Finite element methods in scientific computing

Wolfgang Bangerth, Colorado State University

Lecture 42:

Beyond computational methods

Part 1:

Workflows in Scientific Computing

The bigger picture

Numerical analysis and finite element/difference/volume methods are only one piece in the scientific computing world.

The *goal* is always the simulation of real processes for *prediction and optimization*.

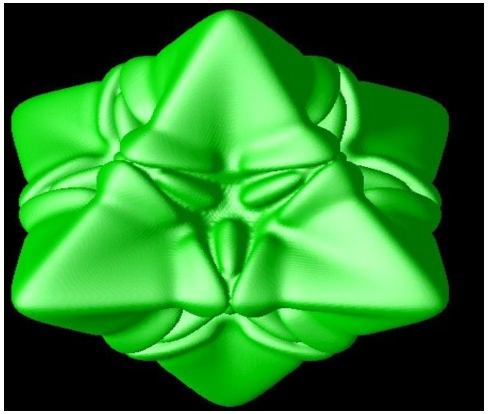
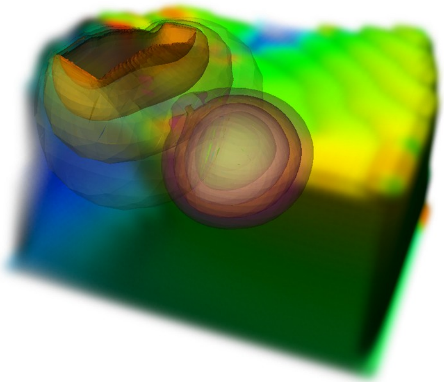
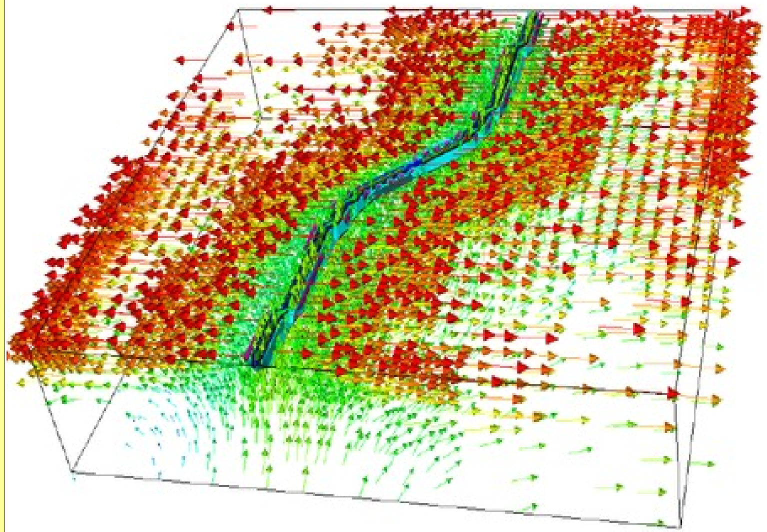
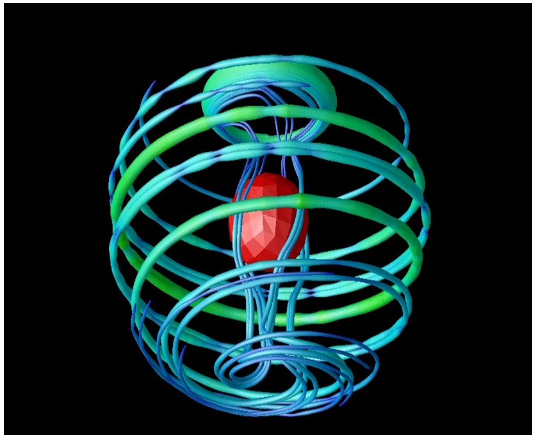
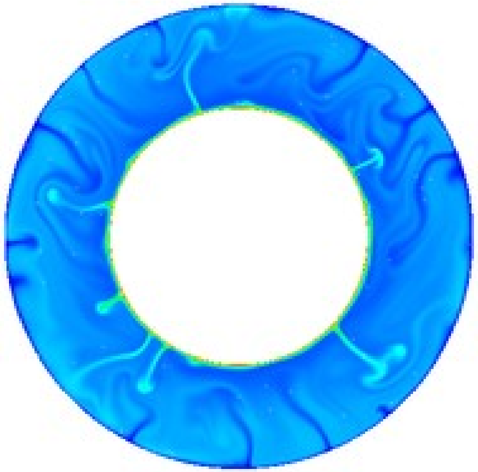
This also involves:

- Understanding the application
- Implementation of numerical methods
- Understanding the complexity of algorithms
- Understanding the hardware characteristics
- Interfacing with pre- and postprocessing tools

Together, these are called *High Performance Computing.*

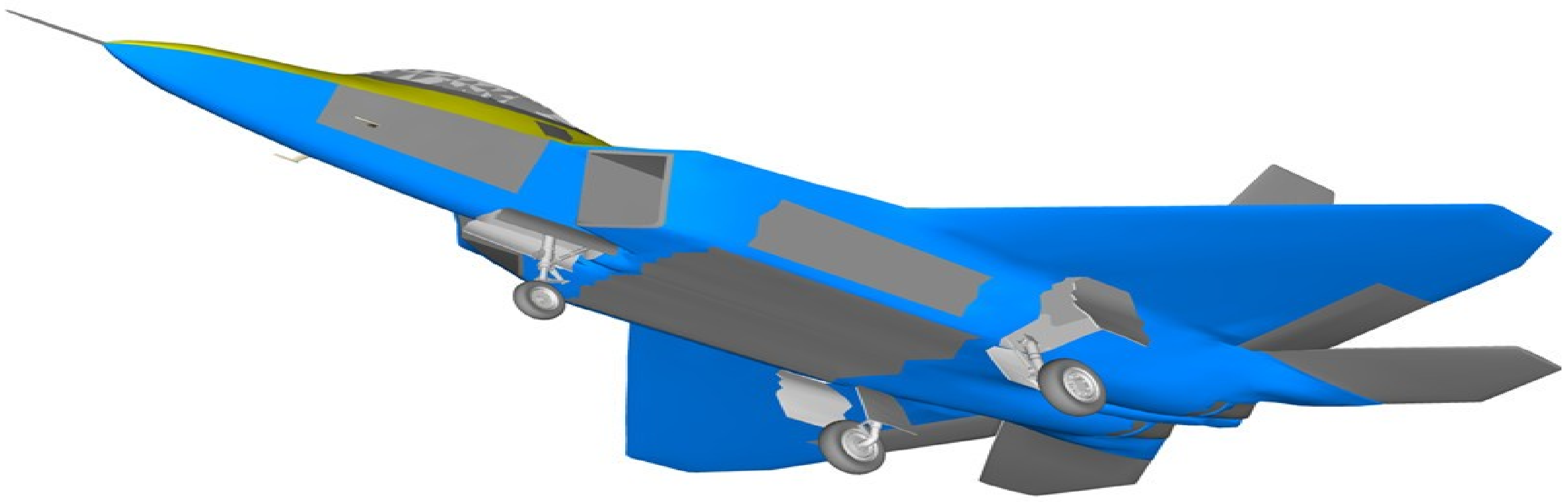
Examples of FEM applications in HPC

Examples from a variety of fields:

Workflow for HPC in PDEs

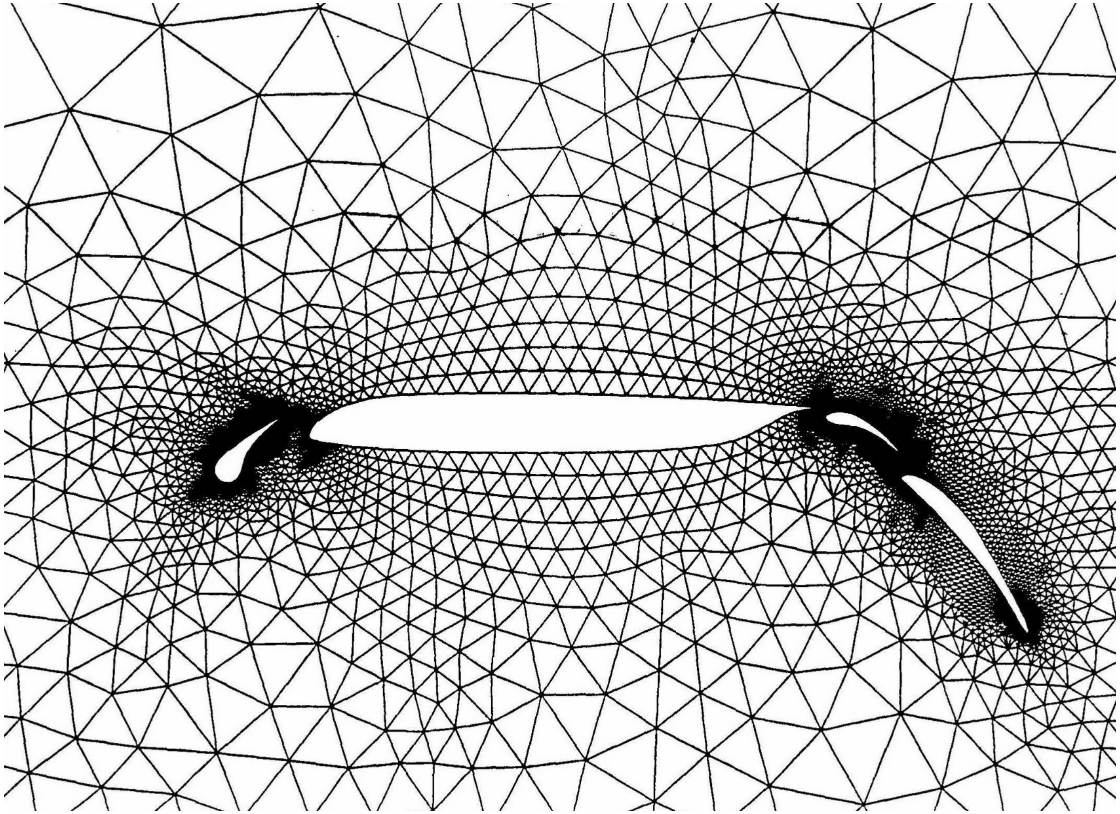
Step 1: Identify geometry and details of the model



