THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

deal.II, IBAMR, and Cardinal: Scalable Software for Difficult Problems

David Wells

University of North Carolina

Cardiovascular Modeling and Simulation Lab

October 2, 2024

Overview

About Me

- PhD in applied mathematics, 2015
- postdoc at RPI, 2015 - 2018
- postdoc at UNC, 2018 - 2023
- research scientist at UNC, 2023 - present

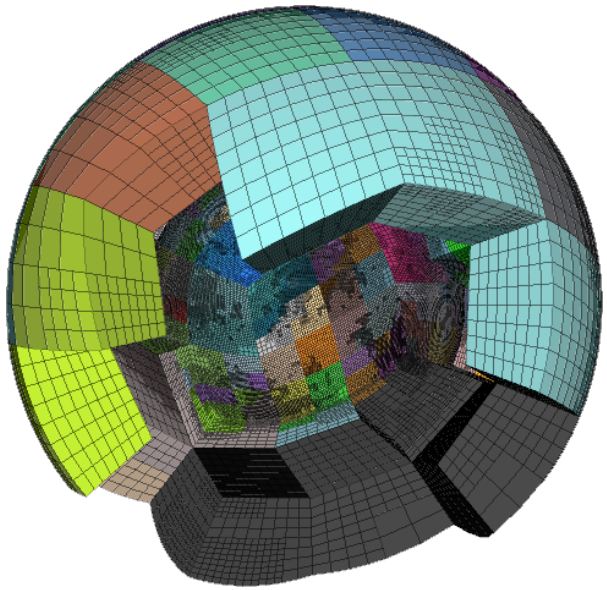
Why?

- Help students on their journeys in scientific software
- Contribute to the greater applied mathematics community by maintaining software, contributing patches to upstream projects
- Solve new and interesting problems with cutting-edge tools

Topics

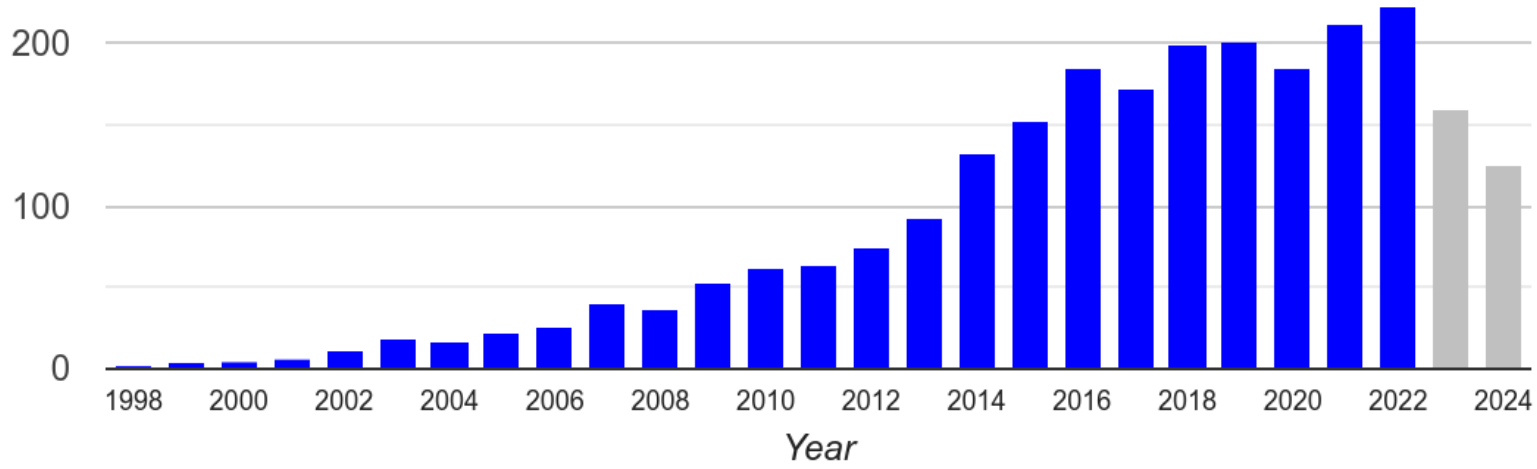
- deal.II
- IBAMR
- Cardinal

deal.II: Overview



- Large C++ library implementing the adaptive finite element method
- Extraordinarily well-documented with an active community, classes, videos, examples, etc.
- Scalable to largest machines today (in use at ORNL and LANL, hetereogeneous compute is WIP)
- Successfully used by students on laptops to solve dissertation-level problems
- Successful industry applications (Siemens, Italian shipbuilding, Canadian lumber industry)
- Does not reinvent the wheel: uses Kokkos, MPI, PETSc, Trilinos, p4est

