MATH 676

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Finite element methods in scientific computing

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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*.

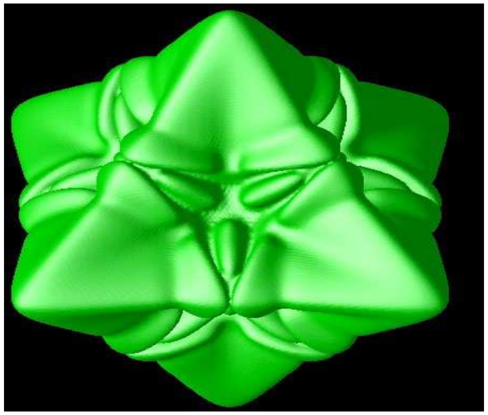
This also involves:

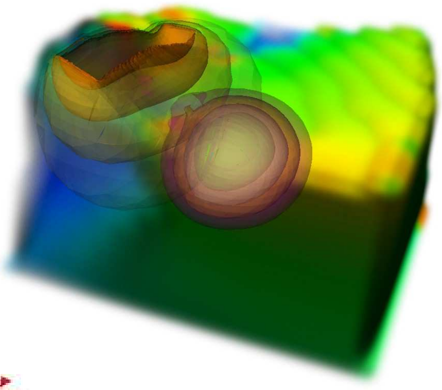
- Understanding the application
- Implementation of numerical methods
- Understanding the complexity of algorithms
- Understanding the hardware characteristics
- Interfacing with pre- and postprocessing tools

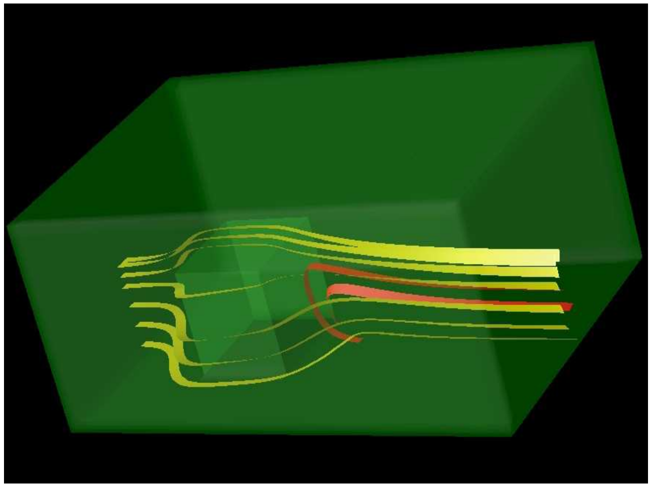
Together, these are called *High Performance Computing.*

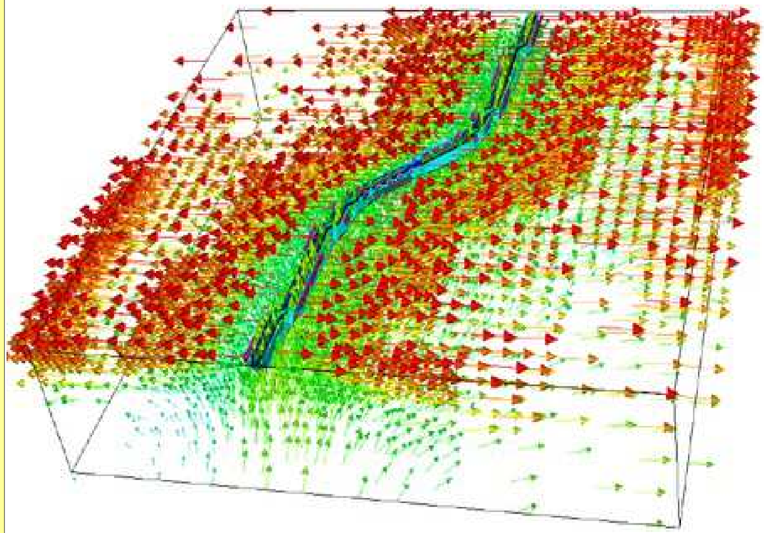
Examples of FEM applications in HPC

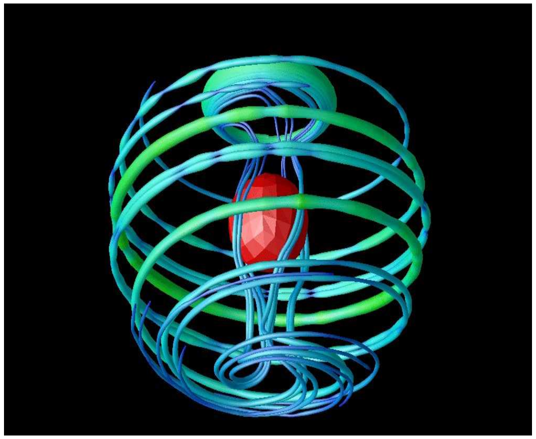
Examples from a wide variety of fields:





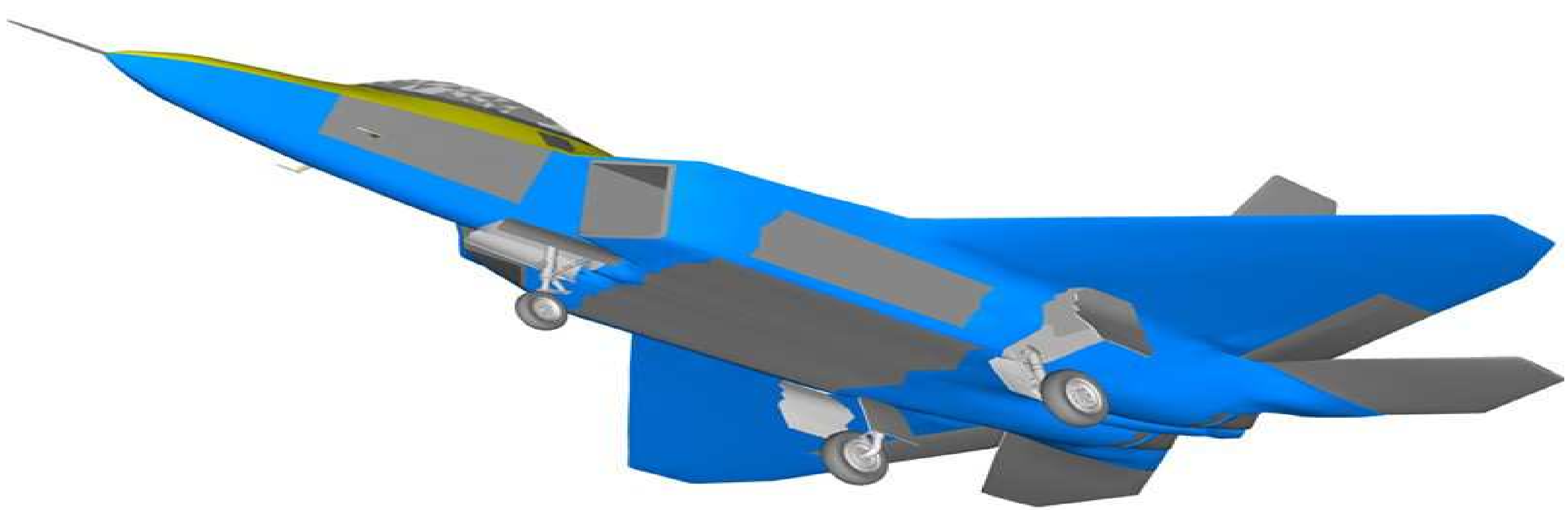






Workflow for HPC in PDEs

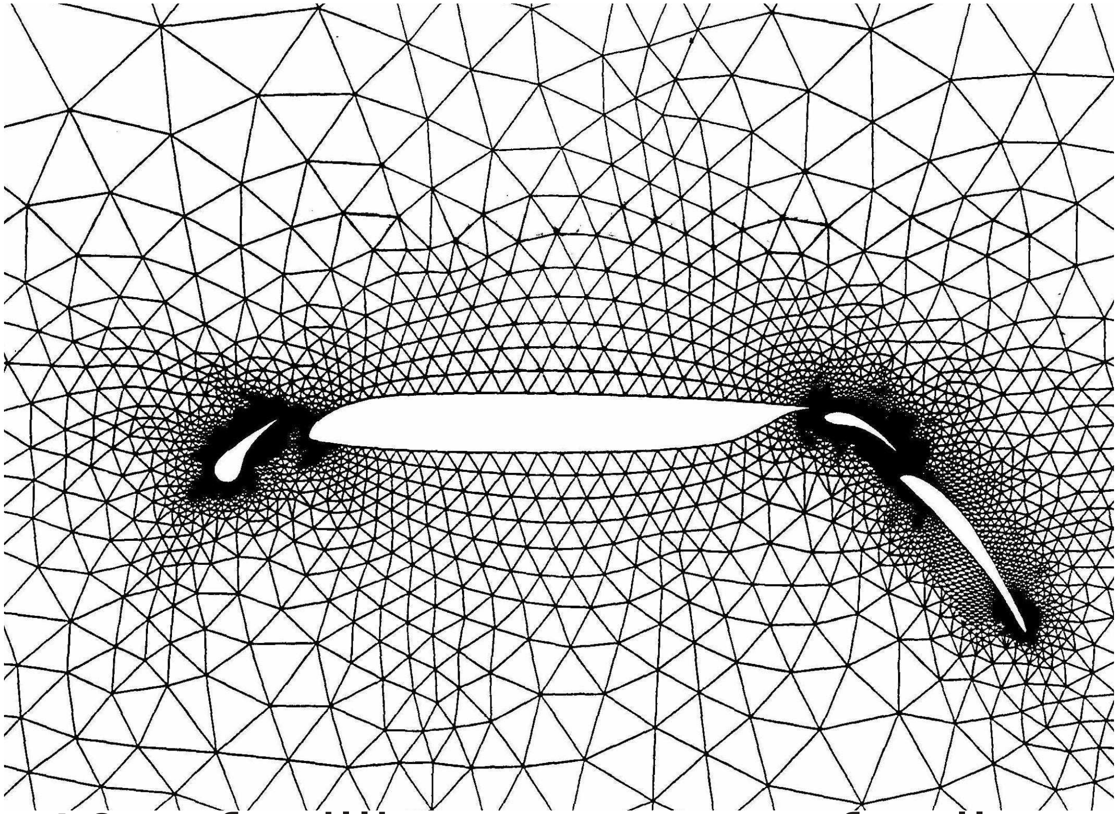
Step 1: Identify geometry and details of the model



