www.dealii.org

Supporting complex simulations with open source finite element software

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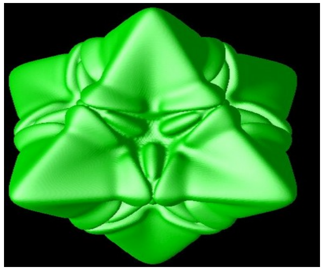
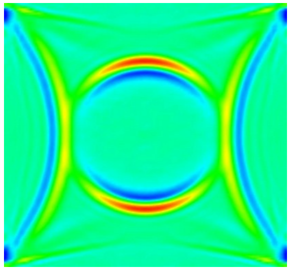
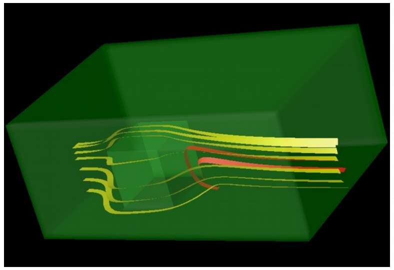
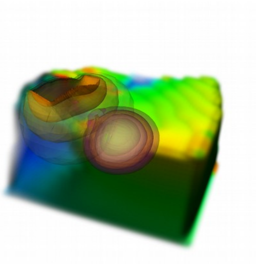
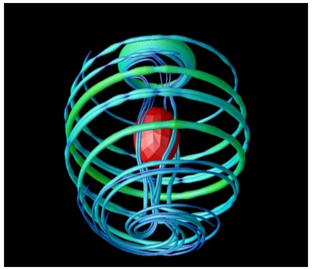
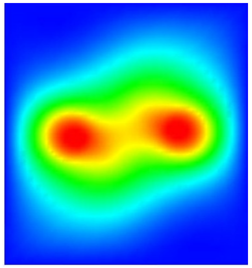
In collaboration with many many others around the world.

National Science Foundation
WHERE DISCOVERIES BEGIN

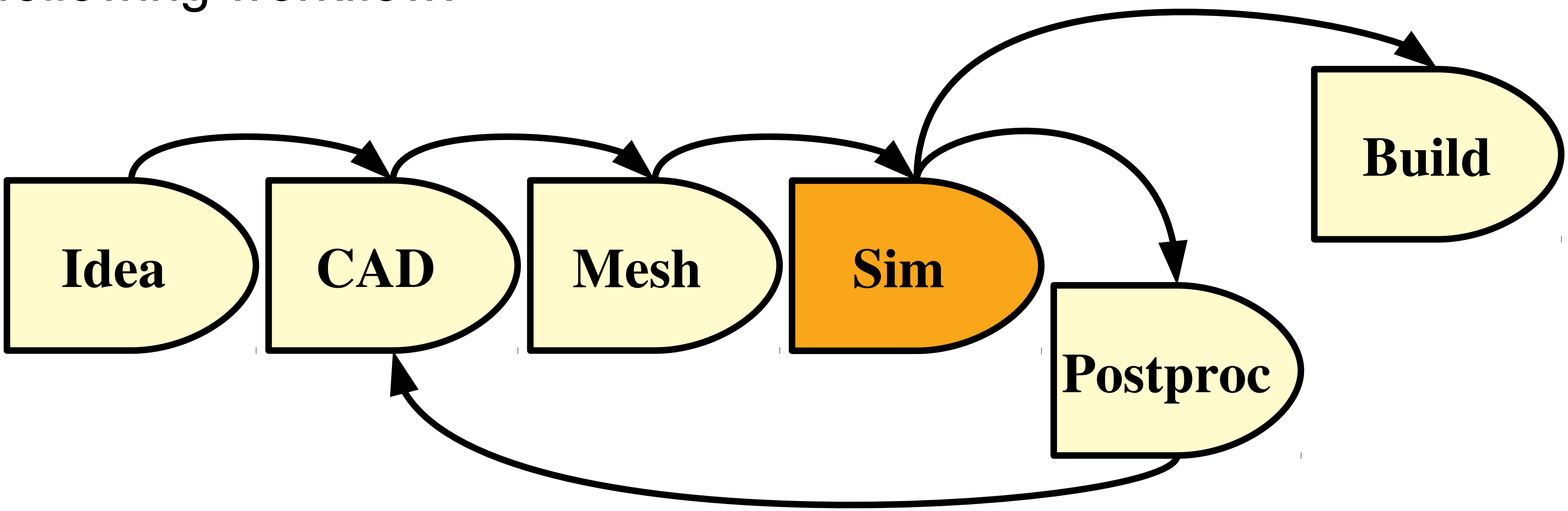
CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

This track

Computer Aided Modeling and Design

Essentially every manufactured object today goes through the following workflow:



Simulation often uses the *finite element method*.

