deal.II: challenges and opportunities of developing an open-source FEM library

Swedish e-Science Academy 2025

Satellite: Common challenges in large-scale code development

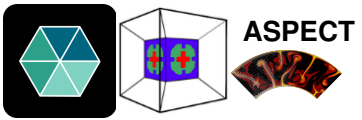
Peter Munch[†]

[†]Institute of Mathematics, Technical University of Berlin, Germany

16. October, 2025

Overview

open-source application codes



▷ FEM library; C++
▷ origin in Heidelberg 1998; 3 developers
▷ 13 principal developers; 418+ contributors
▷ approx. 2,700 publications
▷ free (transition to Apache-2.0 with LLVM-exception)
▷ extensive docu & approx. 90 tutorials

Jethe

+DFT-FE, OpenFCST, life^{x}, ...

About myself: postdoctoral researcher at TU Berlin (2024–, before: Uppsala University), deal.II principal developer (2020–)

Questions to be answered in this presentation:

- Who are the library developing? How do they work? Which resources are used?
- Who are the users? How do the developers interact with them?
- What are challenges/opportunities of developing an open-source library (in academia)?

Part 1:

deal.II: introduction

Introduction

- deal.II[1]: mathematical software for finite-element analysis, written in C++
- origin in Heidelberg 1998: Wolfgang Bangerth, Ralf Hartmann, Guido Kanschat
- 418+ contributors + principal developer team with 13 active members
- more than 2,700 publications (on and with deal.II)
- freely available under Apache-2.0 with LLVM-exception or LGPL-2.1-or-later
- yearly releases; current release: 9.7
- features comprise (supported by **third-party libraries**): matrix-free implementations, parallelization (MPI, threading via TBB & Taskflow, SIMD, GPU support), discontinuous Galerkin methods, AMR via p4est, particles, wrappers for PETSc and Trilinos, ...
- similar libraries: e.g.,
  MFEM, DUNE, FEniCS, libMesh, ...

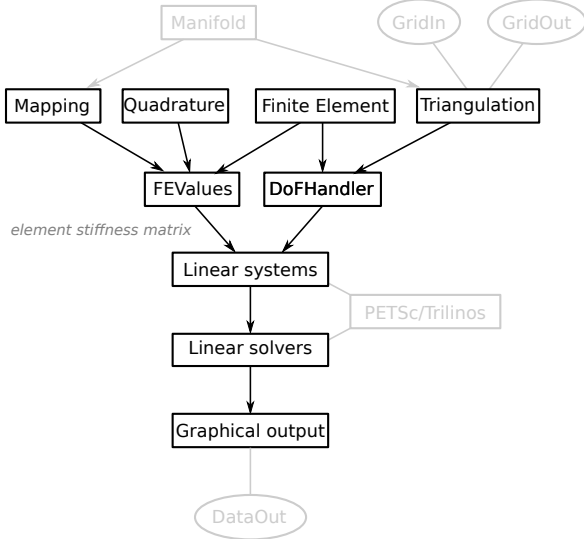
[1] successor of DEAL: **D**ifferential **E**quations **A**nalysis **L**ibrary

Main modules

needed from a FEM library:

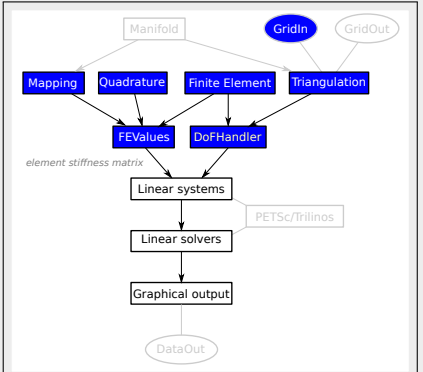
- mesh handling
- finite elements
- quadrature rules
- mapping rules
- assembly procedure
- linear solver

