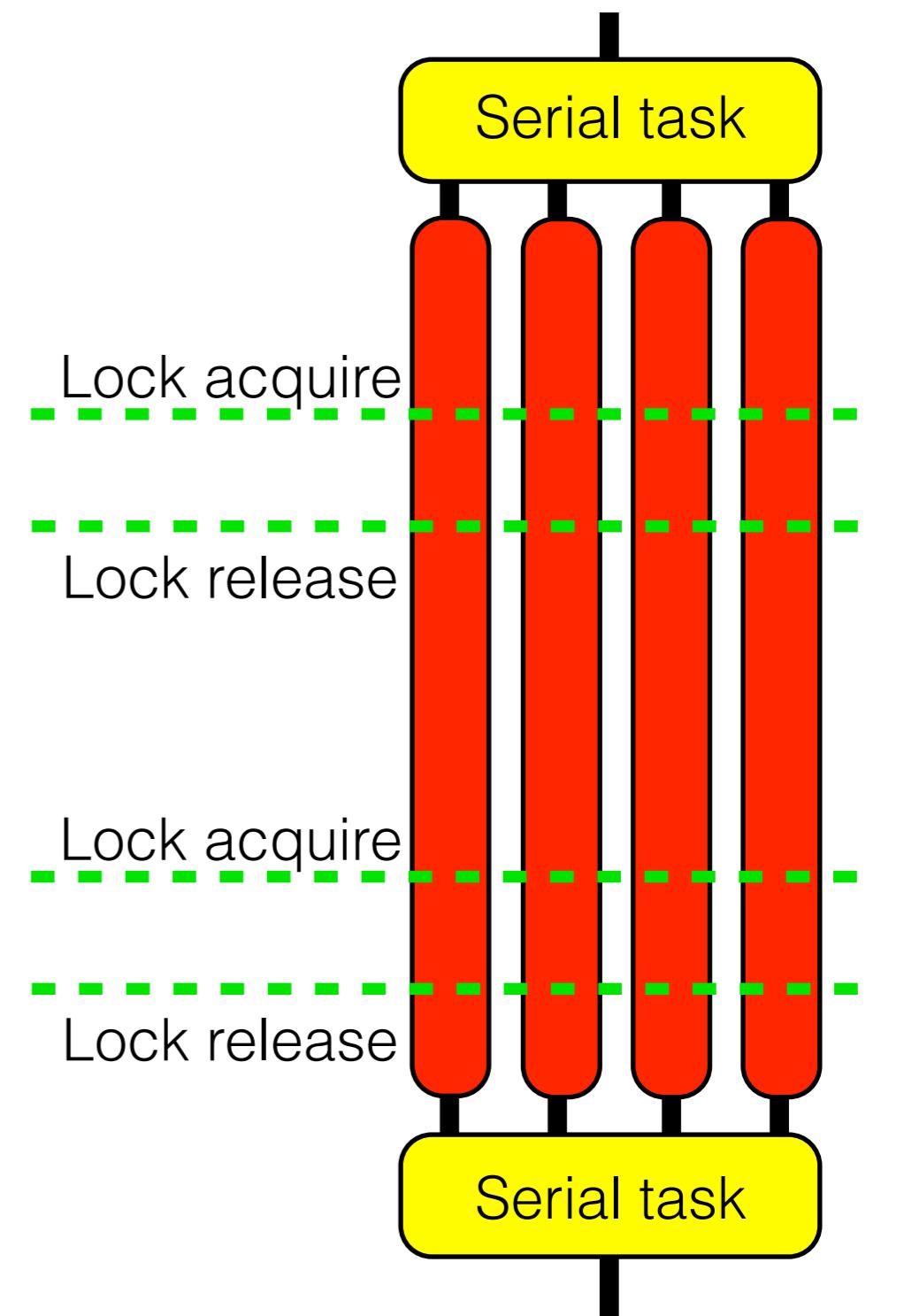
- “Embarrassingly parallelizable tasks”

```
template <int dim>
void MyProblem<dim>::assemble_system () {
    ...
    for (auto cell : dof_handler.active_cells()) {
        fe_values.reinit (cell);
        ...assemble local contribution...
        ...copy local contribution into global matrix/rhs vector...
    }
}
```

- Many more cells than machine cores
- Computations of local matrices/vectors are mutually independent
- **Accumulation into global system matrix/vector is not!**

# Independent threaded tasks: Option 1

- Code divergence with / without barriers (global / in-thread locks)
- Best used for small number of completely independent tasks
- Inside each thread: Shared data
  - Reading is a safe operation!
  - Use locks to allow data writing
    - Convergence point for threads (bottleneck)
    - Potential for deadlocks



# Creating independent threaded tasks: the Thread class

```
template <int dim>
void MyProblem<dim>::setup_system (){
    dof_handler.distribute_dofs();

    Threads::Thread<void> thread1, thread2, thread3;

    thread1 = Threads::new_thread (&DoFTools::make_hanging_node_constraints,...);
    thread2 = Threads::new_thread (&DoFTools::make_sparsity_pattern, ...);
    thread3 = Threads::new_thread (&VectorTools::interpolate_boundary_values,,...);

    thread1.join();      // and same for thread2, thread3
    ...
}
```

- The call to join() is a blocking call
- Waits to the thread to finish before continuing

# Creating independent threaded tasks: the ThreadGroup class

```
void MyProblem<dim>::assemble_on_one_cell (cell_iterator &cell) {...}

void MyProblem<dim>::assemble_system () {
    Threads::ThreadGroup<void> threads;

    for (cell=dof_handler.begin_active(); ...)
        threads += Threads::new_thread (
            &MyProblem<dim>::assemble_on_one_cell,
            this, cell);

    threads.join_all ();
}
```

- Why is this inefficient?
- How do we prevent data races?

# Creating independent threaded tasks: Ranged based assembly

- Less threads created = more efficient

```
void MyProblem<dim>::assemble_on_cell_range (
    cell_iterator &range_begin,
    cell_iterator &range_end) {...};

void MyProblem<dim>::assemble_system () {
    Threads::ThreadGroup<void> threads;

    std::vector<std::pair<cell_iterator, cell_iterator> >
        sub_ranges = Threads::split_range (
            dof_handler.begin_active(),
            dof_handler.end(),
            n_virtual_cores);

    for (t=0; t<n_virtual_cores; ++t)
        threads += Threads::new_thread (
            &MyProblem<dim>::assemble_on_cell_range,
            this,
            sub_ranges[t].first,
            sub_ranges[t].second);

    threads.join_all ();
}
```