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

Workflow for HPC in PDEs

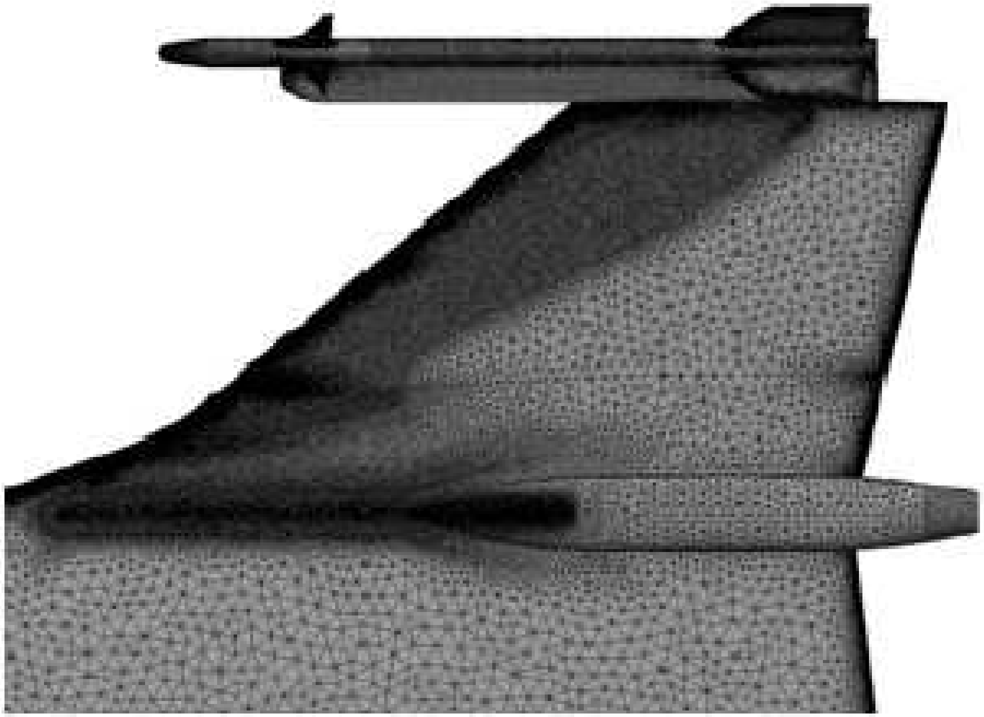
Step 2: Mesh generation and maybe partitioning (preprocessing)



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

Workflow for HPC in PDEs

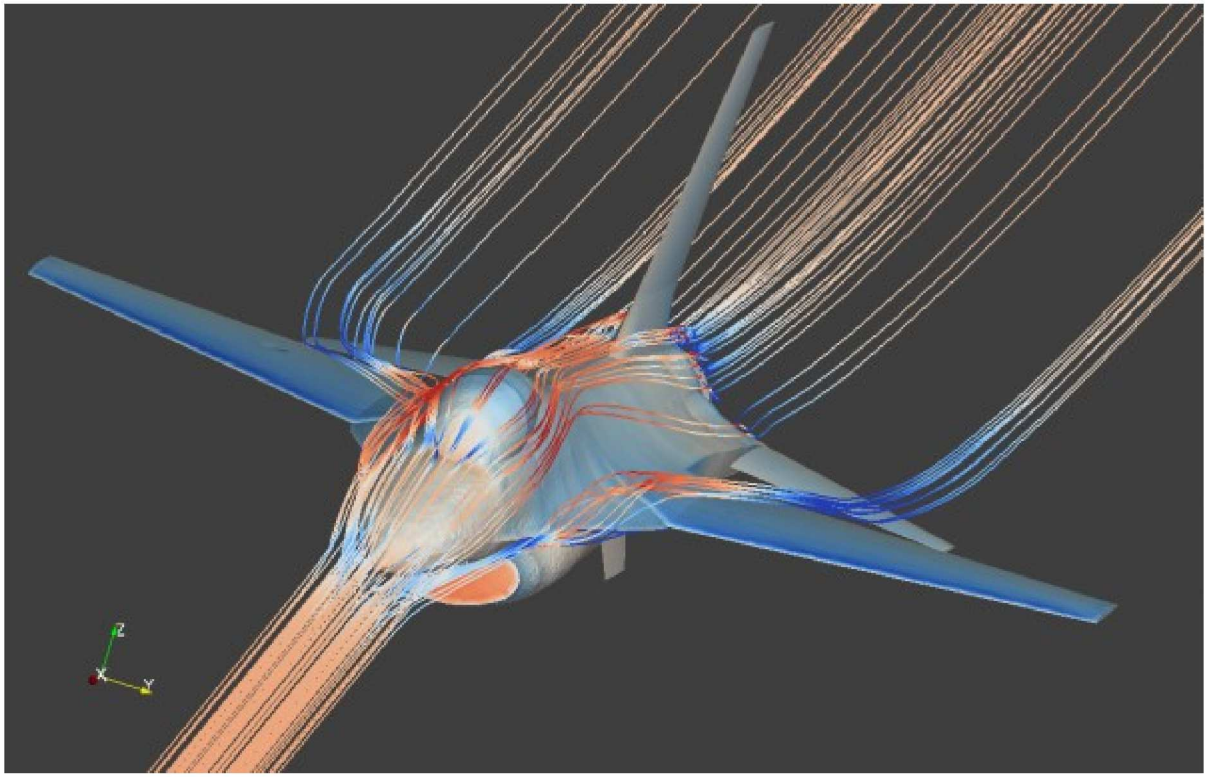
Step 2: Mesh generation and maybe partitioning (preprocessing)



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

Workflow for HPC in PDEs

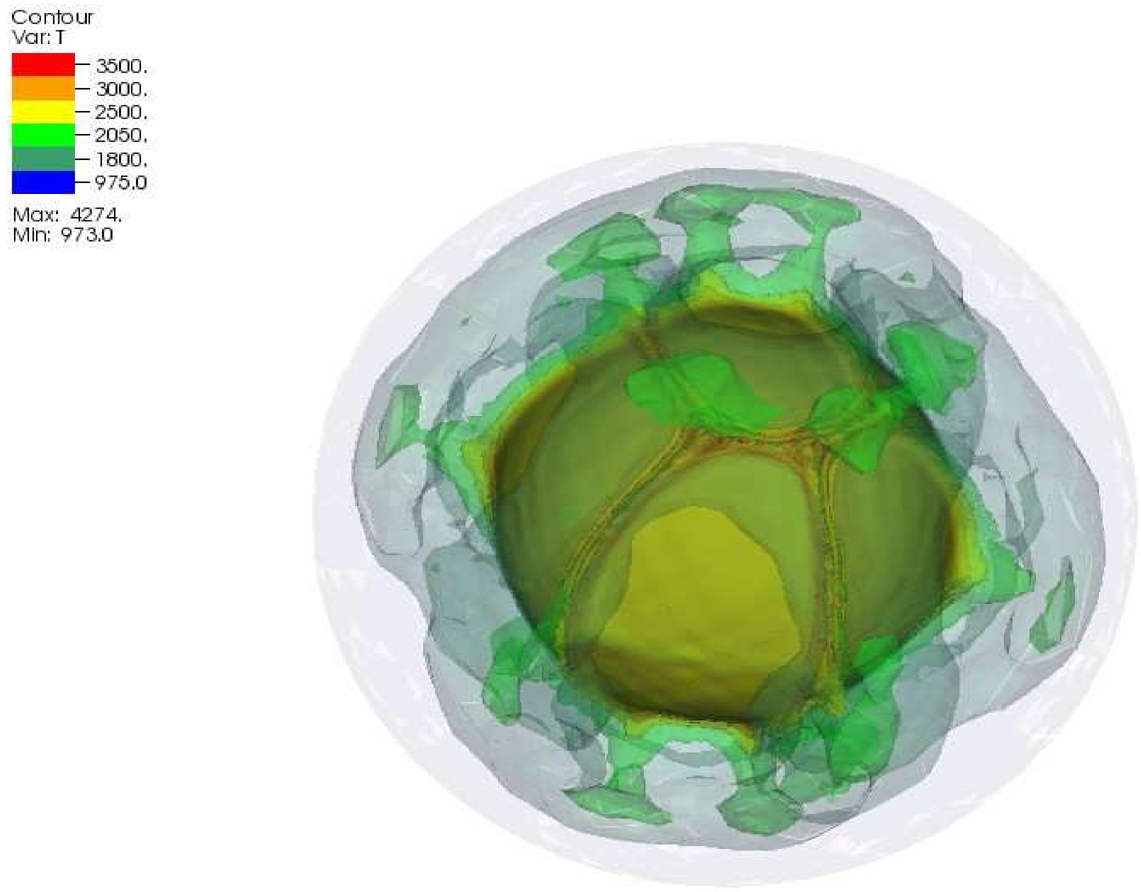
Step 3: Solve model on this mesh using finite elements, finite volumes, finite differences, ...



