Using finite elements via the deal.II library

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Lecture 1:

Course overview.

Why consider software libraries?

Course overview

The topic of this course:

Learn how to solve partial differential equations on computers! *

* Using the finite element method.

Course overview

The numerical solution of partial differential equations is an immensely practical field!

It requires us to know about:

- Partial differential equations
- Methods for discretizations, solvers, preconditioners
- Programming
- Adequate tools

Partial differential equations

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, ...

On why to use existing software

There are times when we need to write computational software ourselves:

- When developing new computational methods
- When solving non-standard problems

In such cases, we could:

- Start from scratch, write everything ourselves
- Build something from existing components
- Adapt existing code written for similar applications

But: Option 1 could be difficult/time consuming/expensive!

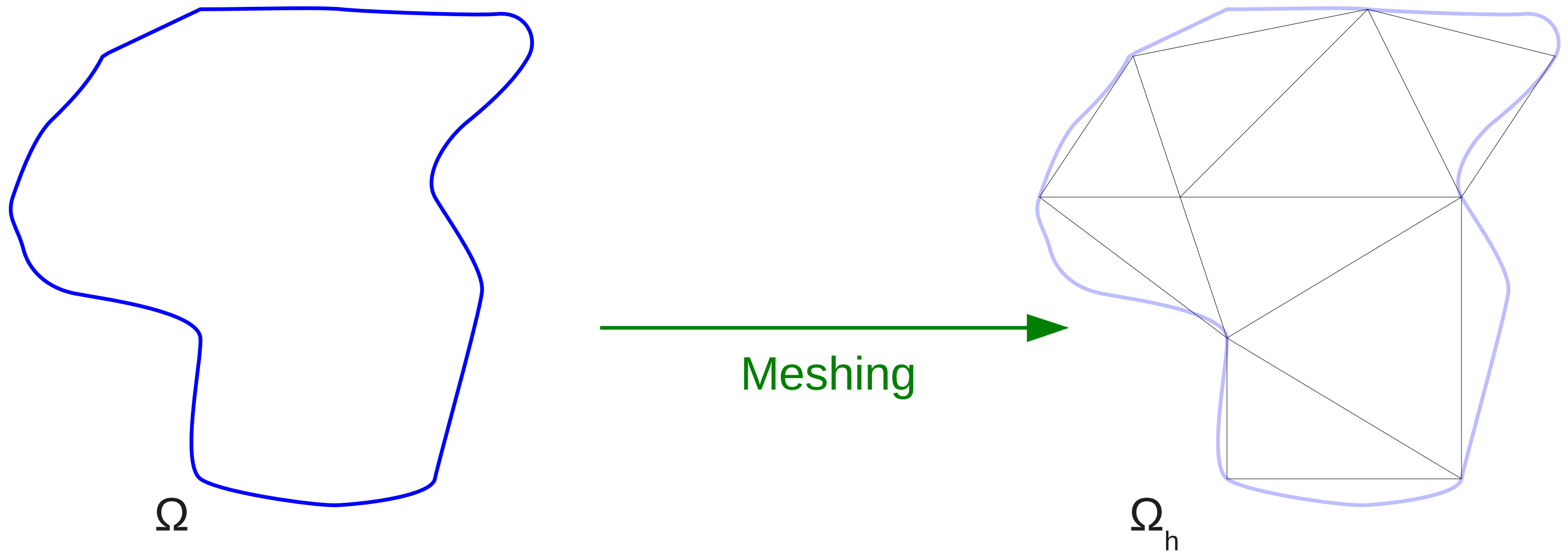
Numerics for PDEs

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)



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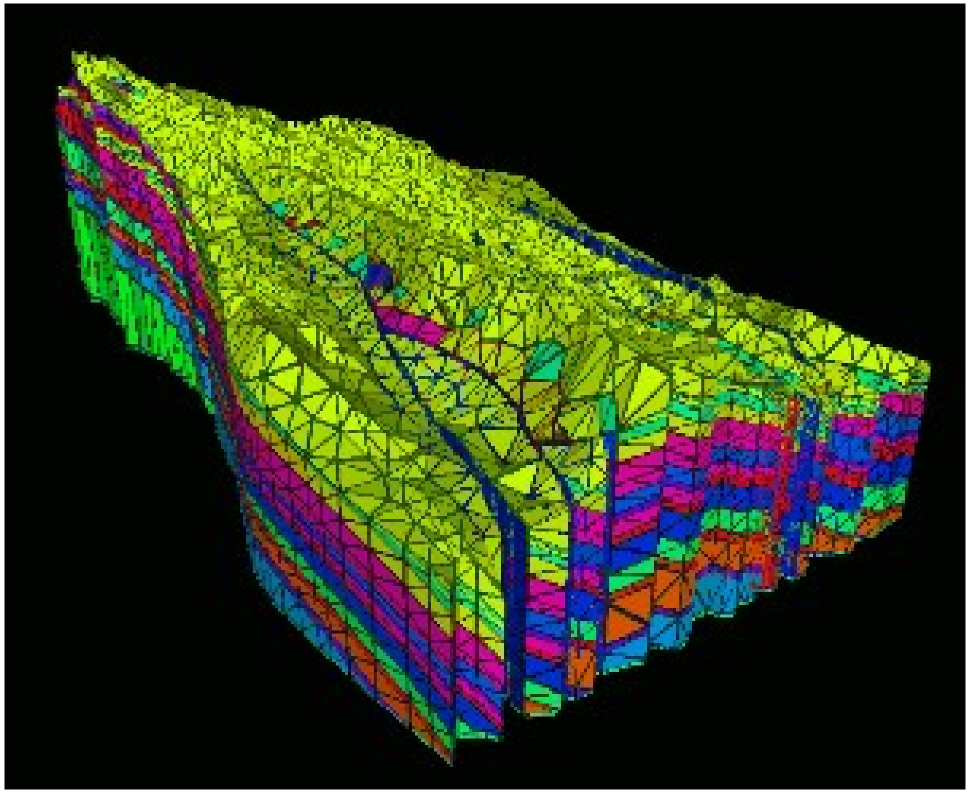

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In addition:

- We don't just want a simple algorithm
- We want state-of-the-art methods for everything

Numerics for PDEs

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?