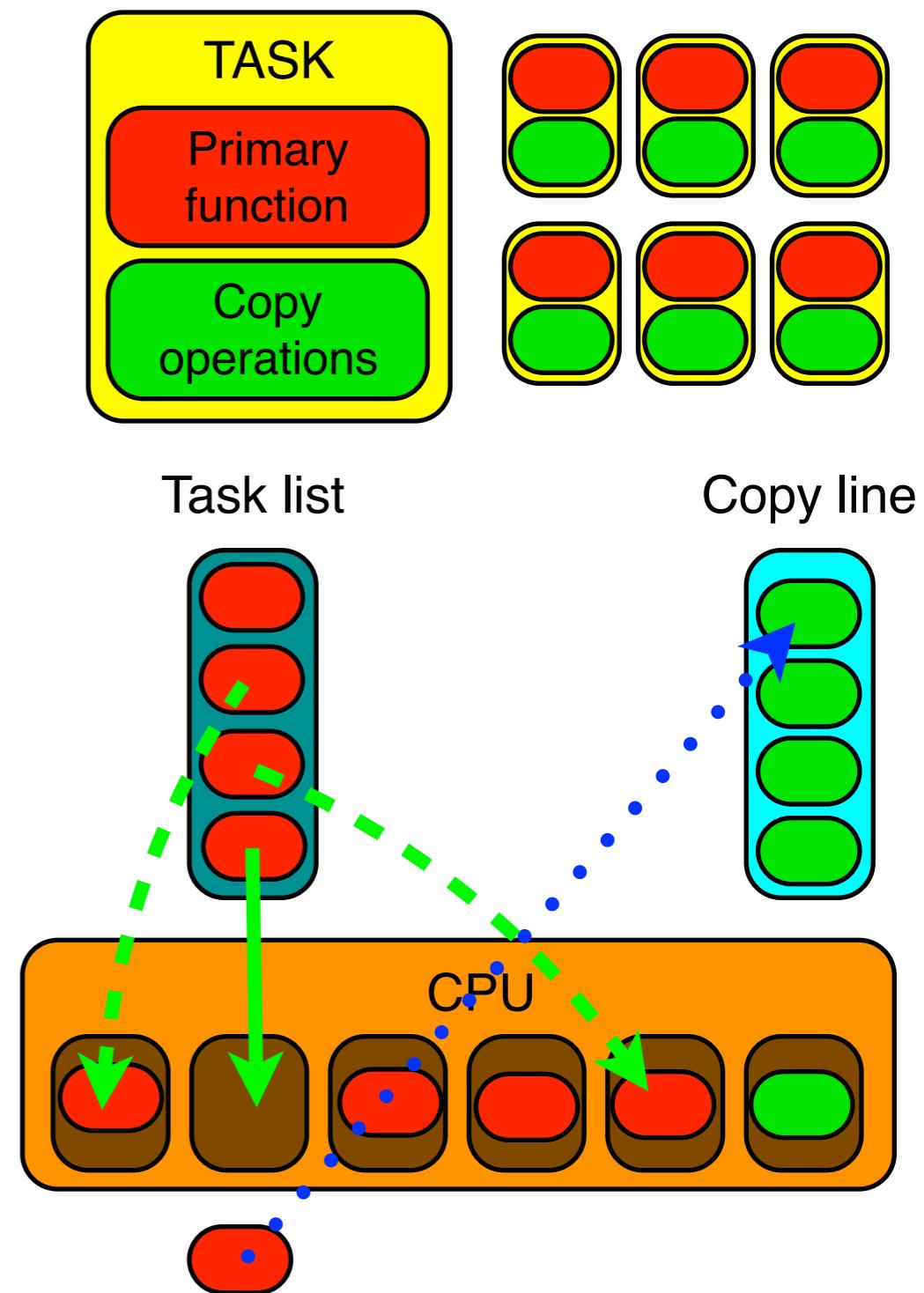
# Independent threaded tasks

- How do we prevent data races?

```
void MyProblem<dim>::assemble_on_one_cell (cell_iterator &cell) {  
  
    static Threads::Mutex mutex;  
  
    mutex.acquire ();  
    for (unsigned int i=0; i<fe.dofs_per_cell; ++i)  
        for (unsigned int j=0; j<fe.dofs_per_cell; ++j)  
            system_matrix.add (dof_indices[i], dof_indices[j],  
                               cell_matrix(i,j));  
    ...same for rhs...  
    mutex.release ();  
}
```

# Creating independent threaded tasks: the WorkStream class

- Task-based threading
  - Continuous use of free CPU cores
  - Create a list of tasks
  - When core free, use it to perform next task
    - Expensive operations continually executed
  - Perform blocking tasks independently
    - Data copied to shared objects serially
  - Optimizations:
    - “Automatic” load balancing
    - Overhead reduction: Works on data chunks



# Creating independent threaded tasks: parallelization of (per-cell) assembly

```
template <int dim>
void MyClass<dim>::assemble_on_one_cell (
    const typename DoFHandler<dim>::active_cell_iterator &cell)
{
    FEValues<dim> fe_values (...); ← Expensive constructor call

    FullMatrix<double> cell_matrix (...);
    Vector<double>      cell_rhs (...);
    std::vector<double> rhs_values (...);

    rhs_function.value_list (...)

    // assemble local contributions
    fe_values.reinit (cell);
    for (unsigned int i=0; i<fe.dofs_per_cell; ++i)
        for (unsigned int j=0; j<fe.dofs_per_cell; ++j)
            for (unsigned int q=0; q<n_points; ++q)
                cell_matrix(i,j) += ...;
    ...same for cell_rhs...

    // now copy results into global system
    std::vector<unsigned int> dof_indices (...);
    cell->get_dof_indices (dof_indices);
    for (unsigned int i=0; i<fe.dofs_per_cell; ++i)
        for (unsigned int j=0; j<fe.dofs_per_cell; ++j)
            system_matrix.add (...);
    ...same for rhs...
    // or constraints.distribute_local_to_global (...);
}
```

The diagram illustrates the parallelization of the assembly process. The main loop body, which contains the local contribution calculation and the global system update, is identified as an **Independent tasks**. Within this parallel region, several operations are highlighted as **Serial operation**: the expensive constructor call for `FEValues`, repeated memory allocations for `FullMatrix`, `Vector`, and `std::vector`, and the final `system_matrix.add` call.

# Threading using WorkStream: the ScratchData class

- Assistant struct / class
- Contains reused data structures
  - FEValues objects
  - Helper vectors and storage containers
  - Precomputed data
- Needs a constructor and a copy constructor
  - Some objects must be manually reconstructed
  - We create one initial instance of the class
  - TBB duplicates as required (queue\_length)

```
struct ScratchData {  
    std::vector<double>           rhs_values;  
    FEValues<dim>                 fe_values;  
  
    ScratchData (  
        const FiniteElement<dim> &fe,  
        const Quadrature<dim>     &quadrature,  
        const UpdateFlags          update_flags)  
        : rhs_values (quadrature.size()),  
          fe_values (fe, quadrature, update_flags)  
    {}  
  
    ScratchData (const ScratchData &rhs)  
        : rhs_values (rhs.rhs_values),  
          fe_values (rhs.fe_values.get_fe(),  
                     rhs.fe_values.get_quadrature(),  
                     rhs.fe_values.get_update_flags())  
    {}  
}
```

# Threading using WorkStream: the PerTaskData class

- Contains data structures required for serial operations
  - Multiple copies made (`queue_length*chunk_size`)
  - Must be “self-contained”
- Used in two places
  - Threaded function
    - Bound to an instance of the threaded function
    - Used as a “data-in” object
  - Serial function
    - A used instance is passed to this function
    - Used as a “data-out” object

```
struct PerTaskData {  
    FullMatrix<double> cell_matrix;  
    Vector<double> cell_rhs;  
    std::vector<unsigned int> dof_indices;  
  
    PerTaskData (const FiniteElement<dim> &fe)  
        : cell_matrix (fe.dofs_per_cell,  
                      fe.dofs_per_cell),  
          cell_rhs (fe.dofs_per_cell),  
          dof_indices (fe.dofs_per_cell)  
    {}  
}
```

# Threading using WorkStream: Revised assembly

```
template <int dim>
void MyClass<dim>::assemble_on_one_cell (
    const typename DoFHandler<dim>::active_cell_iterator &cell,
    ScratchData &scratch,
    PerTaskData &data)
{
    // reinitialise data
    scratch.fe_values.reinit (cell);
    rhs_function.value_list (scratch.fe_values.get_quadrature_points,
                             scratch.rhs_values);
    ...
    data.cell_matrix = 0;
    data.cell_rhs    = 0;

    // assemble local contributions
    for (unsigned int i=0; i<fe.dofs_per_cell; ++i)
        for (unsigned int j=0; j<fe.dofs_per_cell; ++j)
            for (unsigned int q=0; q<fe_values.n_quadrature_points; ++q)
                data.cell_matrix(i,j) += ...;
    ...
}
```

- Now use objects contained within ScratchData and PerTaskData structs

# Threading using WorkStream: Serial copy operation

```
template <int dim>
void MyClass<dim>::copy_local_to_global (const PerTaskData &data)
{
    for (unsigned int i=0; i<fe.dofs_per_cell; ++i)
        for (unsigned int j=0; j<fe.dofs_per_cell; ++j)
            system_matrix.add (data.dof_indices[i], data.dof_indices[j],
                               data.cell_matrix(i,j));
    ...same for rhs...
    // or constraints.distribute_local_to_global (...);
}
```

- Uses writes “fixed” data in PerTaskData to single class object system\_matrix (and whatever else)
- Has to be a serially performed operation

# Threading (not) using WorkStream: Manual assembly using these data structures

```
ScratchData scratch_data (...);  
PerTaskData per_task_data (...);  
  
DoFHandler<deal_II_dimension>::active_cell_iterator  
    cell = dof_handler.begin_active(),  
    endc = dof_handler.end();  
    for (; cell != endc; ++cell)  
{  
    assemble_system_one_cell(cell,  
                            scratch_data,  
                            per_task_data);  
    copy_local_to_global(per_task_data);  
}
```

- This performs the same serial assembly as we had before
  - More efficient though (use of ScratchData)

# Threading using WorkStream

```
ScratchData scratch_data (...);  
PerTaskData per_task_data (...);  
  
WorkStream::run ( dof_handler.begin_active(),  
                  dof_handler.end(),  
                  *this,  
                  &MyClass::assemble_system_one_cell,  
                  &MyClass::copy_local_to_global,  
                  scratch_data,  
                  per_task_data );
```

- Execute function in threaded manner
- Only operates on functions with a specific prototype
  - Threadable function:  
void function\_name(cell, scratch, per\_task\_data)
  - Serial function:  
void function\_name(per\_task\_data)

