Lecture 4: Solving Poisson's Equation

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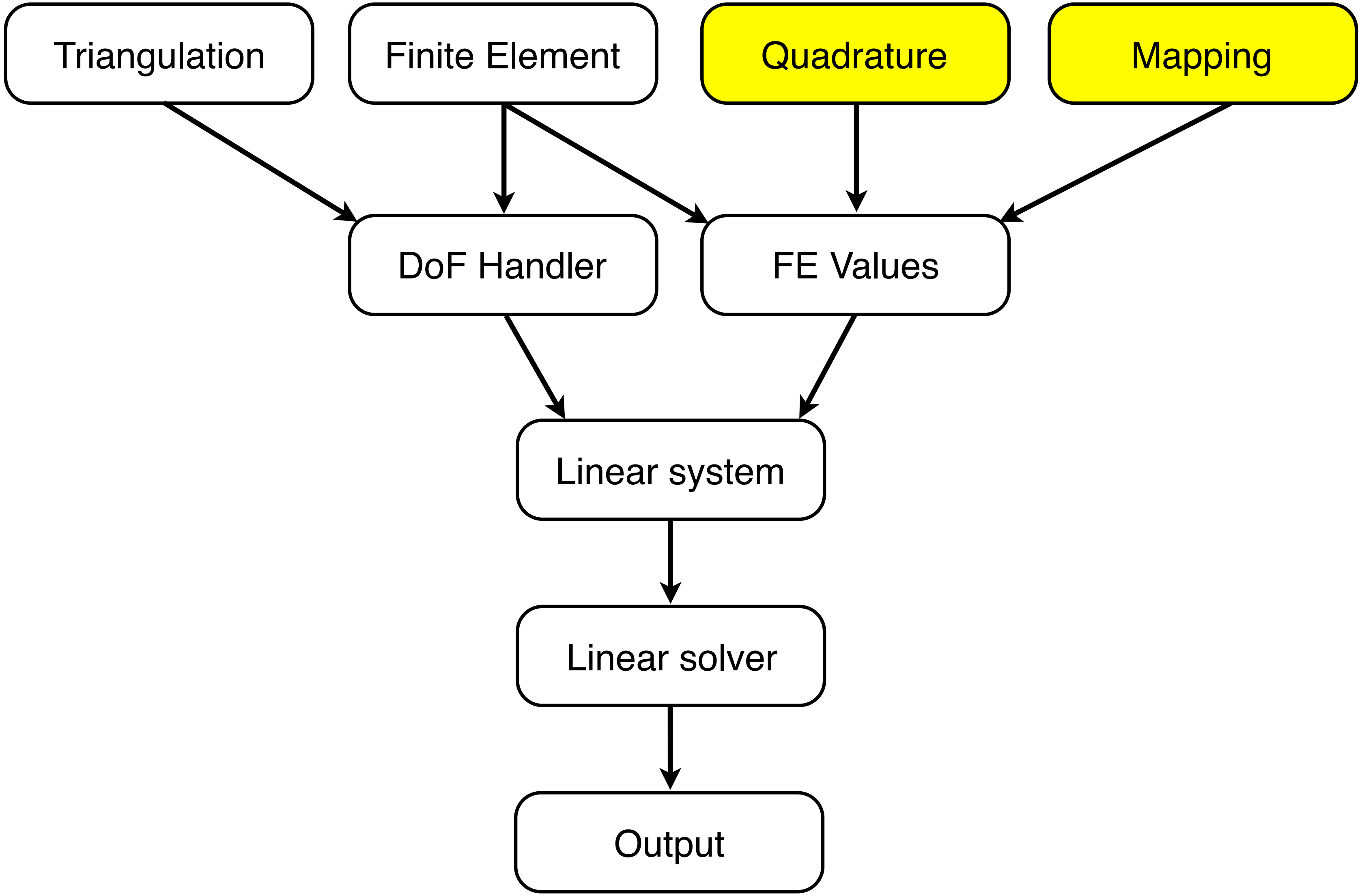
Aims for this module

- 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/current/doxygen/deal.II/step_3.html
- Documentation
  - https://www.dealii.org/current/doxygen/deal.II/group__FE__vs__Mapping__vs__FEValues.html
  - https://www.dealii.org/current/doxygen/deal.II/group__UpdateFlags.html