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

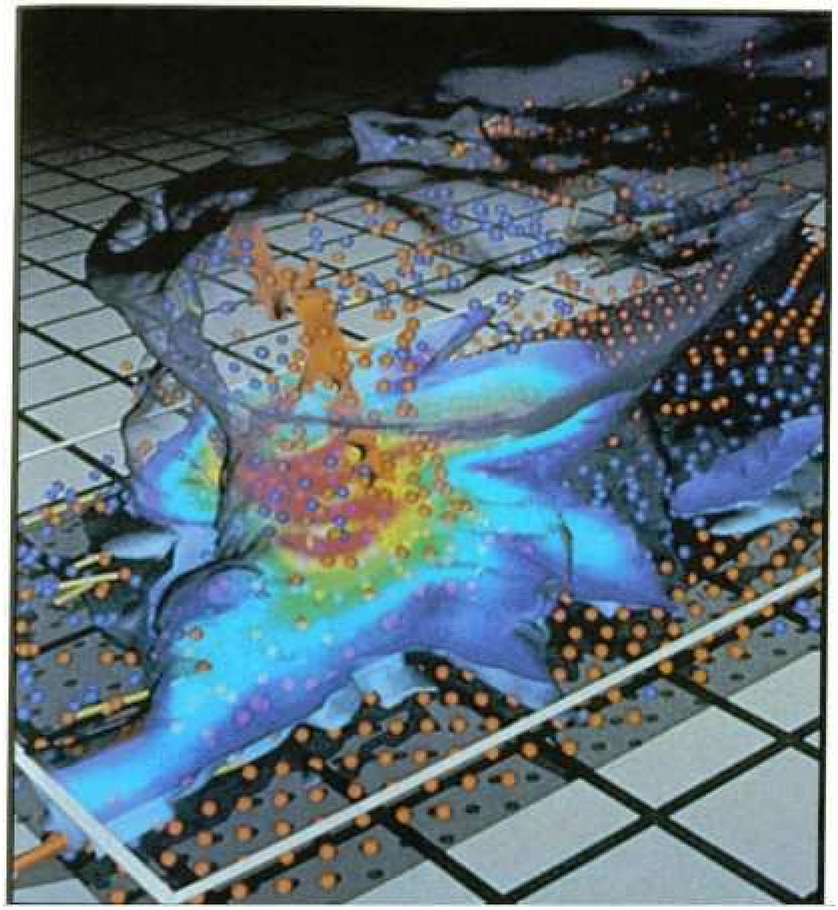
Step 4: Visualization to learn from the numerical results



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*!

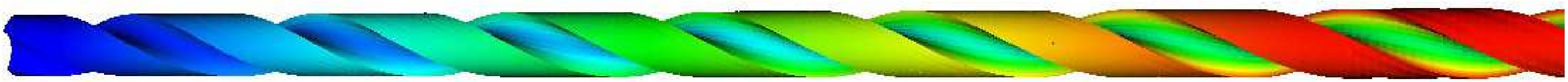
Workflow for HPC in PDEs

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



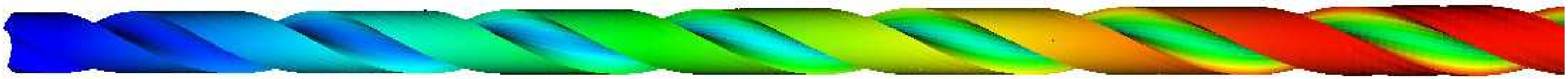
Data produced by *Patrik Boettcher*:

- 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

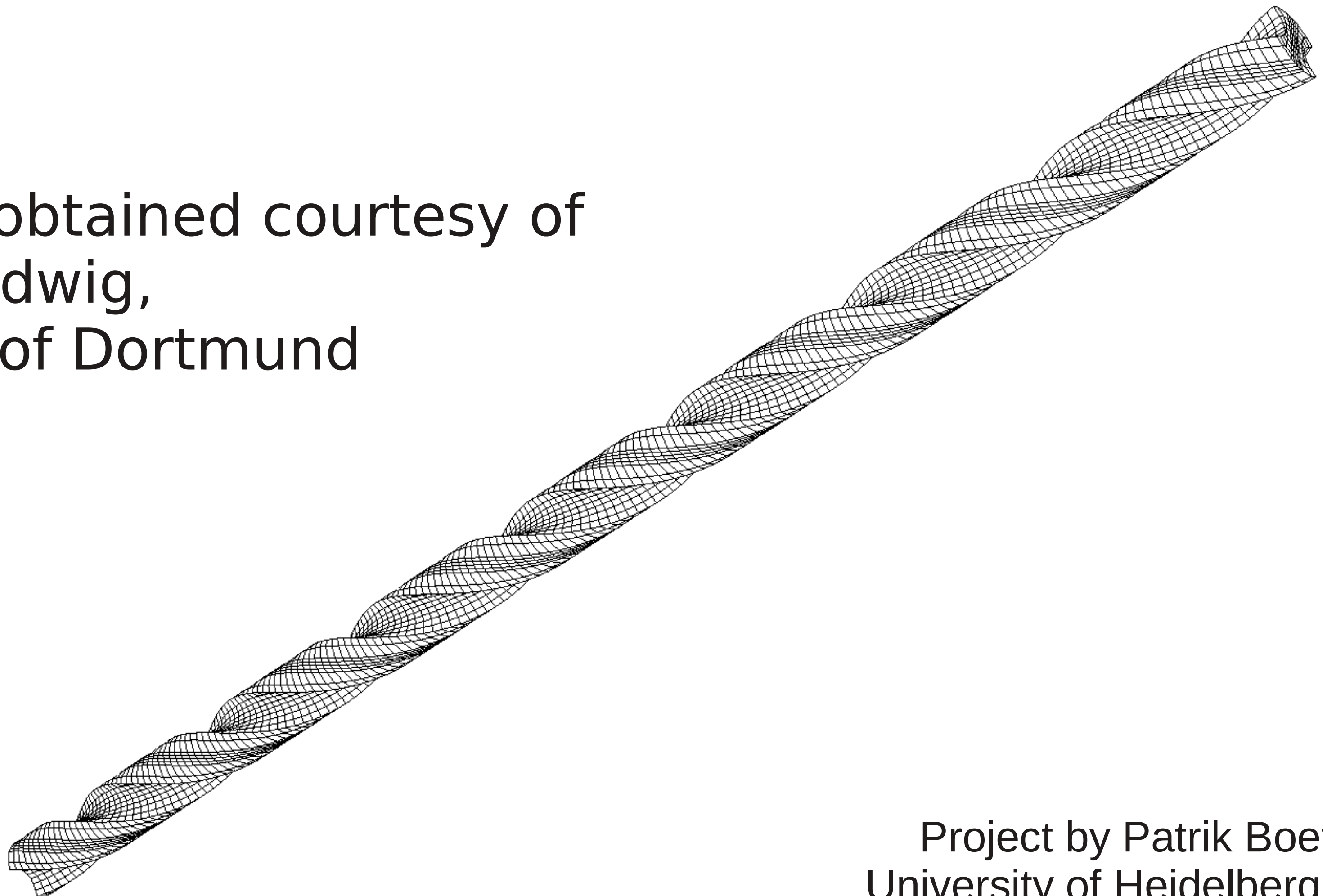
(8) Visualize

(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:

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

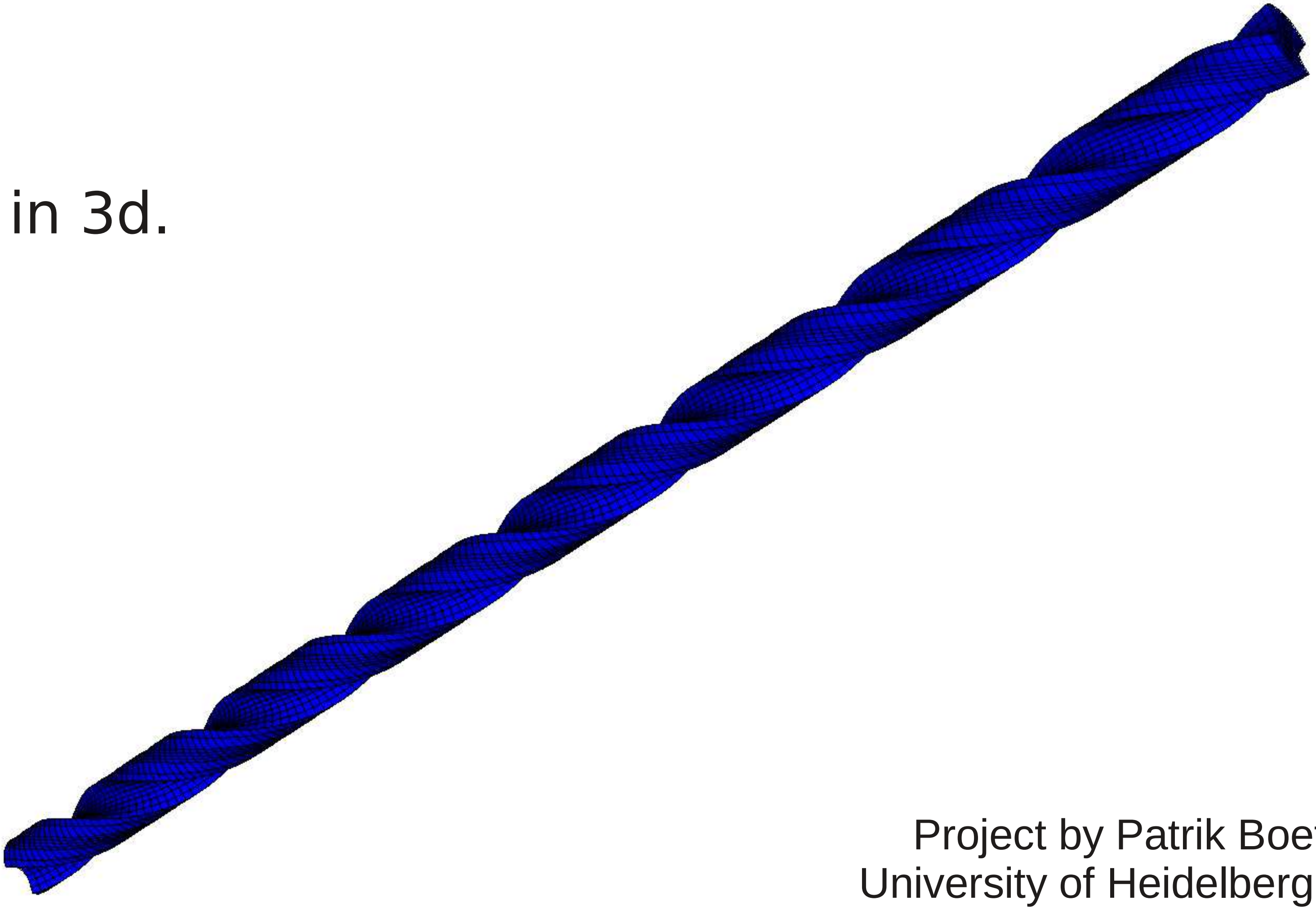
- Justified because displacements will be <0.3mm on domain sizes of >20mm