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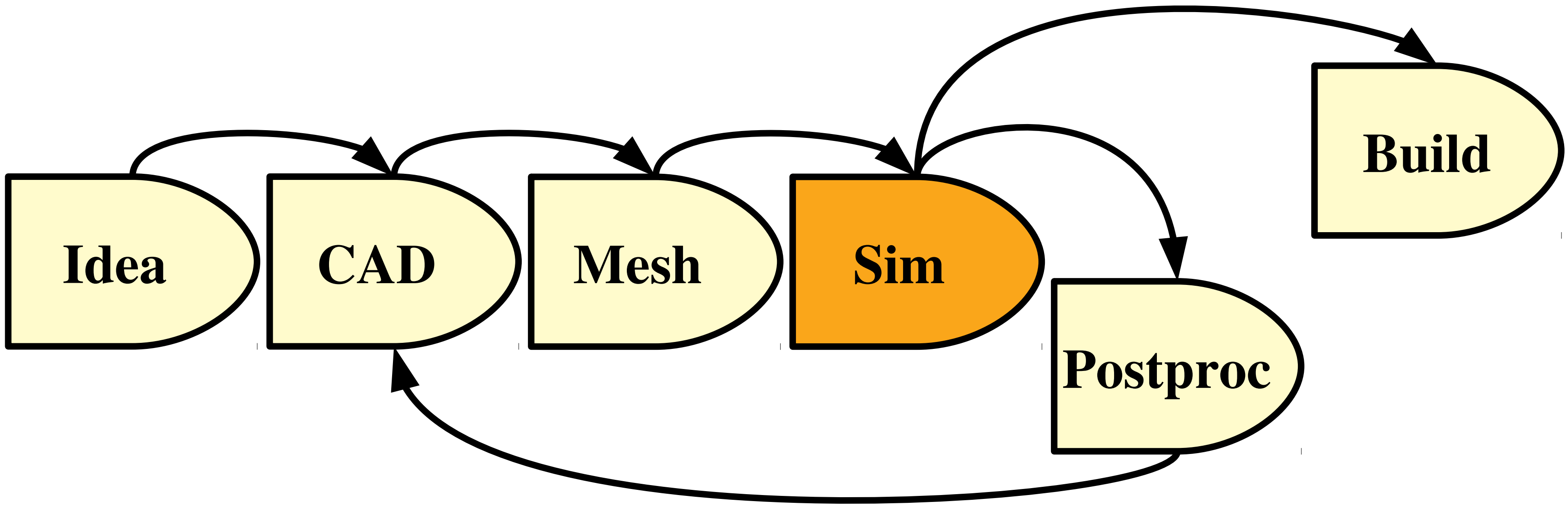
Computer Aided Modeling and Design



Simulation:

Computationally predict the physical response to external stimuli of interest.

Typical areas:

- Solid mechanics (statics + dynamics)
- Fluid dynamics
- Electrodynamics

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Available tools

Many commercial packages for “common” problems:

- Fluent
- Abaqus
- Comsol
- …

- Covers most problems of “traditional engineering”
- Provide GUIs and integration in typical workflows

- Generally does it well and reliably, though:
  – does not use modern mathematical methods
  – scales poorly to parallel computers

Essentially no open source software in this arena.

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Available tools

Large collection of open source software libraries:

- deal.II
- libmesh
- FEniCS
- …

- Serve as the basis for
  – method development
  – **solving “non-standard” problems**

- The biggest of these libraries are
  – high quality
  – provide modern mathematical methods
  – some scale very well to parallel computers

Generally no GUIs; integration in typical workflows via external interfaces.

Available tools

One example: deal.II (*https://www.dealii.org*)

- 100s to 1000s of users
- Used in 1,400+ scientific publications we know of

- 1.4M lines of C++
- One major release per year:
  – 30-50 contributors to each release
  – 5-10 pull requests per day, every day

- Big focus on documentation:
  – 1000s of pages of doxygen-generated HTML
  – ~70 tutorial programs
  – 68 video lectures
  – short courses around the world

- Runs efficiently from laptops → 300,000 processor cores.

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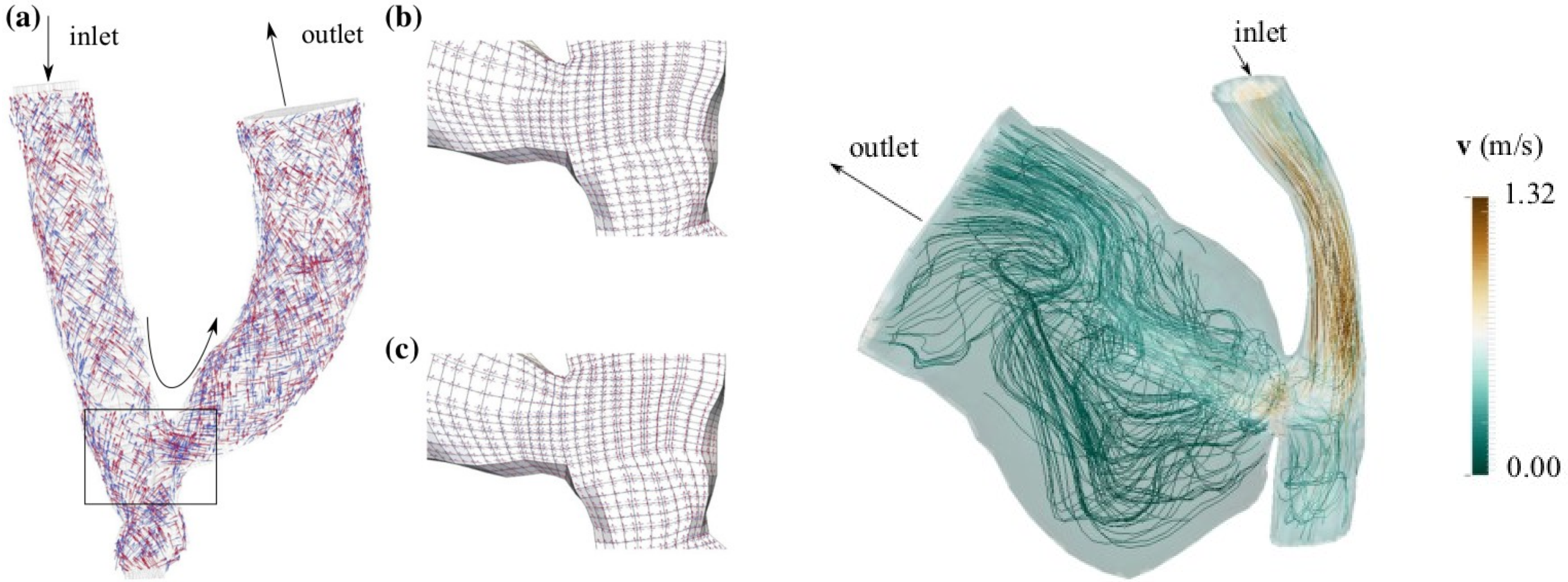
Example applications: Aortic stents



