Master in High Performance Computing

Numerical Solution of PDEs using the Finite Element Method

A Poisson solver - deal.II step-3

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Aims for this Lecture

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

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

Recap of Poisson Problem

Variational, continuous problem, infinte dimensional space:

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f v \qquad \forall v \in H^1_0(\Omega)$$

Variational, discrete problem, finite dimensional space:

$$\int_\Omega \nabla u_h \cdot \nabla v_h = \int_\Omega f v_h \qquad \forall v_h \in V_h \subset H^1_0(\Omega)$$

Recap of Poisson Problem

$$\int_\Omega \nabla u_h \cdot \nabla v_h = \int_\Omega f v_h \qquad \forall v_h \in V_h = \text{span}\{v_i\}_{i=1}^N$$

$$\Longleftrightarrow$$

$$A_{ij} u^j = F_i \qquad u_h := u^i v_i$$

$$A_{ij} := \int_\Omega \nabla v_j \nabla v_i \qquad F_i := \int_\Omega f v_i$$

Split Assembly on cells

$$A_{ij} := \int_\Omega \nabla v_j \cdot \nabla v_i d\Omega \qquad F_i := \int_\Omega f v_i d\Omega$$

$$A_{ij} = \sum_m \int_{T_m} \nabla v_j \cdot \nabla v_i dT_m$$

To make this efficiently, we need a smart way to map local dofs to global dofs

Split Assembly on cells

$$A_{ij} = \sum_m \int_{T_m} \nabla v_j \cdot \nabla v_i dT_m = \sum_m \int_{\hat{T}} [(\nabla v_j) \circ F_m] \cdot [(\nabla v_i) \circ F_m] J_m d\hat{T}$$

$$v_i \circ F_m |_{T_m} = \sum_\alpha P_{mi\alpha} \hat{v}_\alpha$$

$$P_{mi\alpha} = \begin{cases} 1 & \text{if local dof } \alpha \text{ on element } T_m \text{ maps to global dof } i \\ 0 & \text{otherwise} \end{cases}$$

Split Assembly on cells

$$A_{ij} = \sum_m \int_{T_m} \nabla v_j \cdot \nabla v_i dT_m = \sum_m \int_{\hat{T}} [(\nabla v_j) \circ F_m] \cdot [(\nabla v_i) \circ F_m] J_m d\hat{T}$$

$$A_{ij} = \sum_m \sum_\alpha \sum_\beta P_{mi\alpha} \int_{\hat{T}} [(DF_m^{-T} \hat{\nabla} \hat{v}_\alpha)] \cdot [DF_m^{-T} (\hat{\nabla} \hat{v}_\beta)] J_m d\hat{T} \; P_{mj\beta}$$

$$A_{ij} = \sum_m \sum_\alpha \sum_\beta \sum_q P_{mi\alpha} [(DF_m^{-T} \hat{\nabla} \hat{v}_\alpha)](\hat{x}_q) \cdot [DF_m^{-T} (\hat{\nabla} \hat{v}_\beta)](\hat{x}_q) J_m(\hat{x}_q) w_q \; P_{mj\beta}$$

$m \in [0, N_{\text{cell}})$ $\alpha, \beta \in [0, N_{\text{localdofs}})$ $i, j \in [0, N_{\text{dofs}})$ $q \in [0, N_{\text{qpoints}})$

Local VS global matrix

$$A_{ij} = \sum_m \int_{T_m} \nabla v_j \cdot \nabla v_i dT_m = \sum_m \int_{\hat{T}} [(\nabla v_j) \circ F_m] \cdot [(\nabla v_i) \circ F_m] J_m d\hat{T}$$

$$A_{ij} = \sum_m \sum_\alpha \sum_\beta \sum_q P_{mi\alpha} [(DF_m^{-T} \hat{\nabla} \hat{v}_\alpha)](\hat{x}_q) \cdot [DF_m^{-T} (\hat{\nabla} \hat{v}_\beta)](\hat{x}_q) J_m(\hat{x}_q) w_q \; P_{mj\beta}$$

$$a_{m\;\alpha\beta} := \sum_q [(DF_m^{-T} \hat{\nabla} \hat{v}_\alpha)](\hat{x}_q) \cdot [DF_m^{-T} (\hat{\nabla} \hat{v}_\beta)](\hat{x}_q) J_m(\hat{x}_q) w_q$$