# Threading using WorkStream

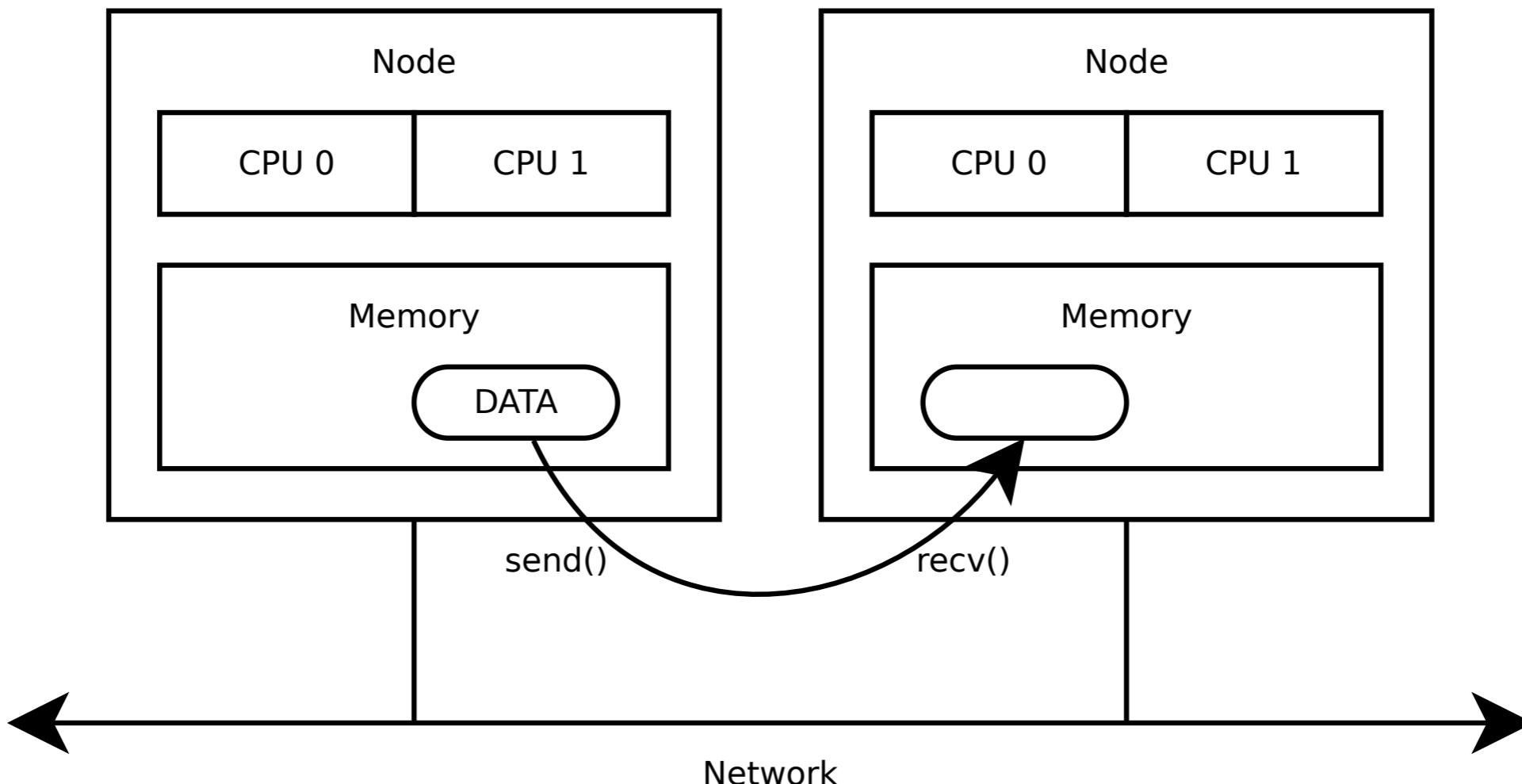
```
WorkStream::run ( dof_handler.begin_active(),
                  dof_handler.end(),
                  std::bind(&Solid::assemble_residual_one_cell,
                            this,
                            _1, // cell
                            _2, // scratch
                            _3), // data
                  std::bind(&Solid::copy_local_to_global_residual,
                            this,
                            _1, // data
                            &in_vector),
                  scratch_data,
                  per_task_data_residual);
```

- copy\_local\_to\_global\_F function prototype:  
void function (per\_task\_data, vector)
- std::bind only binds memory addresses
  - Will make copies of objects not sent in via memory address
  - Need to send in pointers if wish to work on an existing object
  - “std::\_1, \_2, \_3” are placeholders for expected data

[https://www.dealii.org/8.5.1/doxygen/deal.II/  
namespaceWorkStream.html](https://www.dealii.org/8.5.1/doxygen/deal.II/namespaceWorkStream.html)

NOTE: If your data objects are large, or their constructors are expensive, it is helpful to keep in mind that queue\_length copies of the ScratchData object and queue\_length\*chunk\_size copies of the CopyData object are generated.

# Parallel computing model: MPI

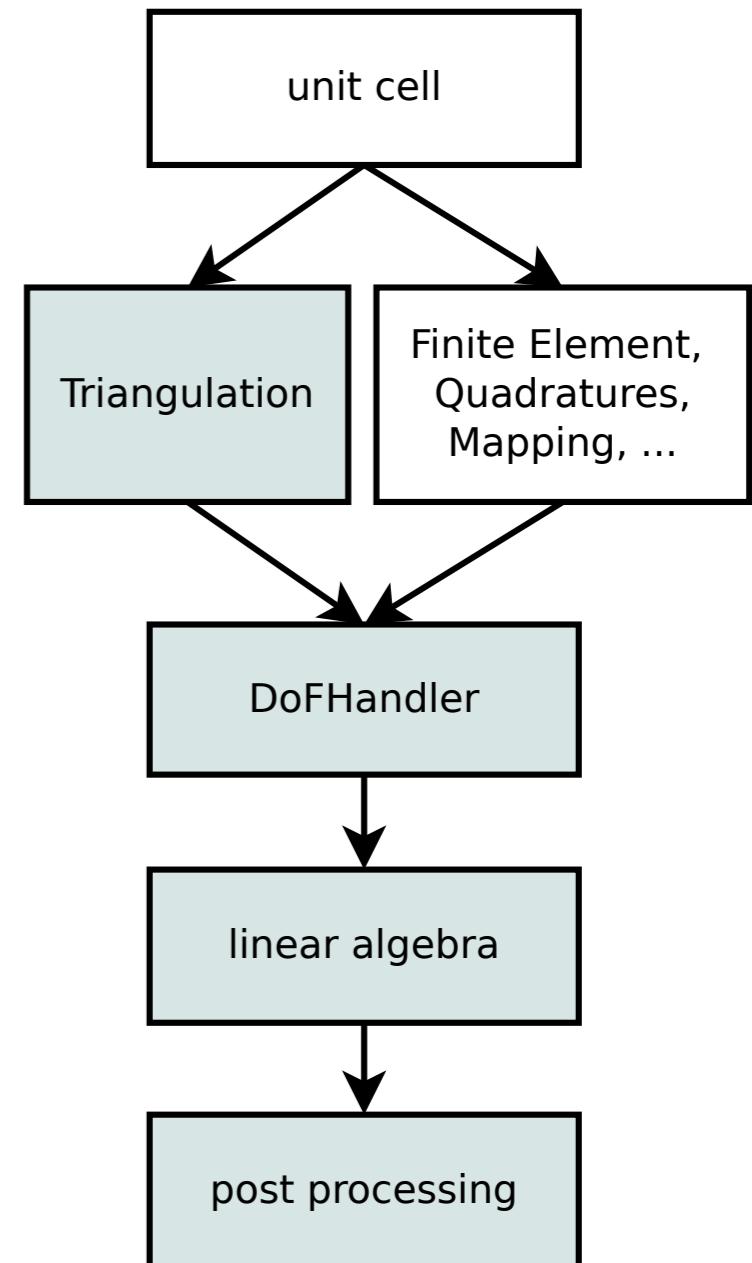


# General Considerations

- Goal: get the solution faster!
- If FEM with <500.000 dofs, and 2d, use direct solver!
- If you need more, then you have to **SPLIT** the work
  - **Distributed data storage** everywhere
    - need special data structures
  - **Efficient algorithms**
    - not depending on total problem size
  - **“Localize” and “hide” communication**
    - point-to-point communication, nonblocking sends and receives

## C Needs to be parallelized:

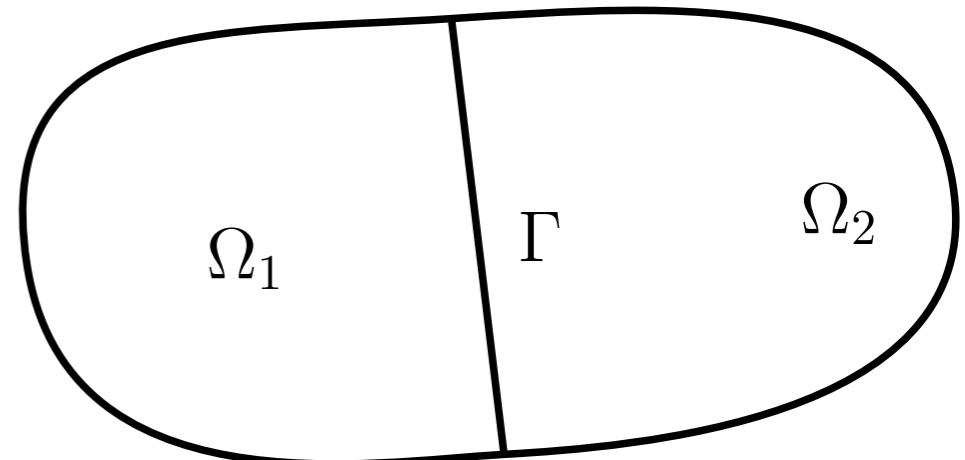
1. Triangulation (mesh with associated data)
  - hard: distributed storage, new algorithms
2. DoFHandler (manages degrees of freedom)
  - hard: find global numbering of DoFs
3. Linear Algebra (matrices, vectors, solvers)
  - use existing library
4. Postprocessing (error estimation, solution transfer, output, . . . )
  - do work on local mesh, communicate