Patient-specific fluid-structure interaction with realistic material models for vascular modeling

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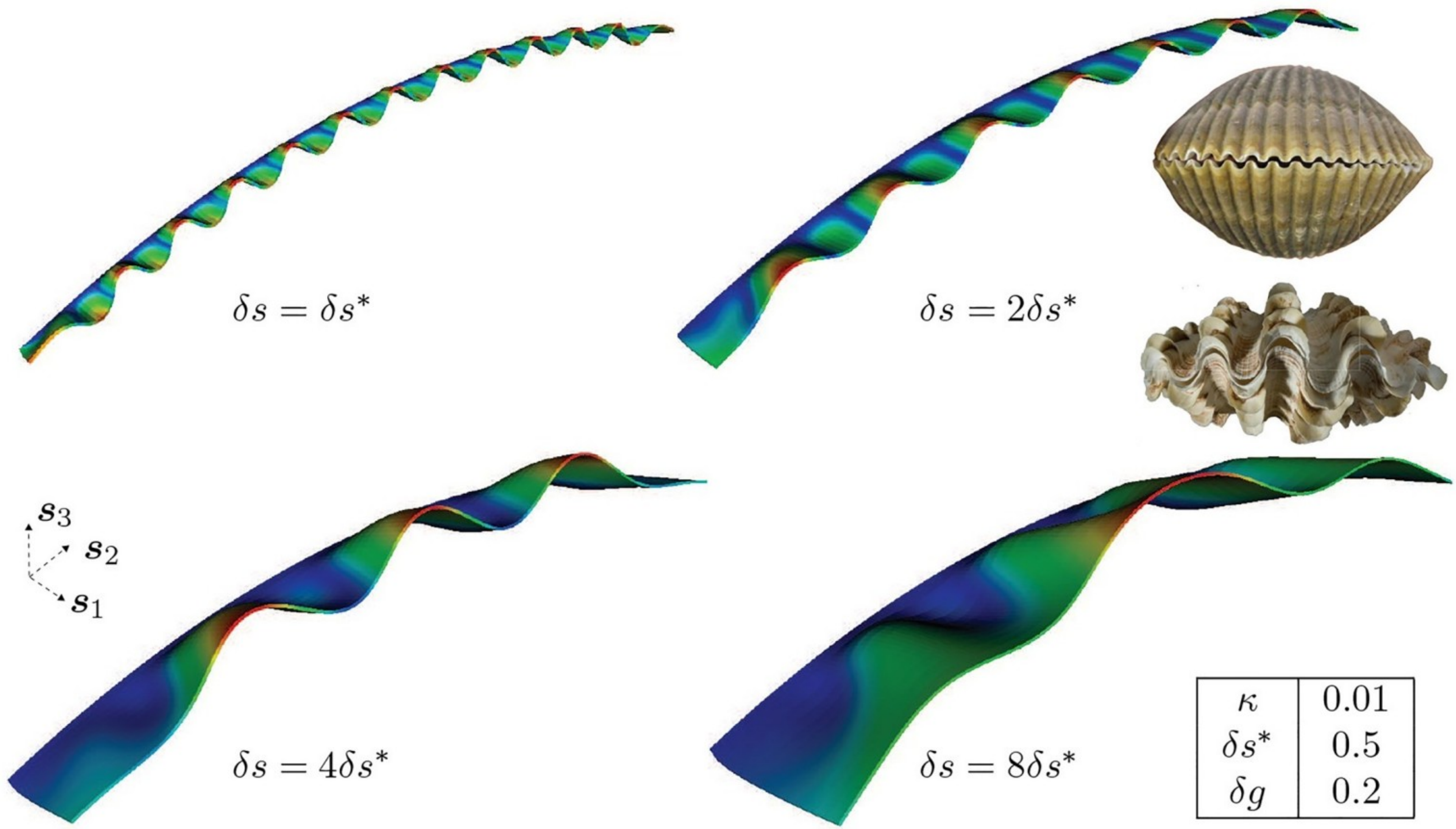
Example applications: Biomorphic growth