$$A = \sum_m P_m^T a_m P_m$$

Local VS global right-hand-side

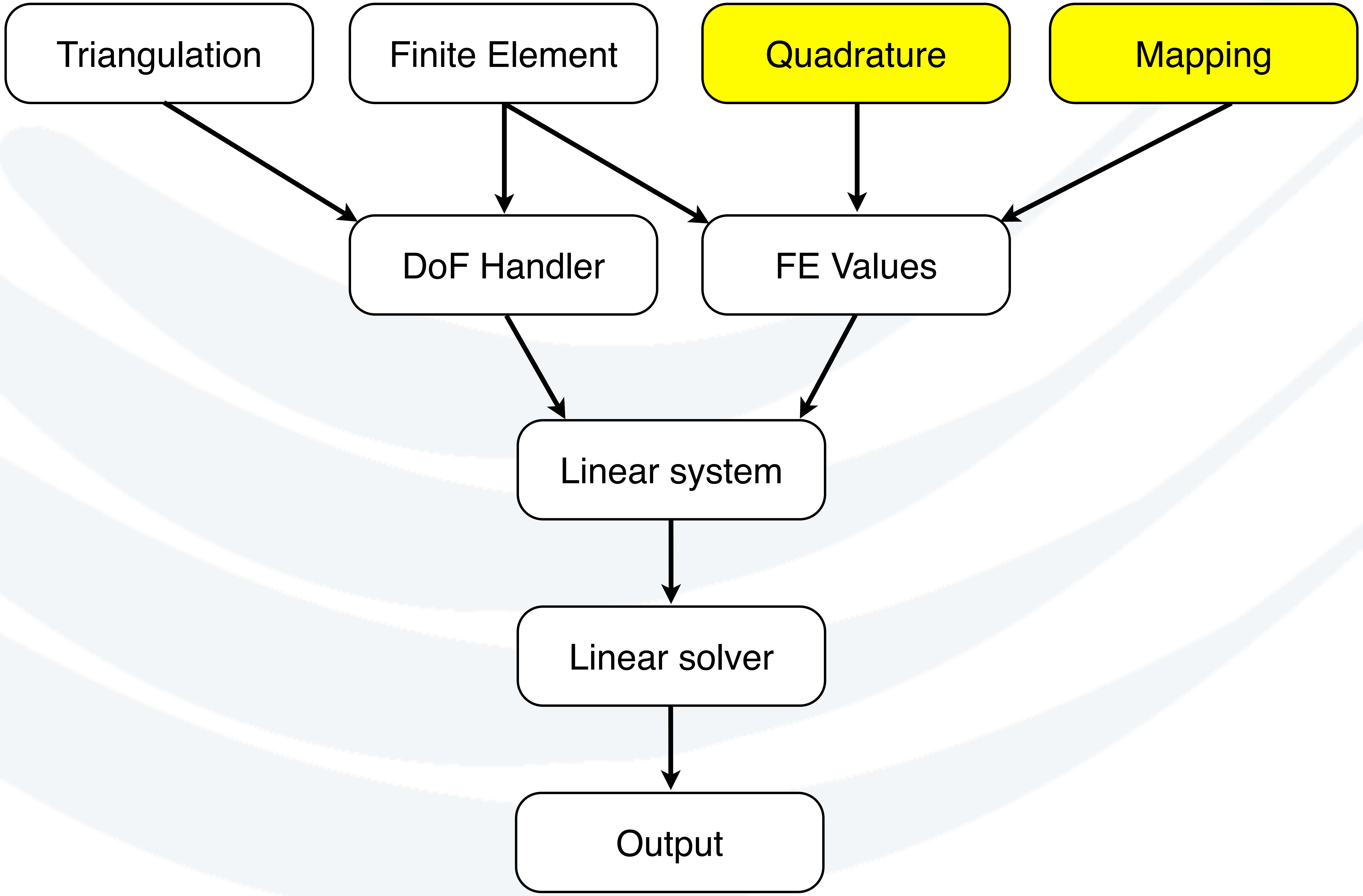
$$F_i = \sum_m \int_{T_m} f v_i dT_m = \sum_m \int_{\hat{T}} [f \circ F_m][v_i \circ F_m] J_m d\hat{T}$$

$$F_i = \sum_m \sum_\alpha \sum_q P_{mi\alpha} [f \circ F_m](\hat{x}_q) \hat{v}_\alpha(\hat{x}_q) J_m(\hat{x}_q) w_q$$

$$f_{m\ \alpha} := \sum_\alpha \sum_q [f \circ F_m](\hat{x}_q) \hat{v}_\alpha(\hat{x}_q) J_m(\hat{x}_q) w_q$$