# How to Parallelize?

## Option 1: Domain Decomposition

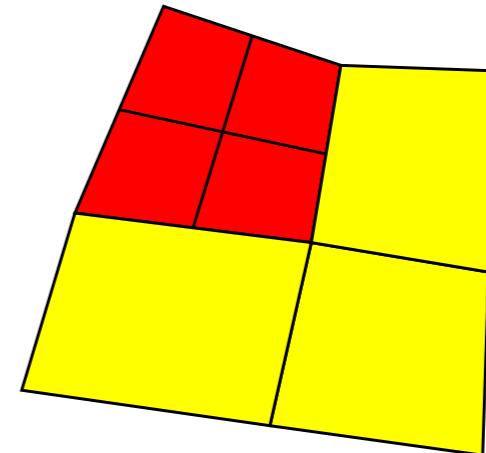
- ❖ Split up problem on PDE level
- ❖ Solve subproblems independently
- ❖ Converges against global solution
- ❖ Problems:
  - ❖ Boundary conditions are problem dependent:
    - ~~> sometimes difficult!
    - ~~> no black box approach!
  - ❖ Without coarse grid solver:  
condition number grows with # subdomains
    - ~~> no linear scaling with number of CPUs!



# How to Parallelize?

## Option 2: Algebraic Splitting

- ❖ Split up mesh between processors:



- ❖ Assemble logically global linear system  
(distributed storage):

$$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

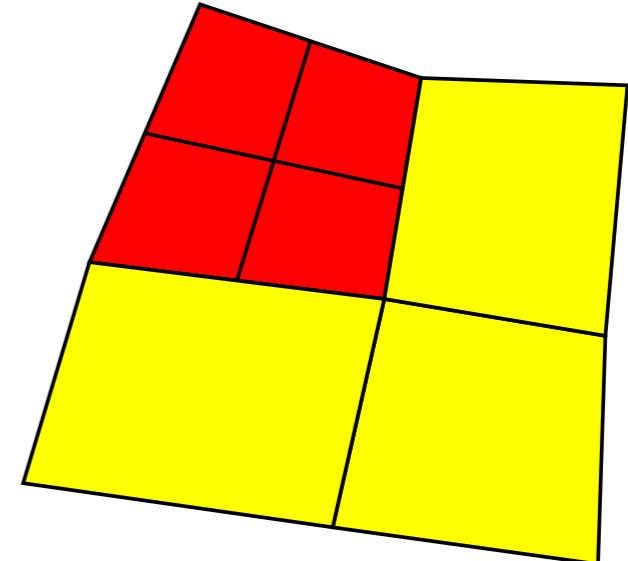
A mathematical equation representing a linear system. It consists of a 3x3 matrix with dots for entries, followed by an equals sign, and a 3x1 vector with dots for entries. The matrix and vector are flanked by thick grey bars.

- ❖ Solve using iterative linear solvers in parallel
- ❖ Advantages:
  - ❖ Looks like serial program to the user
  - ❖ Linear scaling possible (with good preconditioner)

# Partitioning

Optimal partitioning (coloring of cells):

- ❖ same size per region
  - ~~ even distribution of work
- ❖ minimize interface between region
  - ~~ reduce communication

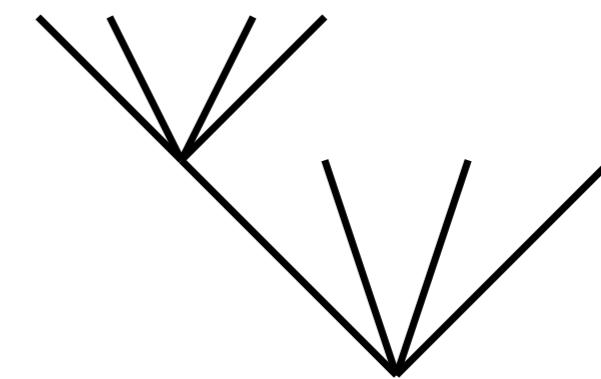
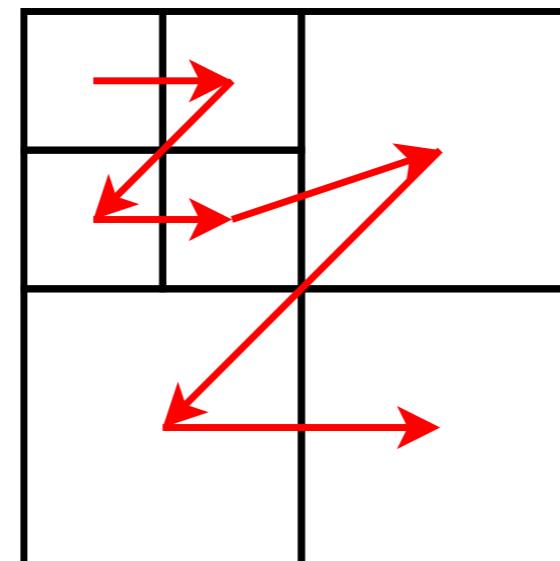
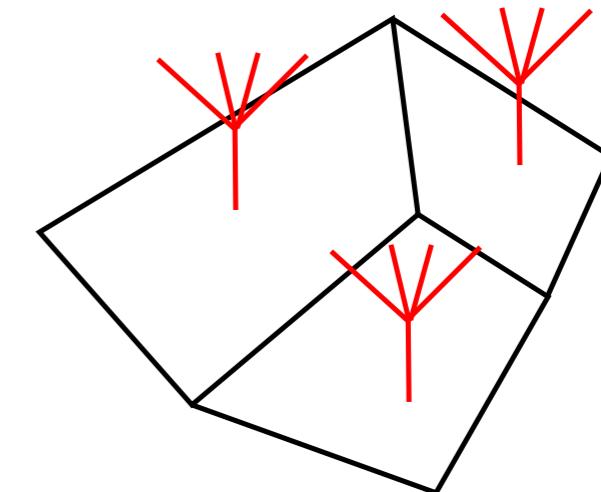


Optimal partitioning is an NP-hard  
**graph partitioning** problem.

- ❖ Typically done: heuristics (existing tools: METIS)
  - ❖ Problem: worse than linear runtime
  - ❖ Large graphs: several minutes, memory restrictions
- ~~ Alternative: avoid graph partitioning

# Partitioning with “Space filling curves”

- *p4est* library: parallel quad-/octrees
- Store refinement flags from a base mesh
- Based on space-filling curves
- Very good scalability



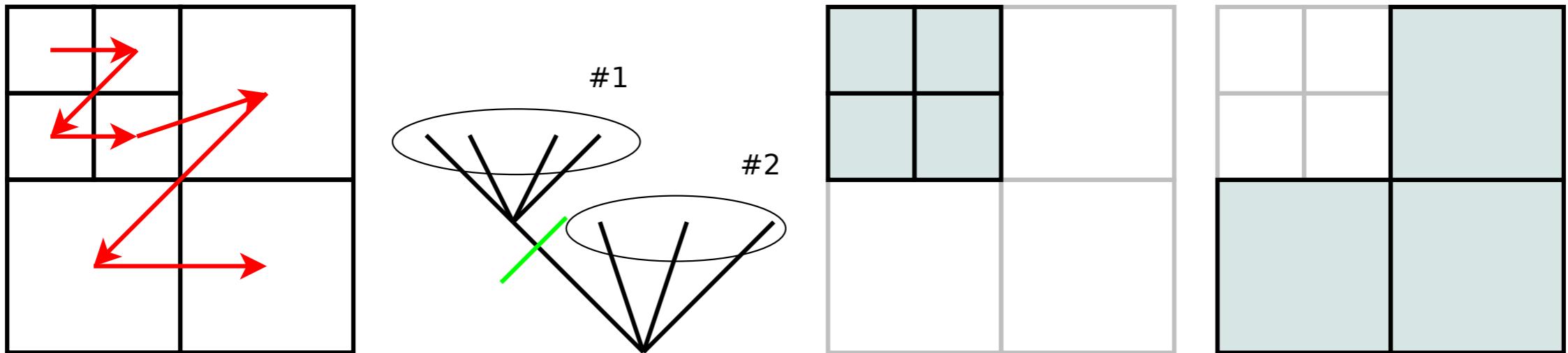
Burstedde, Wilcox, and Ghattas.

*p4est: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees.*

*SIAM J. Sci. Comput.*, 33 no. 3 (2011), pages 1103-1133.

