Numerical Solution of PDEs Using the Finite Element Method

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Motivations

Many of the big problems in scientific computing are described by partial differential equations (PDEs):

- Structural statics and dynamics
  – Bridges, roads, cars, …
- Fluid dynamics
  – Ships, pipe networks, …
- Aerodynamics
  – Cars, airplanes, rockets, …
- Plasma dynamics
  – Astrophysics, fusion energy
- But also in many other fields: Biology, finance, epidemiology, ...

Numerics for PDEs

There are 3 standard tools for the numerical solution of PDEs:

- Finite element method (FEM)
- Finite volume method (FVM)
- Finite difference method (FDM)

Common features:

- Split the domain into small volumes (cells)
- Define balance relations on each cell
- Obtain and solve very large (non-)linear systems

Problems:

- Every code has to implement these steps
- There is only so much time in a day
- There is only so much expertise anyone can have

Ideal Characteristics

Examples of what we would like to have:

- Adaptive meshes
- Realistic, complex geometries

- Quadratic or even higher order elements

- Multigrid solvers
- Scalability to 1000s of processors
- Efficient use of current hardware

- Graphical output suitable for high quality rendering

Q: How can we make all of this happen in a single code?

Main Question!

Q: How can we make all of this happen in a single code?

Not a question of feasibility but of how we develop software:

- Is every student developing their own software?
- Or are we re-using what others have done?

- Do we insist on implementing everything from scratch?
- Or do we build our software on existing libraries?

There has been a major shift on how we approach the second question in scientific computing over the past 10-15 years!

Main Answer…

The secret to good scientific software is (re)using existing libraries!

Existing Software

There is excellent software for almost every purpose!

Basic linear algebra (dense vectors, matrices):

- BLAS
- LAPACK

Parallel linear algebra (vectors, sparse matrices, solvers):

- PETSc
- Trilinos

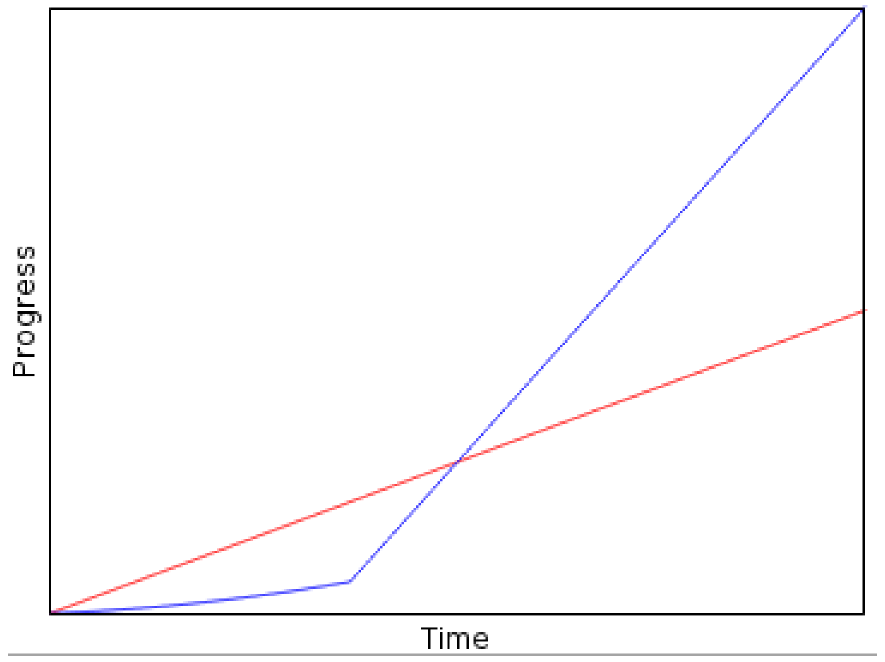
Meshes, finite elements, etc:

- deal.II – the topic of this class
- …

Visualization, dealing with parameter files, ...