May involve tens of thousands of pieces, very labor intensive, interface to designers and to manufacturing

Workflow for HPC in PDEs

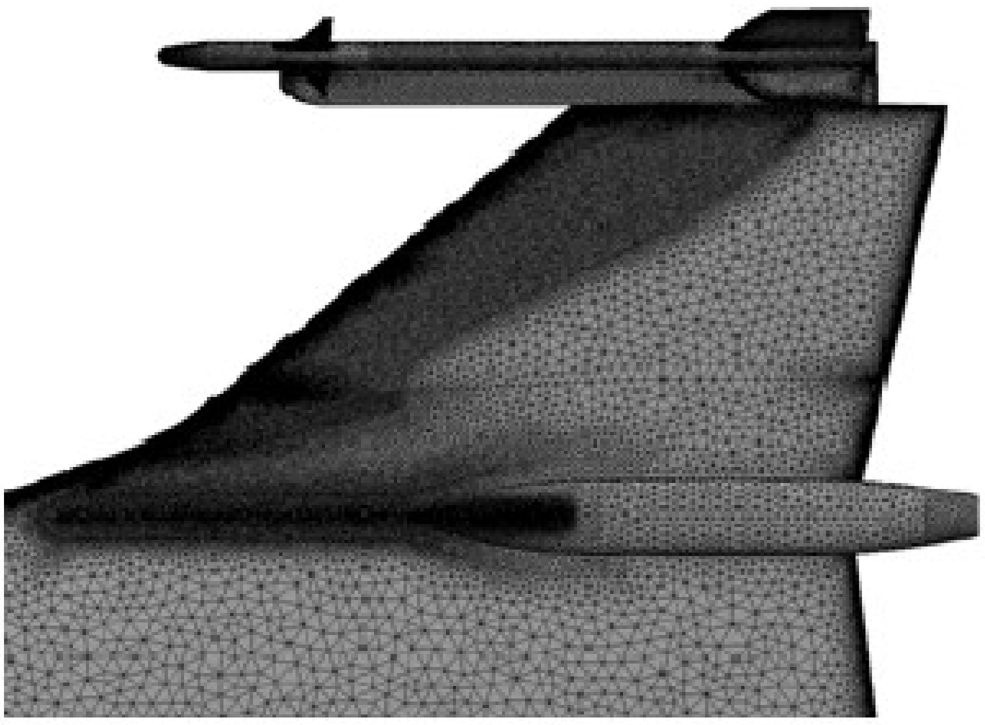
Step 2: Mesh generation and maybe partitioning (preprocessing)



May involve 10s of millions or more of cells; requires lots of memory; very difficult to parallelize

Workflow for HPC in PDEs

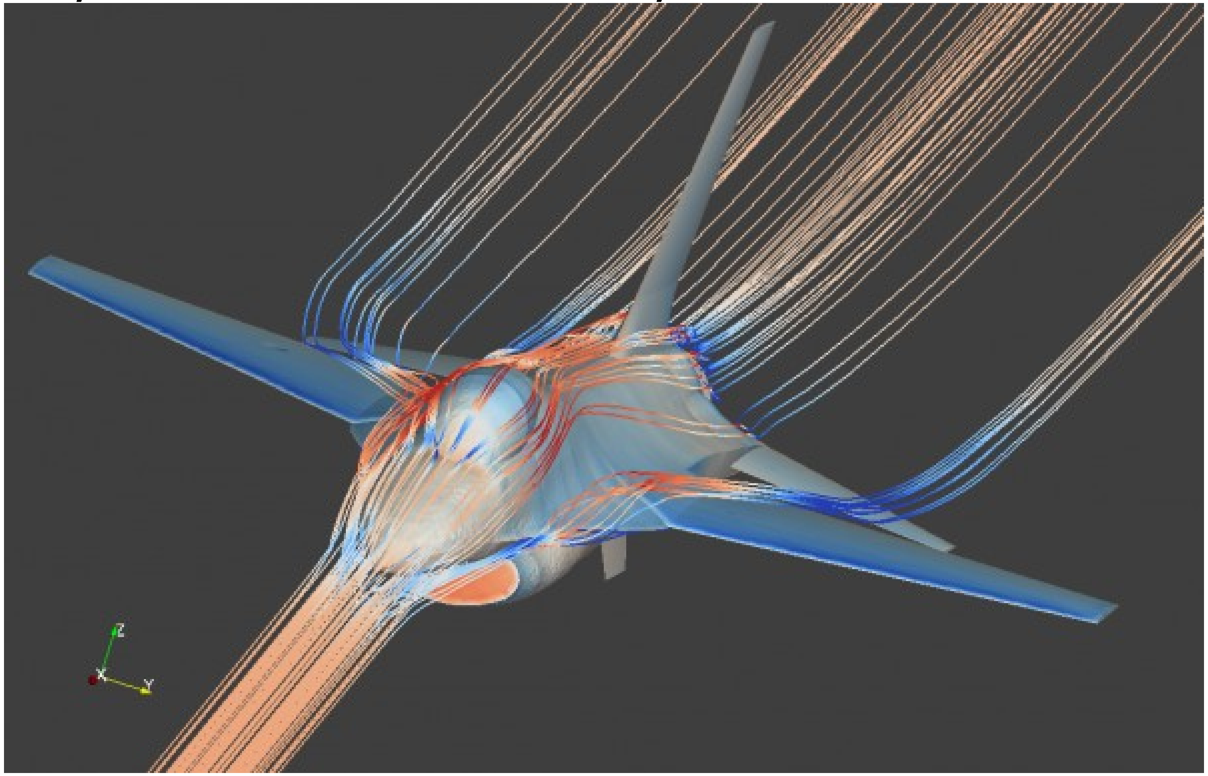
Step 2: Mesh generation and maybe partitioning (preprocessing)



May involve 10s of millions or more of cells; requires lots of memory; very difficult to parallelize

Workflow for HPC in PDEs

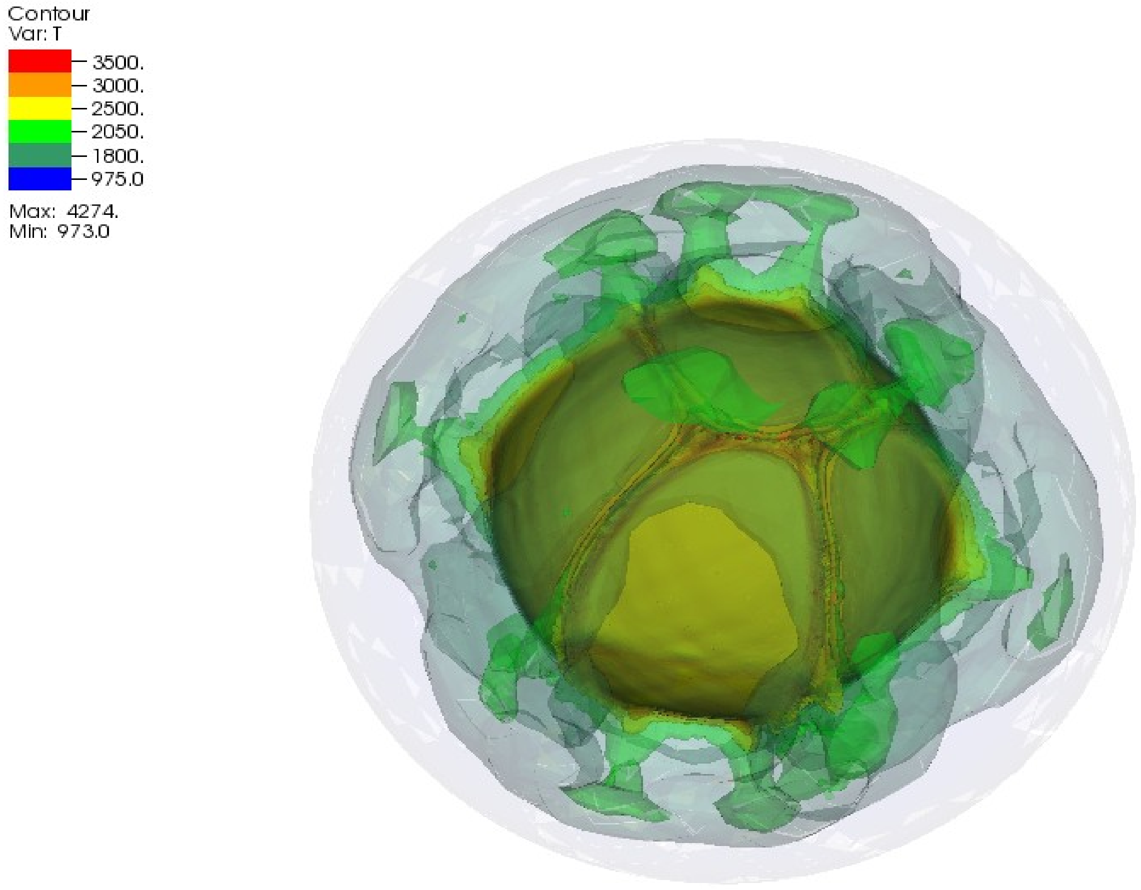
Step 3: Solve model on this mesh using finite elements, finite volumes, finite differences, …