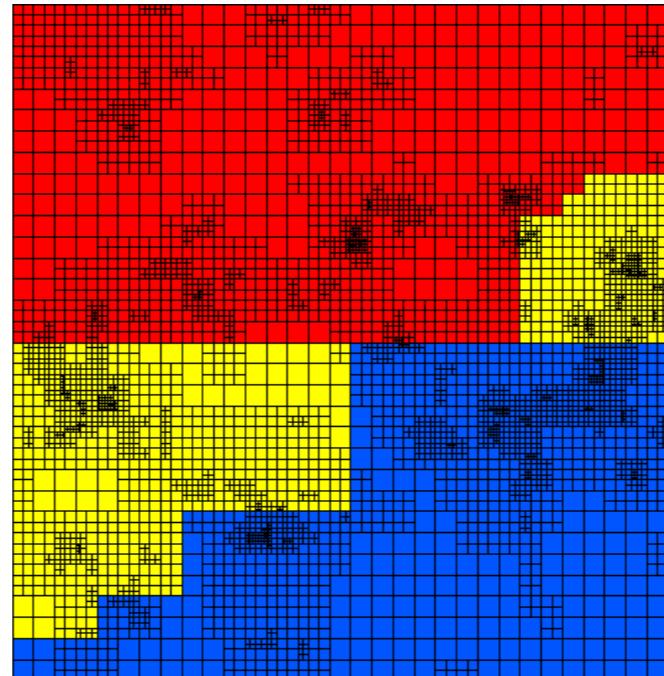
# Triangulation

- Partitioning is cheap and simple:

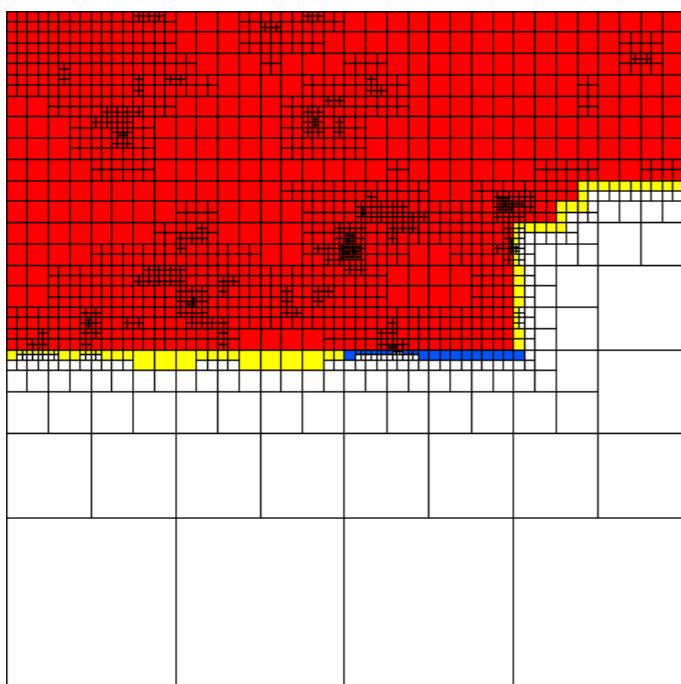


- Then: take *p4est* refinement information
- Recreate rich *deal.II* Triangulation only for local cells  
(stores coordinates, connectivity, faces, materials, . . .)
- How? recursive queries to *p4est*
- Also create ghost layer (one layer of cells around own ones)

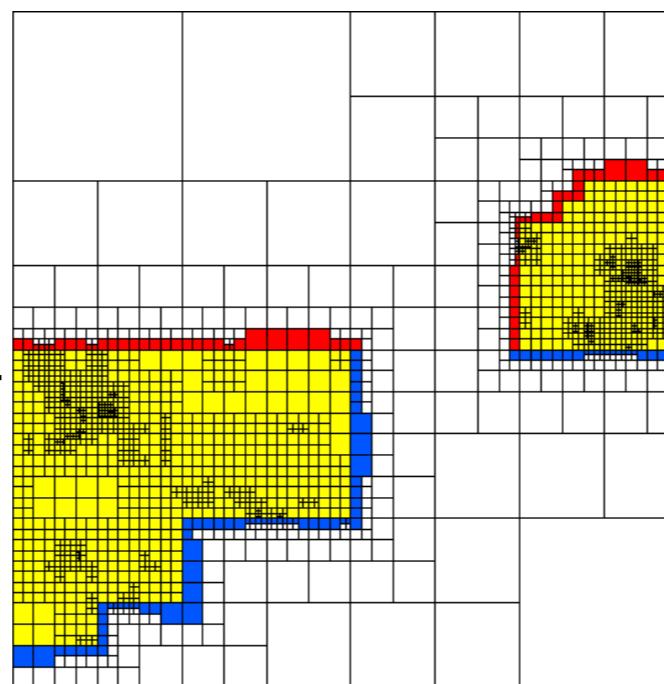
# Example (color by CPU ID)



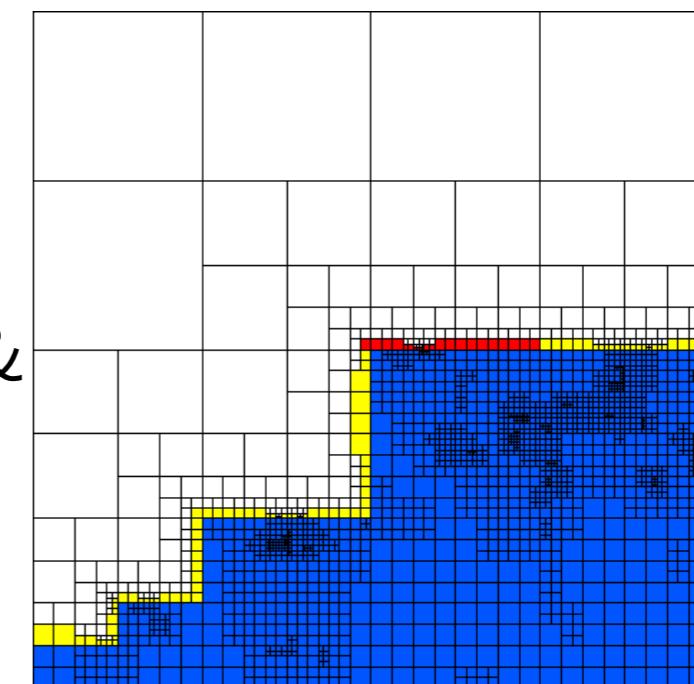
=



&



&



# What's needed?

## How to use?

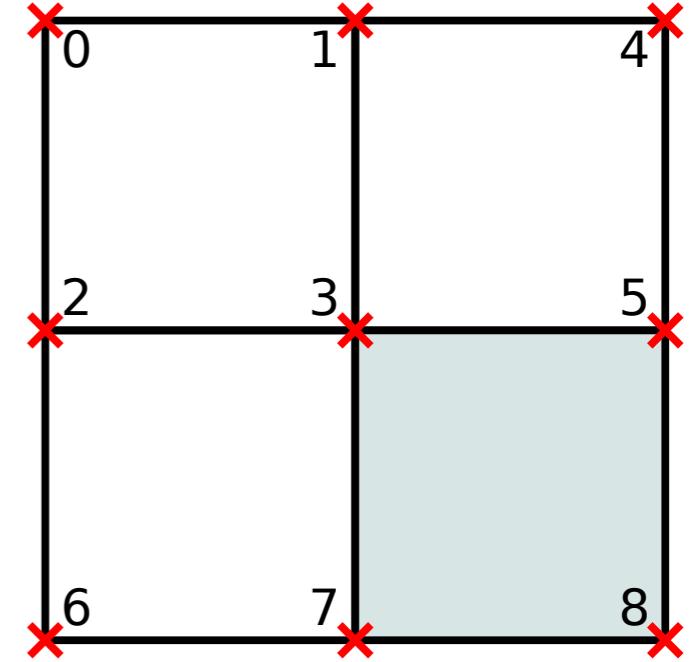
- ▶ Replace Triangulation by  
`parallel::distributed::Triangulation`
- ▶ Continue to load or create meshes as usual
- ▶ Adapt with `GridRefinement::refine_and_coarsen*` and  
`tr.execute_coarsening_and_refinement()`, etc.
- ▶ You can only look at own cells and ghost cells:  
`cell->is_locally_owned()`, `cell->is_ghost()`, or  
`cell->is_artificial()`
- ▶ Of course: dealing with DoFs and linear algebra changes!

# What's needed?

	serial mesh	dynamic parallel mesh	static parallel mesh
name	Triangulation	parallel::distributed ::Triangulation	(just an idea)
duplicated	everything	coarse mesh	nothing
partitioning	METIS	p4est: fast, scalable	offline, (PAR)METIS?
part. quality	good	okay	better?
hp?	yes	(planned)	yes?
geom. MG?	yes	in progress	?
Aniso. ref.?	yes	no	(offline only)
Periodicity	yes	in progress	?
Scalability	100 cores	16k+ cores	?