Existing Software

Progress over time:

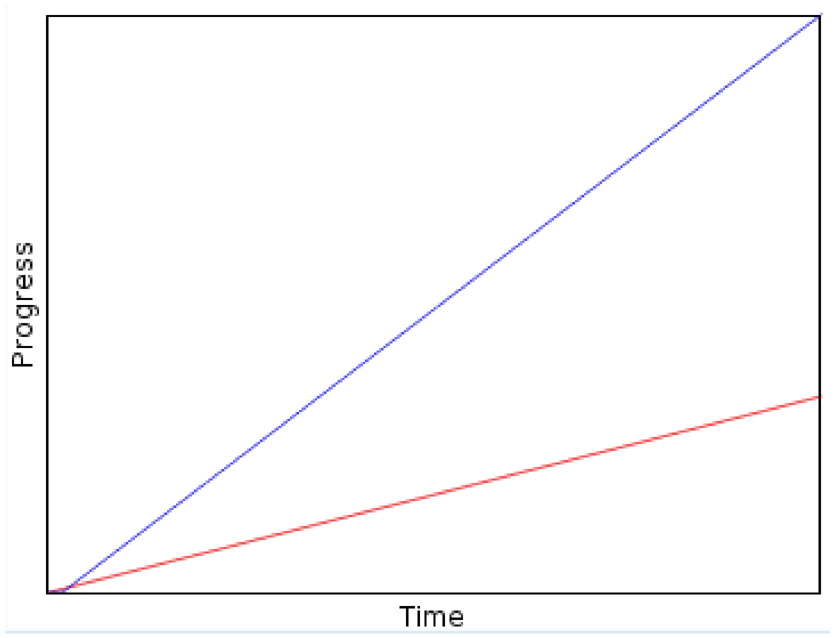


Red: Do it yourself. Blue: Use existing software.

Question: Where is the cross-over point?

Existing Software

Progress over time, the real picture:



Red: Do it yourself.   Blue: Use existing software.

Answer: Cross-over is after 2–4 weeks! A PhD takes 3–4 years.

Existing Software

Experience:

It is realistic for a student developing numerical methods to have a code at the end of a PhD time that:

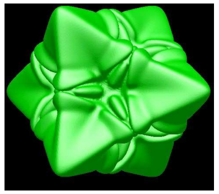
- Works in 2d and 3d
- On complex geometries
- Uses higher order finite element methods
- Uses multigrid solvers or preconditioners
- Solves a nonlinear, time dependent problem

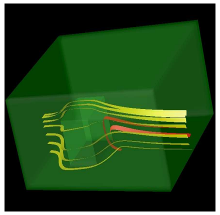
Doing this from scratch would take 10+ years.

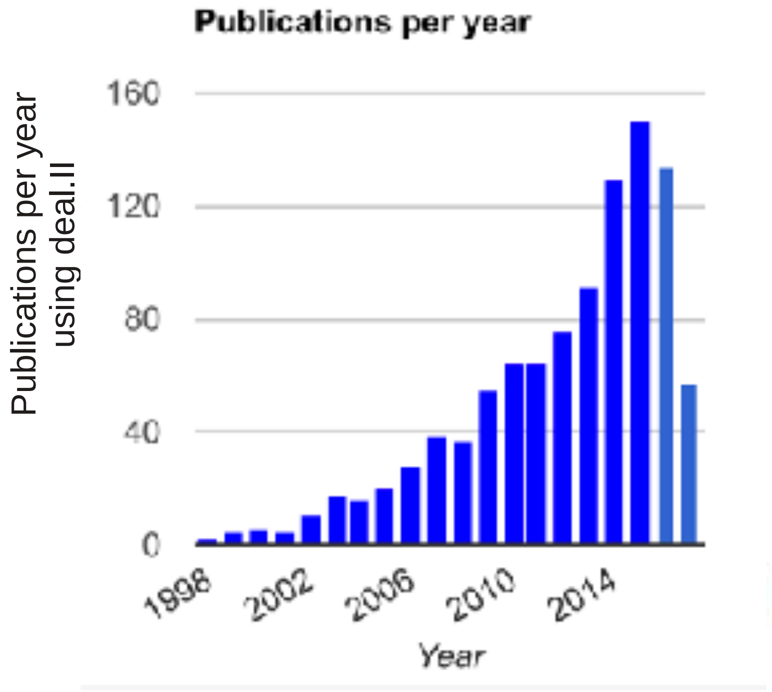
Why Deal.II?

deal.II is probably the largest FEM library:

- Presently ~600,000 lines of C++ code
- 10,000+ pages of documentation
- ~45 tutorial programs
- Fairly widely distributed:
  20,000+ downloads in 2012
- At least 65+ publications in 2012,
  996 - overall, that use it
- Used in teaching at a number
  of universities
- 2007 Wilkinson prize.







Why Deal.II?