How we develop software

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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 on existing libraries?

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

How we develop software

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 course
- …

Visualization, dealing with parameter files, ...

Existing software

Arguments against using other people's packages:

I would need to learn a new piece of software, how it works, its conventions. I would have to find my way around its documentation. Etc.

I think I'll be faster writing the code I want myself!

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> I think I'll be faster writing the code I want myself!

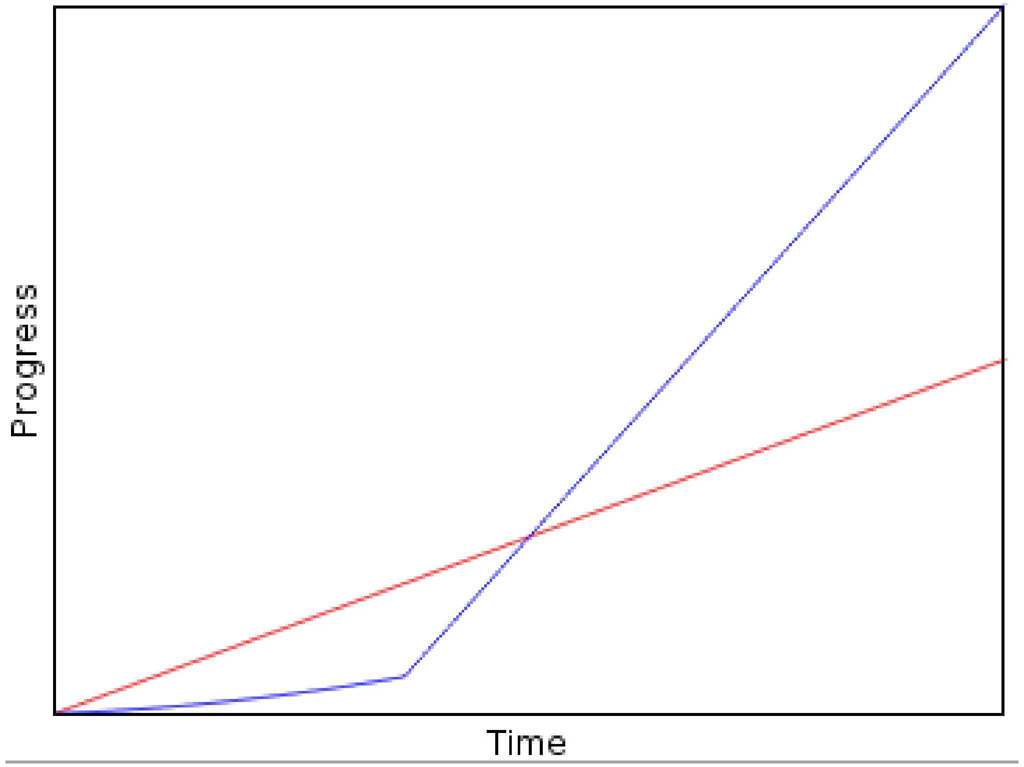
Answers:

- The first part is true.
- The second is not!

- You get to use a lot of functionality you could never in a lifetime implement yourself.
- Think of how we use Matlab today!

Existing software

Progress over time:

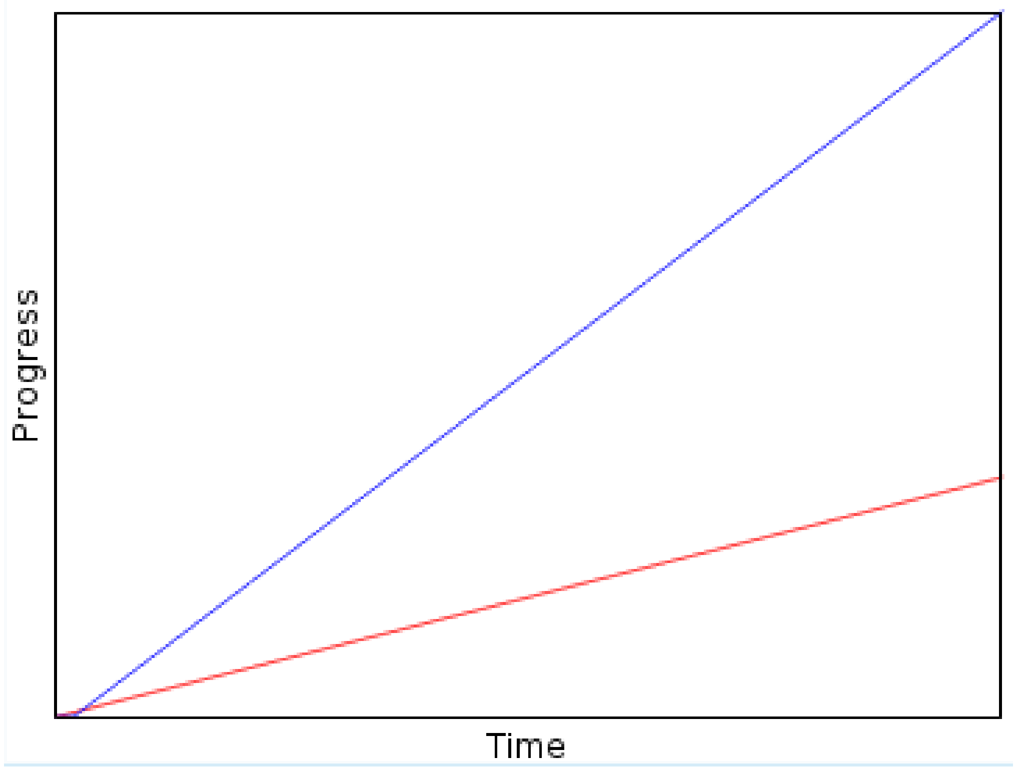


Red: Do it yourself. Blue: Use existing software.