# Sketch...

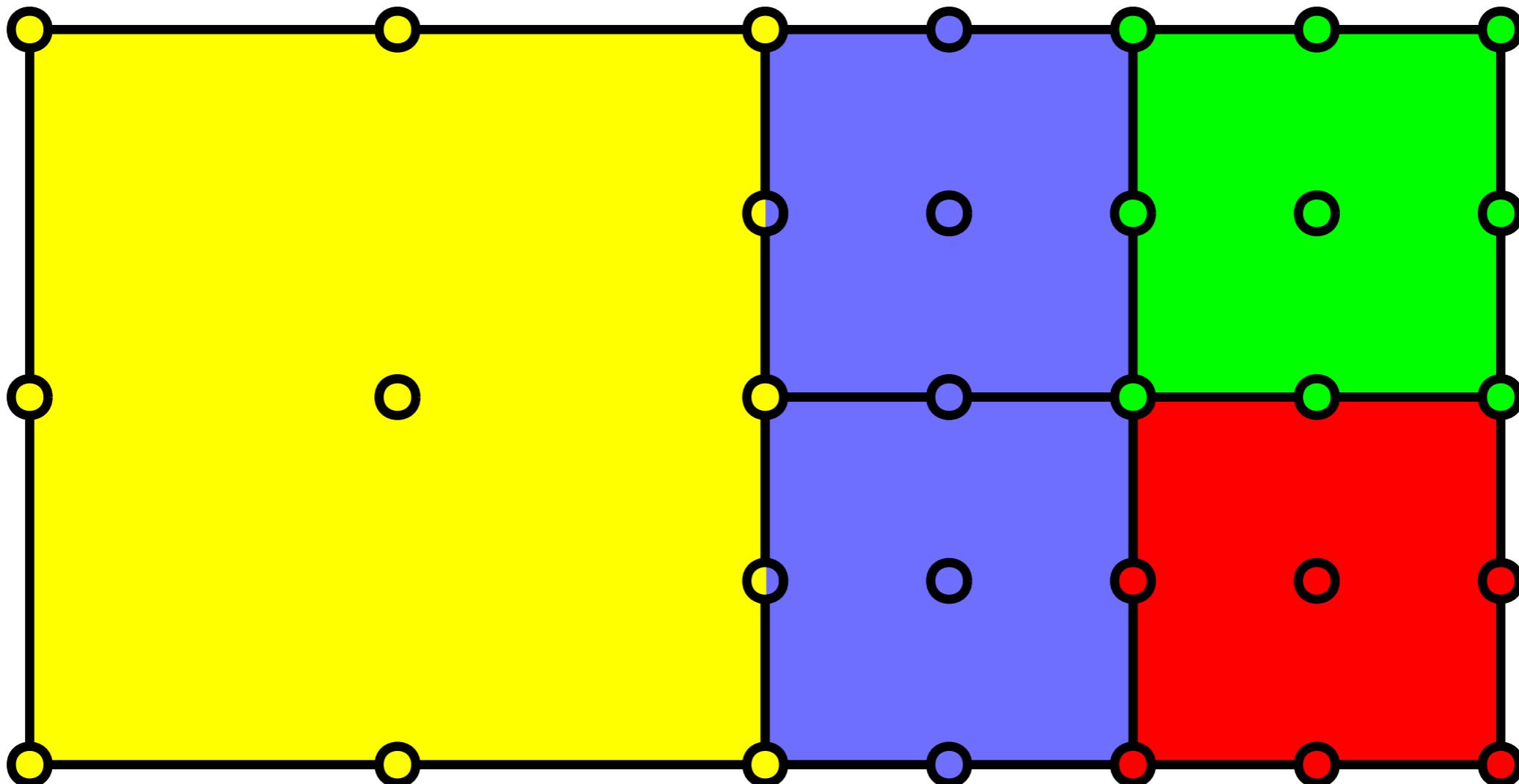
- ❖ Create global numbering for all DoFs
- ❖ Reason: identify shared ones
- ❖ Problem: no knowledge about the whole mesh



Sketch:

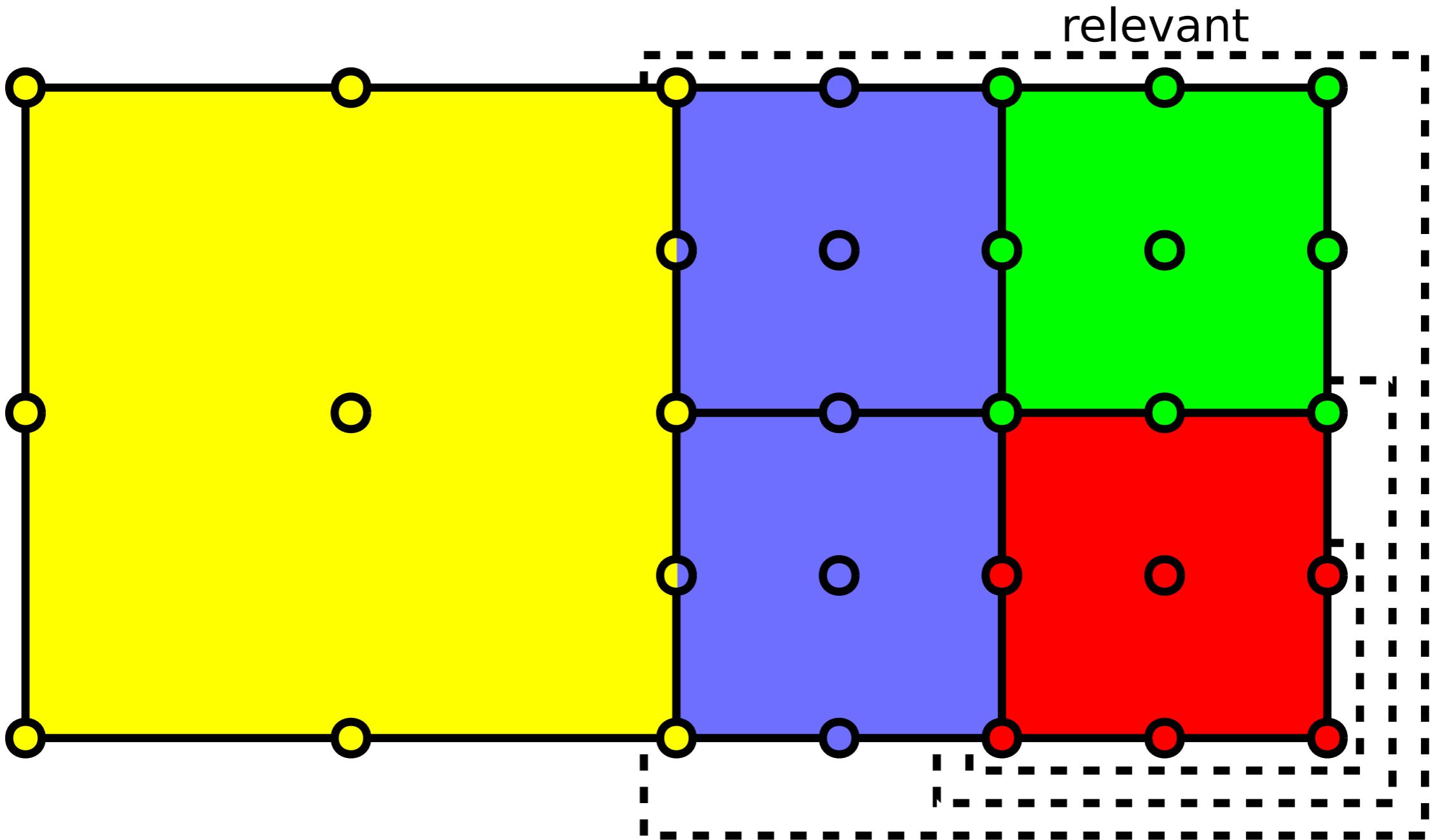
1. Decide on ownership of DoFs on interface (no communication!)
2. Enumerate locally (only own DoFs)
3. Shift indices to make them globally unique (only communicate local quantities)
4. Exchange indices to ghost neighbors

# Sketch...



- ❖ Example: Q2 element and ownership of DoFs
- ❖ What might red CPU be interested in?

# Sketch...



(perspective of the red CPU)

# Sketch...

- ❖ Each CPU has sets:
  - ❖ owned: we store vector and matrix entries of these rows
  - ❖ active: we need those for assembling, computing integrals, output, etc.
  - ❖ relevant: error estimation
- ❖ These set are subsets of  $\{0, \dots, n\_global\_dofs\}$
- ❖ Represented by objects of type IndexSet
- ❖ How to get? `DoFHandler::locally_owned_dofs()`,  
`DoFTools::extract_locally_relevant_dofs()`,  
`DoFHandler::locally_owned_dofs_per_processor()`, ...

# Sketch...

- reading from owned rows only (for both vectors and matrices)
- writing allowed everywhere (more about compress later)
- what if you need to read others?
- Never copy a whole vector to each machine!
- instead: **ghosted vectors**

# Sketch...

- ❖ read-only
- ❖ create using  
`Vector(IndexSet owned, IndexSet ghost, MPI_COMM)`  
where ghost is relevant or active
- ❖ copy values into it by using `operator=(Vector)`
- ❖ then just read entries you need



# Compressing

## 🐾 Why?

- 🐾 After writing into foreign entries communication has to happen
- 🐾 All in one go for performance reasons

## 🐾 How?

- 🐾 `object.compress (VectorOperation::add);` if you added to entries
- 🐾 `object.compress (VectorOperation::insert);` if you set entries
- 🐾 This is a collective call

## 🐾 When?

- 🐾 After the assembly loop (with `::add`)
- 🐾 After you do `vec(j) = k;` or `vec(j) += k;` (and in between add/insert groups)
- 🐾 In no other case (all functions inside deal.II compress if necessary)!  
**(this is new!)**



# Trilinos VS PETSc

What should I use?