Linear algebra in deal.II:

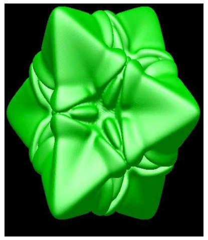
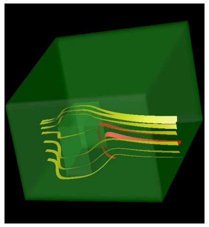
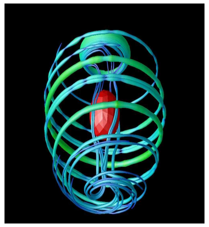
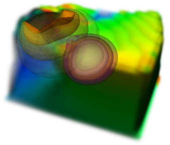
- Has its own sub-library for dense + sparse linear algebra
- Interfaces to PETSC, Trilinos, UMFPACK

Pre- and postprocessing:

- Can read most mesh formats
- Can write almost any visualization file format

Parallelization:

- Uses threads and tasks on multicore machines
- Uses MPI, up to 10,000s of processors

Why Deal.II?

Professional-level software management:

- Globally accessible repository
- Mailing lists with significant volume
  – for user questions
  – for developer discussions
- ~2,700 tests run after every change
- Multi-platform build systems
  – Linux/Unix
  – Mac OS X
  – Windows
- Web sites tracking changes, tests, builds, ...

Prerequisites

Operating system:

- Linux or other Unix
- Mac OS X
- Windows

C++ Compiler:

- GNU Compiler Collection (GCC)
- Intel C++
- Clang++

Other software: Perl, CMake, viz software, IDE

Disk space: 1–2GB

Obtaining deal.II

Development sources

Fork our repository on github:

https://github.com/dealii/dealii.git

Building

Detailed instructions:

http://www.dealii.org/developer/readme.html

Basic instructions:

- Create build directory:
  cd deal.II ; mkdir build ; cd build
- Determine properties of the system and compilers:
  cmake -DCMAKE_INSTALL_PREFIX=/a/b/c ..
- Compile the entire library (~1 hour):
  make ; make install
- Verify that everything works:
  cd examples/step-1
  cmake -DDEAL_II_DIR=/a/b/c . ; make run

Building

There are many flags other than

- the installation directory
- the source directory

that can be given to *cmake*. For example:

- Paths to PETSc, Trilinos and other libraries
- Whether to build documentation locally
- Whether to disable or enable multithreading

Detailed instructions:

http://www.dealii.org/developer/readme.html

Basis of FEM!

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

We start with the strong form:

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

Basis of FEM!

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:

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

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

Basis of FEM!

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

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

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

$$(\nabla \phi_i, \nabla u_h) = (\phi_i, f) \quad \forall i = 1 \ldots N$$

If basis functions are linearly independent, this yields *N* equations for *N* coefficients.
This is called the *Galerkin* method.

Basis of FEM!

Practical question 1: How to define the basis functions?

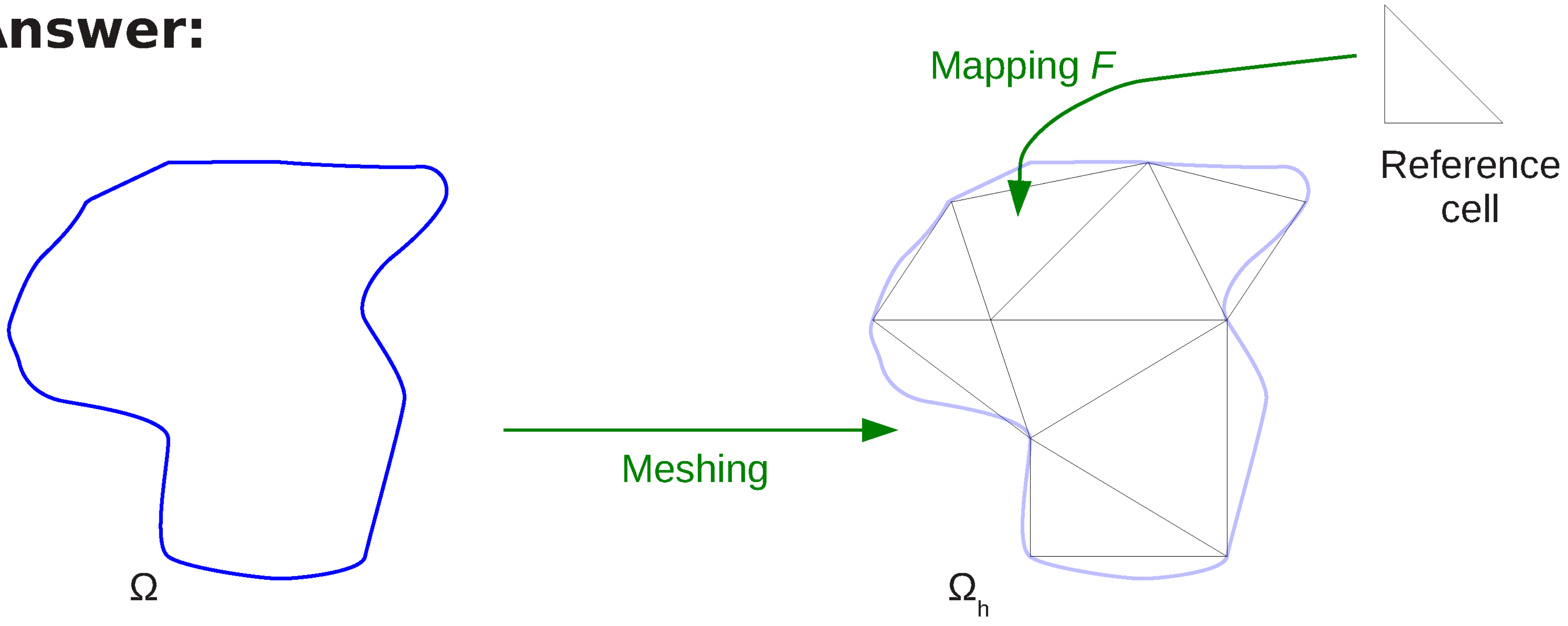
Answer: In the finite element method, this is done using the following concepts:

- 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

Basis of FEM!

Practical question 1: How to define the basis functions?

Answer:



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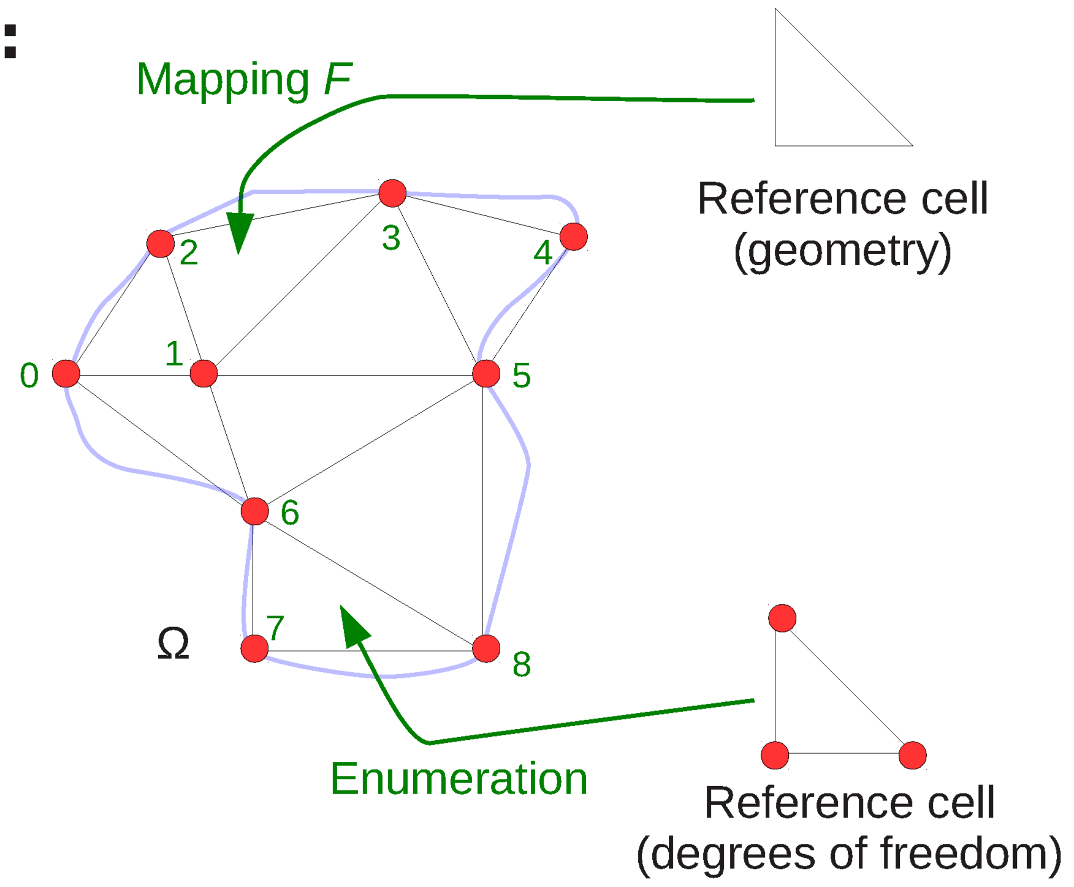

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Concepts in red will correspond to things we need to implement in software, explicitly or implicitly.