deal.II main modules $\rightarrow$



Main modules (cont.)

```
const unsigned int dim = 2, degree = 3;

parallel::distributed::Triangulation<dim> tria(MPI_COMM_WORLD);
util::create_reentrant_corner(tria);

FE_Q<dim>            fe(degree);
QGauss<dim>          quad(degree + 1);
MappingQGeneric<dim> mapping(1);

DoFHandler<dim> dof_handler(tria);
dof_handler.distribute_dofs(fe);

// deal with boundary conditions
AffineConstraints<double> constraints;
VectorTools::interpolate_boundary_values(mapping, dof_handler, 0,
  Functions::ZeroFunction<dim>(), constraints);
constraints.close();

// initialize vectors and system matrix
LinearAlgebra::distributed::Vector<double> x, b;
TrilinosWrappers::SparseMatrix             A;
util::initialize_dof_vector(dof_handler, x); util::initialize_dof_vector(dof_handler, b);
util::initialize_system_matrix(dof_handler, constraints, A);
```




```
// assemble right-hand side and system matrix
FullMatrix<double>                   cell_matrix;
Vector<double>                       cell_rhs;
std::vector<types::global_dof_index> local_dof_indices;

FEValues<dim> fe_values(mapping, fe, quad, update_values | update_gradients | update_JxW_values);
```

$$\sum_q (\nabla N_{iq}, \nabla N_{jq}) \cdot |J_q| \times w_q, \quad \sum_q (N_{iq}, f) \cdot |J_q| \times w_q$$

Main modules (cont.)

```
for (const auto &cell : dof_handler.active_cell_iterators()) // loop over all locally-owned cells
  {
    if (cell->is_locally_owned() == false) continue;
    fe_values.reinit(cell);

    const auto dofs_per_cell = cell->get_fe().n_dofs_per_cell();  // allocate memory for element matrix/vector
    cell_matrix.reinit(dofs_per_cell, dofs_per_cell);             //
    cell_rhs.reinit(dofs_per_cell);                               //

    for (const auto q : fe_values.quadrature_point_indices())  // compute element matrix/vector
      for (const auto i : fe_values.dof_indices())             //
        for (const auto j : fe_values.dof_indices())           //
          cell_matrix(i, j) += (fe_values.shape_grad(i, q) *   //
                                fe_values.shape_grad(j, q) *   //
                                fe_values.JxW(q));             //
                                                               //
    for (const auto q : fe_values.quadrature_point_indices())  //
      for (const auto i : fe_values.dof_indices())             //
        cell_rhs(i) += (fe_values.shape_value(i, q) *          //
                        1. *                                   //
                        fe_values.JxW(q));                     //

    local_dof_indices.resize(cell->get_fe().dofs_per_cell);                                  // assembly
    cell->get_dof_indices(local_dof_indices);                                                //
    constraints.distribute_local_to_global(cell_matrix, cell_rhs,  local_dof_indices, A, b); //
  }                                                                                          //
                                                                                             //
b.compress(VectorOperation::add); A.compress(VectorOperation::add);                          //
```

$$\sum_q (\nabla N_{iq}, \nabla N_{jq}) \cdot |J_q| \times w_q \to \mathbf{K}_{ij}^{(e)}$$

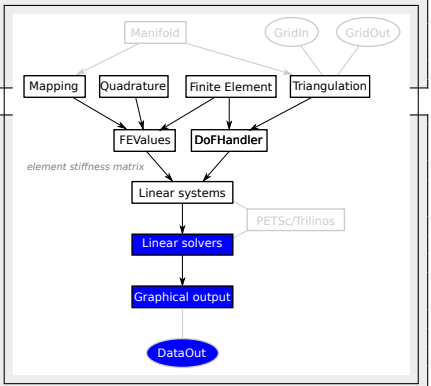
$$\sum_q (N_{iq}, f) \cdot |J_q| \times w_q \to \mathbf{f}_i^{(e)}$$

$$\mathop{\mathbf{A}}_{e} \mathbf{K}^{(e)}, \mathop{\mathbf{A}}_{e} \mathbf{f}^{(e)}$$