Involves some of the biggest computations ever done, 10,000s of processors, millions of CPU hours, wide variety of algorithms

Workflow for HPC in PDEs

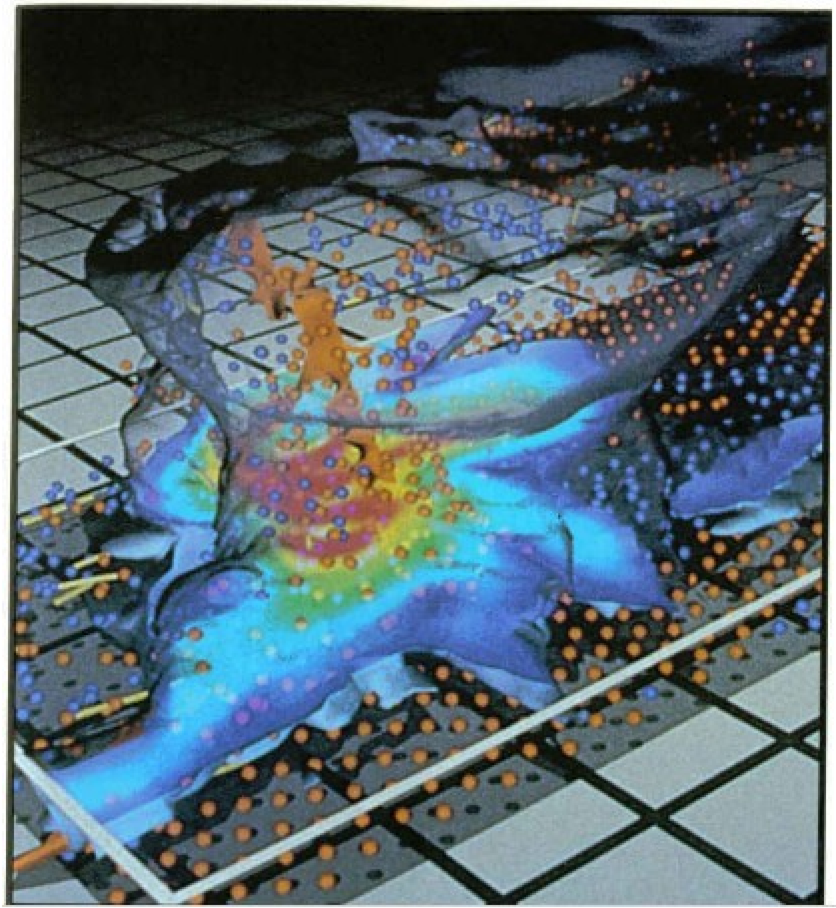
Step 4: Visualization to learn from the numerical results



Can be done in parallel, difficulty is amount of data.

Workflow for HPC in PDEs

Step 4: Visualization to learn from the numerical results



Goal: Not to *plot data*, but to *provide insight*!

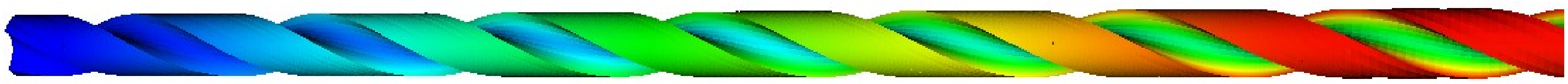
Workflow for HPC in PDEs

Step 5: Repeat

- To improve on the design
- To investigate different conditions (speed, altitude, angle of attack, …)
- To vary physical parameters that may not be known exactly
- To vary parameters of the numerical model (e.g. mesh size)
- To improve match with experiments

A complete example

Goal: Simulating the deformation of a drill



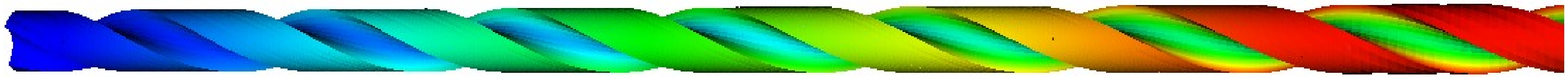
Data produced by *Patrik Boettcher*:

- Created during a 2-week deal.II course
- Time needed: approximately 50 hours, including learning deal.II

Geometry and mesh provided by *Hannah Ludwig*.

A complete example

Goal: Simulating the deformation of a drill



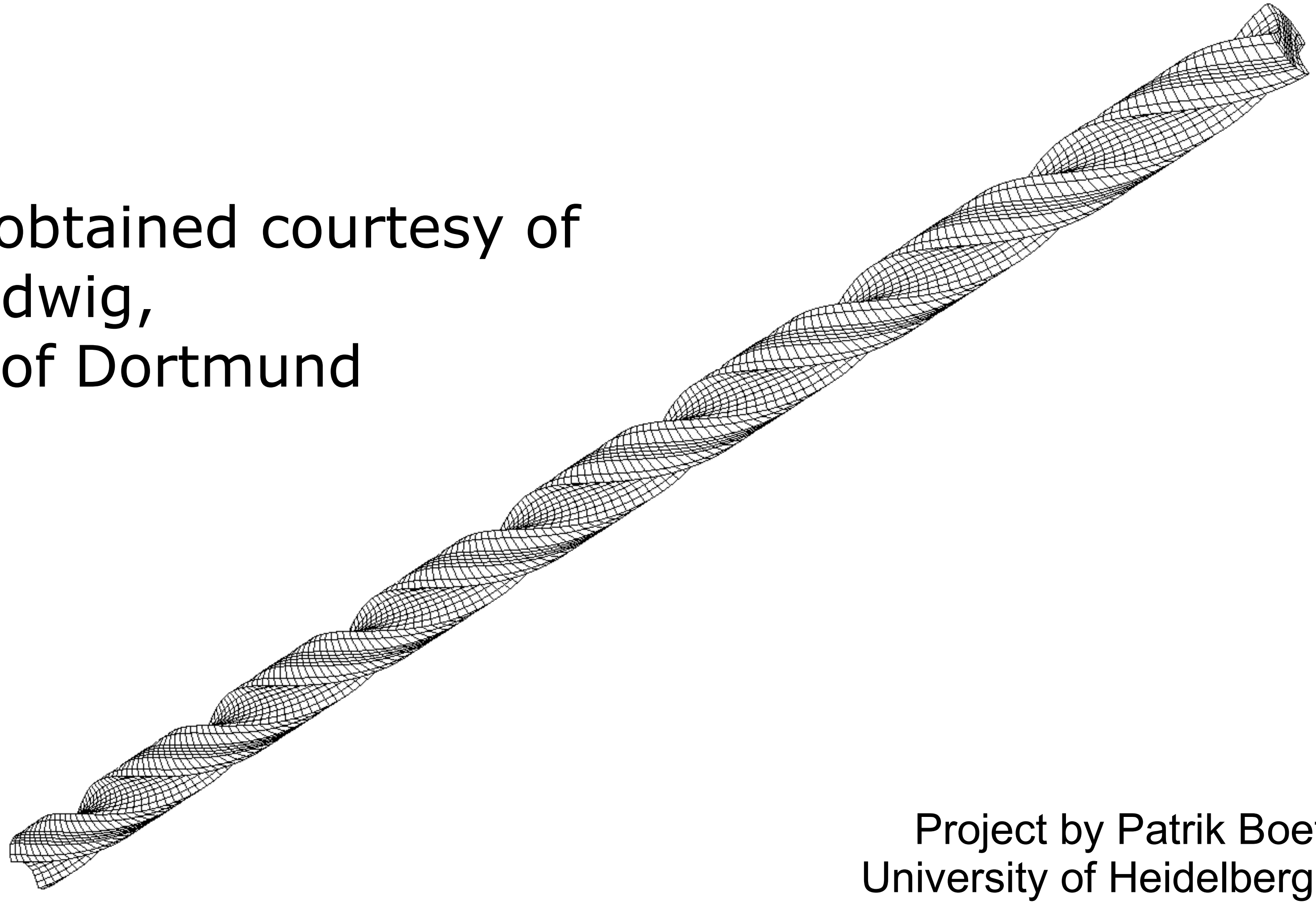
Steps:

(1) Create or obtain a coarse mesh
(2) Identify the model (elasticity) and implement a solver
(3) Obtain material parameters for steel used in the drill
(4) Mark up geometry: Where do which forces act
(5) Identify magnitude of forces
(6) Mark up geometry: Describe boundary approximation
(7) Postprocess for quantities of interest
(8) Visualize
(9) Start over: Optimization of drill and validation

A complete example

Step 1: Create or obtain a coarse mesh

Here:
Mesh was obtained courtesy of
Hannah Ludwig,
University of Dortmund



Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 2: Identify the model

Here:

- Linear, small deformation elasticity model 3d:

$$
\begin{aligned}
-\nabla(\lambda \nabla \cdot \boldsymbol{u}) - 2\nabla \cdot (\mu\, \varepsilon(\boldsymbol{u})) &= \boldsymbol{f} && \text{in } \Omega \\
\boldsymbol{u} &= \boldsymbol{g}_D && \text{on } \Gamma_D \\
\boldsymbol{n} \cdot (\lambda (\nabla \cdot \boldsymbol{u}) I + 2\mu\, \varepsilon(\boldsymbol{u})) &= \boldsymbol{g}_N && \text{on } \Gamma_N
\end{aligned}
$$