Structure of a prototypical FE problem



Master in High Performance Computing

Matrix form

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

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

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

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

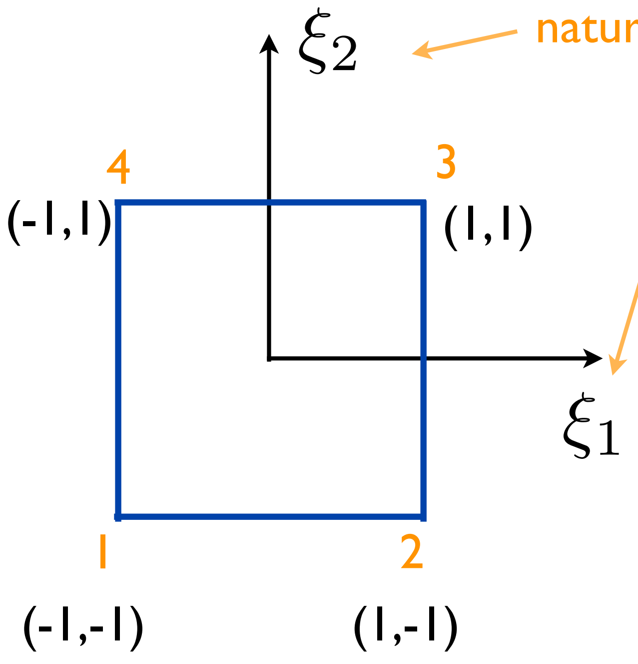
need to evaluate integrals numerically

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

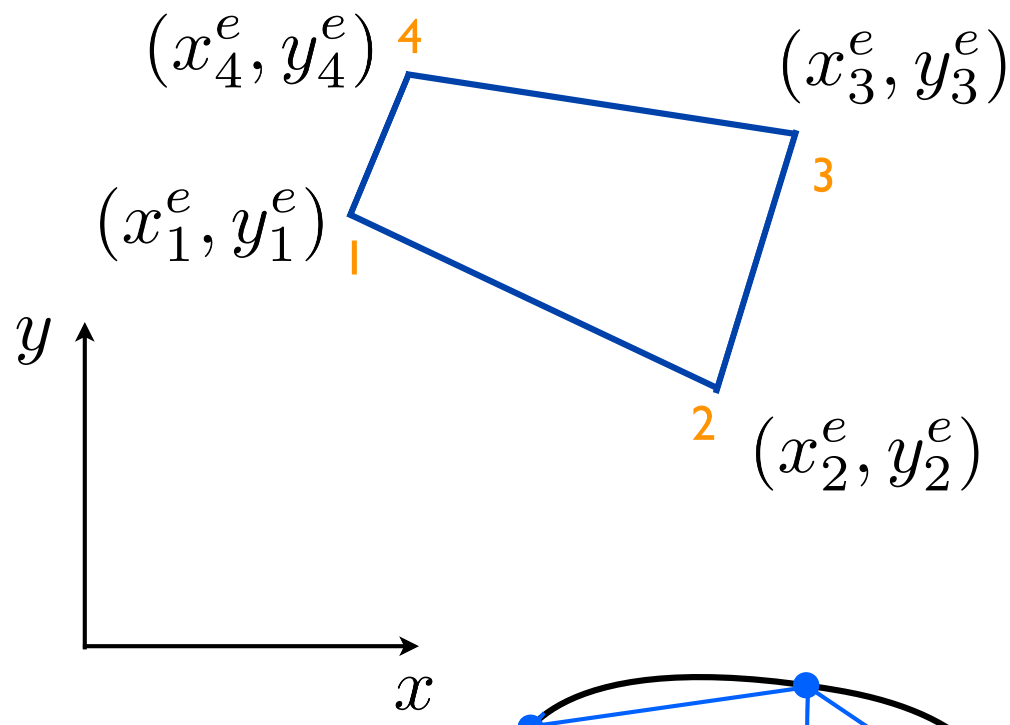
$$(N_i, f) := \sum_K \int_{\Omega_K} N_i f(\mathbf{x}) \mathrm{d}v \qquad (w, h)_{\partial\Omega} := \sum_K \int_{\partial\Omega_K^N} whds$$