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

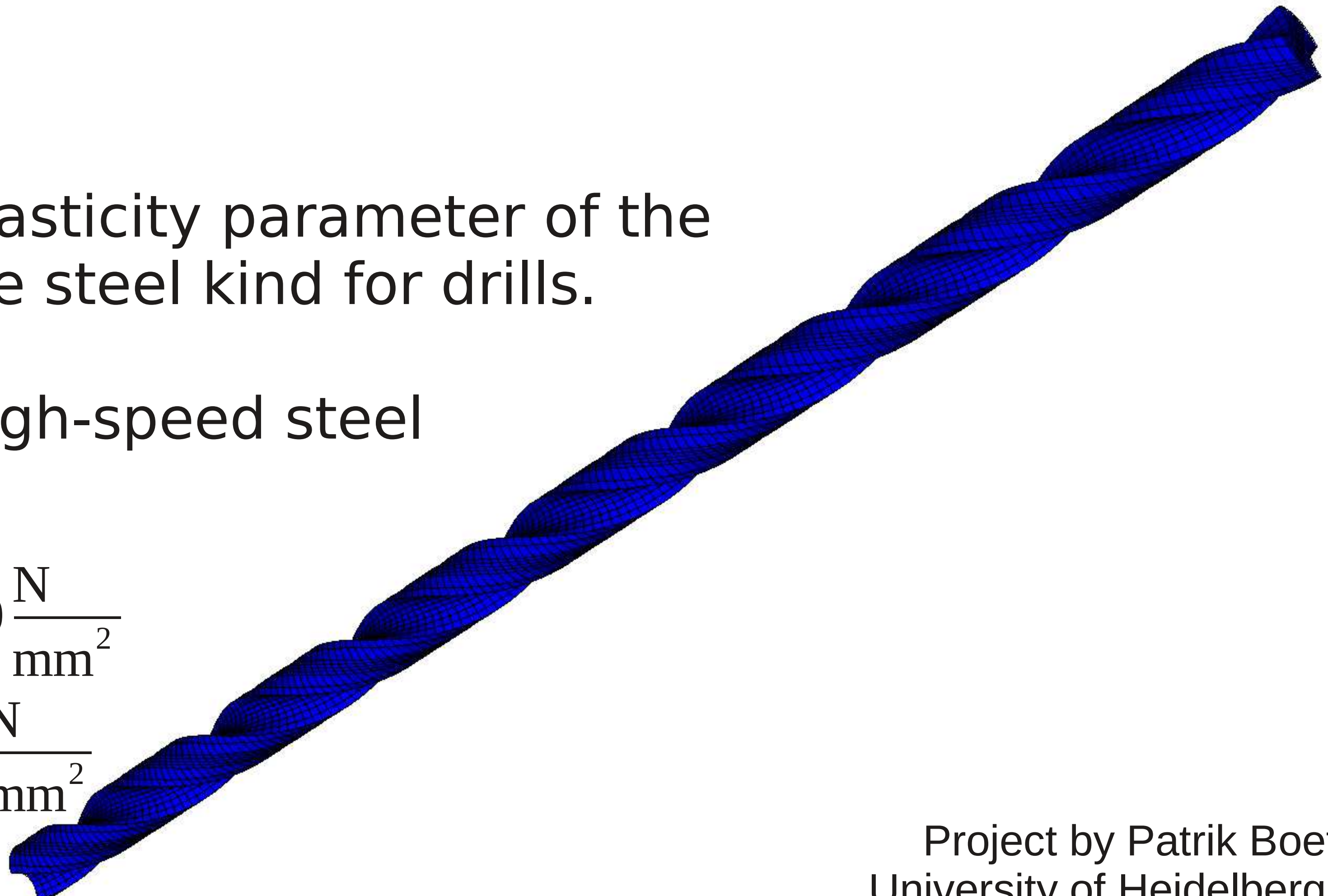
Step 3: Identify material parameters

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

Choose: High-speed steel
HS-30 with

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

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



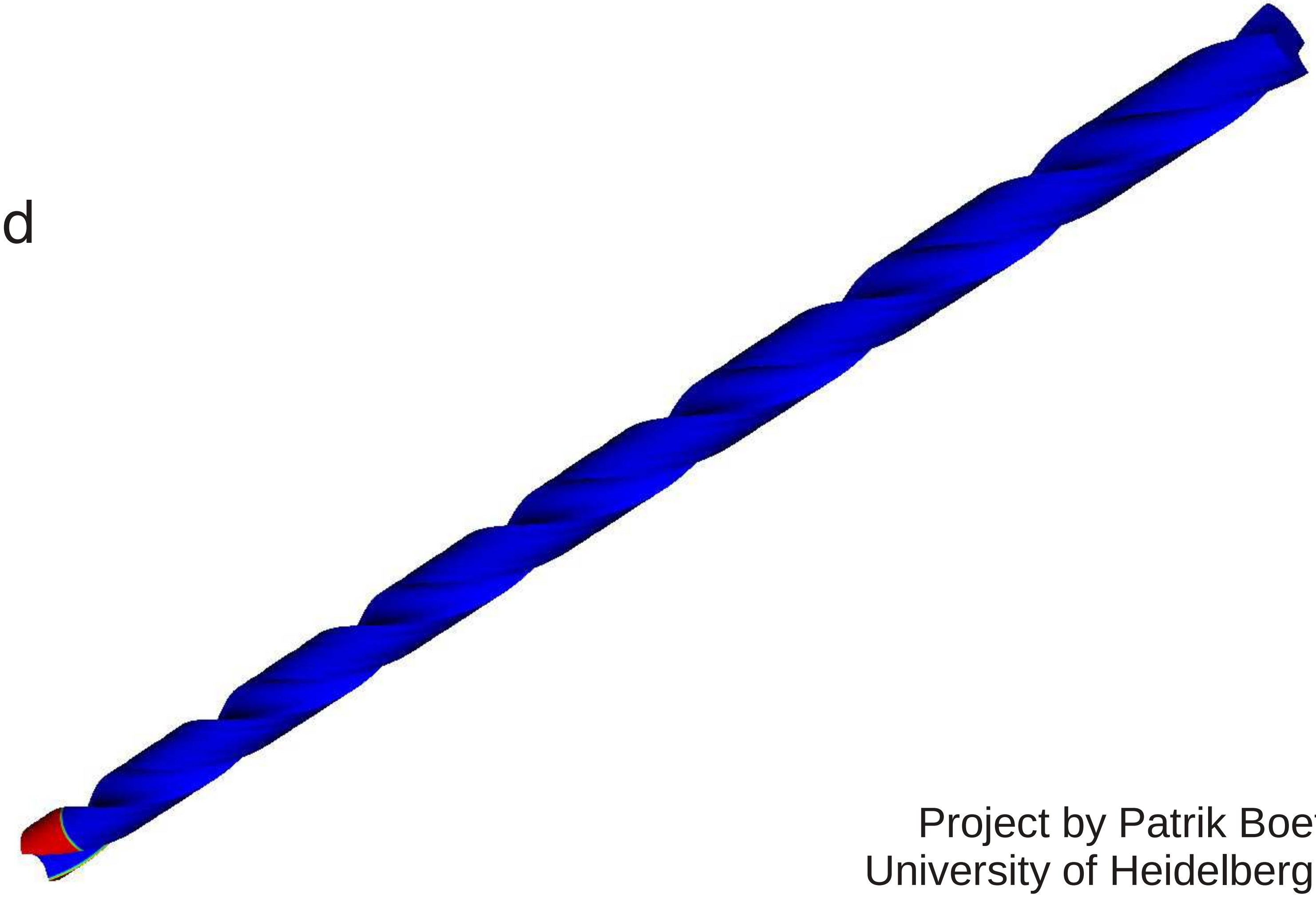
Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