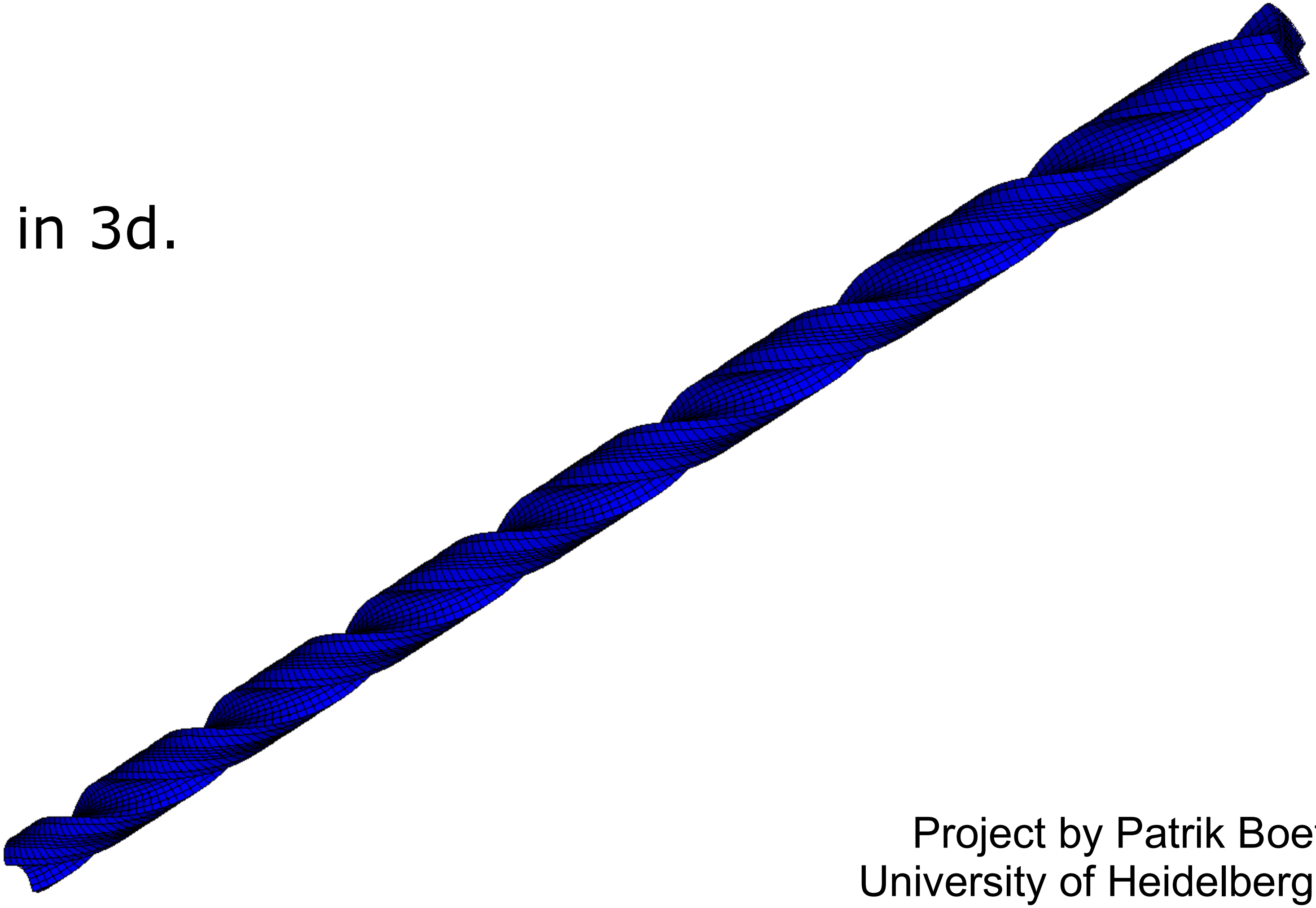
- Justified because displacements will be <0.3mm on domain sizes of >20mm

Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 2: Implement an elasticity solver

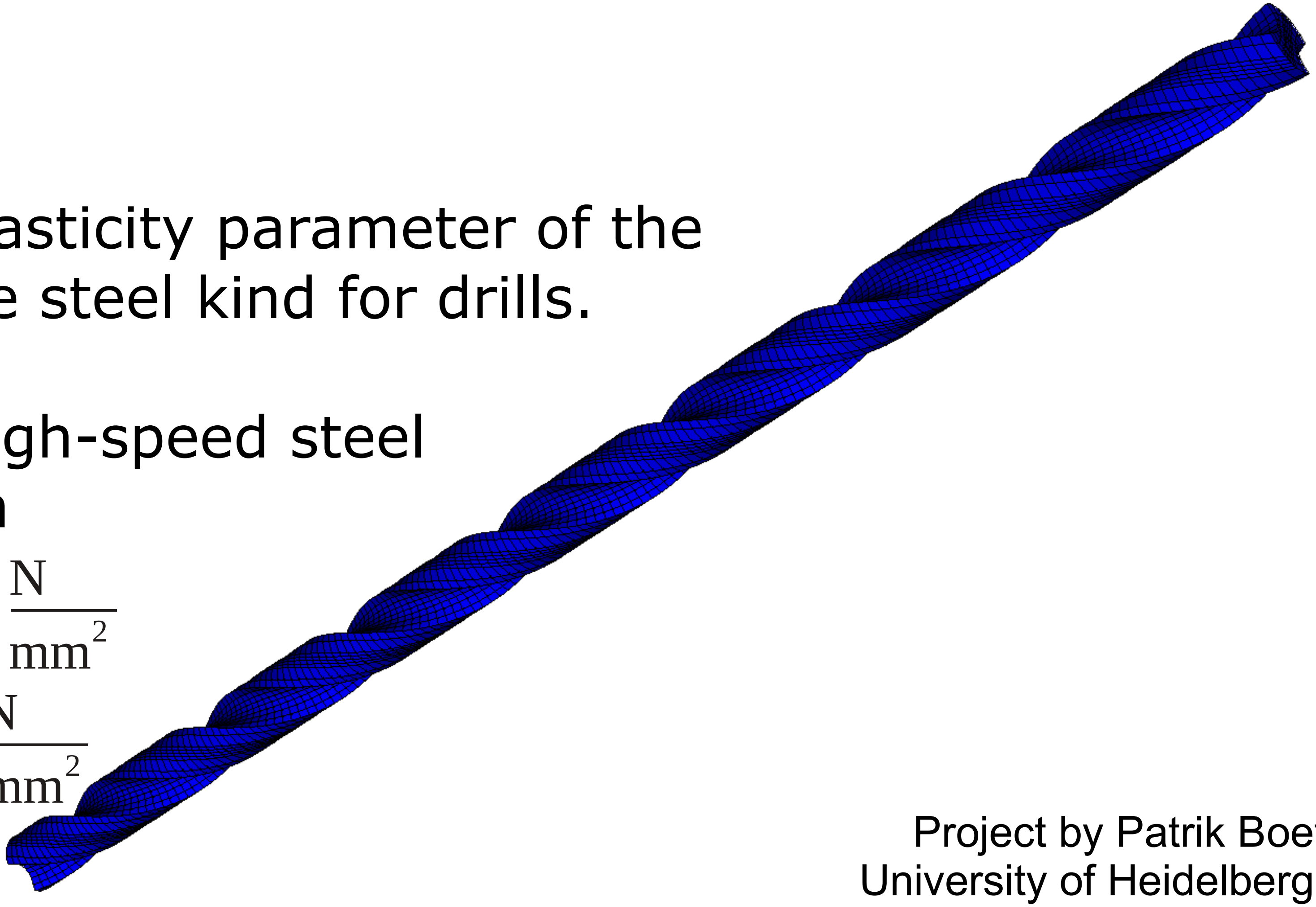
Here:
Use step-8 in 3d.



Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 3: Identify material parameters



Here:
Find the elasticity parameter of the appropriate steel kind for drills.