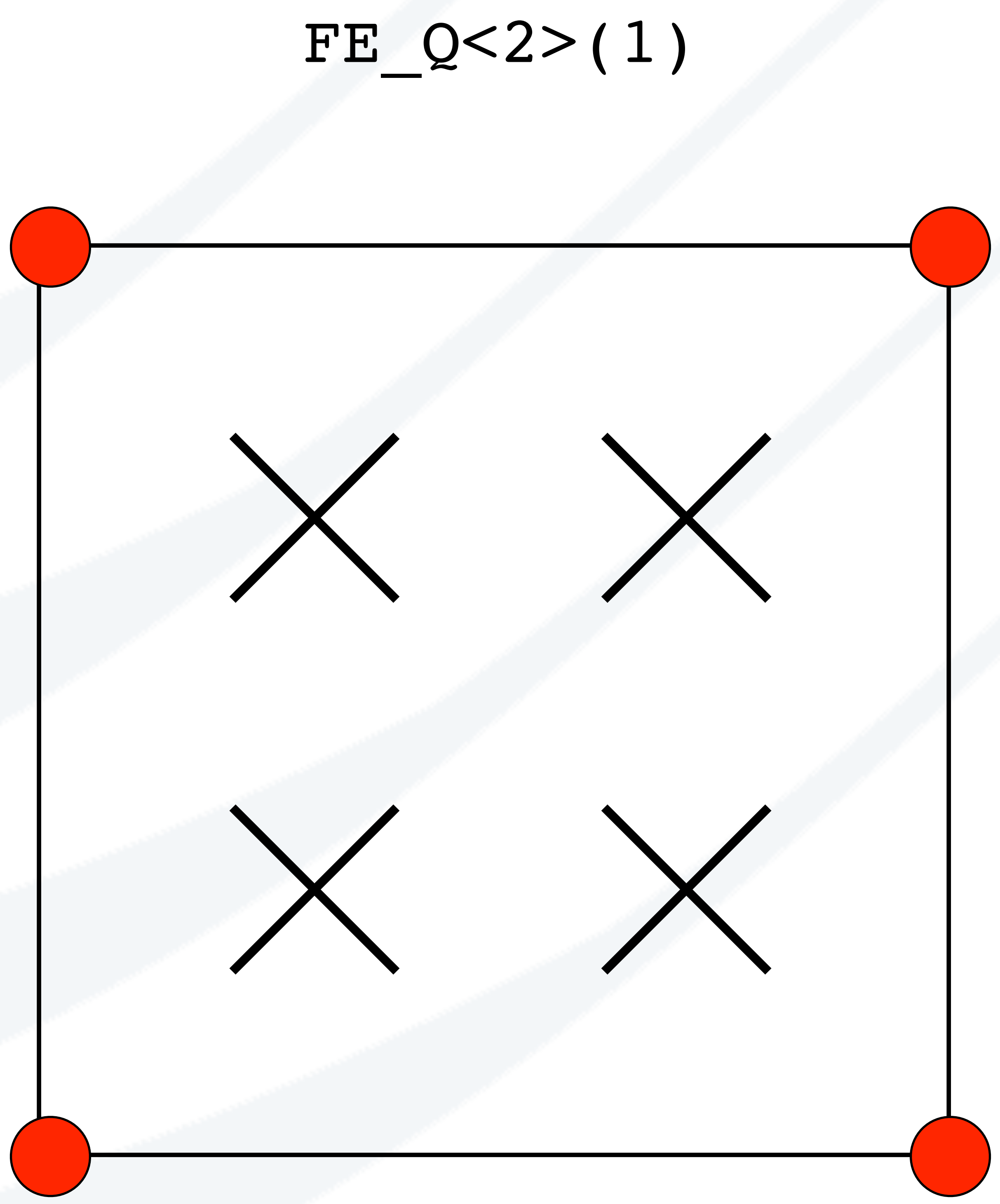
$$F = \sum_m P_m^T f_m$$

Structure of a prototypical FE problem