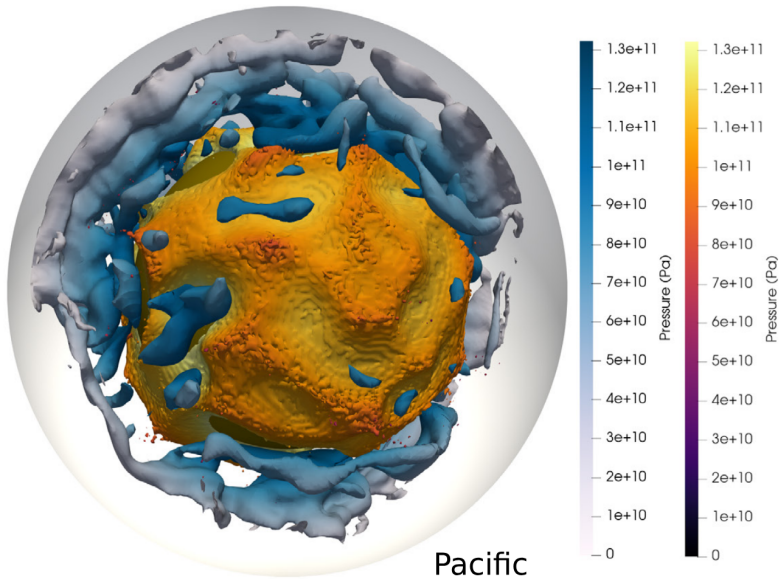
deal.II: Community Impact



Known publications using deal.II. Total: **2462**. (Gray bars: Incomplete data.)

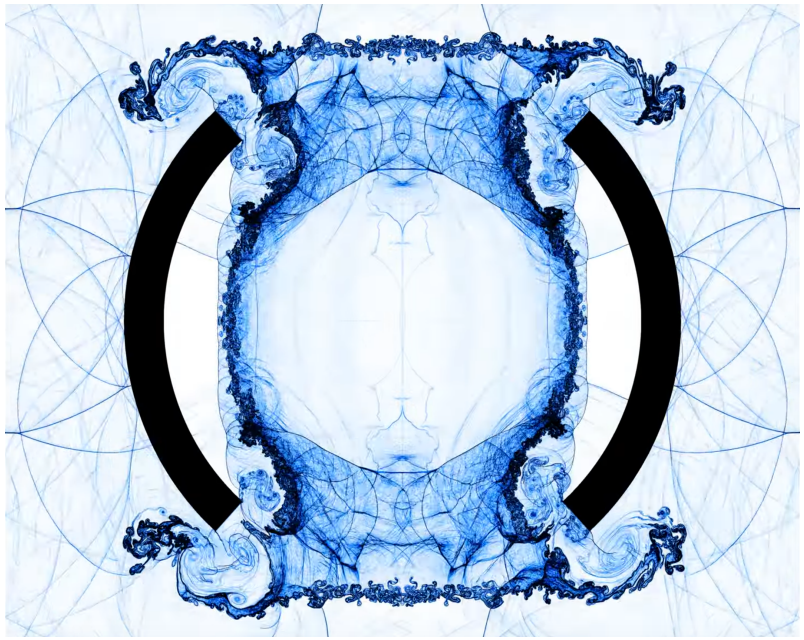
- I've been a principal developer since 2015 (one of fourteen)
- Large, quantifiable impact on science
- S-tier finite element library
- If you need to solve a PDE, deal.II can help