Morphoelastic development of mollusk shells

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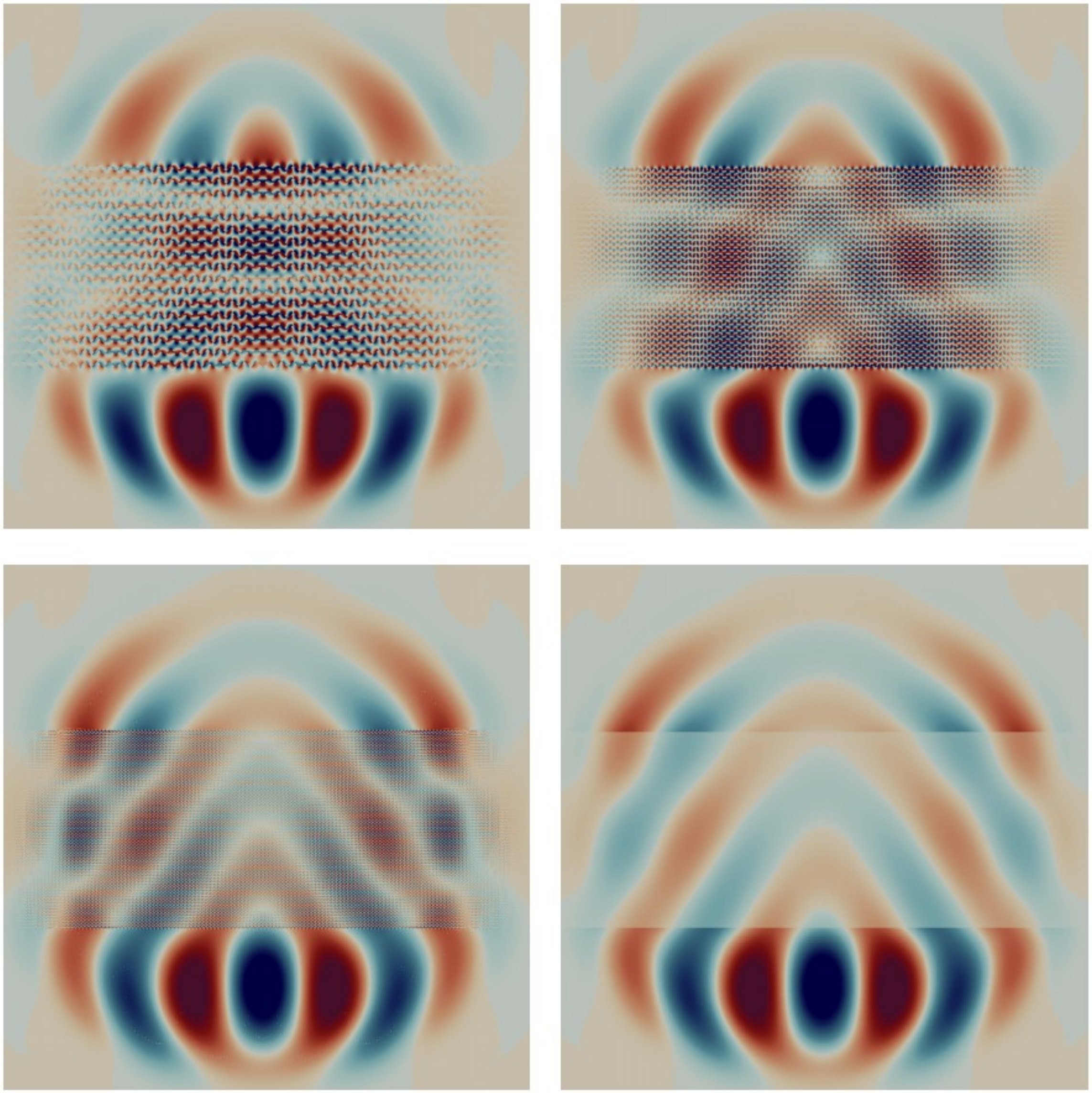
Example applications: Microscopic antennae