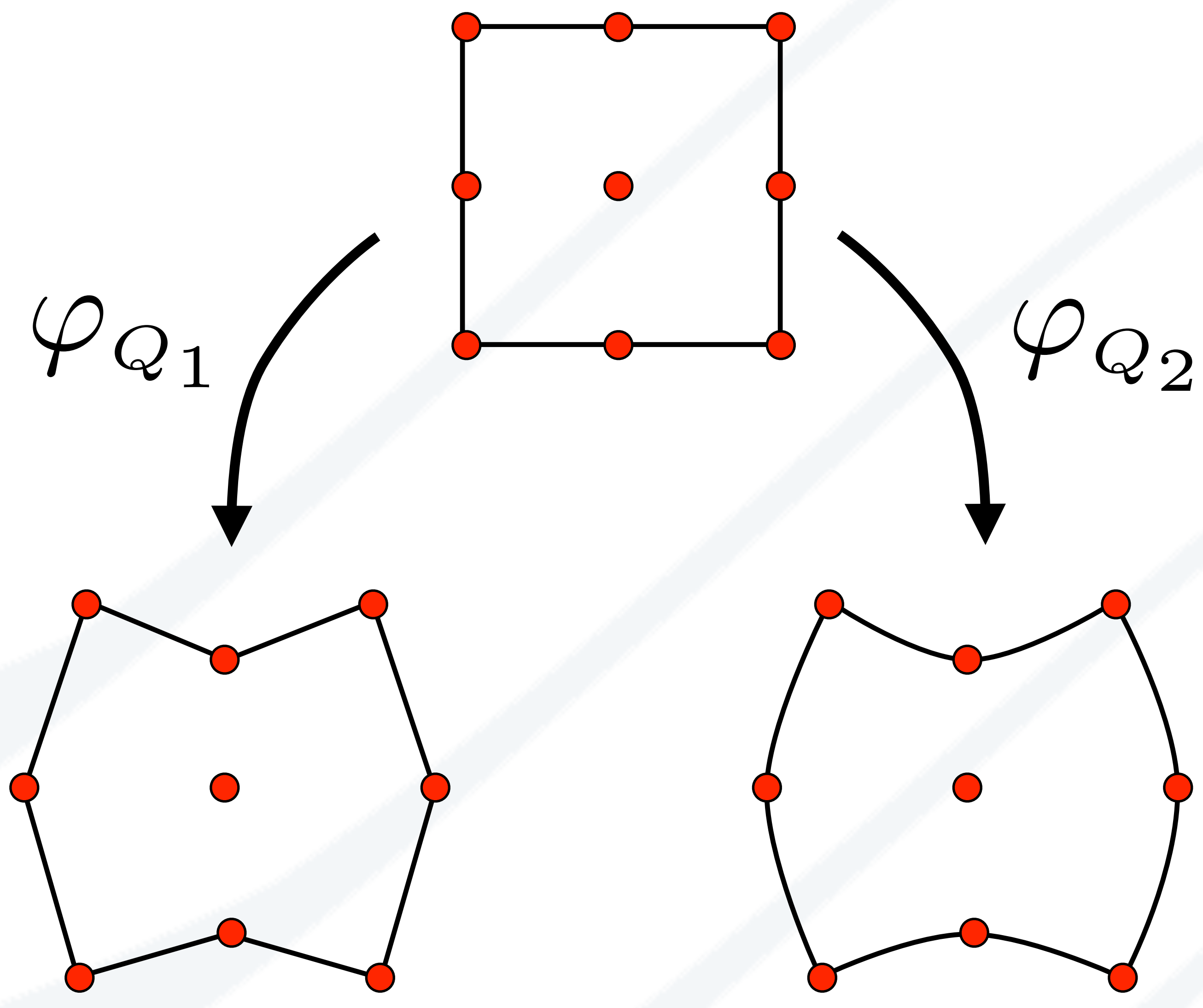
Integration on a cell: the Quadrature classes