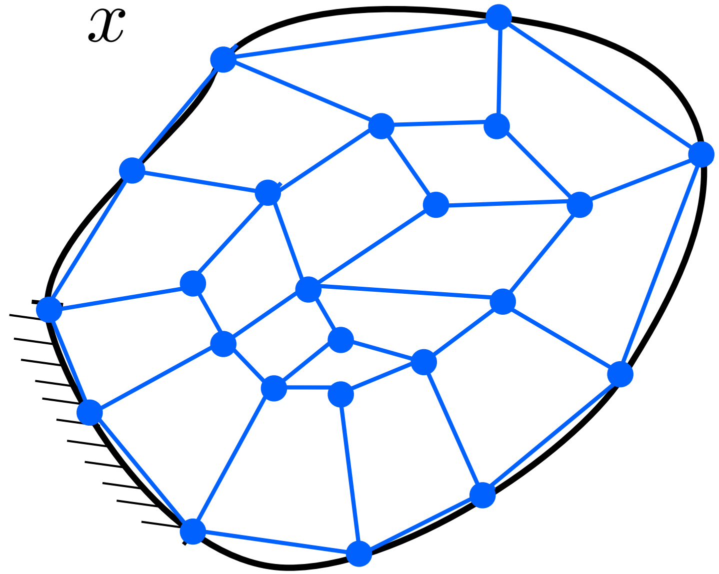
Q1 mapping

natural coordinates



reference element





we can construct the mapping
between the two elements

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

Bilinear Quadrilateral Element

Bilinear expansion

$$x(\xi_1,\xi_2) =: \alpha_0 + \alpha_1\xi_1 + \alpha_2\xi_2 + \alpha_3\xi_1\xi_2$$
$$y(\xi_1,\xi_2) =: \beta_0 + \beta_1\xi_1 + \beta_2\xi_2 + \beta_3\xi_1\xi_2$$

+

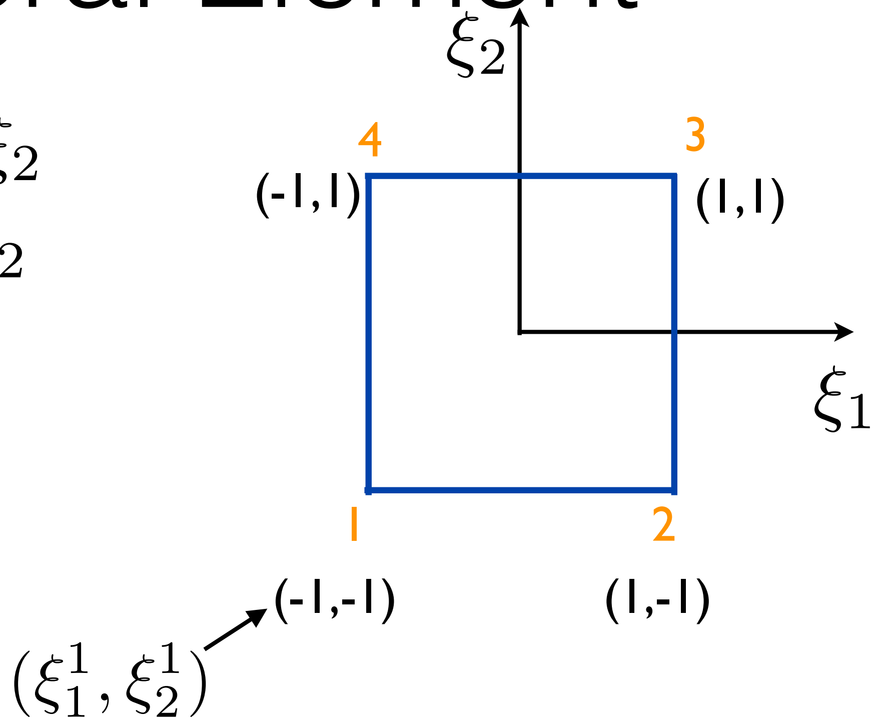
$$x(\xi_1^a,\xi_2^a) = x_a^e \qquad a = \overline{1,4}$$
$$y(\xi_1^a,\xi_2^a) = y_a^e$$