Main modules (cont.)

```
// solve linear equation system
ReductionControl                                        reduction_control;
SolverCG<LinearAlgebra::distributed::Vector<double>> solver(reduction_control);
solver.solve(A, x, b, PreconditionIdentity());

if (Utilities::MPI::this_mpi_process(util::get_mpi_comm(tria)) == 0)
  printf("Solved in %d iterations.\n", reduction_control.last_step());

constraints.distribute(x);
```

$$\mathbf{K}\mathbf{x} = \mathbf{f} \rightarrow \mathbf{x} = \mathbf{K}^{-1}\mathbf{f}$$



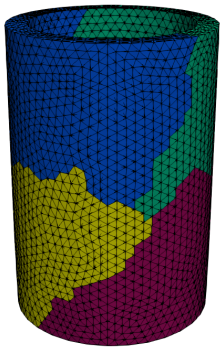

```
// output results (e.g. VTK, VTU, Tecplot, HDF5, svg, gnuplot, ...)
DataOutBase::VtkFlags flags;
flags.write_higher_order_cells = true;

DataOut<dim> data_out;
data_out.set_flags(flags);
data_out.attach_dof_handler(dof_handler);
x.update_ghost_values();
data_out.add_data_vector(dof_handler, x, "solution");
data_out.build_patches(mapping, degree + 1);
data_out.write_vtu_with_pvtu_record("./", "result", 0, MPI_COMM_WORLD);
```

Full code: `https://github.com/peterrum/dealii-examples/blob/master/poisson.cc`

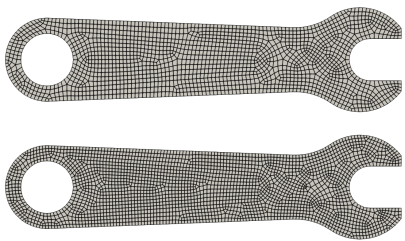
Active development

- yearly release (current release: 9.7)
- major additions in the last years, e.g., particles,

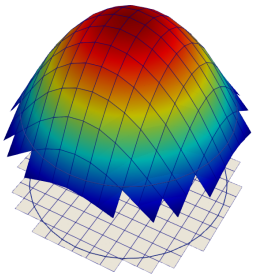
simplex meshes



non-nested multigrid



CutFEM



... and 24 new tutorials over the last 5 years

- each release is accompanied by a release paper (mostly in Journal of Numerical Mathematics)

Successful?

Winner of “SIAM/ACM Prize in Computational Science and Engineering 2025”

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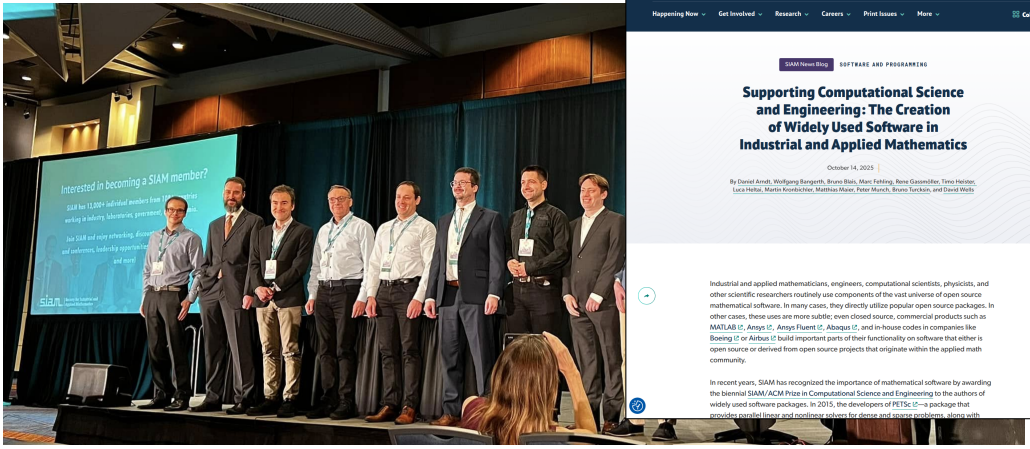
Wolfgang Bangerth’s acceptance speech [1]

Successful?