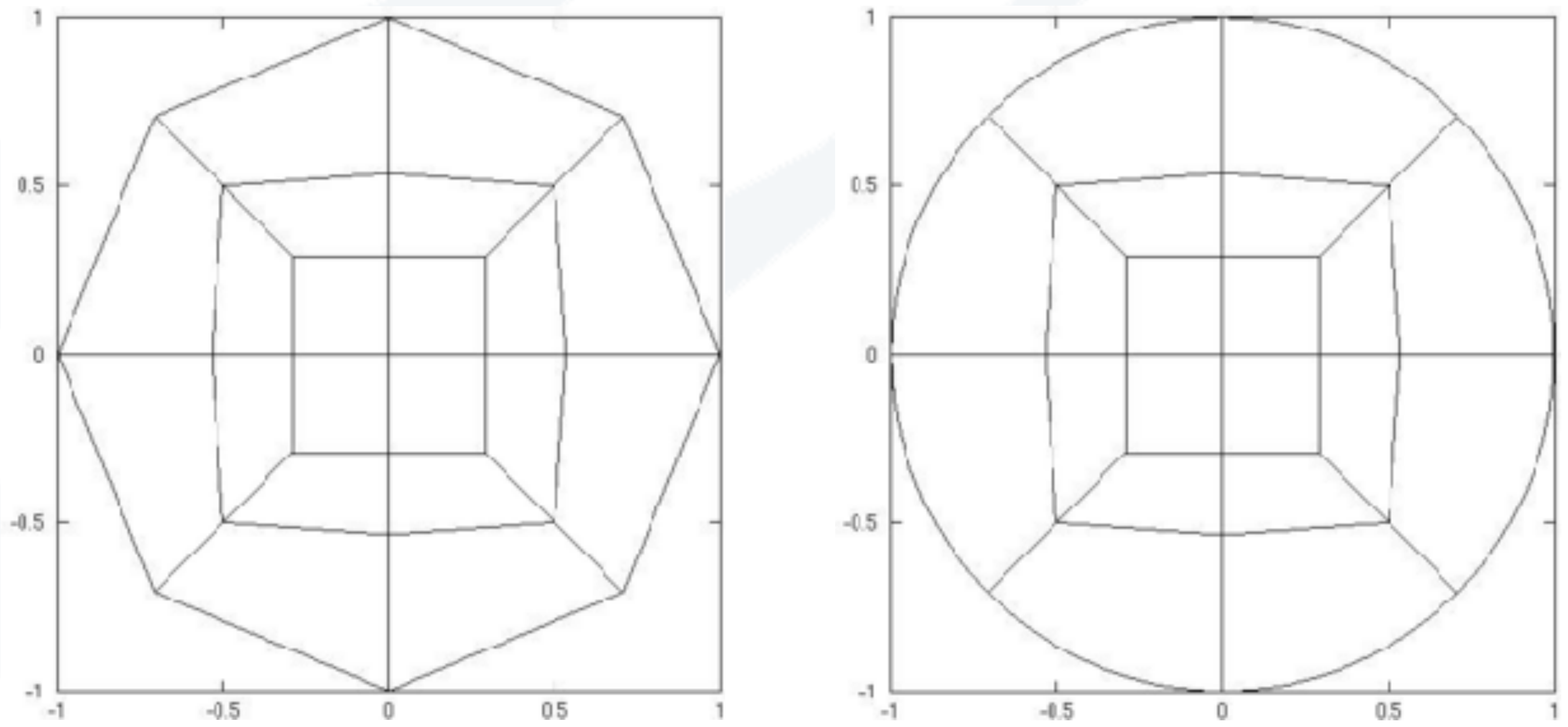
- n-Order Gauss quadrature
- Other rules
  - Gauss Lobatto
  - Simpson
  - Trapezoidal
  - Midpoint
  - A few others
- Anisotropic
  - Tensor product