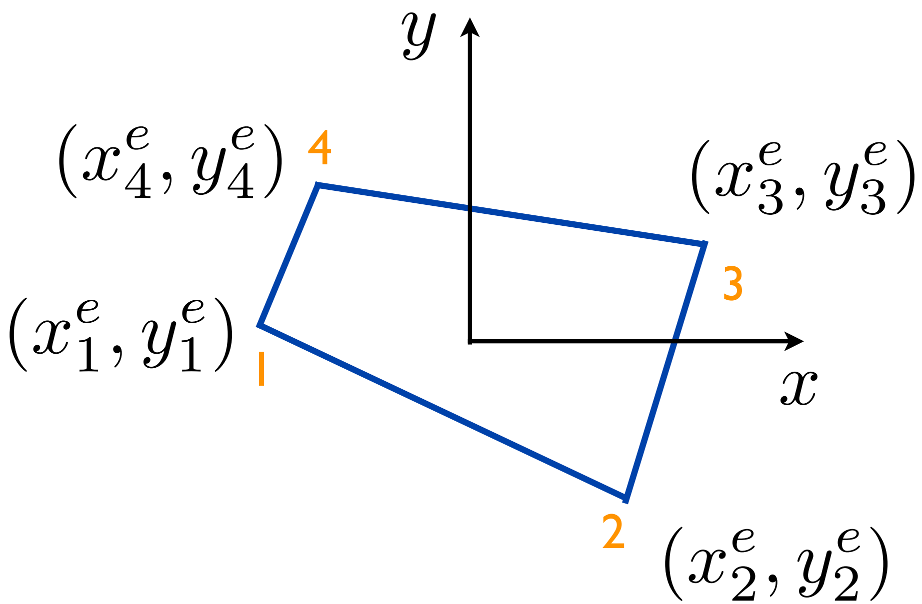
=

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

maps any point in the reference element to the actual element

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





Mapping to the reference element:

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

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

$$\mathrm{d}v = \det(\mathbf{J}_K)\mathrm{d}\hat{v}$$

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

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

$$a(N_i, N_j) = \sum_K \int_{\Omega_K} \mathrm{grad}\, N_i(\mathbf{x}) \cdot \mathrm{grad}\, N_j(\mathbf{x})\mathrm{d}v$$

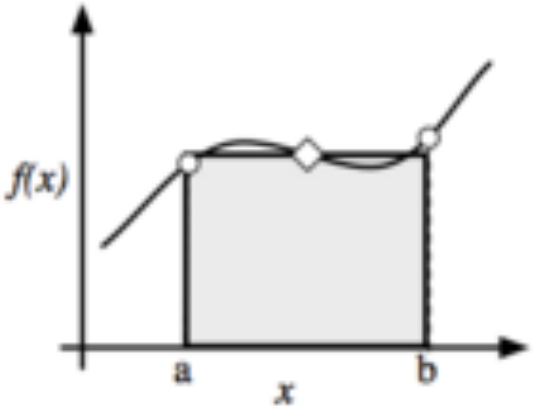
$$= \sum_K \int_{\hat{\Omega}_K} [\widehat{\mathrm{grad}}\ \widehat{N}_i(\xi)\cdot\mathbf{J}_K^{-1}(\xi)]\cdot[\widehat{\mathrm{grad}}\ \widehat{N}_j(\xi)\cdot\mathbf{J}_K^{-1}(\xi)]\det(\mathbf{J}_K(\xi))\mathrm{d}\hat{v}$$

$$\approx \sum_K \sum_q [\widehat{\mathrm{grad}}\ \widehat{N}_i(\xi_q)\cdot\mathbf{J}_K^{-1}(\xi_q)]\cdot[\widehat{\mathrm{grad}}\ \widehat{N}_j(\xi_q)\cdot\mathbf{J}_K^{-1}(\xi_q)]\det(\mathbf{J}_K(\xi_q))w_q$$

do not depend on a particular cell

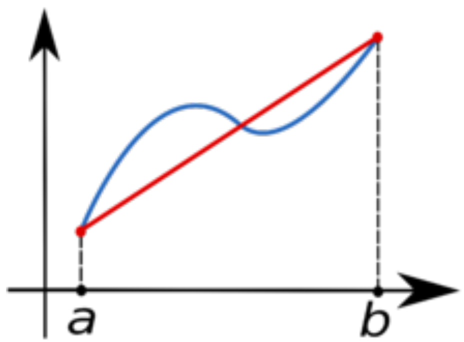
Integration rules:

1. midpoint



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

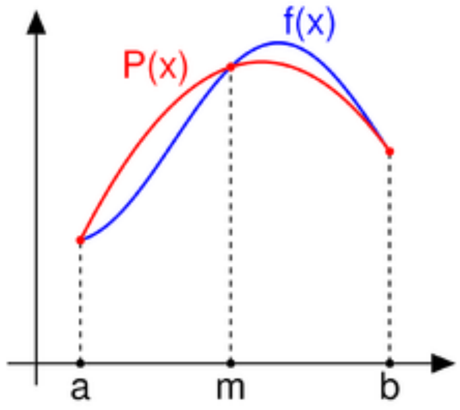
2. trapezoidal



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

Integration rules:

3. Simpson



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

4. Gauss quadrature rule

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

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

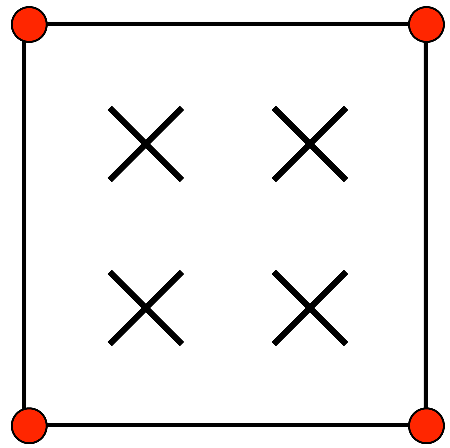
n_q	x_1	x_2	x_3	w_1	w_2	w_3
1	0			2		
2	$-1/\sqrt{3}$	$1/\sqrt{3}$		1	1	
3	$-\sqrt{3/5}$	0	$\sqrt{3/5}$	$5/9$	$8/9$	$5/9$

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

Integration on a cell: the Quadrature classes

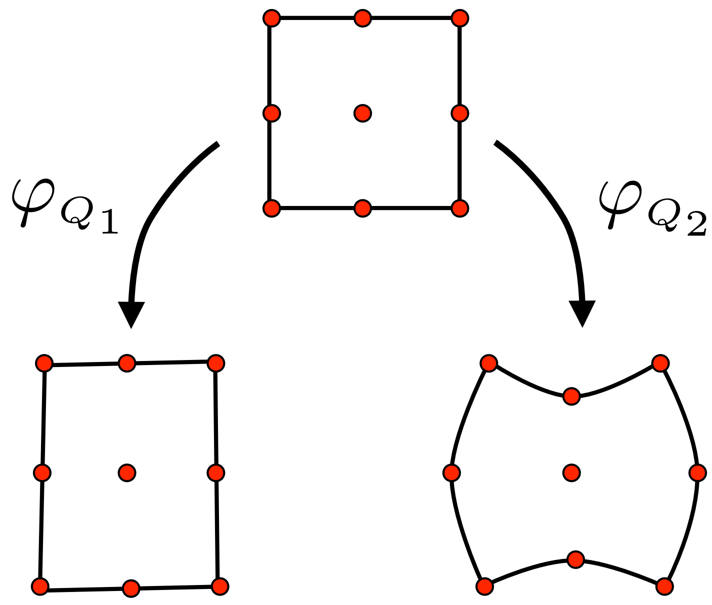
- QGauss<dim> n-Order Gauss quadrature
- Other rules
  - QGaussLobattom<dim> Gauss Lobatto
  - QSimpson<dim> Simpson
  - QTrapez<dim> Trapezoidal
  - QMidpoint Midpoint
  - …