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:

Students developing numerical methods can realistically expect 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.

Existing software

Arguments against using other people's packages:

How do I know that that software I'm supposed to use doesn't have bugs? How can I *trust* other people's software?

With my own software, at least I know that I don't have bugs!

Existing software

Arguments against using other people's packages:

How do I know that that software I'm supposed to use doesn't have bugs? How can I *trust* other people's software?

With my own software, at least I know that I don't have bugs!

Answer 1:

- You can't be serious to think that your own software has no bugs!

Existing software

Arguments against using other people's packages:

How do I know that that software I'm supposed to use doesn't have bugs? How can I *trust* other people's software?

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Answer 2:

- deal.II is developed by professionals with a lot of experience
- It has an extensive testsuite:

  We run 2,800+ tests after every single change!

Conclusions

- When having to implement software for a particular problem, re-use what others have done already
- There are many high-quality, open source software libraries for every purpose in scientific computing
- Use them:
  – You will be far more productive
  – You will be able to use state-of-the-art methods
  – You will have far fewer bugs in your code

If you are a graduate student:
Use them because you will be able to impress your adviser with quick results!

Lecture 2:

A real short overview of deal.II

deal.II

Deal.II is a finite element library. It provides:

- Meshes
- Finite elements, quadrature,
- Linear algebra
- Most everything you will ever need when writing a finite element code

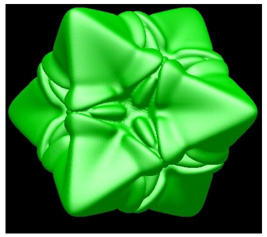
On the web at

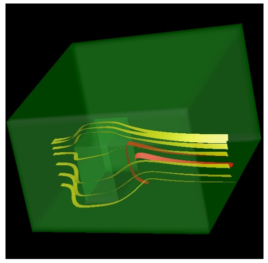
http://www.dealii.org/

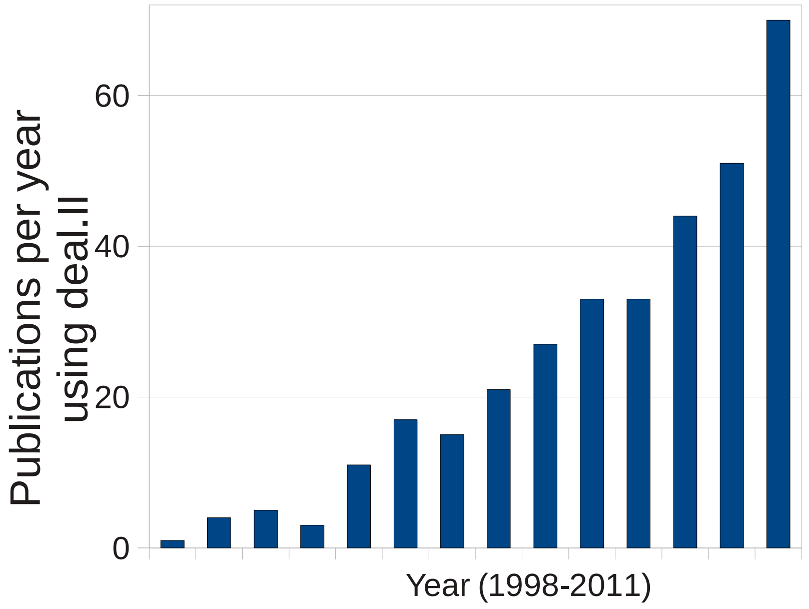
deal.II

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,
  400+ overall, that use it
- Used in teaching at a number
  of universities
- 2007 Wilkinson prize.



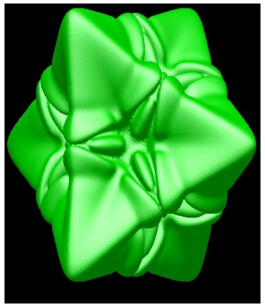


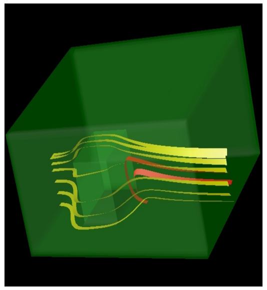


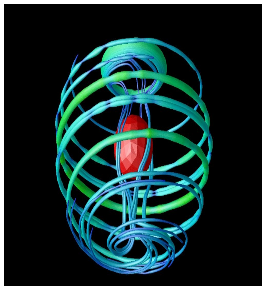
What's in deal.II

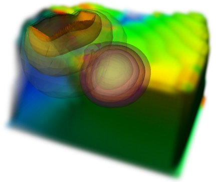
Meshes and elements:

- Supports adaptive meshes in 1d, 2d, and 3d
- Easy ways to adapt meshes: Standard refinement indicators already built in
- Many standard finite element types (continuous, discontinuous, mixed, Raviart-Thomas, ...)
- Low and high order elements
- Full support for multi-component problems





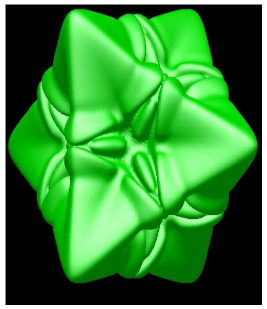


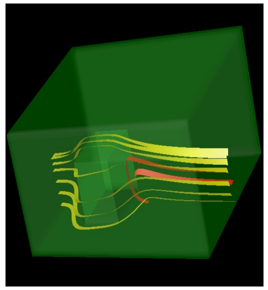


What's in deal.II

Linear algebra in deal.II:

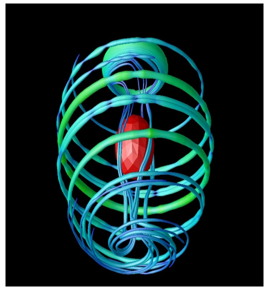
- Has its own sub-library for dense + sparse linear algebra
- Interfaces to PETSC, Trilinos, UMFPACK





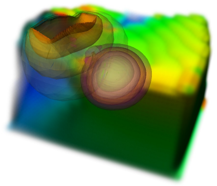
Pre- and postprocessing:

- 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



What deal.II is used for

Apparently any PDE can be solved with deal.II.

In 2008–2010, papers were published that simulate:

- Biomedical imaging
- Heart muscle fibers

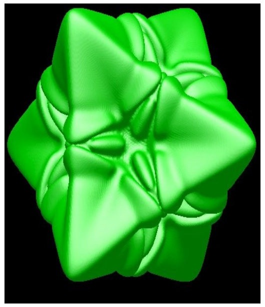
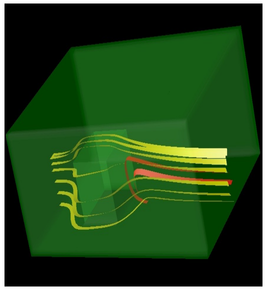
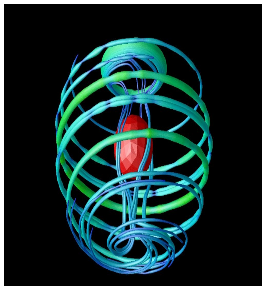
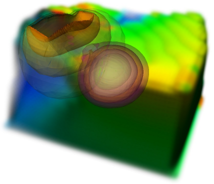
- Microfluidics
- Oil reservoir flow
- Fuel cells
- Aerodynamics

- Quantum mechanics
- Neutron transport

- Numerical methods research

- Fracture mechanics
- Damage models
- Sedimentation
- Biomechanics
- Root growth of plants
- Solidification of alloys
- Glacier mechanics

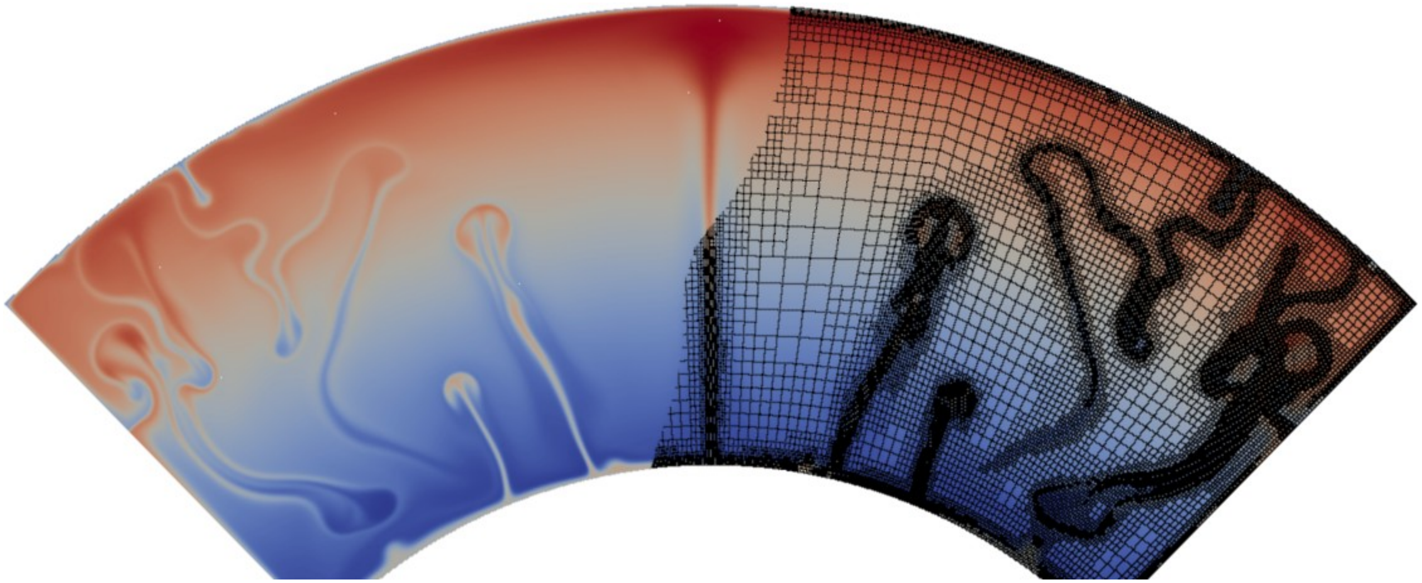
- Deterioration of statues due to air pollution

What deal.II is used for

Example: The mantle convection code ASPECT

http://aspect.dealii.org/



Methods:

- 2d, 3d, adaptive meshes, multigrid solvers
- Higher order finite elements
- Fully parallel