- Similar features and performance
- Pro Trilinos: more development, some more features (automatic differentiation, . . . ), cooperation with deal.II
- Pro PETSc: stable, easier to compile on older clusters
- But: being flexible would be better! – “why not both?”
  - you can! Example: new step-40
  - can switch at compile time
  - need #ifdef in a few places (different solver parameters TrilinosML vs BoomerAMG)
  - some limitations, somewhat work in progress



# Trilinos VS PETSc

```

#include <deal.II/lac/generic_linear_algebra.h>
#define USE_PETSC_LA // uncomment this to run with Trilinos

namespace LA
{
#ifndef USE_PETSC_LA
    using namespace dealii::LinearAlgebraPETSc;
#else
    using namespace dealii::LinearAlgebraTrilinos;
#endif
}

// ...
LA::MPI::SparseMatrix system_matrix;
LA::MPI::Vector solution;

// ...
LA::SolverCG solver(solver_control, mpi_communicator);
LA::MPI::PreconditionAMG preconditioner;

LA::MPI::PreconditionAMG::AdditionalData data;

#ifndef USE_PETSC_LA
    data.symmetric_operator = true;
#else
    // trilinos defaults are good
#endif
    preconditioner.initialize(system_matrix, data);

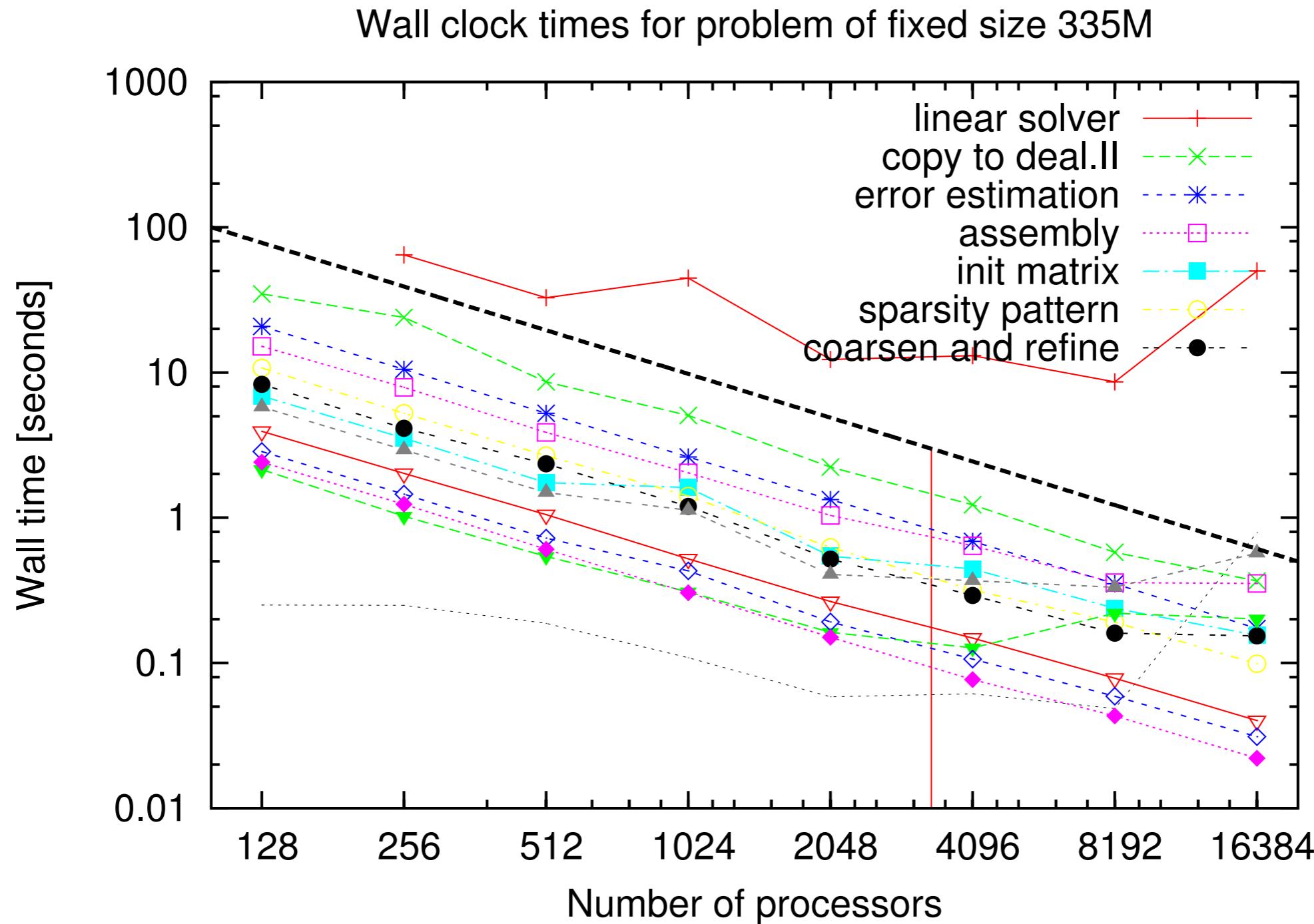
// ...

```

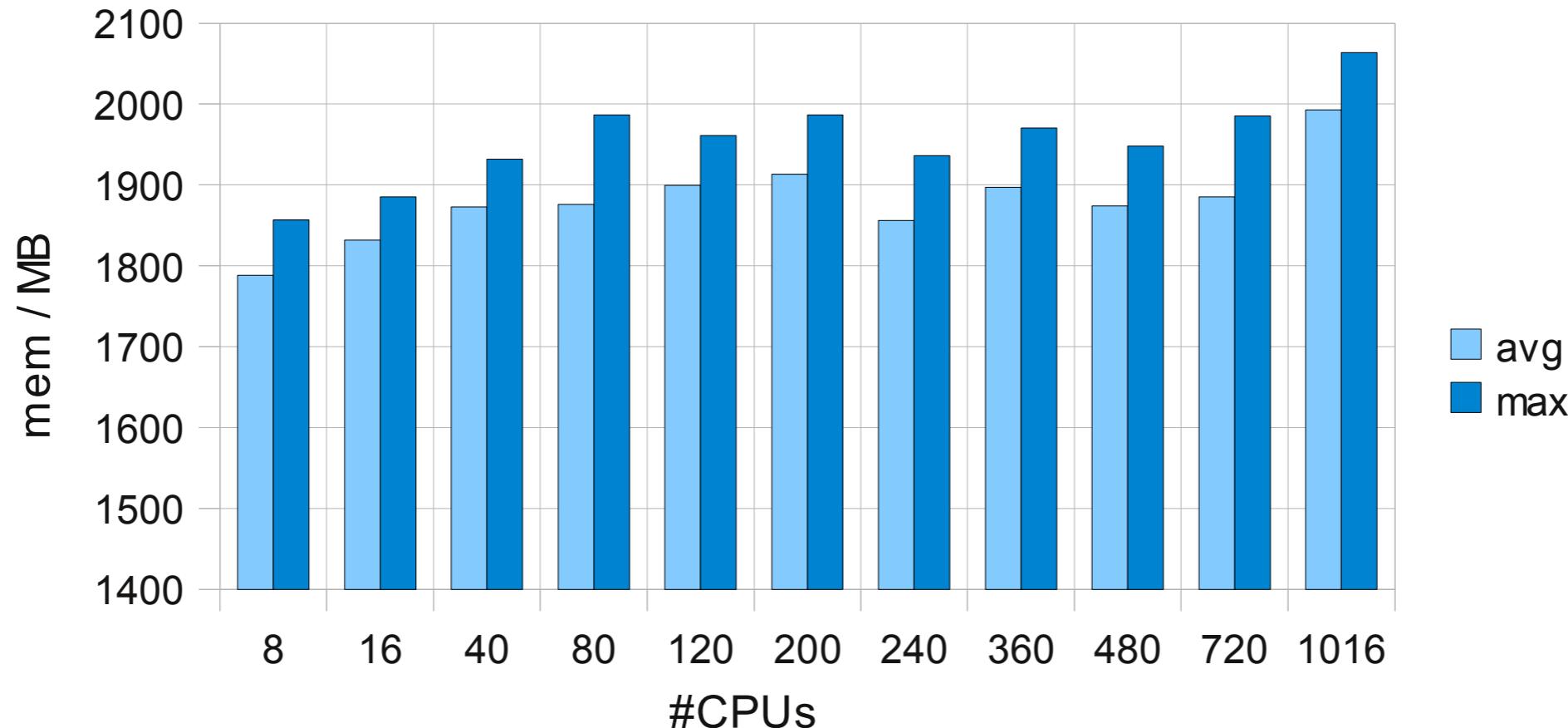
# Solvers

- ✿ Iterative solvers only need Mat-Vec products and scalar products  
~~> equivalent to serial code
- ✿ Can use templated deal.II solvers like GMRES!
- ✿ Better: use tuned parallel iterative solvers that hide/minimize communication
- ✿ Preconditioners: more work, just operating on local blocks not enough