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

Here:

- Clamped



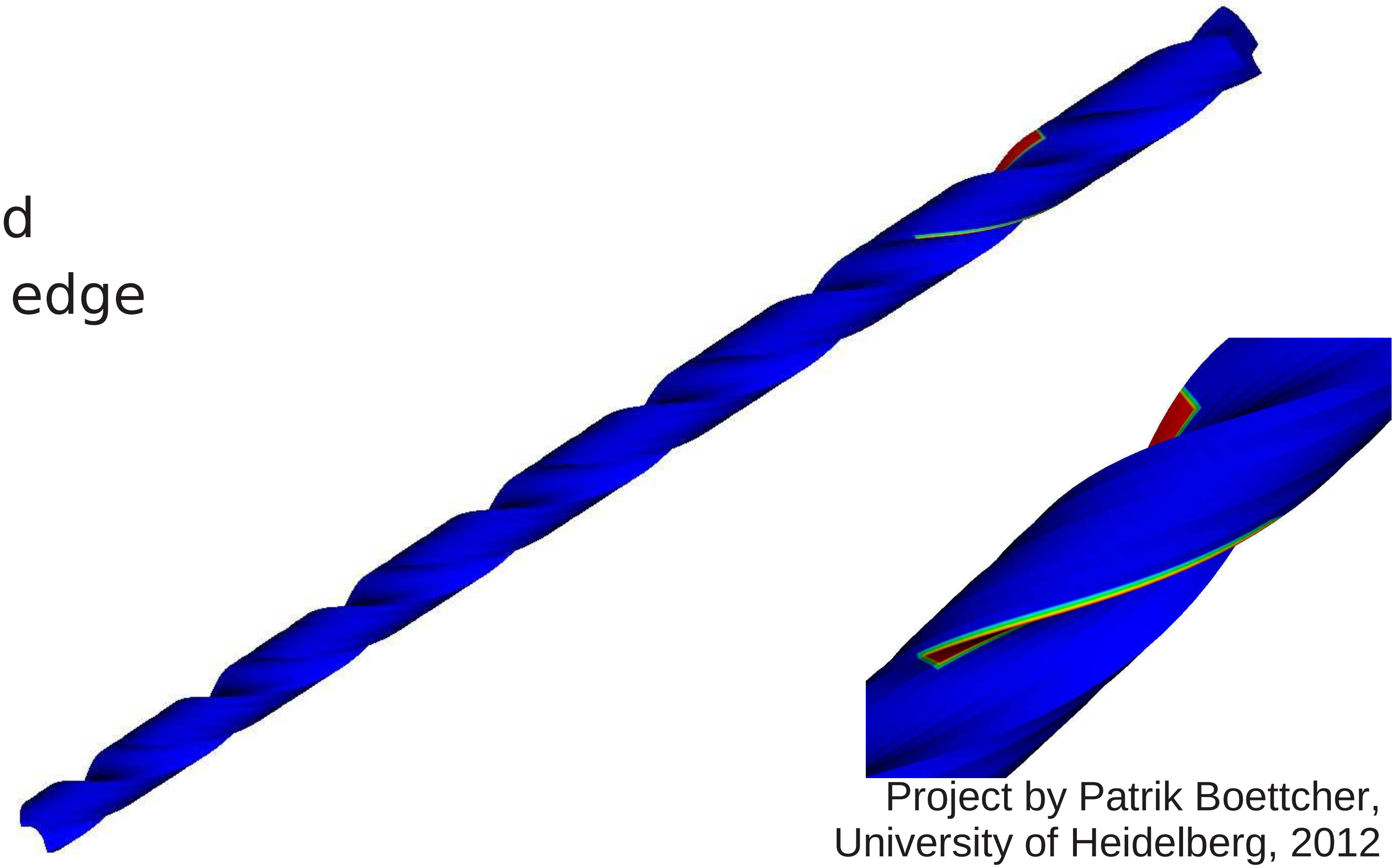
Project by Patrik Boettcher,
University of Heidelberg, 2012

A complete example

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

Here:

- Clamped
- Cutting edge



Project by Patrik Boettcher,
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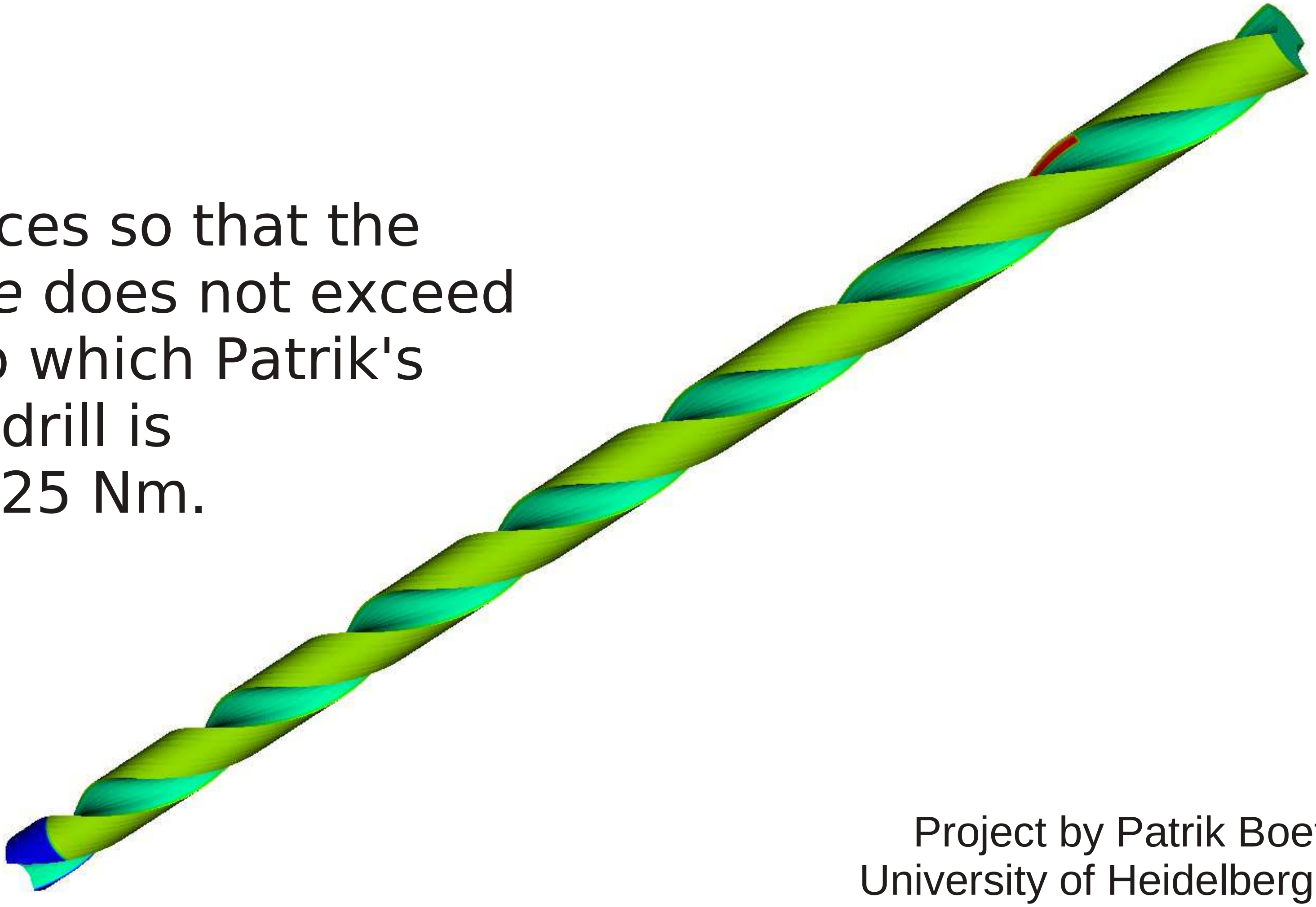
A complete example

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.