How deal.II is developed

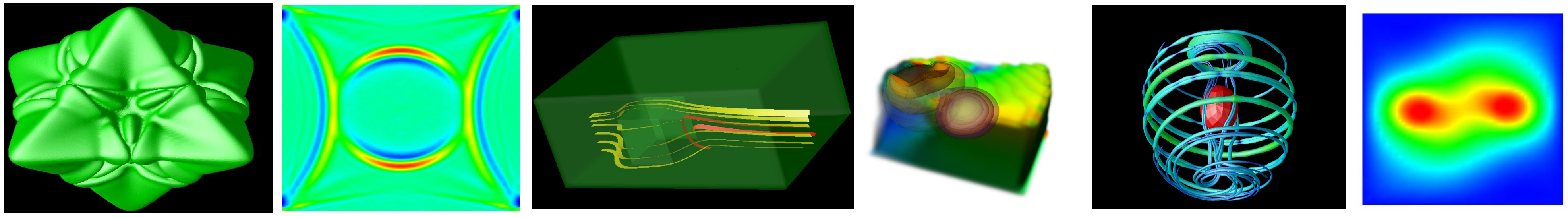
Development:

- 4–6 core developers (in the US, South Africa, Germany)
- ~10 occasional contributors (around the world)
- 100+ people have contributed over the past 10 years
- ~3000 lines of new code per month

deal.II is a typical open source project:

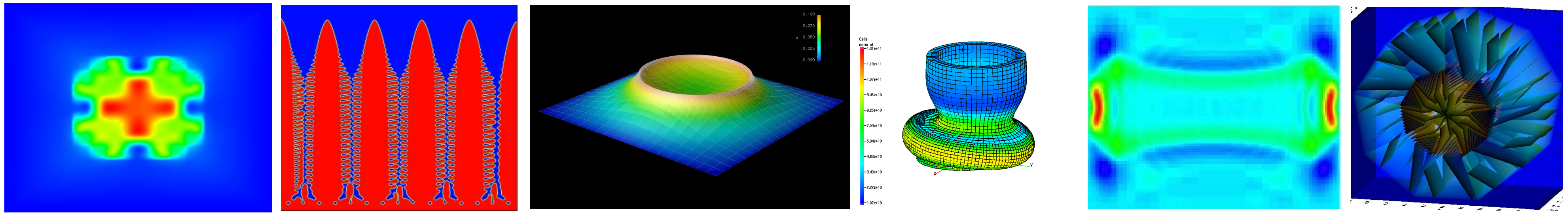
- People primarily develop what they need
- Open culture:
  – All development happens in the open
  – We (really) welcome everyone's contributions!

On the web



Visit the deal.II library:

http://www.dealii.org/



Conclusions

- **Mission:**
  To provide everything that is needed in finite element computations.

- **Development:**
  As an open source project

  As an inviting community to all who want to contribute

  As professional-grade software to users

Lecture 3:

The building blocks of a finite element code

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:

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

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

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

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.

Note: This is called the *Galerkin* method.

Implementing the finite element method

Practical question 1: How to define the basis functions?

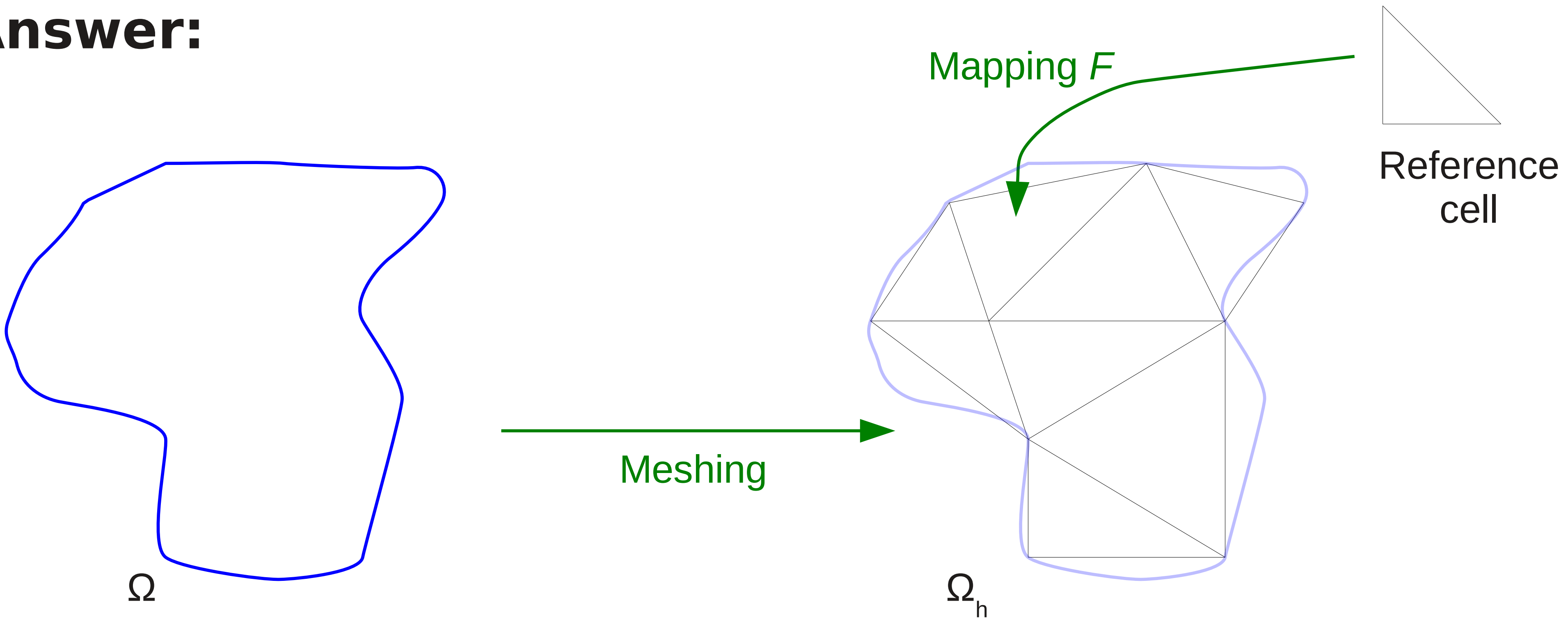
Answer: In the finite element method, this is done using the following concepts:

- Subdivision of the domain into a mesh
- Each cell of the mesh is mapped from 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

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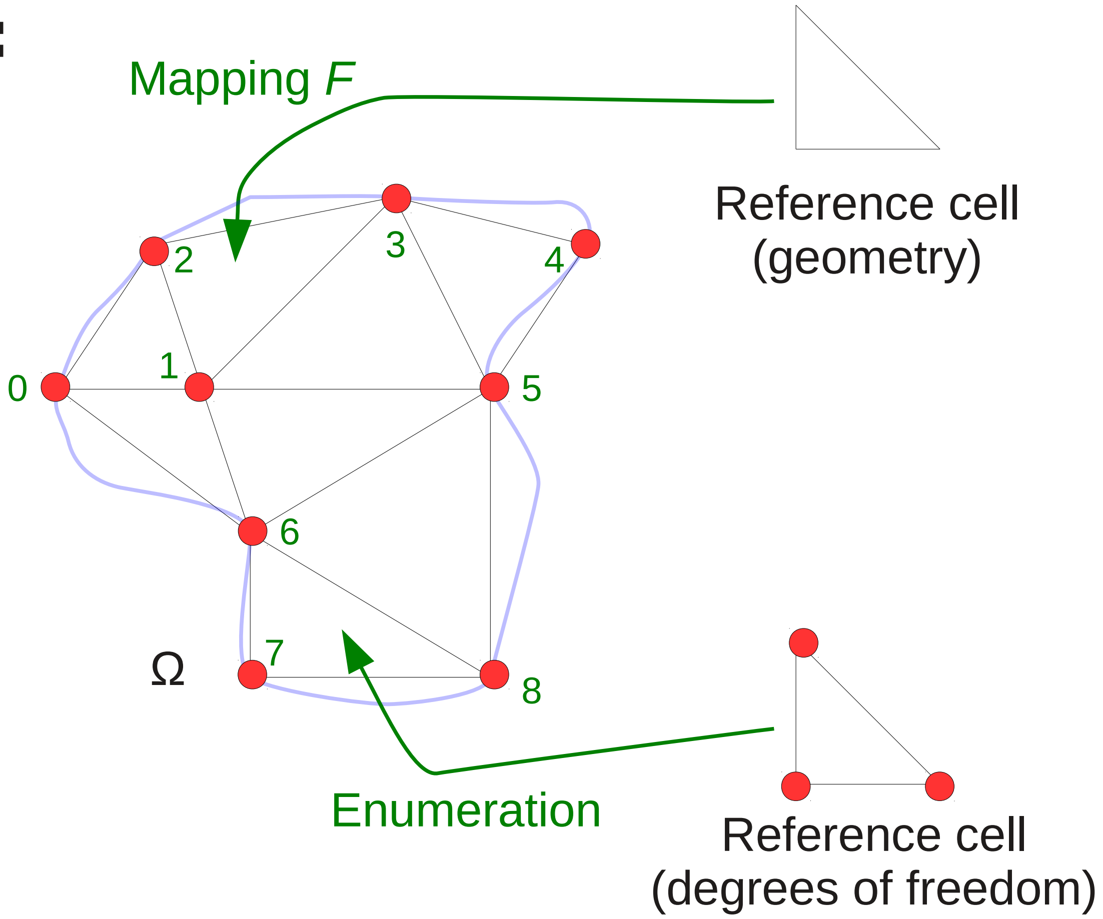

Implementing the finite element method

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

Implementing the finite element method

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

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

Implementing the finite element method

Practical question 2: How to compute

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

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*.

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

$$AU=F$$

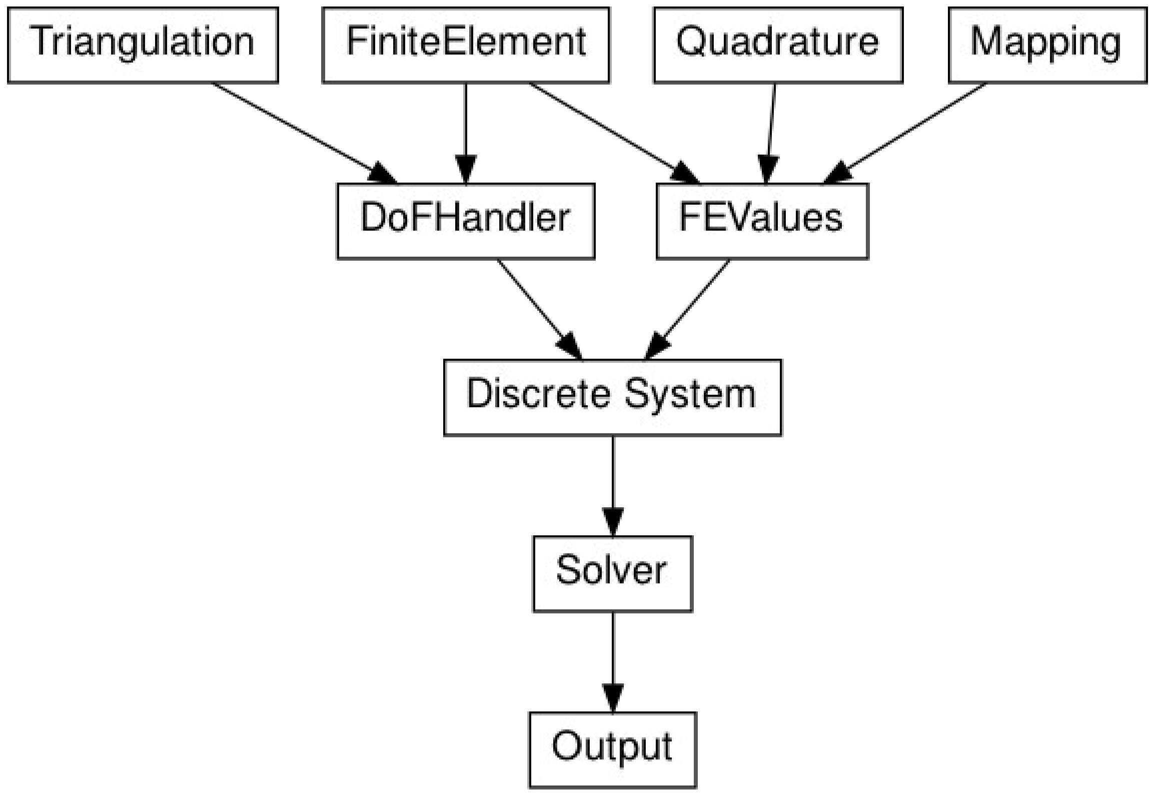
Answers: The goal is not to solve the linear system, but to do something with its solution:

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

These steps are often called *postprocessing the solution*.

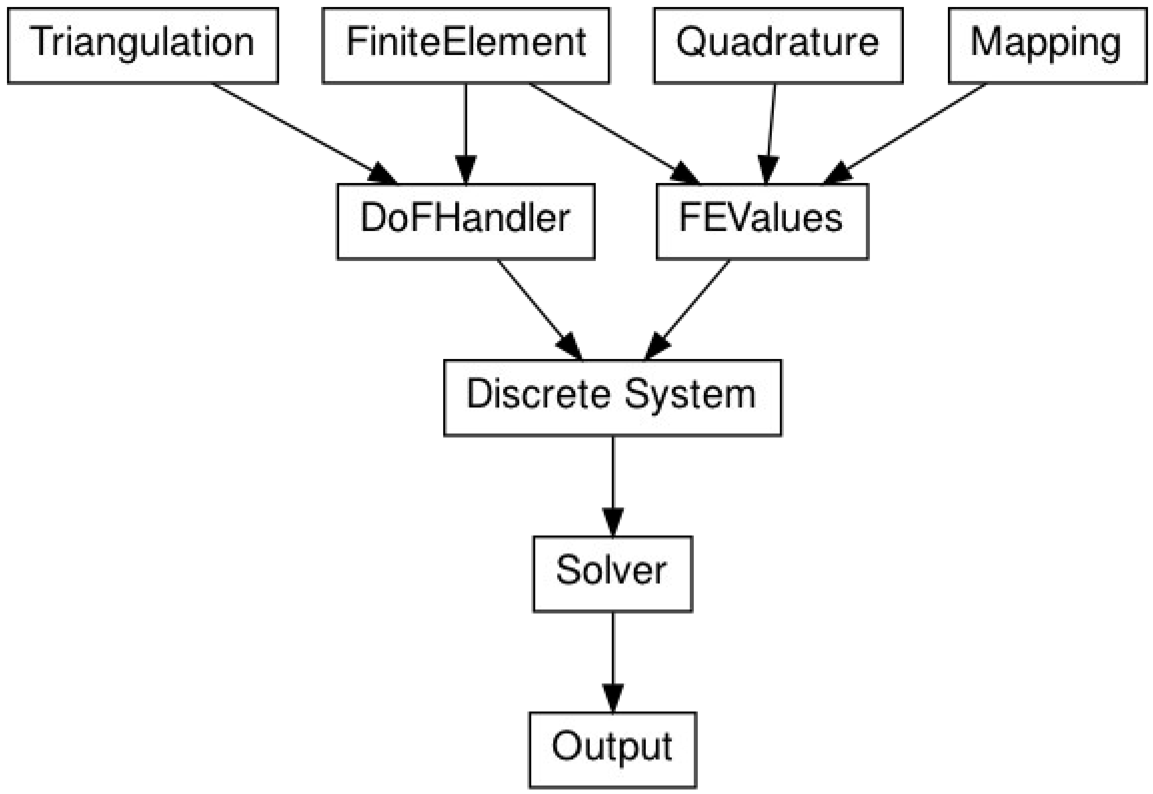
Implementing the finite element method

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

Each one of the components in this chart...



... can also be found in the *manual* at

http://www.dealii.org/7.2.0/index.html

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.

Lecture 4:

A first example

–

The *step-1* tutorial program: Triangulations

step-1

Step-1 shows:

- The *Triangulation* class
- How to think of a triangulation: as a collection of cells
- How to query cells for information, and what to do with them
- How to output a mesh, and a way to visualize it.

step-1

Tutorial programs have the following structure:

- Introduction:
  - lays out the problem to be solved
  - discusses the numerical method
  - introduces basics of the implementation
- Thoroughly documented code, processed for better readability
- Results section, often with suggestions for further extensions
- Copy of the code without the comments

All programs use similar structure and naming convention.

step-1

Read through the commented program at
http://www.dealii.org/7.1.0/doxygen/deal.II/step_1.html

Notes when reading:

- Read the introduction!
- If you want to *understand the entire code*, read from the top
- If you just want to *follow the flow* of the program, read from the bottom!
- Think about modifying the code as you read.

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!

Lecture 5:

A second example:

The *step-2* tutorial program
–
Degrees of freedom (DoFs)

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

step-2

Sparsity of system matrices:

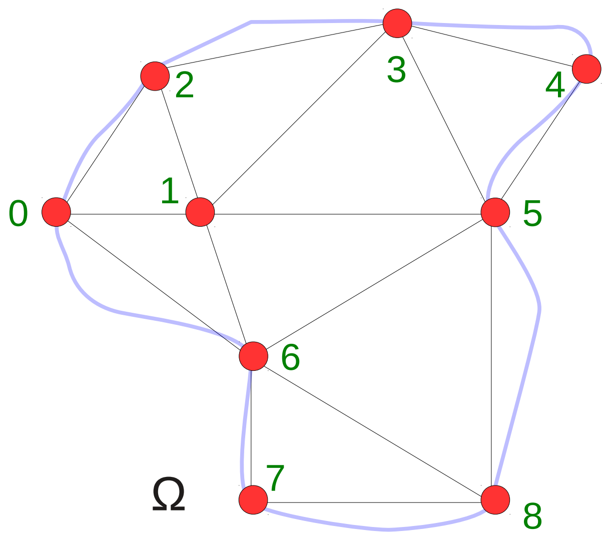
- For PDEs, finite element matrices are *always sparse*
- Result of
  – *local* definition of shape functions
  – *locality* of the differential operator

Sparsity is not a coincidence. It is a design choice of the finite element method.