Choose: High-speed steel HS-30 with

$$\lambda = 207{,}000 \frac{N}{mm^2}$$

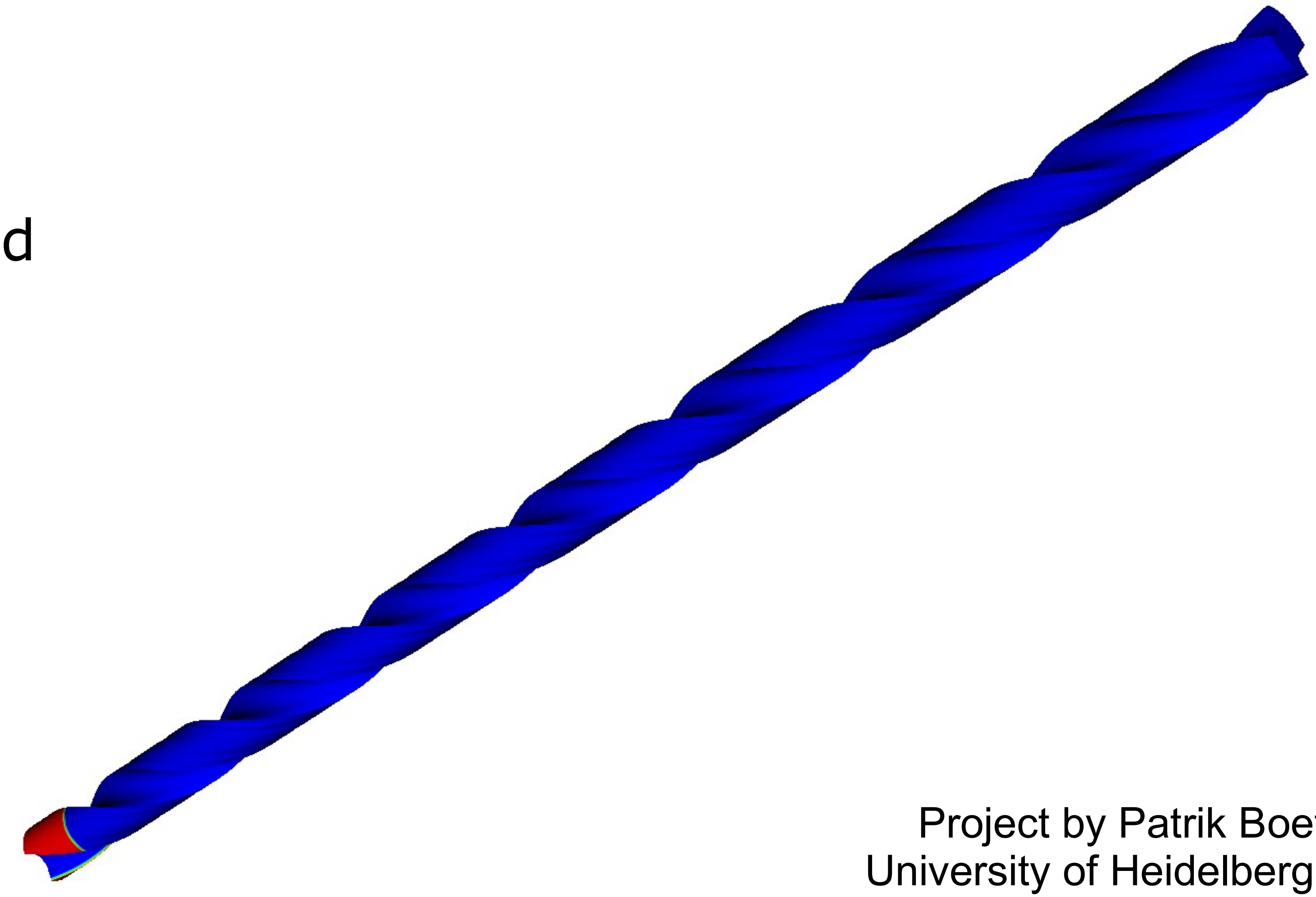
$$\mu = 82{,}800 \frac{N}{mm^2}$$

Project by Patrik Boettcher, University of Heidelberg, 2012

A complete example

Step 4: Mark up geometry – where does which force act?

Here:
- Clamped



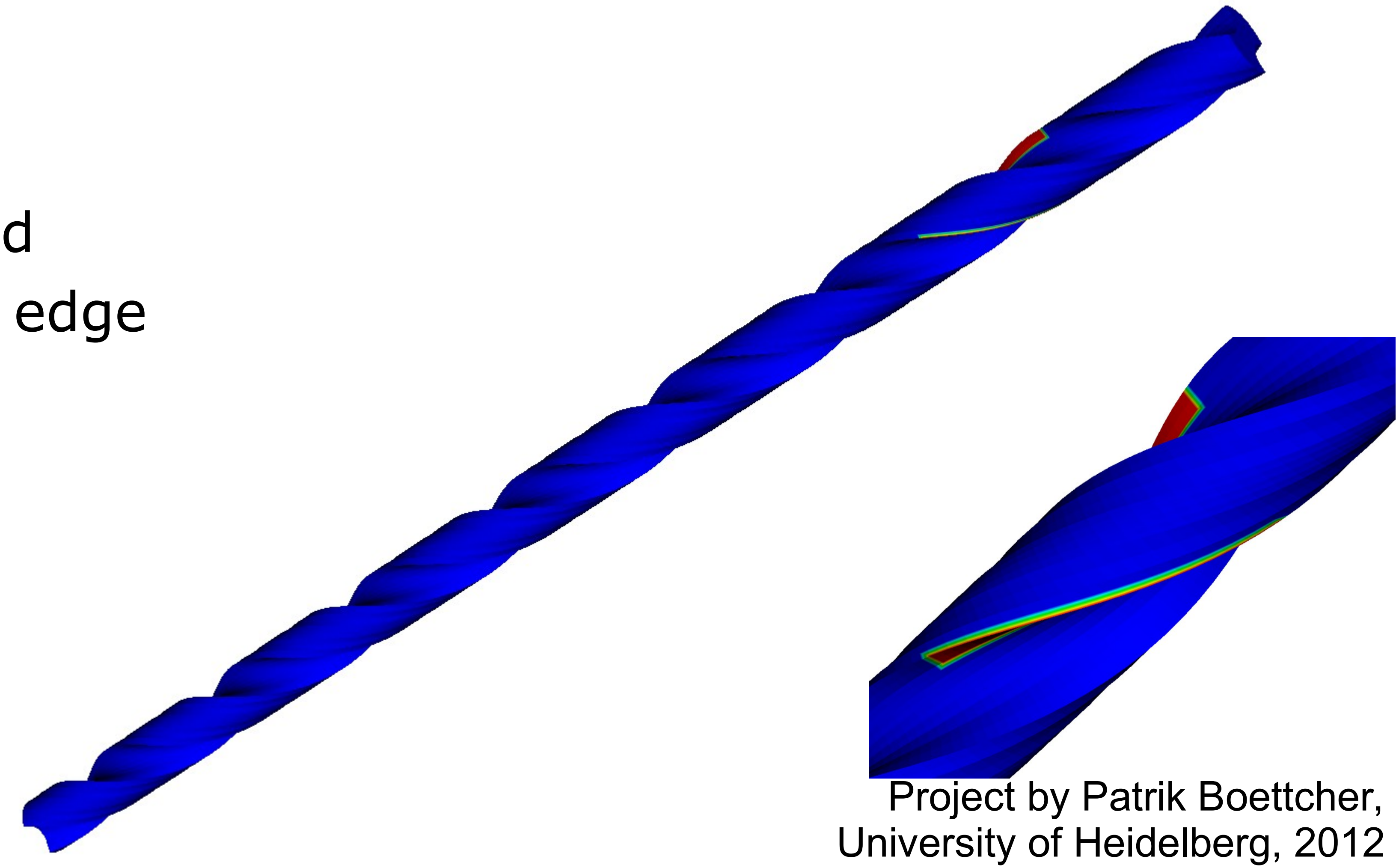
Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 4: Mark up geometry – where does which force act?

Here:

- Clamped
- Cutting edge



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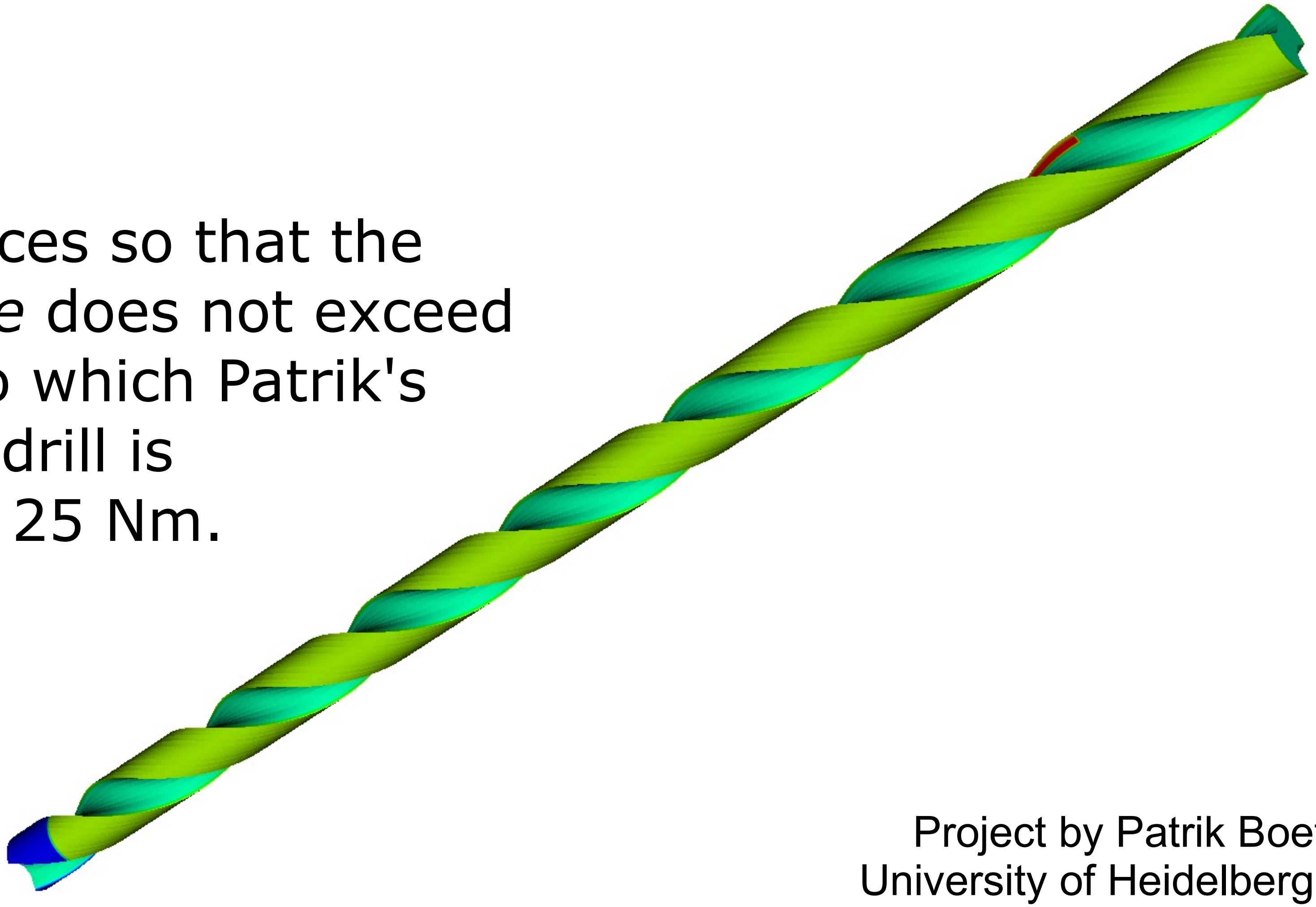
A complete example