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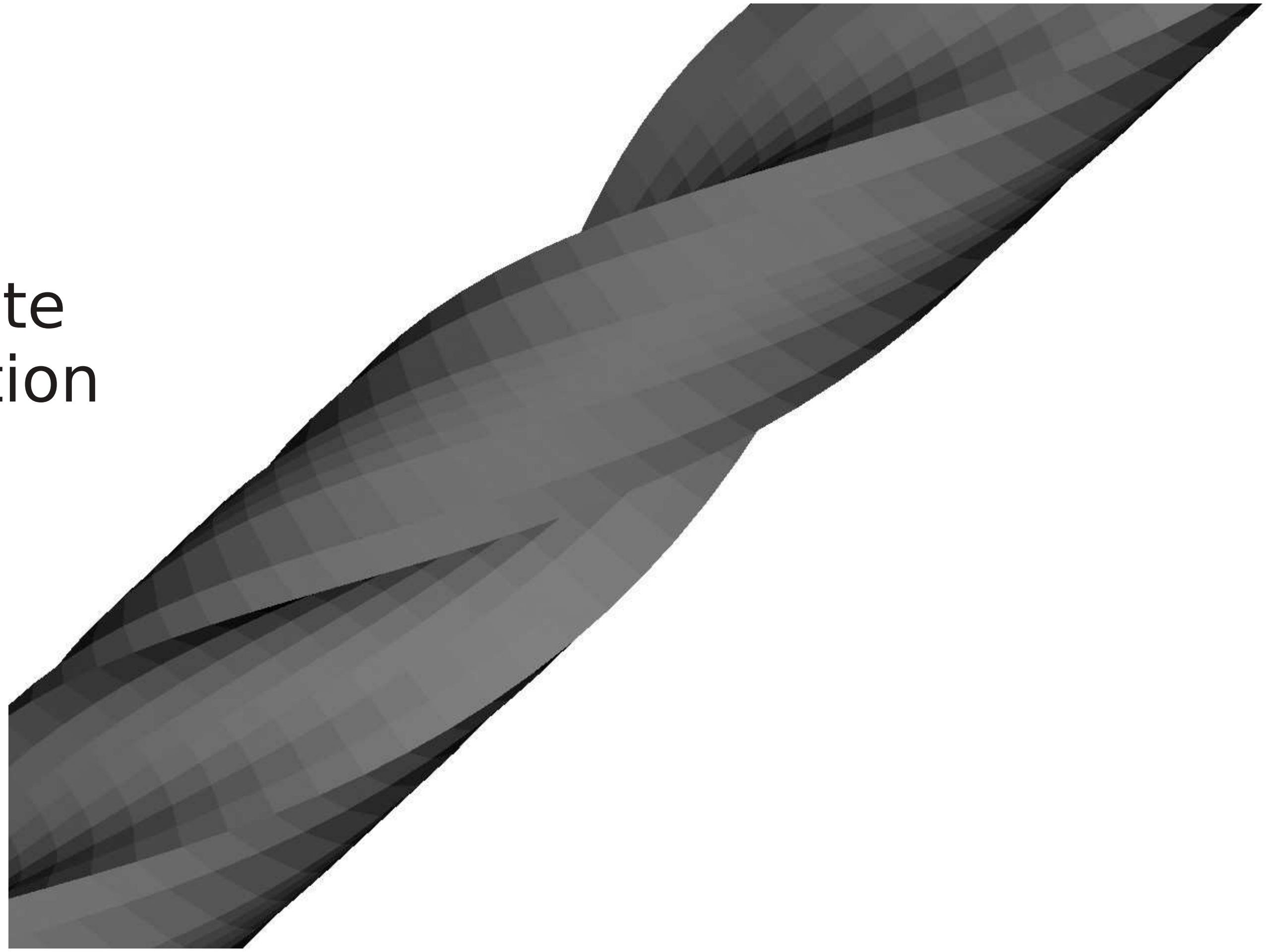
A complete example

Step 6: Mark up boundaries for geometry description

Here:

Without appropriate
boundary description



Project by Patrik Boettcher,
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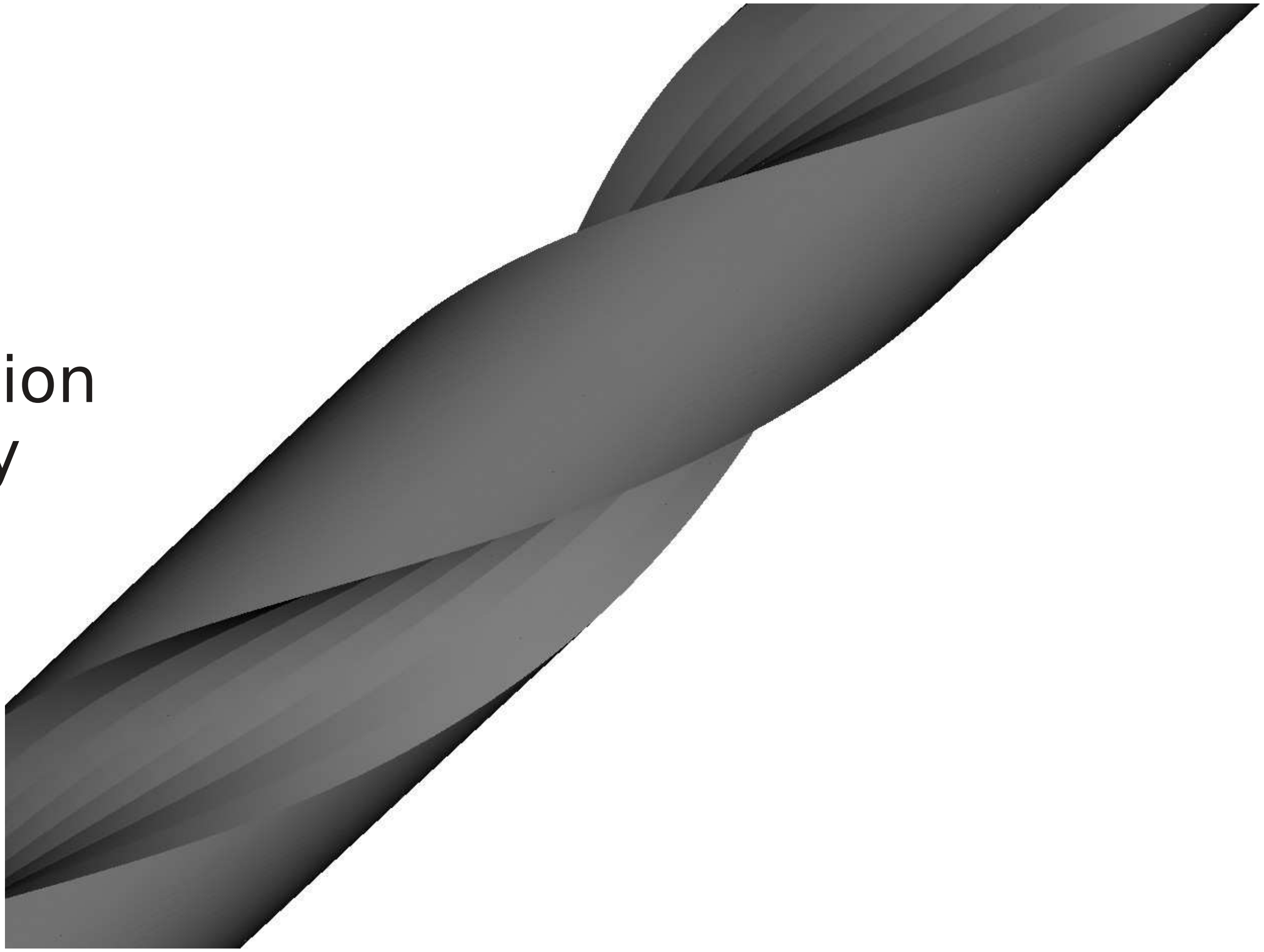
A complete example

Step 6: Mark up boundaries for geometry description

Here:

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



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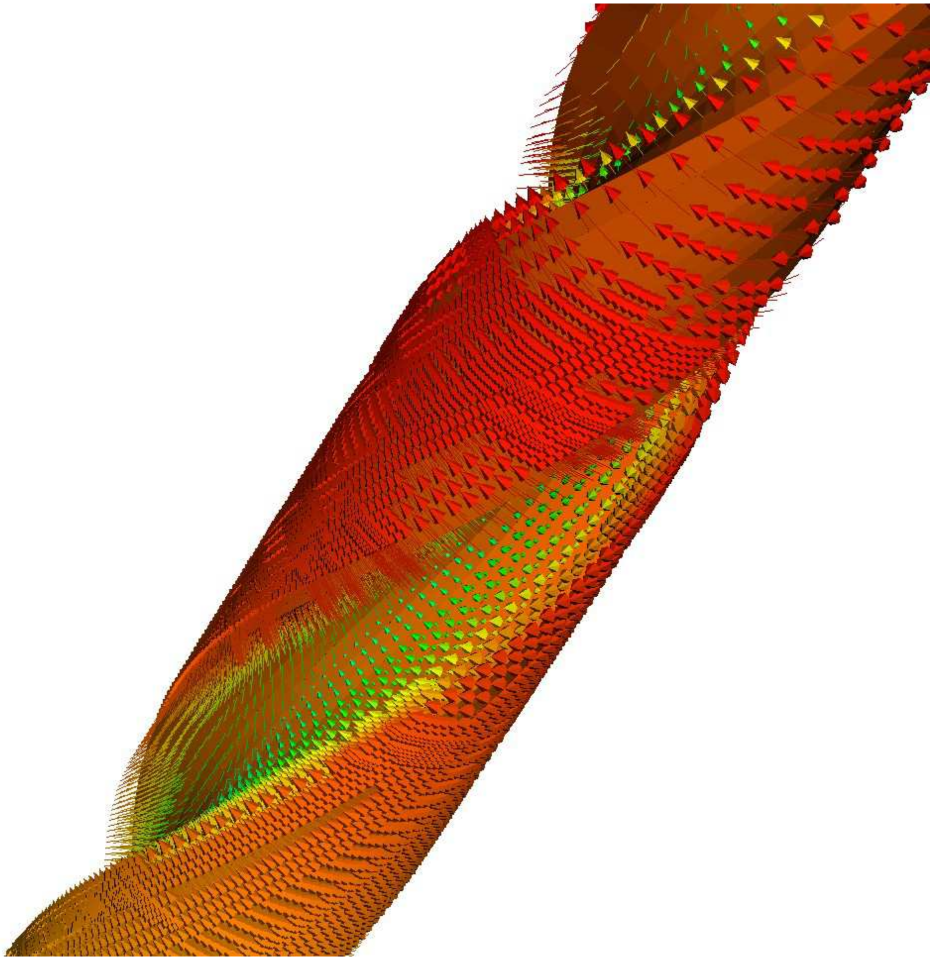
A complete example

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.