Homogenization of models for plasmonic crystals

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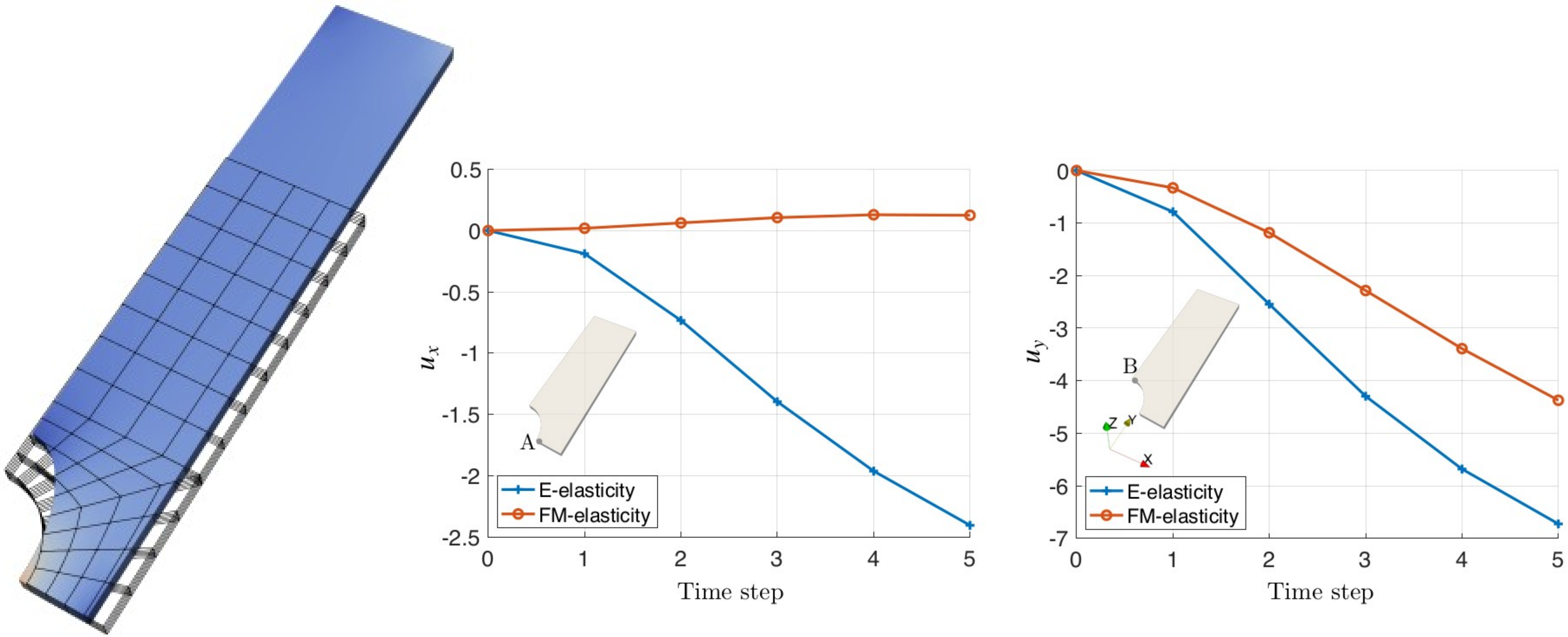
Example applications: Complex models



Micromorphic models for the flexoelectric effect

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A “typical” application in computational mechanics

What we generally need:

- Non-trivial 2d/3d geometries
- Coupled system of nonlinear PDEs
- Efficient non-linear iteration strategy
- Efficient linear solver
- Ways to visualize the solution

What we may need:

- Parallel execution on large systems
- Mixed or higher order finite elements
- Combination of meshes (overlapping domains, micro/macro)
- …

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A “typical” application in computational mechanics

Question:

How can we write such a code?

Surely, it will take 10,000s–100,000s of lines of code!
(Recall: 20k lines of code per man-year.)

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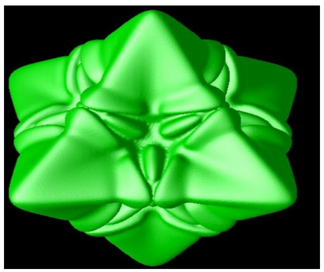
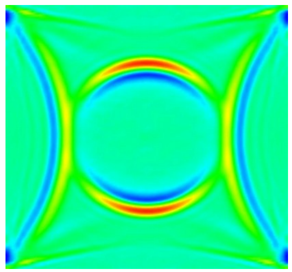
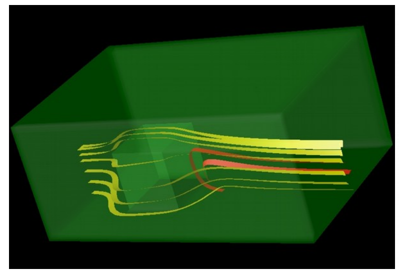
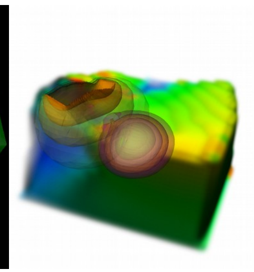
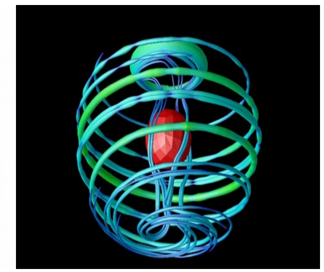
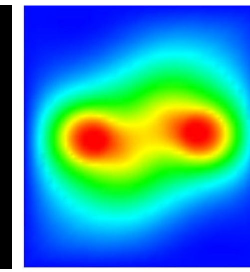
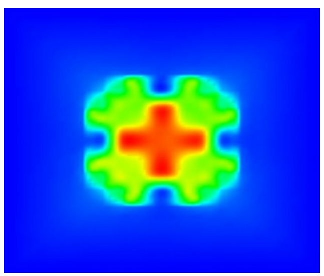
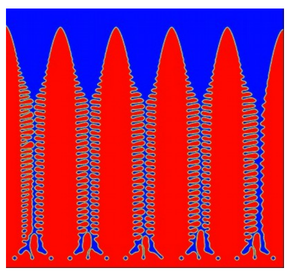
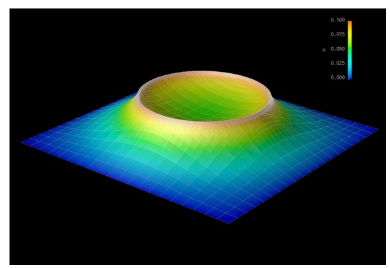
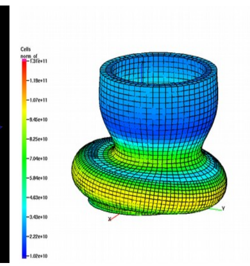
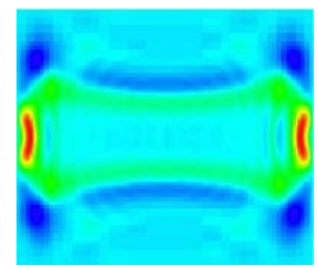
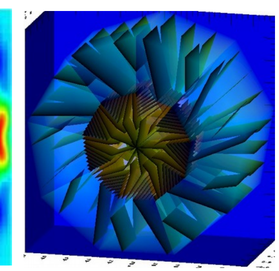
A library for finite element computations that supports...