Winner of “SIAM/ACM Prize in Computational Science a

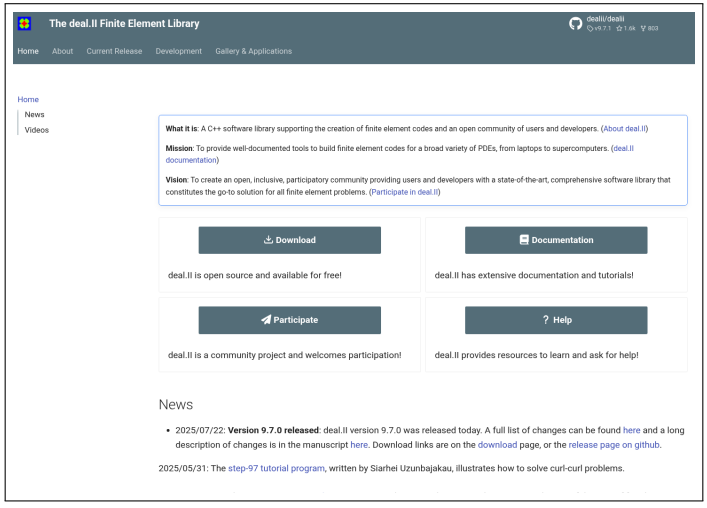


Wolfgang Bangerth’s acceptance speech [1], SIAM News Blog [2].

Part 2:

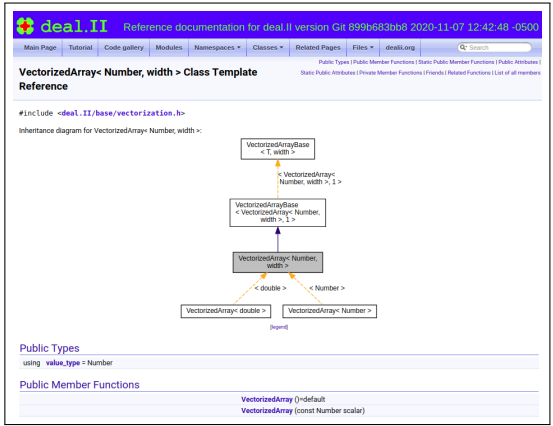
Distributed development: resources

Official webpage

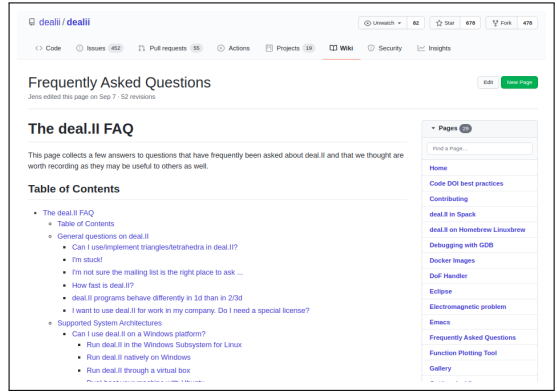


... www.dealii.org

Documentation



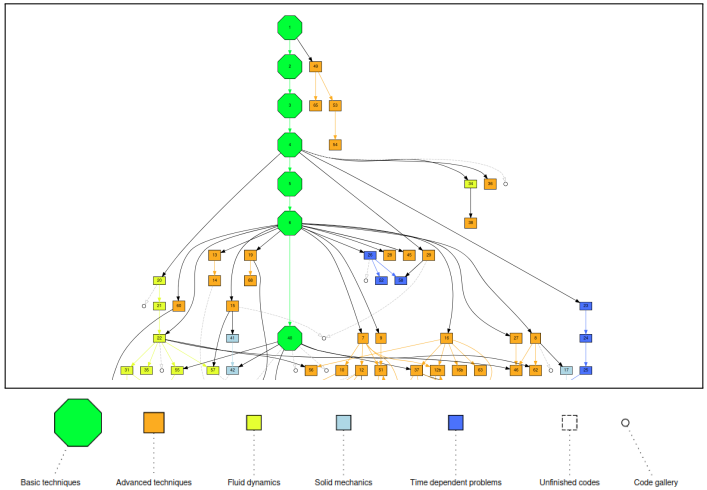
Extensive Doxygen documentation



GitHub Wiki

Documentation (cont.)

87 tutorials and code gallery:



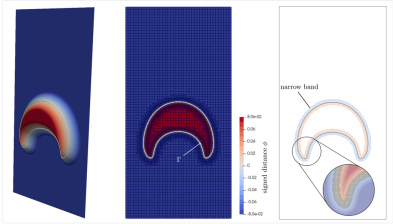
... further 10 tutorials: work in progress

Documentation (cont.)

Example (step-87):

Motivation: two-phase flow

The minimal code examples (short "mini examples") presented in this tutorial are motivated by the application of two-phase-flow simulations formulated in a one-fluid setting using a Eulerian framework. In diffuse interface methods, the two phases may be implicitly described by a level-set function, here chosen as a signed distance function $\phi(\boldsymbol{x})$ in Ω and illustrated for a popular benchmark case of a rising bubble in the following figure.



The discrete interface $\Gamma^{\ast}$ is represented implicitly through a certain isosurface of the level-set function e.g. for the signed-distance function $\Gamma^{\ast} = \{\boldsymbol{x} \in \Omega \mid \phi(\boldsymbol{x}) = 0\}$. We would like to note that deal.II provides a set of analytical signed distance functions for simple geometries in the Functions::SignedDistance namespace. Those can be combined via Boolean operations to describe more complex geometries [58]. The temporal evolution of the level-set field is obtained by the transport equation

$$\frac{\mathrm{d}\,\phi}{\mathrm{d}\,t} + \boldsymbol{u}|_{\Gamma} \cdot \nabla\phi = 0$$

with the transport velocity at the interface $\boldsymbol{u}|_{\Gamma}$, which might be approximated by the local fluid velocity $\boldsymbol{u}|_{\Gamma} \approx \boldsymbol{u}(\boldsymbol{x})$. To reobtain the signed-distance property of the level-set field throughout the numerical solution procedure, PDE-based or, alternatively, also geometric reinitialization methods are used. For the latter, an algorithm for computing the distance from the support points to the discrete interface, e.g., via closest-point point projection [124], is needed. This will be part of one of the mini examples, where we describe how to obtain the closest point $\boldsymbol{x}^{\ast}$ to the interface Γ for an arbitrary point $\boldsymbol{x}$. For the simplest case, the former can be computed from the following equation

$$\boldsymbol{x}^{\ast} = \boldsymbol{x} - \boldsymbol{n}(\boldsymbol{x})\phi(\boldsymbol{x}),$$

assuming that the interface normal vector $\boldsymbol{n}(\boldsymbol{x})$ and $\phi(\boldsymbol{x})$ represent exact quantities. Typically, this projection is only performed for points located within a narrow band region around the interface, indicated in the right panel of the figure above.

Alternatively to the implicit representation of the interface, in sharp interface methods, e.g., via front tracking, the interface Γ is explicitly represented by a surface mesh. The latter is immersed into a background mesh, from which the local velocity at the support points of the surface mesh is extracted and leads to a movement of the support points of the immersed mesh as

$$\boldsymbol{x}_k^{(i+1)} = \boldsymbol{x}_k^{(i)} + \Delta t \cdot \boldsymbol{u}(\boldsymbol{x}_k^{(i)}) \quad \text{for } \boldsymbol{x}_k \in \Gamma$$

which considers an explicit Euler time integration scheme from time step i to $i+1$ with time step-size Δt.