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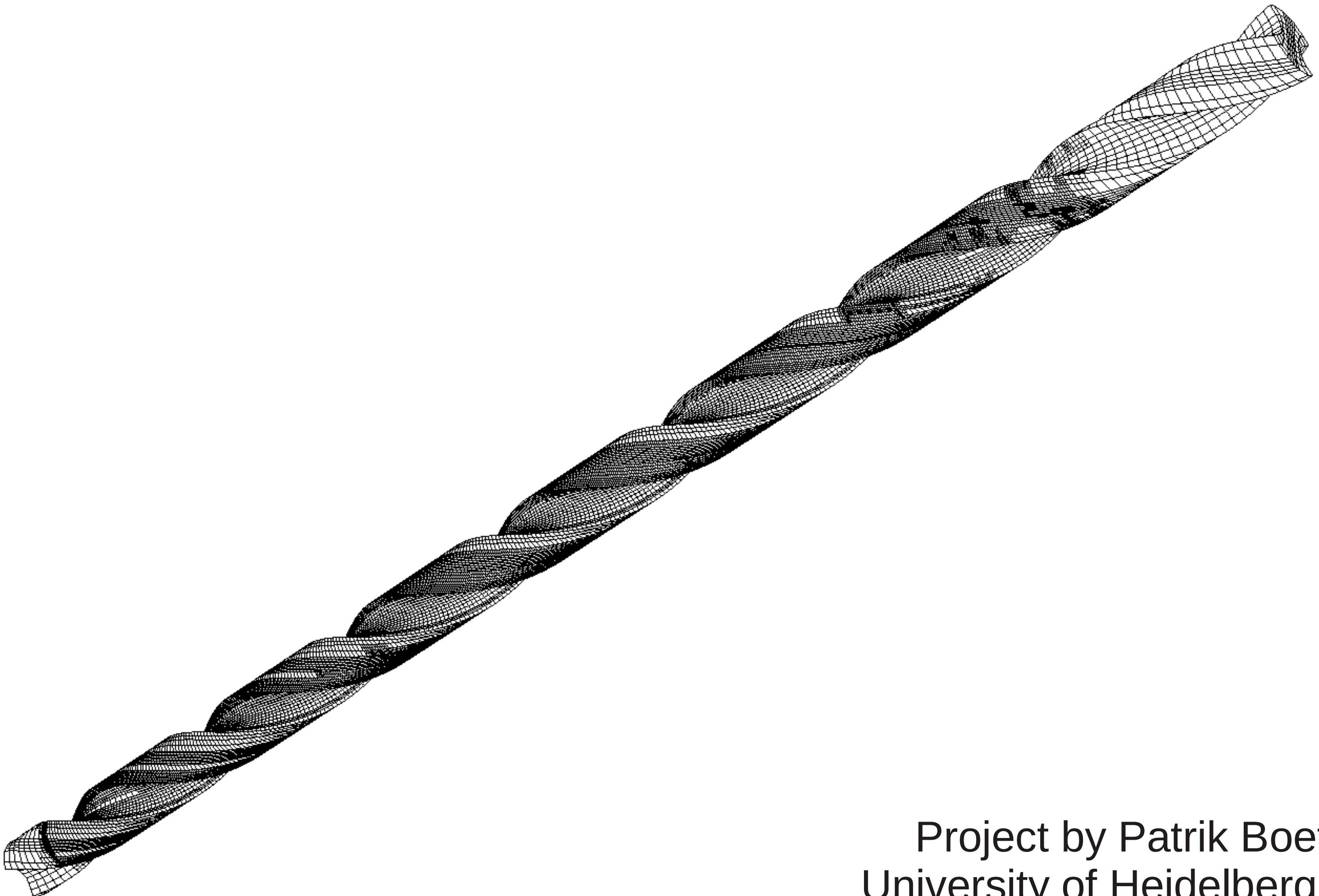
A complete example

Step 8: Visualize

Here:

Mesh



Project by Patrik Boettcher,
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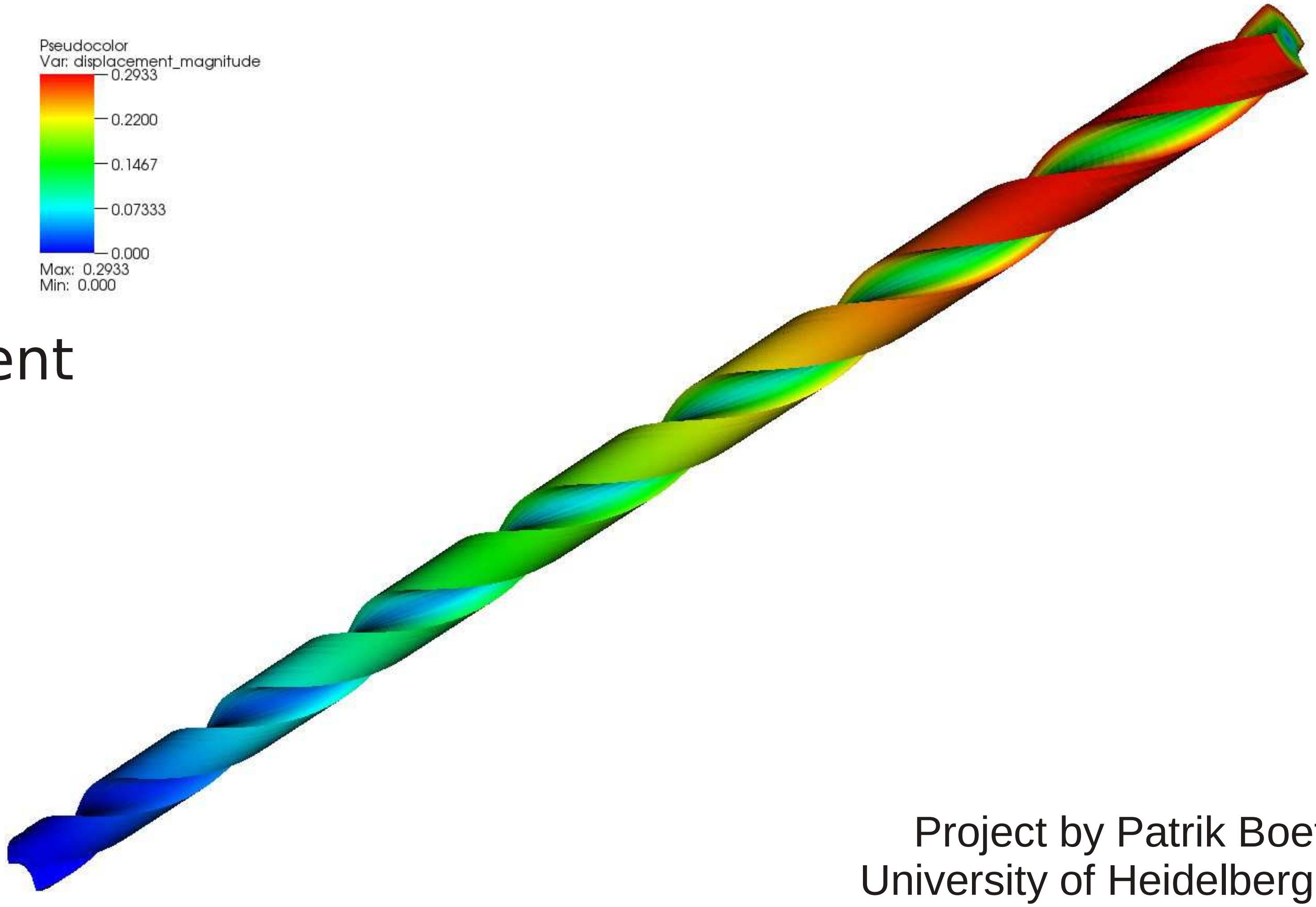
A complete example

Step 8: Visualize

Here:

Magnitude of displacement (in mm)



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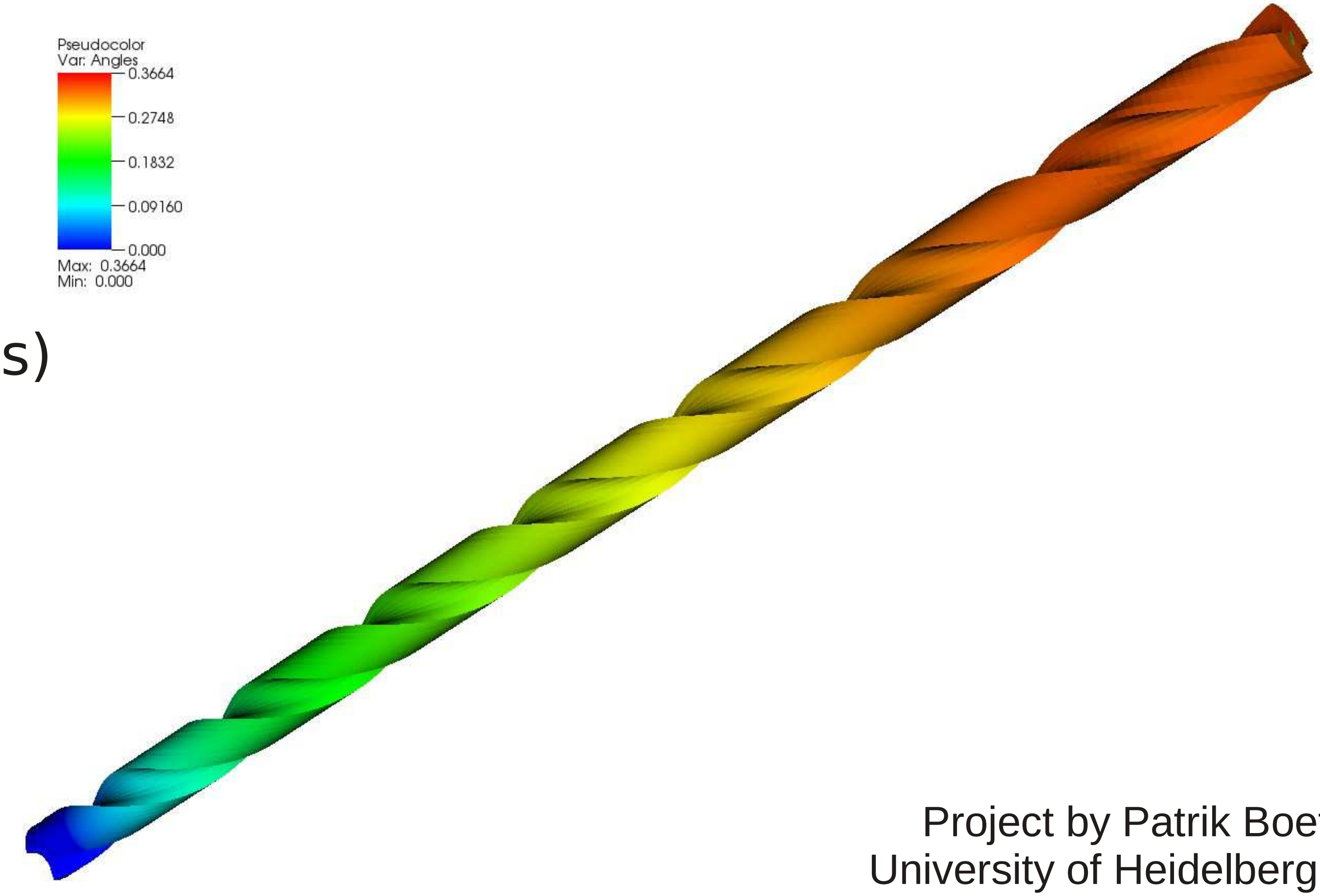
A complete example