...a large variety of PDE applications
tailored to non-experts.

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Goals for this library:

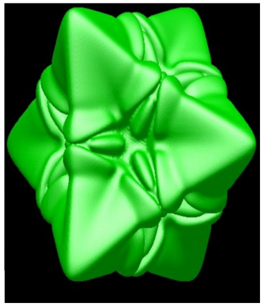
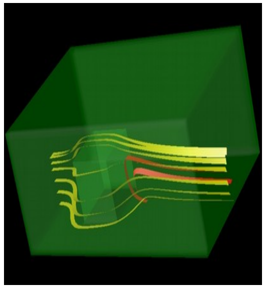
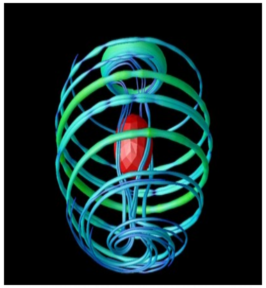
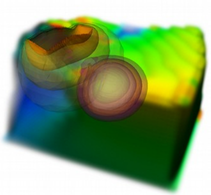
- Supports complex computations in many fields
- Is general (not area-specific)
- Has fully adaptive, dynamically changing 3d meshes
- Scales to 10,000s of processors
- Is efficient on today's multicore machines

Fundamental premise:
Provide building blocks that can be used in many different ways, not a rigid framework.

deal.II

deal.II provides:

- Adaptive meshes in 1d, 2d, and 3d
- Interfaces to all major graphics programs
- Standard refinement indicators built in
- Many standard finite element types (continuous, discontinuous, mixed, Raviart-Thomas, ...)
- Low and high order elements
- Support for multi-component problems
- Its own sub-library for dense + sparse linear algebra
- Interfaces to PETSC, Trilinos, UMFPACK, ARPACK, ...
- Supports SMP + cluster systems

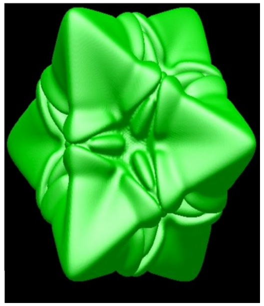





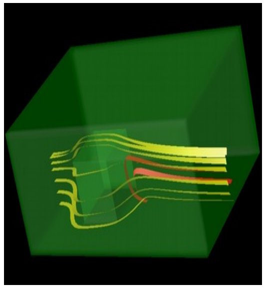
deal.II

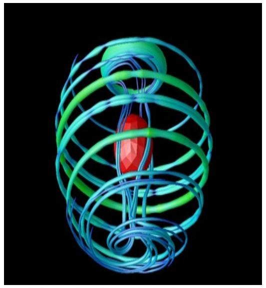
Status today:

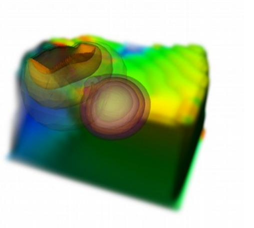
- ~1000 downloads per month
- 1.4M lines of C++ code
- 10,000+ pages of documentation
- Portable build environment
- Used in teaching at many universities

- ~250 people have contributed to it
- ~40 people contribute to each release
- ~10 pull requests merged *each day*









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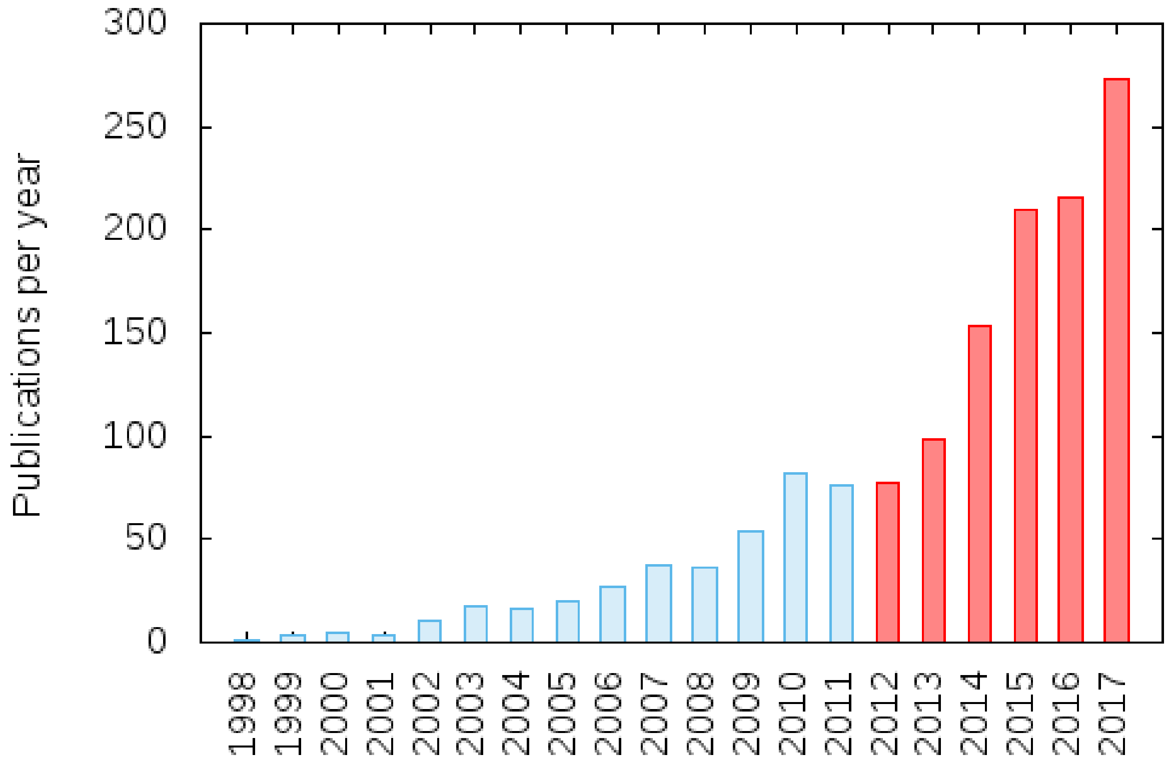
Publications using deal.II:



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Examples

Examples of what can be done with deal.II (2013 only):

- Biomedical imaging
- Brain biomechanics
- E-M brain stimulation

- Microfluidics
- Oil reservoir flow
- Fuel cells
- Transonic aerodynamics
- Foam modeling
- Fluid-structure interactions
- Atmospheric sciences

- Quantum mechanics
- Neutron transport
- Nuclear reactor modeling

- Numerical methods research

- Fracture mechanics
- Damage models
- Solidification of alloys
- Laser hardening of steel
- Glacier mechanics
- Plasticity
- Contact/lubrication models

- Electronic structure
- Photonic crystals

- Financial modeling

- Chemically reactive flow
- Flow in the Earth mantle

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What makes such projects successful?

General observations:

Success or failure of scientific software projects is not decided on technical merit alone.

The *true* factors are beyond the code!
It is not enough to be a good programmer!

In particular, what counts:

- Utility and quality
- Documentation
- Community

All of the big libraries provide this for their users.

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Utility + quality

How deal.II makes itself easy to use:

- Lots of error checking in the code
- Extensive testsuites
- Meaningful error messages and assertions rather than cryptic error codes

- Cataloged use cases
- FAQs
- Well documented examples of debugging common problems

Documentation +education

How we teach using deal.II:

- Installation instructions/README
- Within-function comments
- Function interface documentation
- Class-level documentation
- Module-level documentation
- Worked “tutorial” programs
- Recorded, interactive demonstrations

Example: deal.II has 10,000+ HTML pages. 170,000 lines of code are actually documentation (~10 man years of work). There are 67 recorded video lectures on YouTube.

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Example codes

deal.II comes with ~70 tutorial programs:

- From small Laplace solvers (~100s of lines)
- To medium-sized applications (~1000s of lines)
- Intent:
  - teach deal.II
  - teach advanced numerical methods
  - teach software development skills

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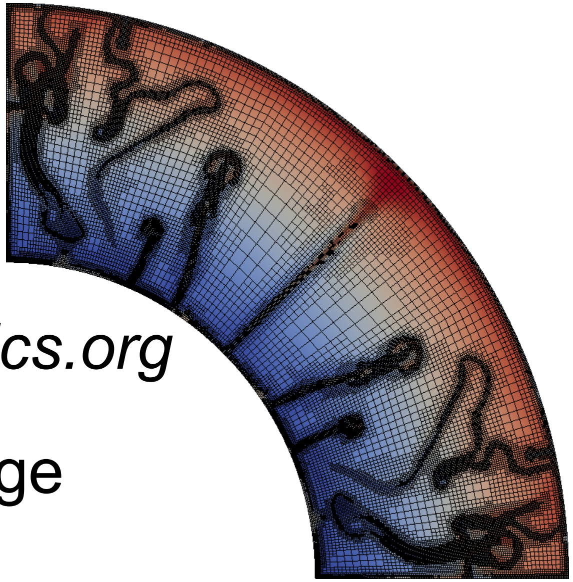
Example applications

There are also a number of large applications built on deal.II:



- *Aspect:* Advanced Solver for Problems in Earth Convection
  – ~140,000 lines of code
  – Open source: *http://aspect.geodynamics.org*

- *OpenFCST:* A fuel cell simulation package
  – Supported by an industrial consortium
  – Open source: *http://www.openfcst.org/*

- DFT-FE: A density functional theory code
  – Open source: *https://sites.google.com/umich.edu/dftfe*

- …

How much work does it take?

Use case: Grad student with 3 years for research

- Solve a complex model
- With realistic geometries, unstructured meshes
- Higher order finite elements
- Multigrid-based solver
- Parallelization
- Output in formats for high-quality graphics
- Results almost from the beginning: a wide variety of tutorials allow a gentle start
- There are ways to share your codes with others

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How much work does it take?