For a two-phase-flow model considering the incompressible Navier-Stokes equations, the two phases are usually coupled by a singular surface-tension force $\boldsymbol{F}_{\Gamma}$, which results, together with the difference in fluid properties, in discontinuities across the interface:

$$\boldsymbol{F}_{\Gamma}(\boldsymbol{x}) = \sigma\kappa(\boldsymbol{x})\boldsymbol{n}(\boldsymbol{x})\delta_{\Gamma}(\boldsymbol{x}).$$

The commented program

Include files

The program starts with including all the relevant header files.

```
#include <deal.II/base/conditional_ostream.h>
#include <deal.II/base/function_lib.h>
#include <deal.II/base/function_signed_distance.h>
#include <deal.II/base/mpi.h>
#include <deal.II/base/mpi.templates.h>

#include <deal.II/distributed/tria.h>

#include <deal.II/dofs/dof_renumbering.h>
#include <deal.II/dofs/dof_tools.h>

#include <deal.II/fe/fe_nothing.h>
#include <deal.II/fe/fe_q.h>
#include <deal.II/fe/fe_system.h>
#include <deal.II/fe/mapping_q1.h>
#include <deal.II/fe/mapping_q_cache.h>

#include <deal.II/grid/grid_generator.h>
#include <deal.II/grid/grid_tools.h>

#include <deal.II/lac/generic_linear_algebra.h>

#include <deal.II/numerics/data_out.h>

#include <iostream>
#include <fstream>
```

The files most relevant for this tutorial are the ones that contain Utilities::MPI::RemotePointEvaluation and the distributed evaluation functions in the VectorTools namespace, which use Utilities::MPI::RemotePointEvaluation.

```
#include <deal.II/base/mpi_remote_point_evaluation.h>
#include <deal.II/numerics/vector_tools.h>
```

The following header file provides the class FEPointEvaluation, which allows us to evaluate values of a local solution vector at arbitrary unit points of a cell.

```
#include <deal.II/matrix_free/fe_point_evaluation.h>
```

We pack everything that is specific for this program into a namespace of its own.

```
namespace Step87
{
  using namespace dealii;
```

Utility functions (declaration)

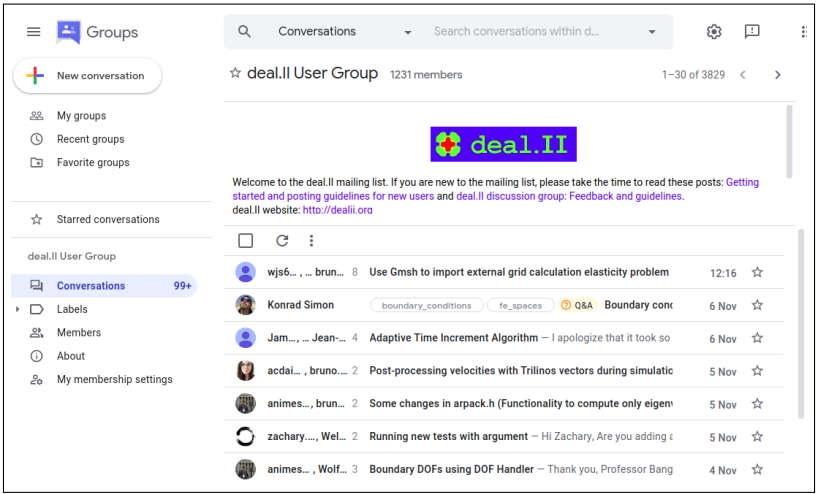
In the following, we declare utility functions that are used in the mini examples below. You find the definitions at the end of the tutorial.