Sparsity can not be overestimated as a factor in the success of the FEM!

step-2

Example: Consider this mesh and bilinear form:



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

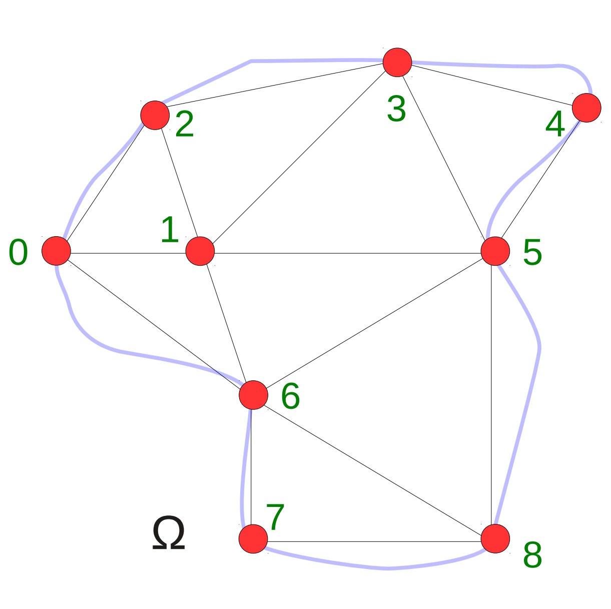
Note: In general we have that

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

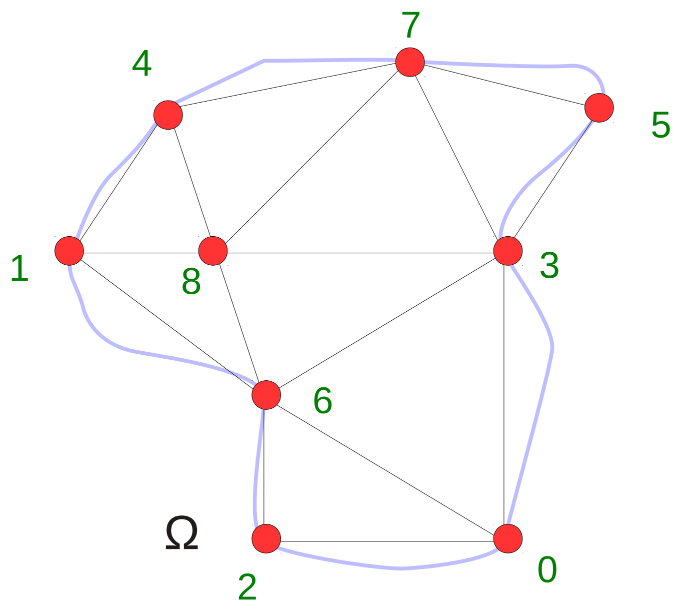
The bigger the mesh, the more zeros there are per row!

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

step-2

Read through the commented program at

http://www.dealii.org/7.1.0/doxygen/deal.II/step_2.html

Then play with the program:

```
cd examples/step-2
cmake -DDEAL_II_DIR=/a/b/c . ; make run
```

This will run the program and generate output files:

```
ls -l
```

Then run *gnuplot* as described in the documentation

```
gnuplot
```

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

Lecture 6:

A third example:

The *step-3* tutorial program – A first Laplace solver

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

step-3

Recall:

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

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

step-3

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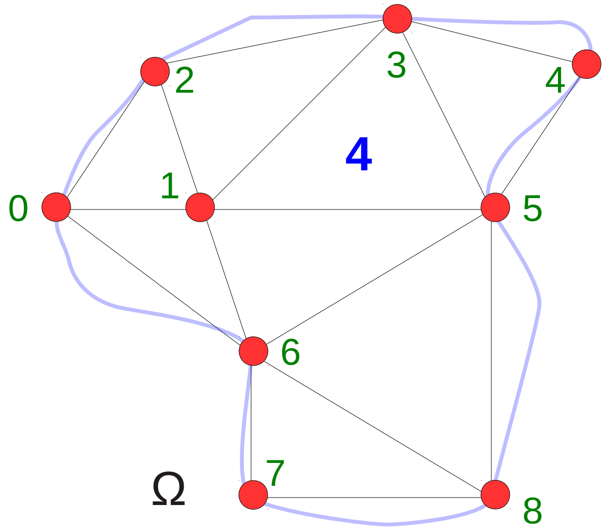
$$\begin{aligned} A_{ij} &= (\nabla \phi_i, \nabla \phi_j) \\ &= \sum_K \int_K \nabla \phi_i(x) \cdot \nabla \phi_j(x) \end{aligned}$$

- 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.

step-3

Example:



- On cell 4, only shape functions 1, 3, 5 are nonzero.
- We get a dense sub-matrix composed of rows and columns 1,3,5 of A.

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 cell

step-3

Read through the commented program at

http://www.dealii.org/7.1.0/doxygen/deal.II/step_3.html

Then play with the program:

```
cd examples/step-3
cmake -DDEAL_II_DIR=/a/b/c . ; make run
```

This will run the program and generate output files:

```
ls -l
```

Then run *visit* to visualize the output

```
visit
```

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