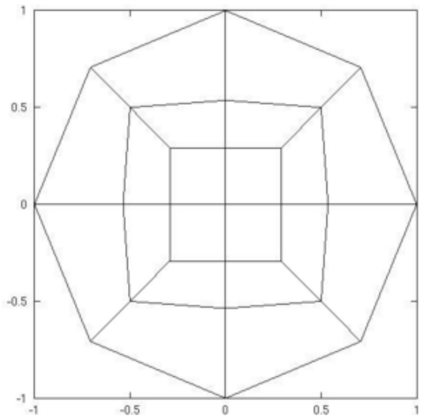
`FE_Q<2>(1)`

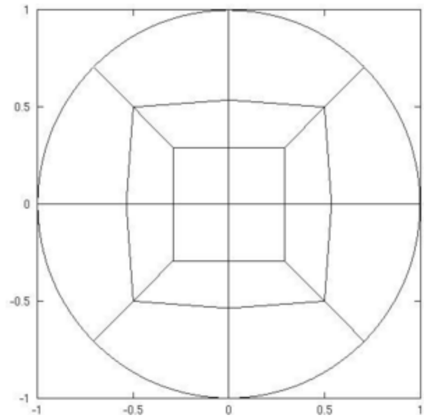


Integration on a cell: the Mapping classes

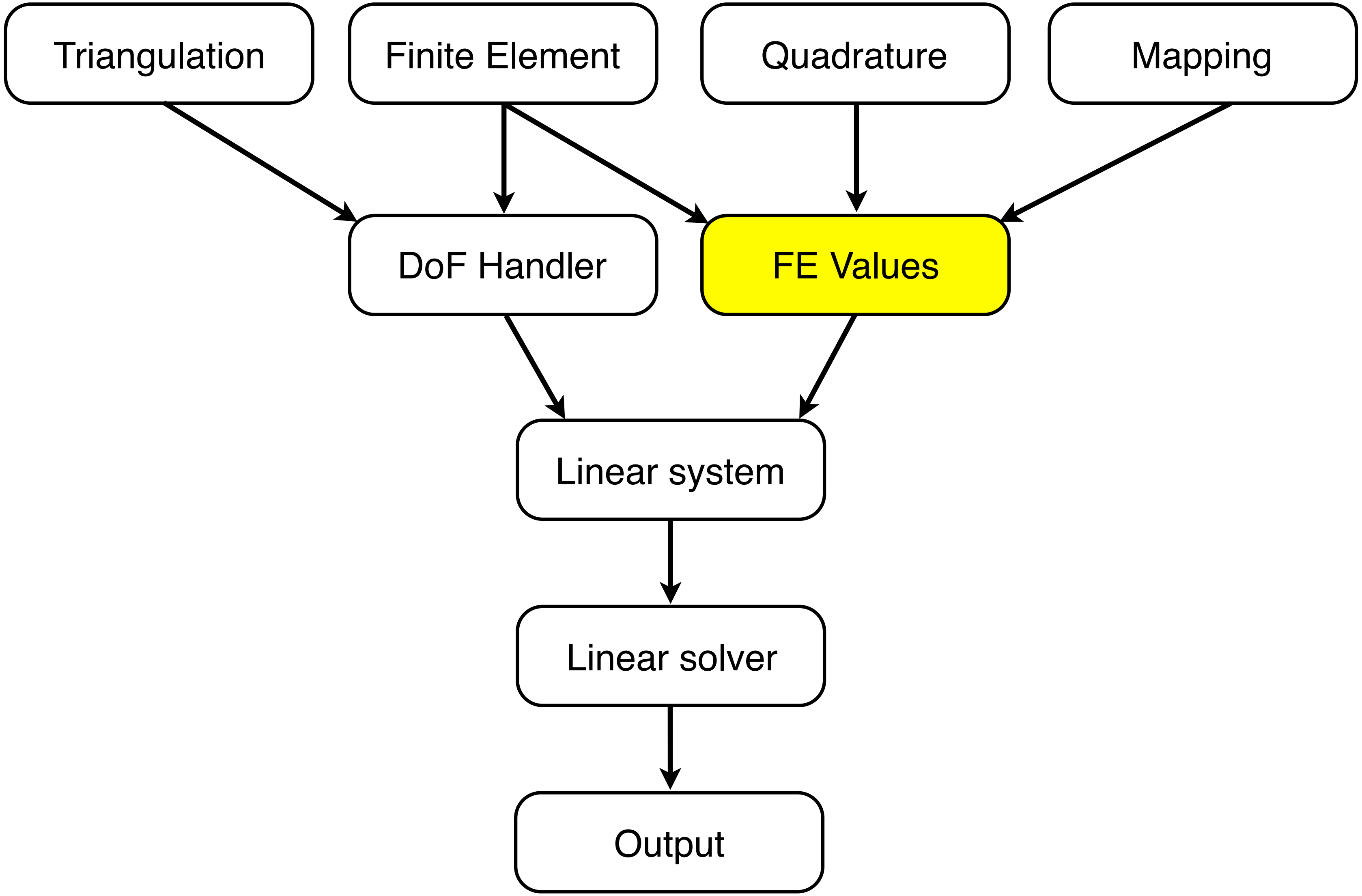
- n-order mappings
  - Increase accuracy of:
    - Integration schemes
    - Surface basis vectors
- Lagrangian / Eulerian
  - Latter useful for fluid and contact problems, data visualization
- Boundary and interior manifolds