Step 5: Identify appropriate magnitude of forces

Here:

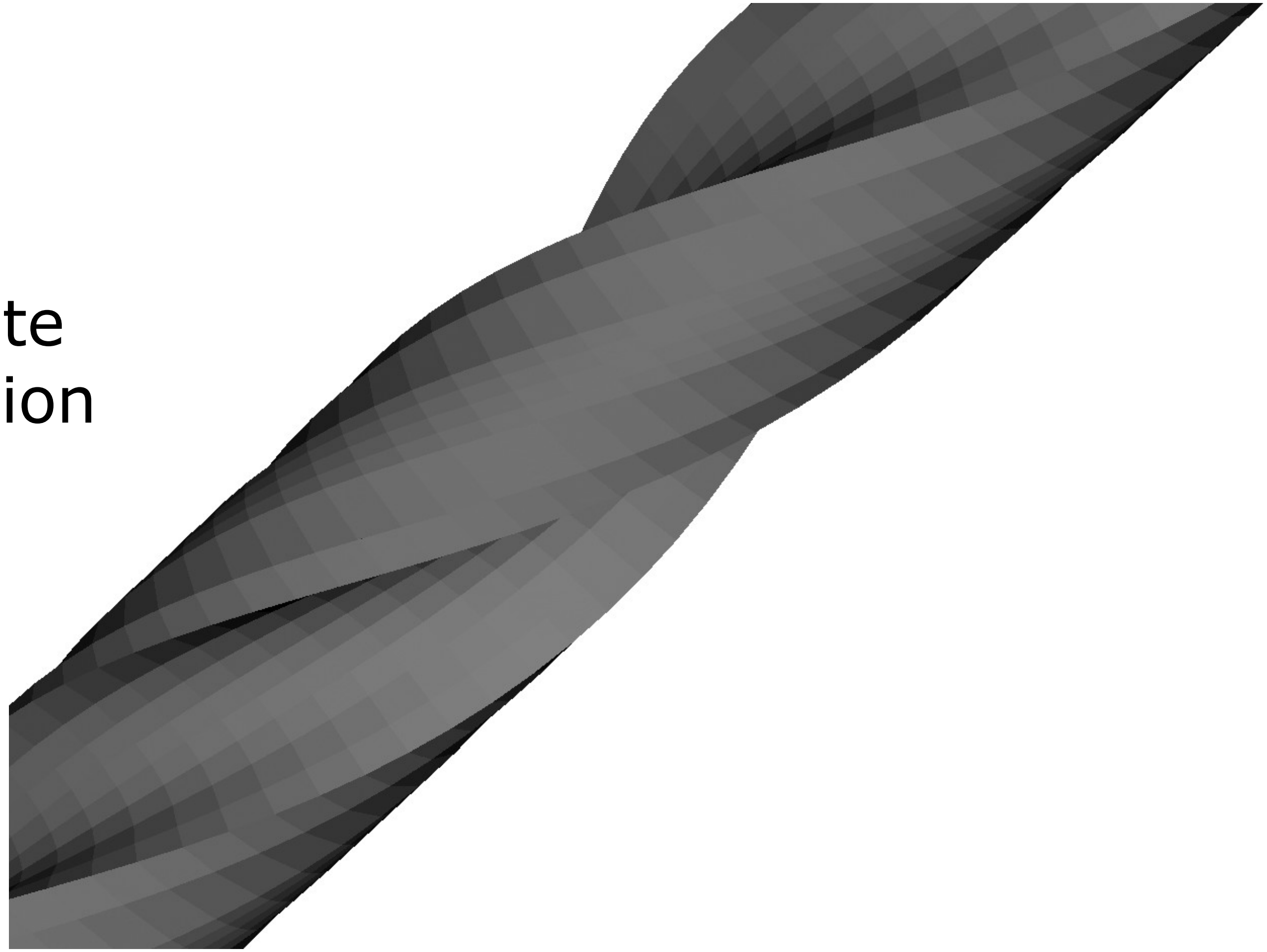
Choose forces so that the *total torque* does not exceed the level to which Patrik's household drill is rated, i.e., 25 Nm.



Project by Patrik Boettcher, University of Heidelberg, 2012

A complete example

Step 6: Mark up boundaries for geometry description



Here:

Without appropriate boundary description

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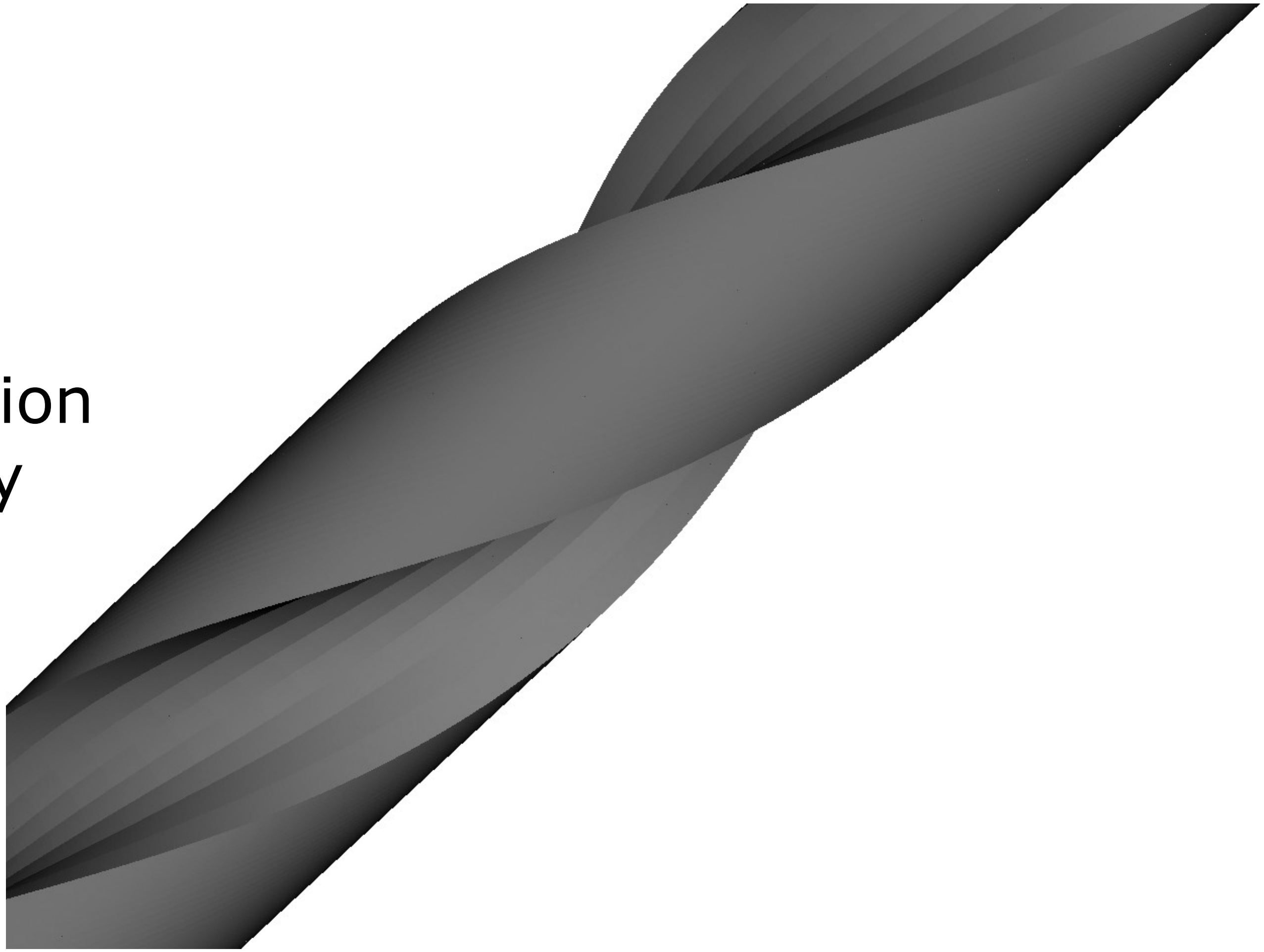
A complete example

Step 6: Mark up boundaries for geometry description

Here:

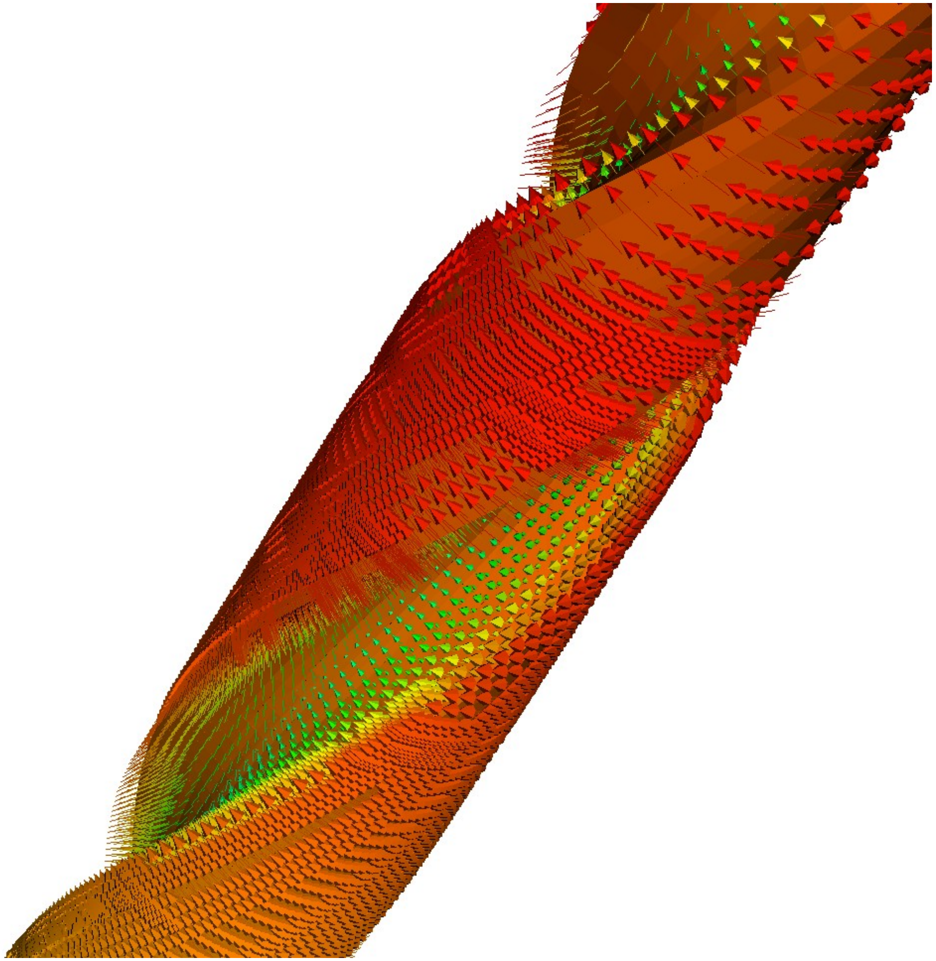
With appropriate boundary description for outer boundary (no description for the inner ones was available)



Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 7: Identify goals of simulation and set up postprocessing needs



Here:

The goal is to determine the torsion angle of the drill from the displacement vector.

Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 8: Visualize

Here:

Mesh

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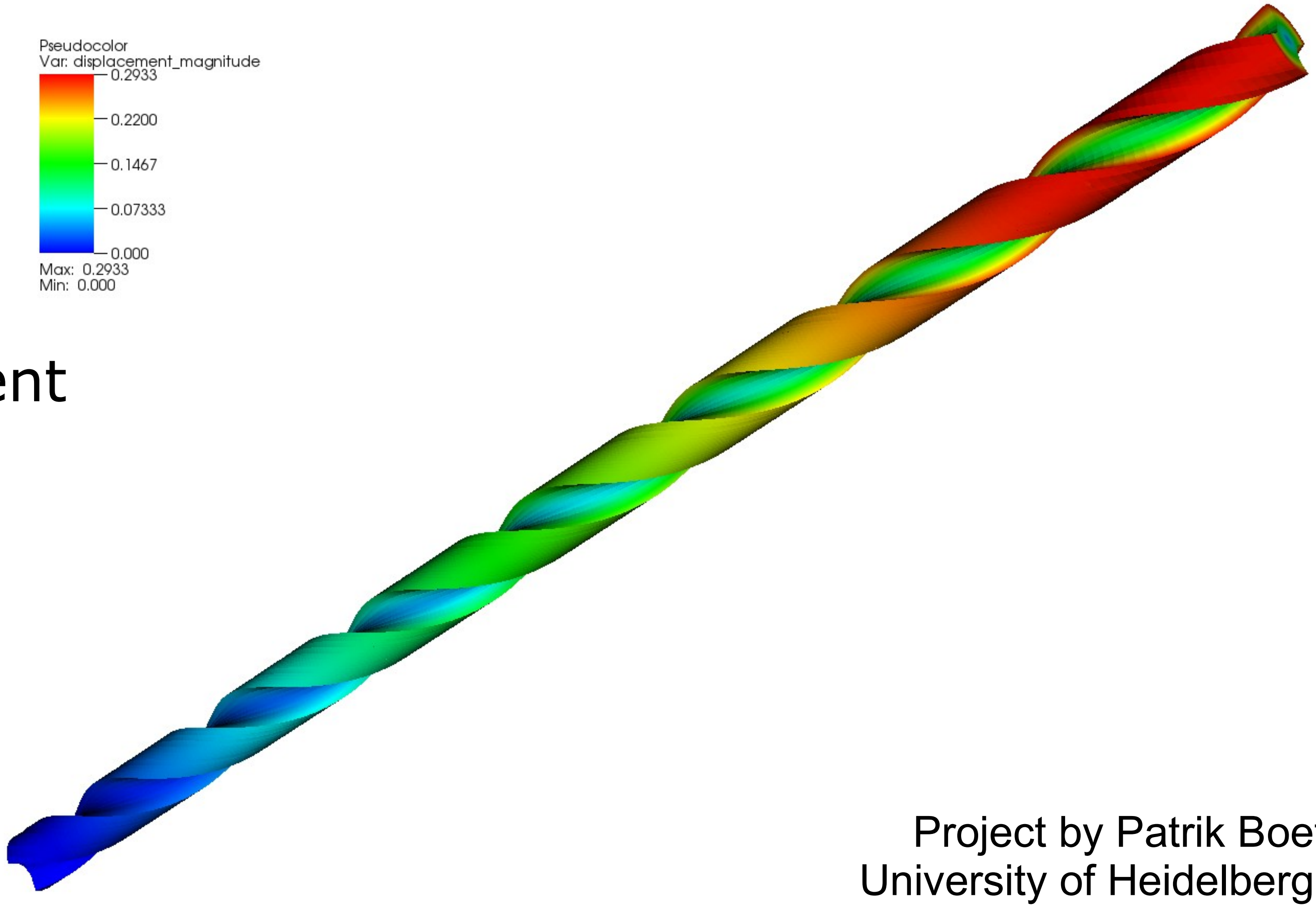
University of Heidelberg, 2012

A complete example

Step 8: Visualize

Here:

Magnitude of displacement (in mm)



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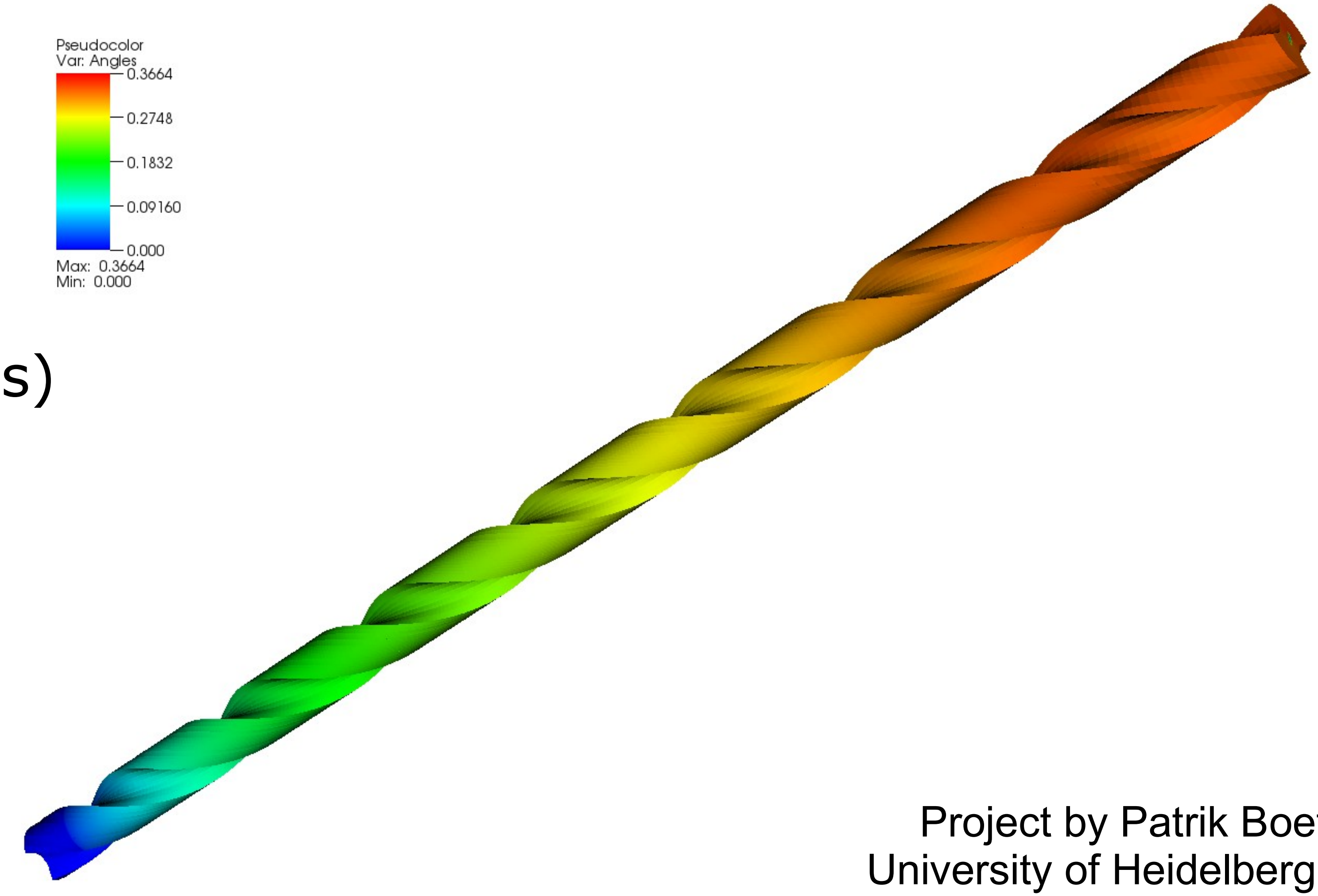
A complete example