Basis of FEM!

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

$$(\nabla \phi_i, \nabla u_h) = (\phi_i, f) \quad \forall i = 1 \ldots N$$

to obtain:

$$\sum_{j=1}^{N} (\nabla \phi_i, \nabla \phi_j) U_j = (\phi_i, f) \quad \forall i = 1 \ldots N$$

This is a linear system

$$AU = F$$

with

$$A_{ij} = (\nabla \phi_i, \nabla \phi_j) \qquad F_i = (\phi_i, f)$$

Basis of FEM!

Practical question 2: How to compute

$$A_{ij} = (\nabla\phi_i, \nabla\phi_j) \qquad F_i = (\phi_i, f)$$

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

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

...and quadrature:

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

Similarly for the right hand side *F*.

Basis of FEM!

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

Basis of FEM!

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

Basis of FEM!

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

$$AU=F$$

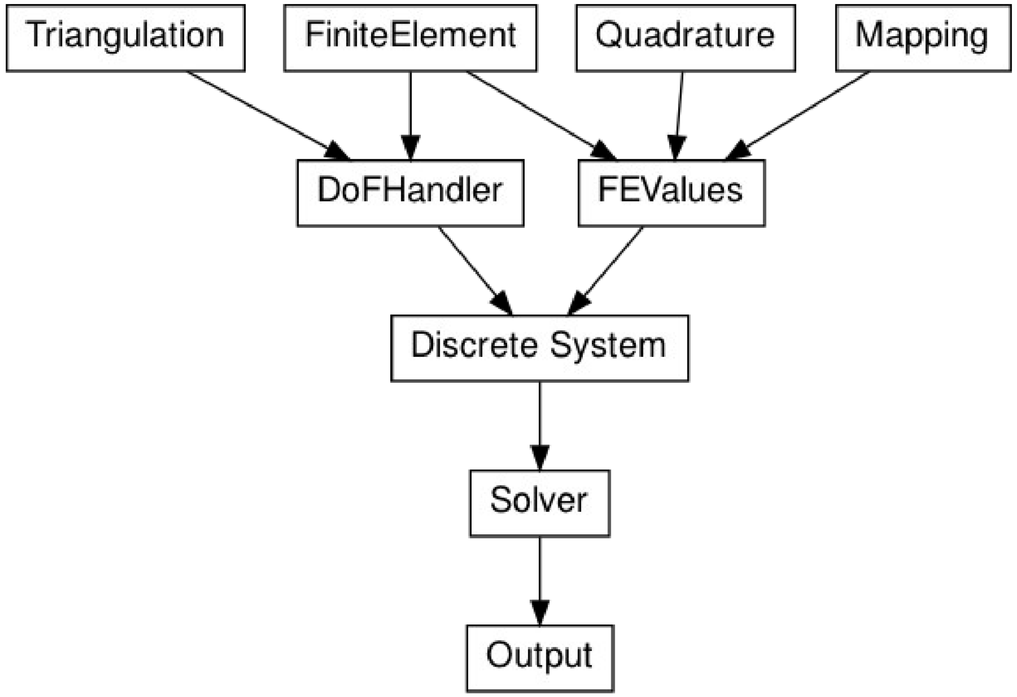
Answers: The goal is not to solve the linear system, but to do something with its solution:

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

These steps are often called *postprocessing the solution*.

Basis of FEM!

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



Start with Tutorial: step-1

After reading, play with the program:

```
cd examples/step-1
cmake -DDEAL_II_DIR=/path/to/deal.II .
make run
```

This will run the program and generate output files:

```
ls -l
okular grid-2.eps
```

Next step: Play by following the suggestions in the results section. This is the best way to learn!