deal.II Showcase: plate tectonics



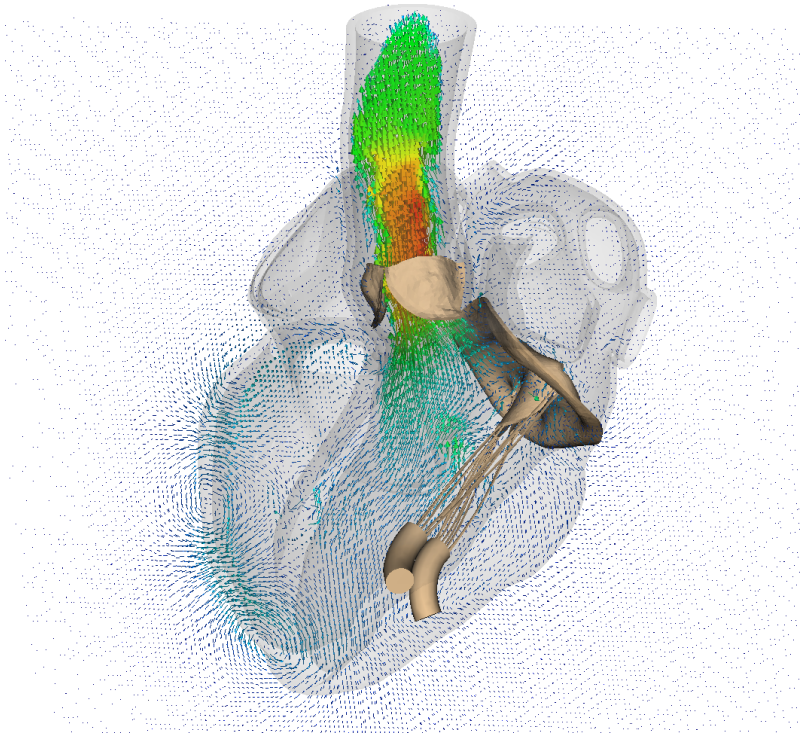
- ASPECT: solve Stokes system at extreme scale (ten trillion DoFs) on Frontera (Gassmoeller et al)
- Picture: *Changes in core-mantle boundary heat flux patterns throughout the supercontinent cycle*, Dannberg et al: how does heat flux inside the earth impact our magnetic field?
- Matrix-free geometric multigrid, adaptive FEM, scalable linear solvers and preconditioners

deal.II Showcase: hypersonic flows



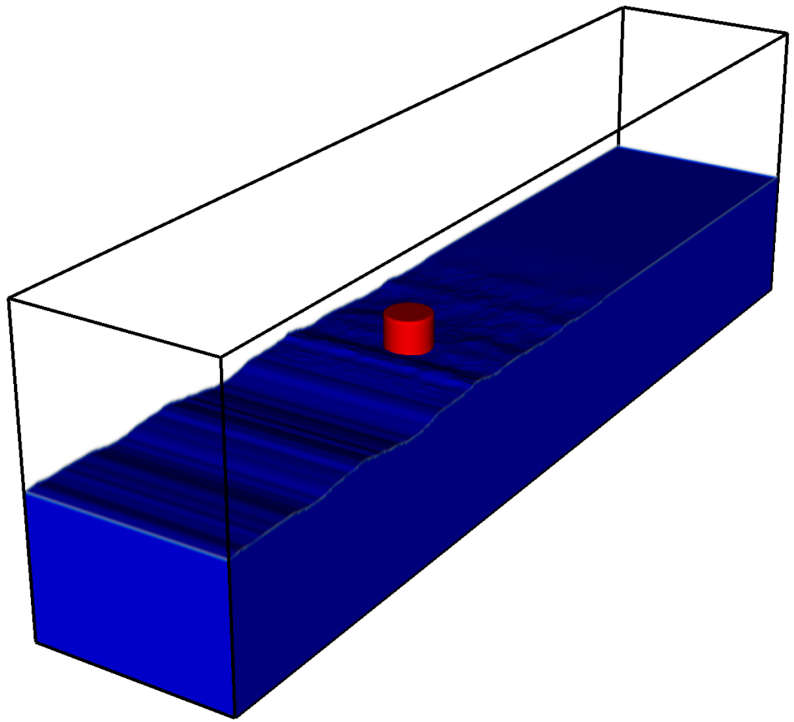
- ryujin: convex limiting, graph viscosity methods (Guermond and Popov) for hyperbolic conservation laws (Maier et al)
- Picture: Compressible Euler equation with Jones-Wilkins-Lee equation of state (Maier et al)
- Not just for EOS-based hypersonic flows: also used to model flooding in Texas with shallow-water equations