# Strong Scaling: 2d Poisson



# Memory Consumption

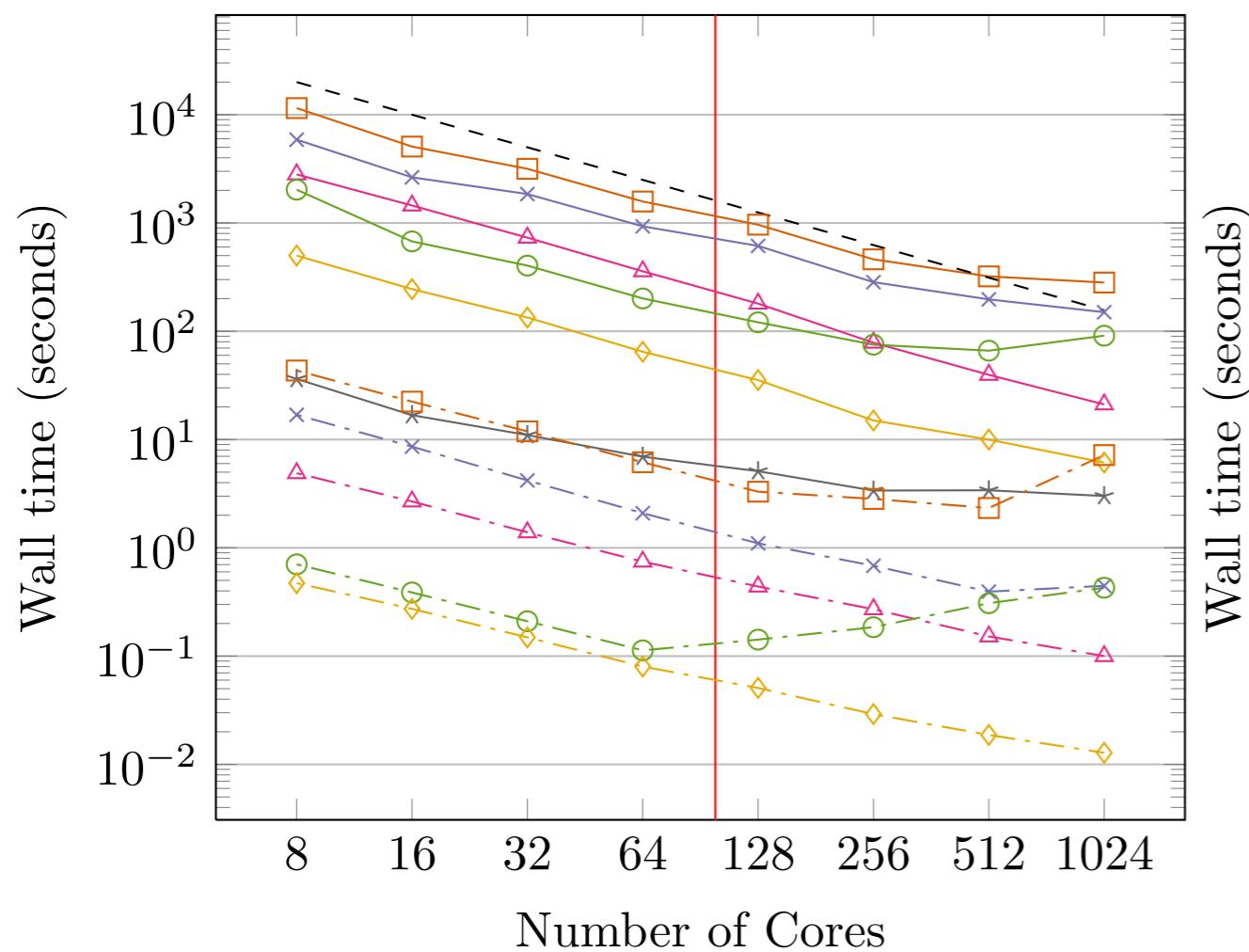


average and maximum memory consumption (VmPeak)  
 3D, weak scalability from 8 to 1000 processors with about 500.000  
 DoFs per processor (4 million up to 500 million total)

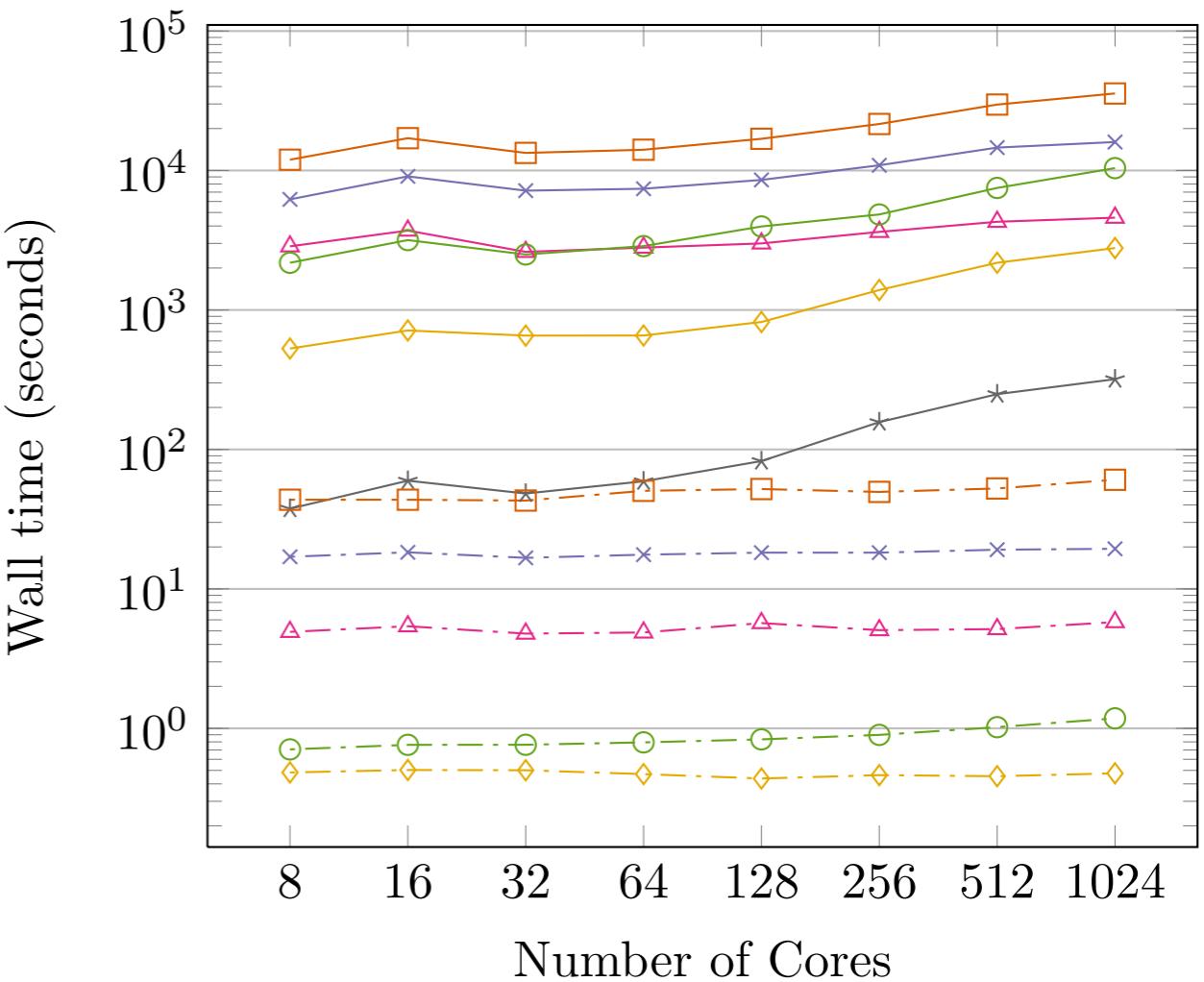
~~> Constant memory usage with increasing  
 # CPUs & problem size

# Step 40

Strong Scaling (9.9M DoFs)



Weak Scaling (1.2M DoFs/Core)



<span style="color: orange;">◻</span>	TOTAL	<span style="color: blue;">✖</span>	Solve: iterate	<span style="color: pink;">▲</span>	Assembling	<span style="color: green;">○</span>	Solve: setup
<span style="color: yellow;">◊</span>	Residual	<span style="color: black;">*</span>	update active set	<span style="color: orange;">□</span>	Setup: refine mesh	<span style="color: blue;">✖</span>	Setup: matrix
<span style="color: pink;">△</span>	Setup: distribute DoFs	<span style="color: green;">○</span>	Setup: vectors	<span style="color: yellow;">◊</span>	Setup: constraints		