Use case: Expert user for a commercial project, 2 weeks of full-time work

- Complex model
- Realistic geometries, unstructured meshes
- Higher order finite elements
- Simple solver
- Parallelization
- Output in formats for high-quality graphics

- Validated against another code/experimental results

Effects

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What this development model means for users:

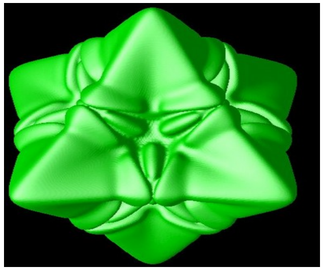
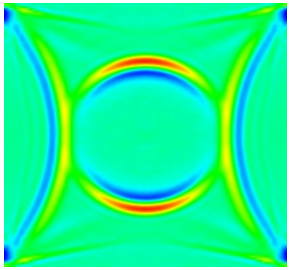
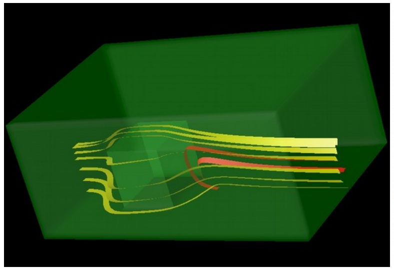
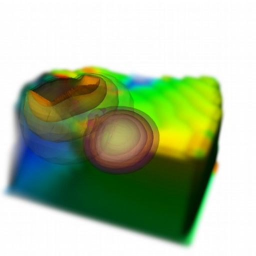
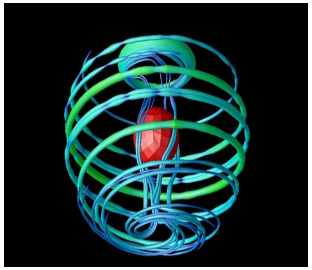
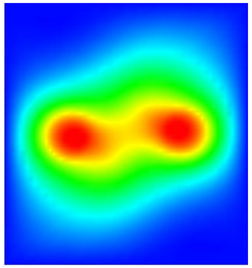
- We can solve problems that were previously intractable
- Methods developers can demonstrate applicability
- Applications scientists can use state of the art methods
- Our codes become **far smaller**:
  – less potential for error
  – less need for documentation

  – lower hurdle for "reproducible" research (publishing the code along with the paper)
- More impact/more citations when publishing one's code

Conclusions

Deal.II is a library that supports building finite element codes:

- Widely used
- High quality, professionally developed
- Allows building codes *much* faster, *much* better
- Used to solve complex, more realistic problems
- Scales far better than almost all commercial software

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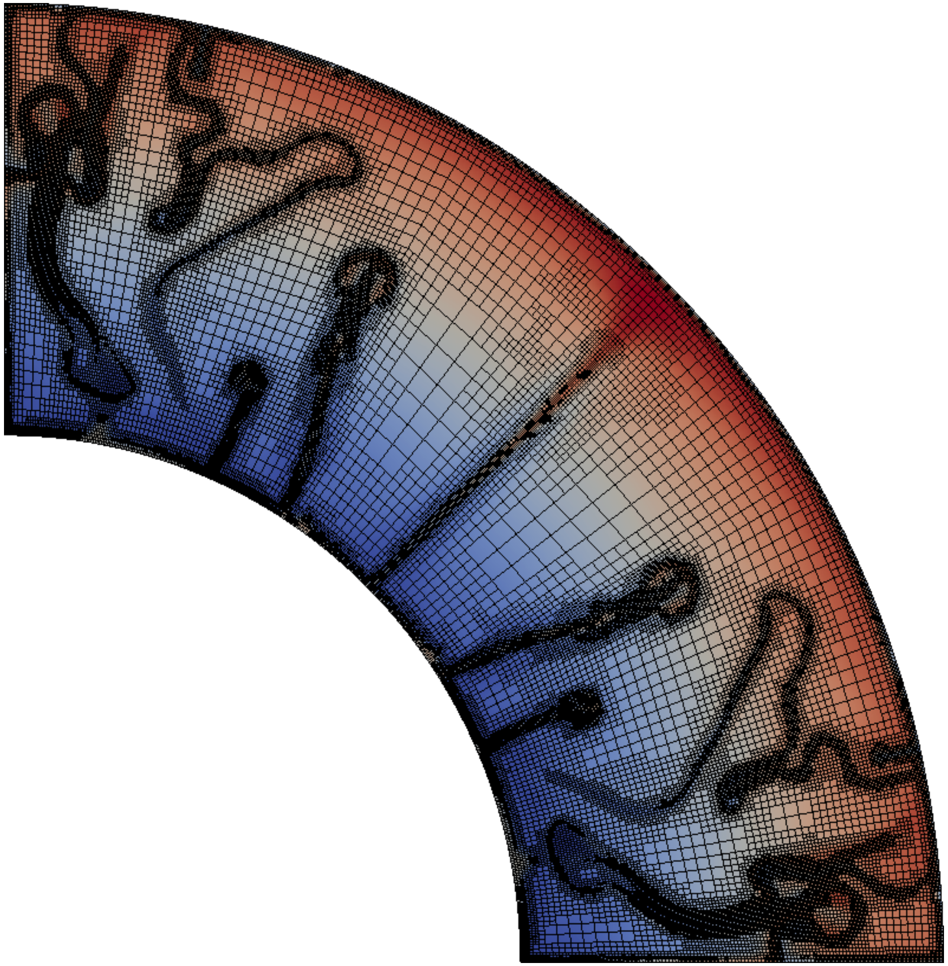

More information:

http://www.dealii.org/