IBAMR: Overview



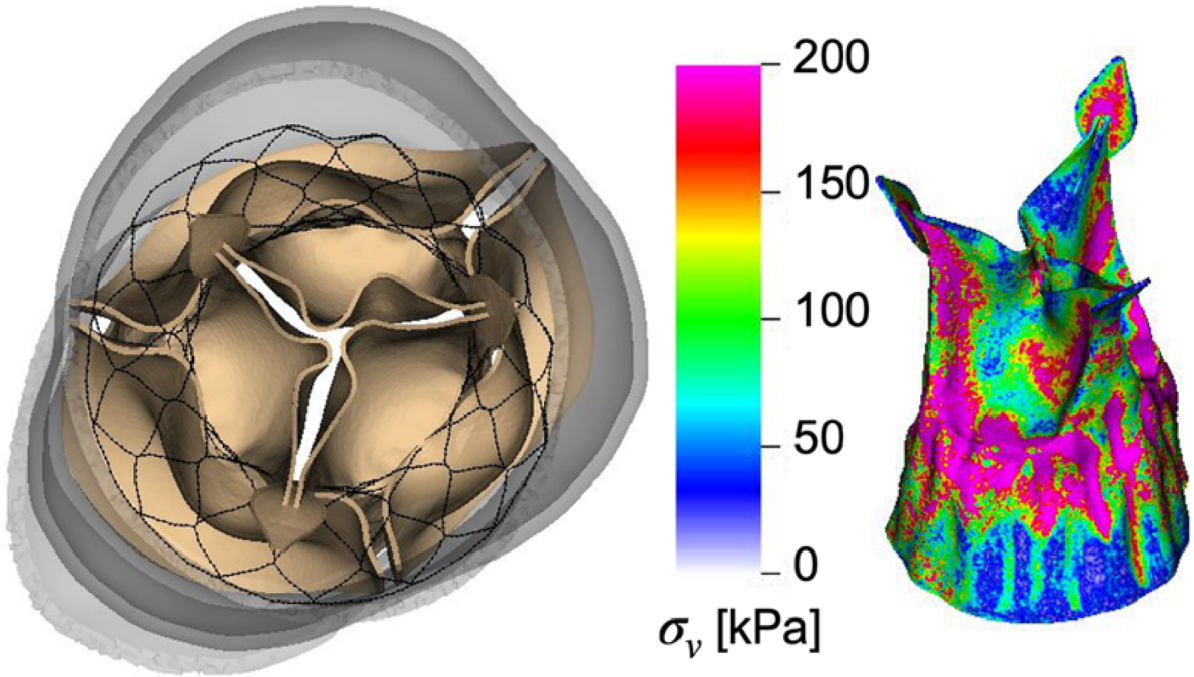
- Large C++ library with both finite differences (FDM) and finite elements (FEM)
- Scalable 2d and 3d implementations of common IB methods
- Major project, lead by Boyce Griffith here at UNC, to solve hard FSI problems, complex fluids, multiphase flows (Bhalla et al at SDSU)
- I have been a co-maintainer since 2018