The minimum requirement of this tutorial is MPI. If deal.II is built with p4est, we use parallel::distributed::Triangulation as distributed mesh. The class parallel::shared::Triangulation is used if deal.II is built without p4est or if the dimension of the triangulation is 1D, e.g., in the case of codim-1 meshes.

```
#ifdef DEAL_II_WITH_P4EST
  template <int dim, int spacedim = dim>
  using DistributedTriangulation = typename std::conditional_t<
```

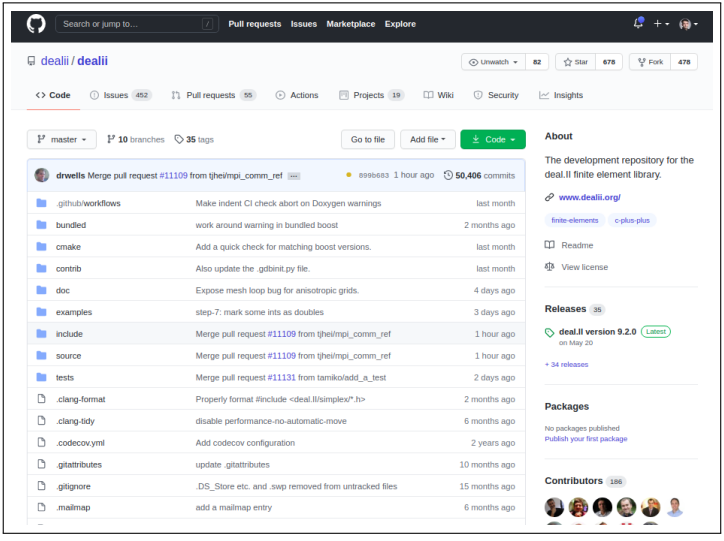
Forum

deal.II user group:



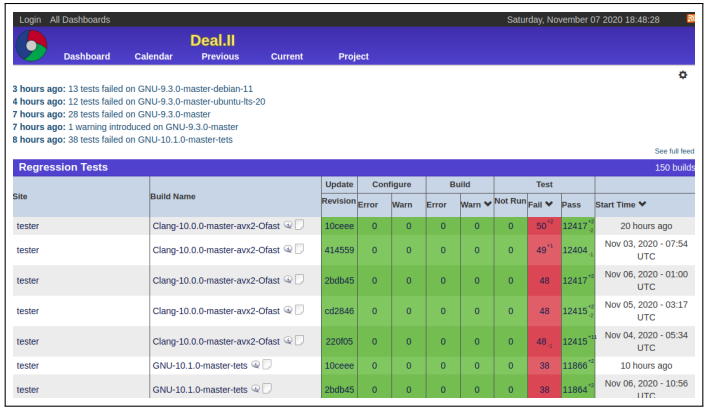
... Q&A by users and developers!

Development on GitHub



- issues
- pull requests
- GitHub actions $\rightarrow$ CI
- required: approval by ≥ 1 principal developer

Continuous integration

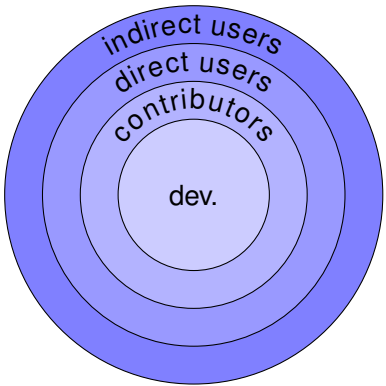


... more than 17,000 tests run for different compilers/hardware/configurations

Part 3:

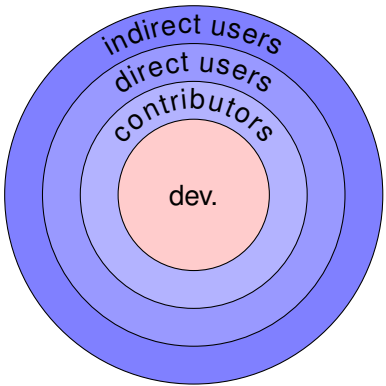
Distributed development: users and developers

User and developer base



- deal.II has a large body of developers and users
- this includes Master students, PhD students, researchers (academia, research centers), industry
- background: Mathematics, Computer Science, Engineering, ...
- location: Europe, China, USA, Canada, India, ...