Structure of a prototypical FE problem



Integration on a cell: the FEValues class

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

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

$$J_K = \frac{\partial \mathbf{X}^\xi}{\partial \mathbf{X}}$$

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

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

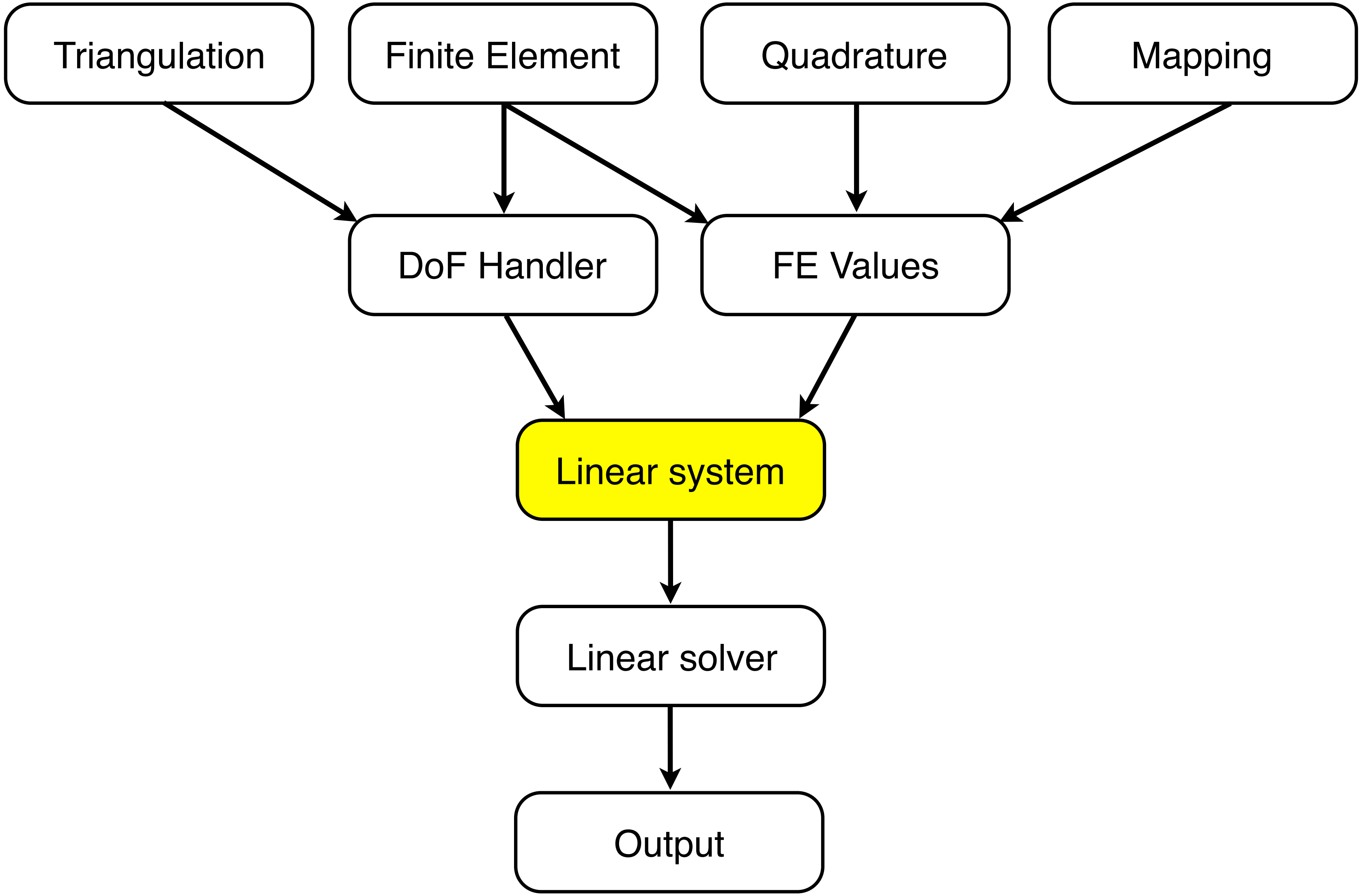
Integration on a cell: the FEValues class