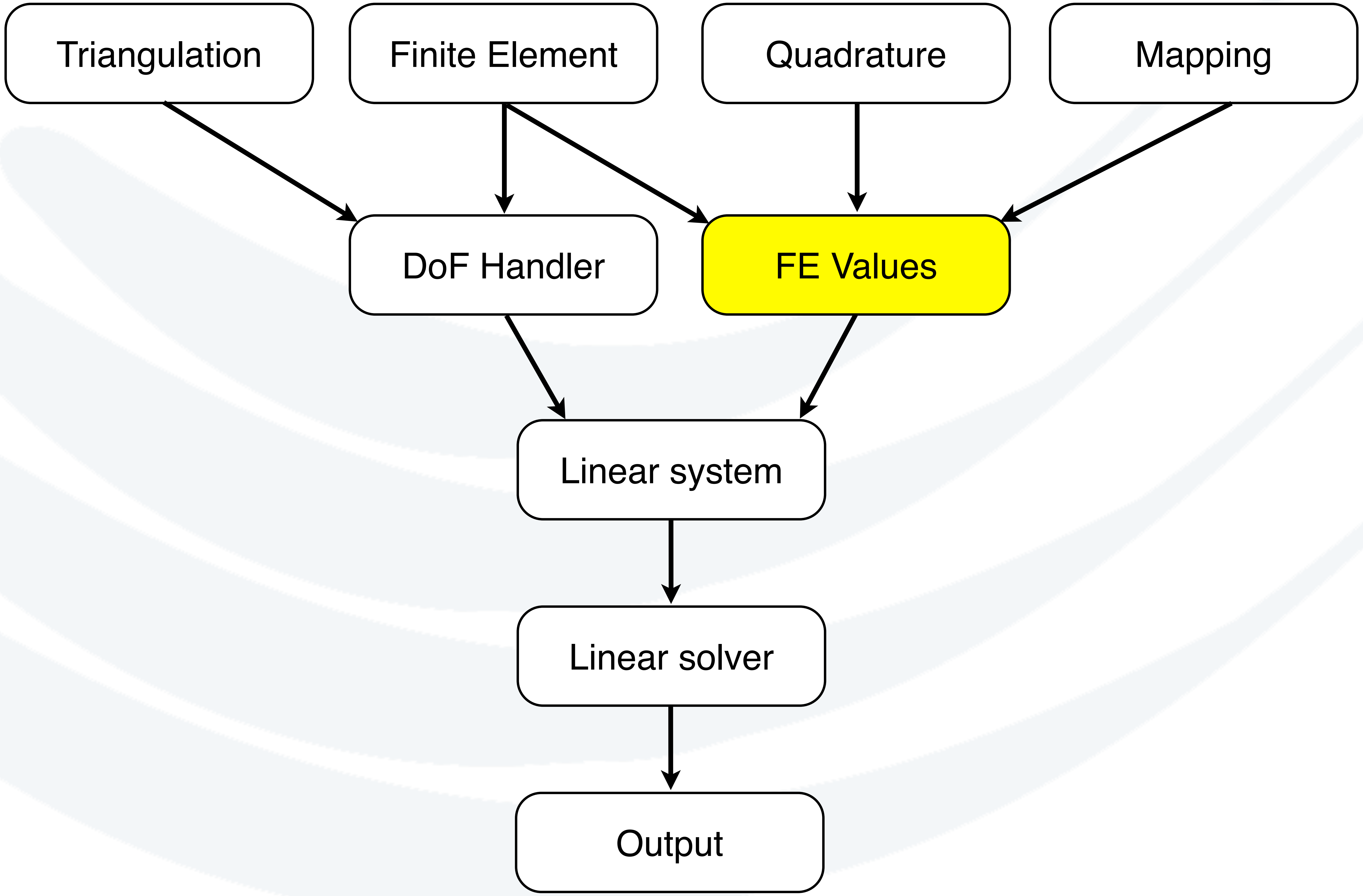
Integration on a cell: the Mapping classes

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





Structure of a prototypical FE problem



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 optimisations

$$a_{IJ} := \sum_q [(DF_m^{-T}\hat{\nabla}\hat{v}_I)](\hat{x}_q) \cdot [DF_m^{-T}(\hat{\nabla}\hat{v}_J)](\hat{x}_q) J_m(\hat{x}_q) w_q$$