Step 8: Visualize

Here:

Torsion angle (in degrees)



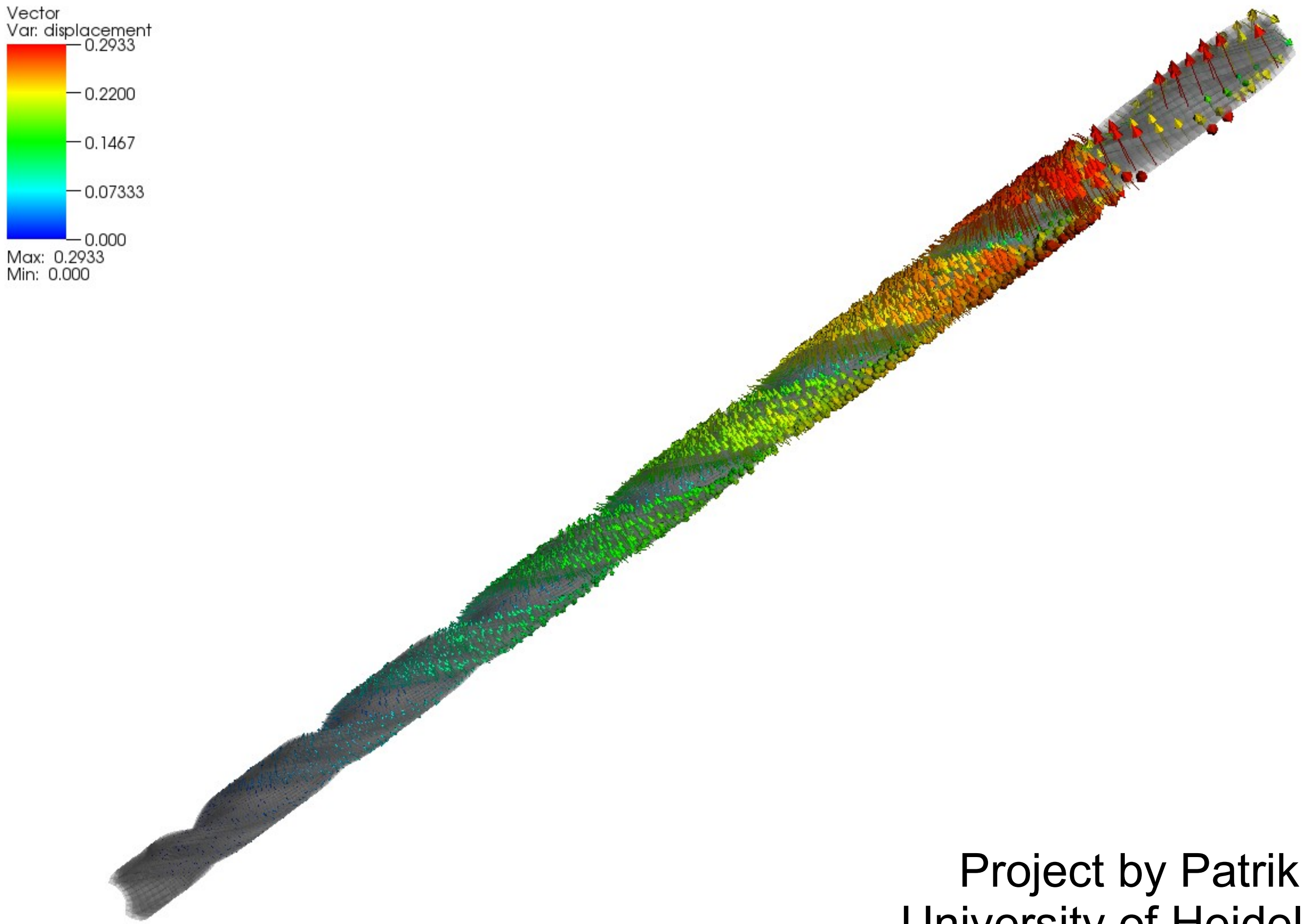
Project by Patrik Boettcher, University of Heidelberg, 2012

A complete example

Step 8: Visualize

Here:

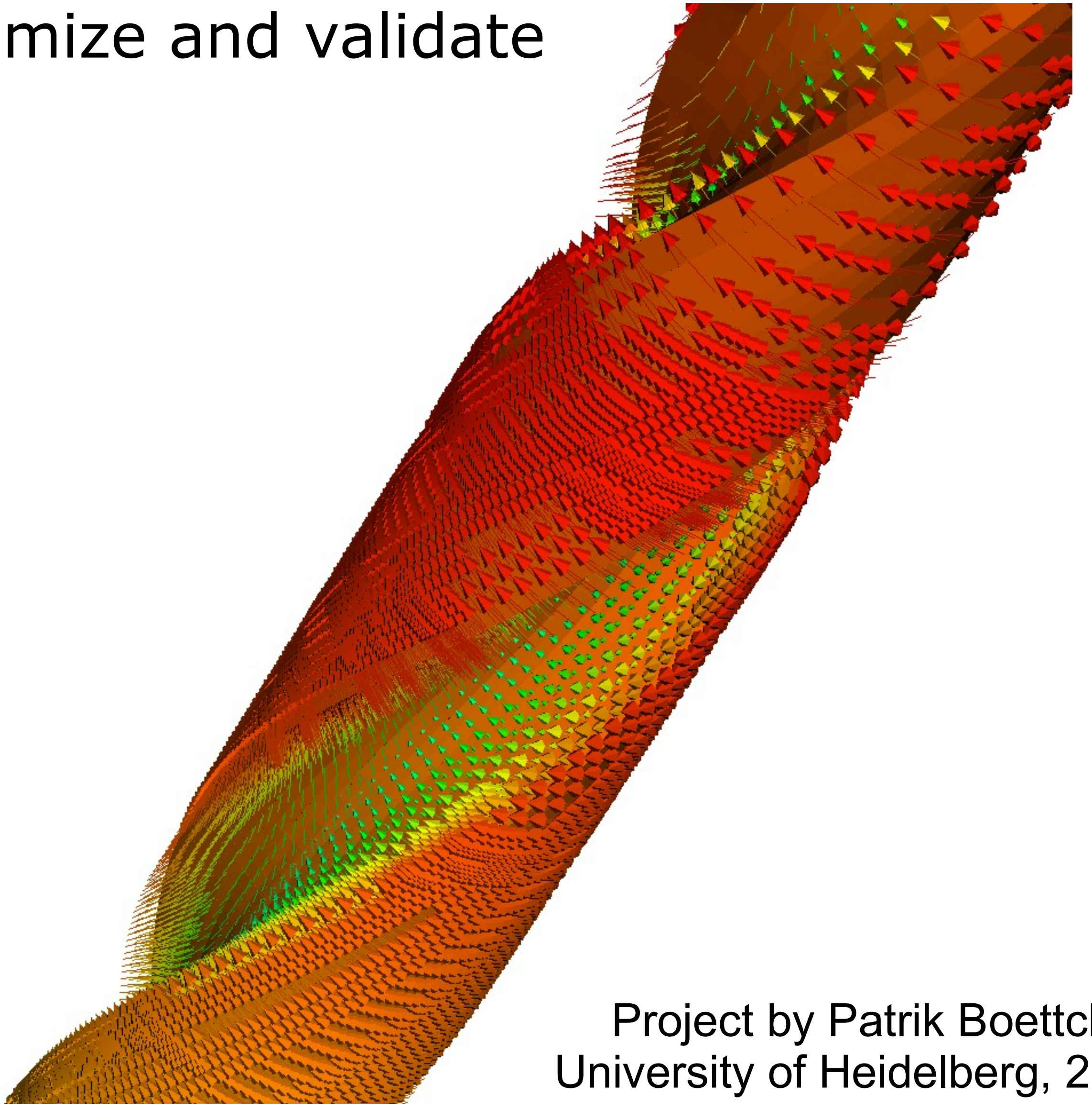
Disp-
lacement
(in mm)



Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

Step 9: Repeat to optimize and validate



Project by Patrik Boettcher,
University of Heidelberg, 2012

Workflow for HPC in PDEs

Each of these steps...

- Identify geometry and details of the model
- Preprocess: Mesh generation
- Solve problem with FEM/FVM/FDM
- Postprocess: Visualize
- Repeat

...needs software that requires:

- domain knowledge
- knowledge of the math. description of the problem
- knowledge of algorithm design
- knowledge of software design and management

Finite element methods in scientific computing

Wolfgang Bangerth, Colorado State University