Step 8: Visualize

Here:

Torsion angle (in degrees)



Project by Patrik Boettcher,
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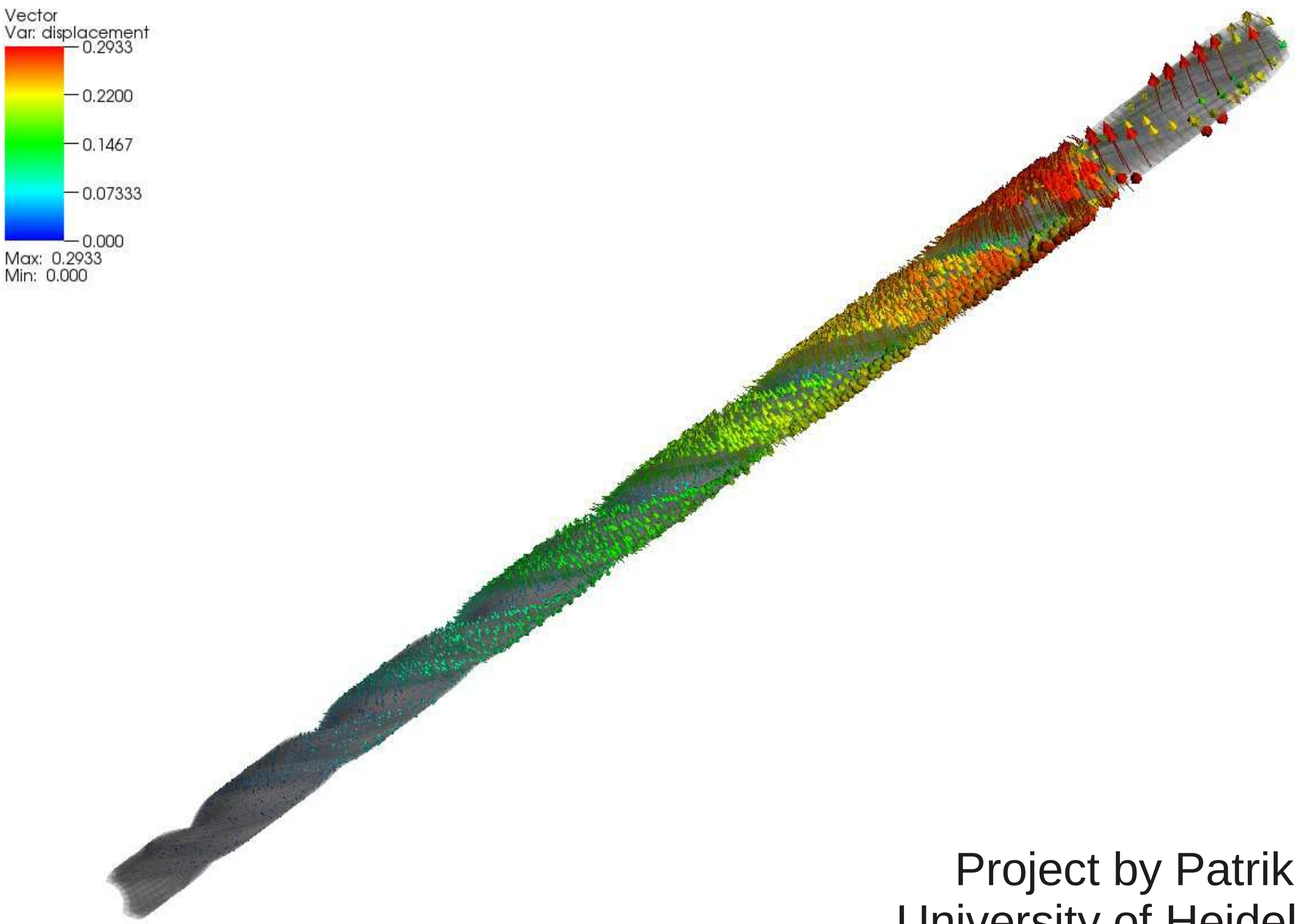
A complete example

Step 8: Visualize

Here:

Disp-
lacement
(in mm)



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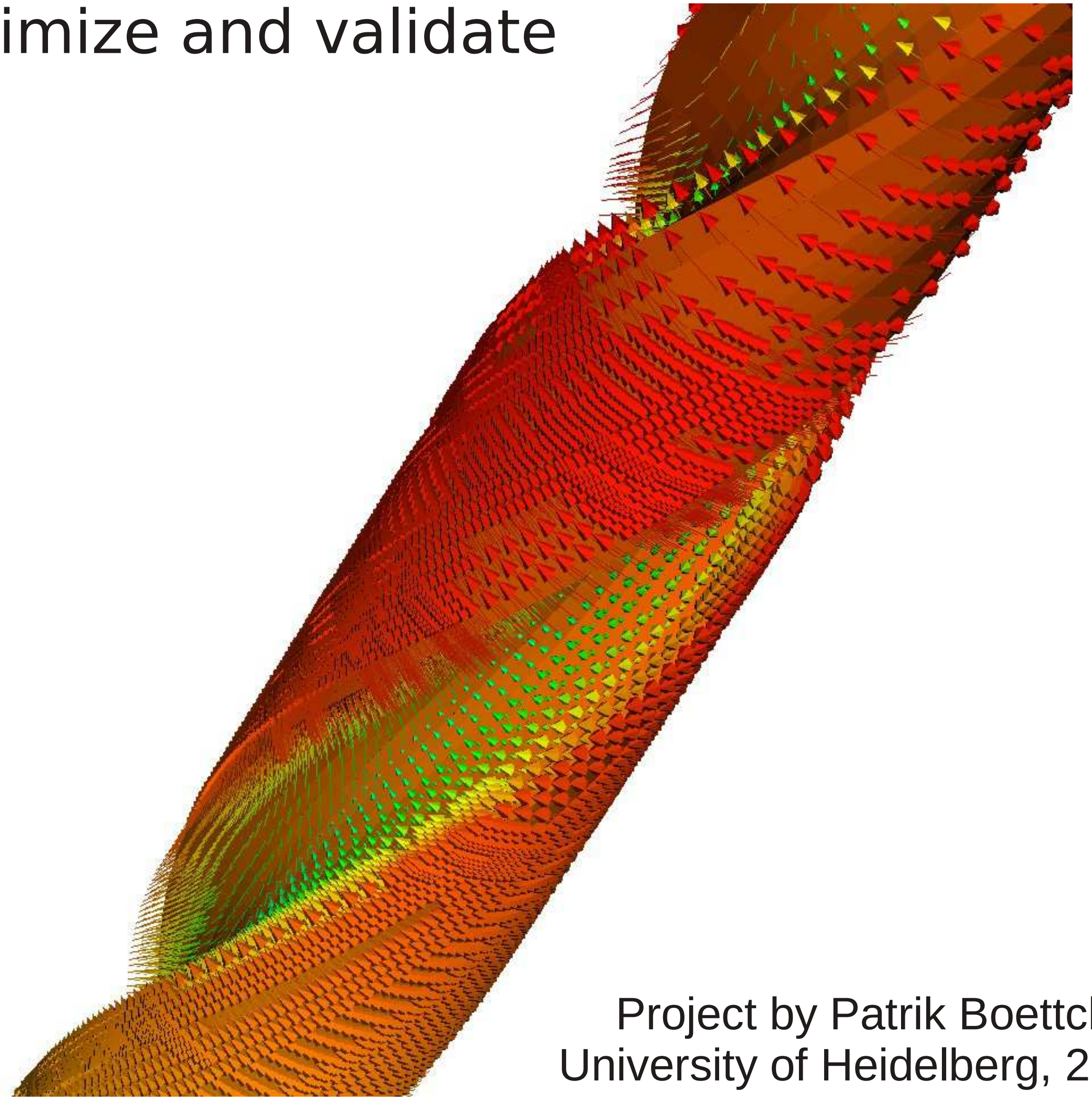
A complete example

Step 9: Repeat to optimize and validate



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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

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