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

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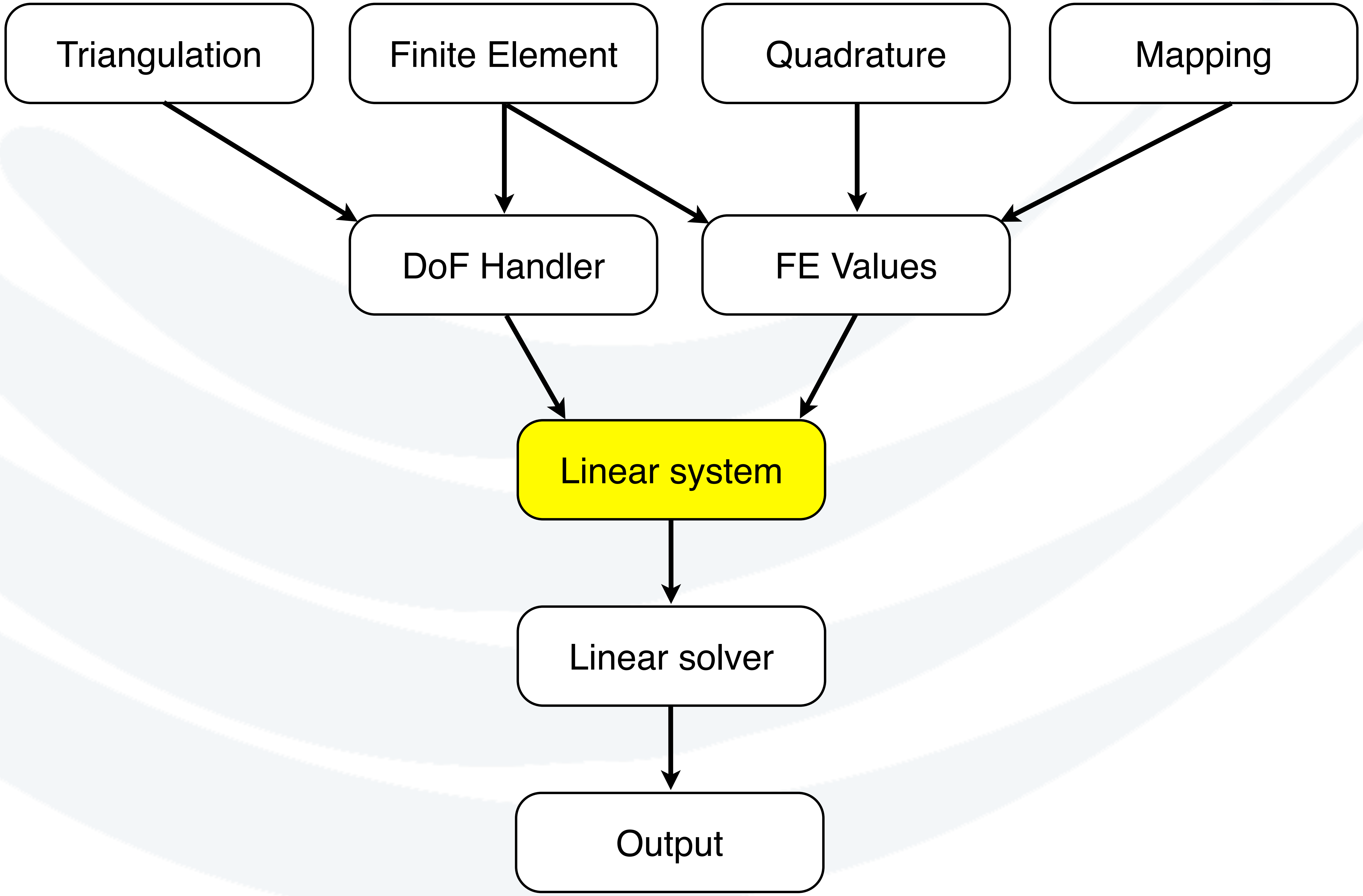
Structure of a prototypical FE problem



Sparse linear systems

- Minimise data storage
  - Evaluate grid connectivity
- Functions to help set up
  - Connectivity
  - 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)

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

$$\left[\begin{array}{c|c} K_{11} & K_{12} \\ \hline K_{21} & K_{22} \end{array}\right] \left\{\begin{array}{c} d_1 \\ \hline d_2 \end{array}\right\} = \left\{\begin{array}{c} F_1 \\ \hline F_2 \end{array}\right\}$$

- $$\left(K_{11} - K_{12}K_{22}^{-1}K_{21}\right) d_1 = F_1 - K_{12}K_{22}^{-1}F_2$$
- $$d_2 = K_{22}^{-1}\left(F_2 - K_{21}d_1\right)$$

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