- 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

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

```
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



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)

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

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

$$\left(K_{11} - K_{12}K_{22}^{-1}K_{21}\right) d_1 = F_1 - K_{12}K_{22}^{-1}F_2$$

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

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

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

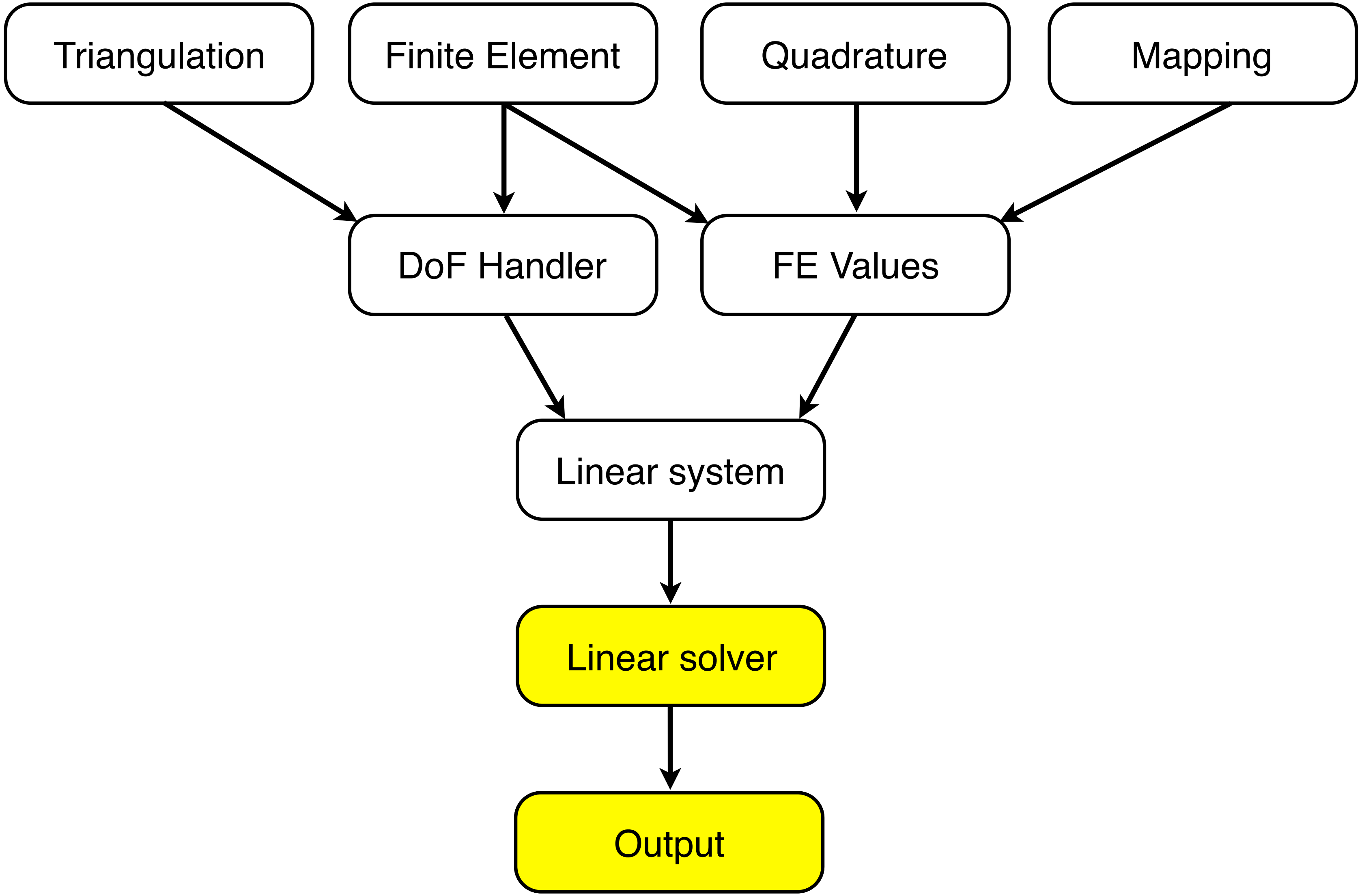
$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \end{Bmatrix} = \begin{Bmatrix} F_1 \\ F_2 \end{Bmatrix}$$

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

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

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

Structure of a prototypical FE problem



Solving Poisson's equation

- Demonstration: Step-3
  https://www.dealii.org/current/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