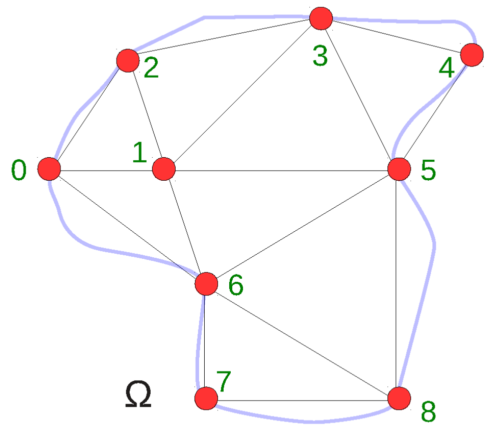
Start with Tutorial: step-2

Step-2 shows:

- How degrees of freedom are defined with finite elements
- The *DoFHandler* class
- How DoFs are connected by bilinear forms
- Sparsity patterns of matrices
- How to visualize a sparsity pattern

Start with Tutorial: step-2

Example: Consider this mesh and bilinear form:



$$A_{ij} = (\nabla \phi_i, \nabla \phi_j) = \int_\Omega \nabla \phi_i \cdot \nabla \phi_j \, dx$$

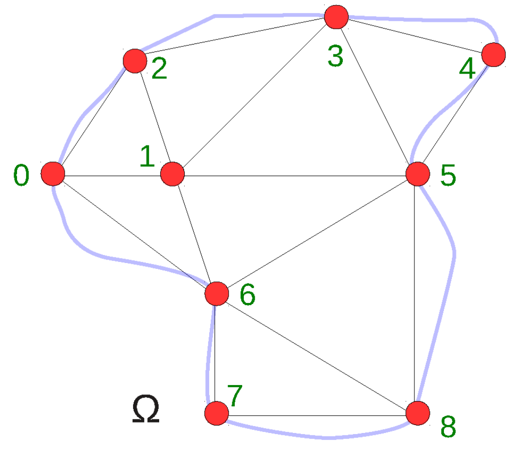
Note: In general we have that

- $A_{00} \neq 0, A_{01} \neq 0, A_{02} \neq 0, A_{06} \neq 0$
- $A_{03} = A_{04} = A_{05} = A_{07} = A_{08} = 0$

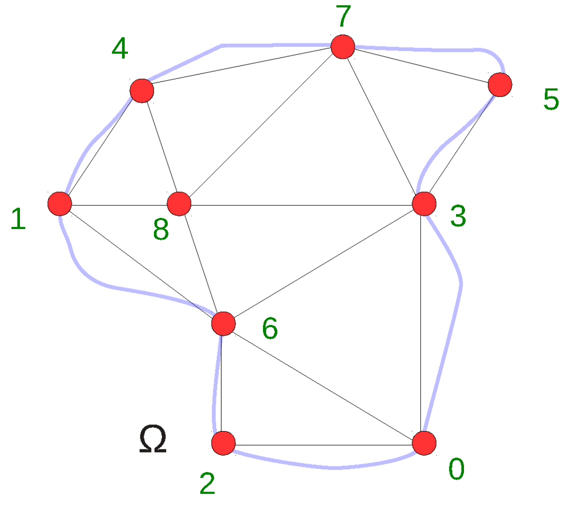
The bigger the mesh, the more zeros there are per row!

Start with Tutorial: step-2

Renumbering: The order of enumerating degrees of freedom is arbitrary



vs.



Notes:

- Resulting matrices are just permutations of each other
- Both sparse, but some algorithms care

Start with Tutorial: step-3

Step-3 shows:

- How to set up a linear system
- How to assemble the linear system from the bilinear form:
  - The loop over all cells
  - The *FEValues* class
- Solving linear systems
- Visualizing the solution

Start with Tutorial: step-3

Recall:

- For the Laplace equation, the bilinear form is written as a sum over all cells:

$$\begin{aligned} A_{ij} &= \left(\nabla\phi_i, \nabla\phi_j\right) \\ &= \sum_K \int_K \nabla\phi_i(x)\cdot\nabla\phi_j(x) \end{aligned}$$

- But on each cell, only few shape functions are nonzero!
- For Q_1, only $16=4^2$ matrix entries are nonzero per cell
- Only compute this (dense) sub-matrix, then “distribute” it to the global A
- Similar for the right hand side vector.

Start with Tutorial: step-3

Recall:

- We use quadrature

$$A_{ij}^{K} = \int_{K} \nabla \hat{\phi}_i(x) \cdot \nabla \hat{\phi}_j \, dx$$
$$\approx \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\phi}_j(\hat{x}_q) \underbrace{|\det J(\hat{x}_q)| \; w_q}_{=:\mathrm{JxW}}$$

- We really only have to evaluate shape functions, Jacobians, etc., at quadrature points – not as functions
- All evaluations happen on the reference cells

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