IBAMR Showcase: Numerical Wave Tank



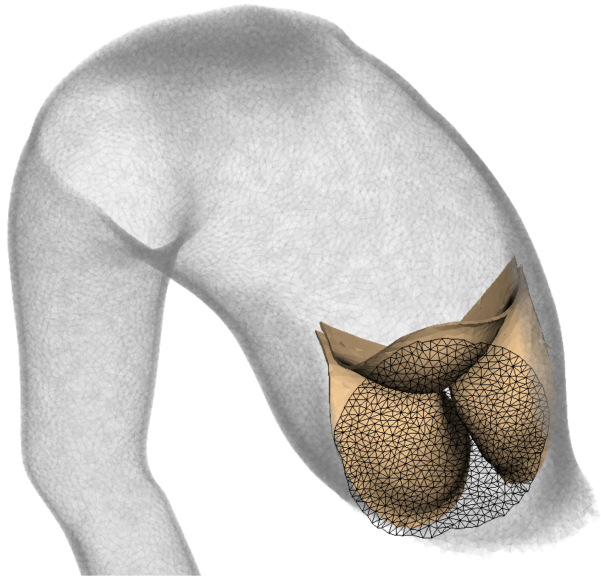
- By the group at SDSU lead by Bhalla
- Picture: *A model predictive control (MPC)-integrated multiphase immersed boundary (IB) framework for simulating wave energy converters (WECs)*, Khedkar et al
- Model solids, liquids, and gasses efficiently to solve a real problem

IBAMR Showcase: Transarterial Valve Replacement



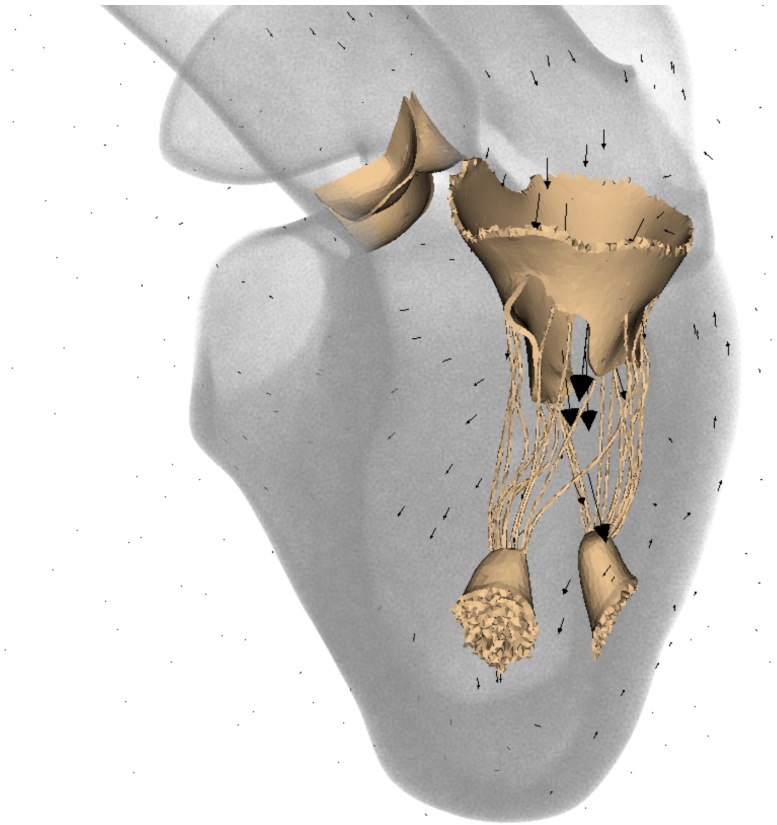
- What happens when we replace someone's tricuspid valve?
- Picture: *Patient–Specific Immersed Finite Element–Difference Model of Transcatheter Aortic Valve Replacement*, Brown et al: stent and valve and von Mises stresses
- Help surgeons understand how these devices work with detailed simulations

Cardinal: IBAMR plus deal.II



- Unified interface to both fluid-structure interaction (FSI) and electrophysiology (EP) models
- Picture: codim 1 meter mesh measuring flow through a tricuspid valve
- Detailed models (HGO, O'Hara-Rudy) practitioners care about
- Group here with Wells, Abdala, Davey, Griffith, and others
- Builds on deal.II's scalable FE infrastructure and IBAMR's IB and incompressible Navier-Stokes (INS) solvers

Cardinal: IBAMR plus deal.II



- Picture: flow around mitral valve and chordae
- Project 1: fully distributed data structures for IB (Wells)
- Project 2: better patch-based load balancers (Davey, Wells)
- Project 3: right heart model (Davey, collaboration with UC Irvine)
- Project 4: fully coupled EP-FSI (Abdala)
- Project 5: distributed Lagrange multipliers (TBA)