User and developer base: principal developers



- team of 13 principal developers
- know a significant fraction of the library
- review and merge PRs
- answer questions/issues
- responsible for infrastructure/testing
- organization of workshops
- not payed for work on deal.II
- discussion via GitHub/Element
- regular Zoom meetings

User and developer base: principal developers (cont.)

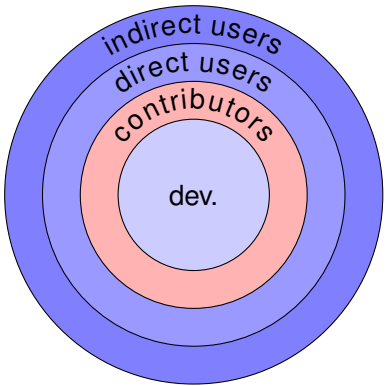
Developers emeriti: Denis Davydov (2015-2020), Ralf Hartmann (1998-2012), Guido Kanschat (1997-2022), Toby D. Young (2013-2017)

User and developer base: principal developers (cont.)

- Daniel Arndt, Oak Ridge National Laboratory, TN, USA (since 2016)
- Wolfgang Bangerth, Colorado State University, CO, USA (since 1997)
- Bruno Blais, Polytechnique Montréal, Canada (since 2023)
- Marc Fehling, Charles University, Czech Republic (since 2021)
- Rene Gassmoeller, GEOMAR Helmholtz Centre for Ocean Research, Kiel, Germany (since 2023)
- Timo Heister, Clemson University, SC, USA (since 2012)
- Luca Heltai, University of Pisa, Italy (since 2013)
- Martin Kronbichler, Ruhr University Bochum, Germany (since 2013)
- Matthias Maier, Texas A&M University, College Station, TX, USA (since 2013)
- Peter Munch, Technical University of Berlin, Germany (since 2020)
- Jean-Paul Pelteret, industry, Germany (since 2016)
- Bruno Turcksin, Oak Ridge National Laboratory, TN, USA (since 2013)
- David Wells University of North Carolina, Chapel Hill, NC, USA (since 2015)

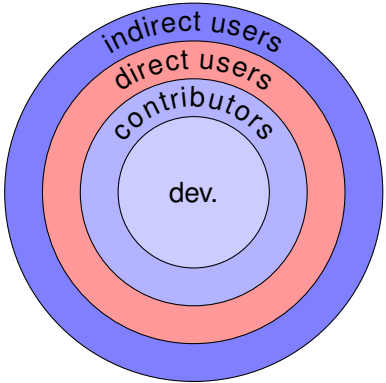
Summary: PhD students (0) vs. postdocs (7) vs. professors (6), Europe (6) vs. USA/Canada (7), male (13) vs. female (0), academia (9) vs. research centers (3) vs. industry (1), math (7) vs non-math (6)

User and developer base: contributors

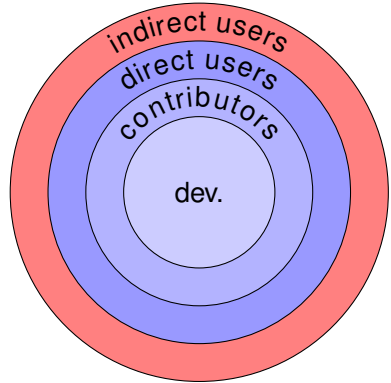


- use deal.II extensively
- read/write deal.II code
- contribute: bug fixes, fixes in documentation, features
- total: 418+
- last release: 88 contributors
- award: co-author of release paper

User and developer base: users



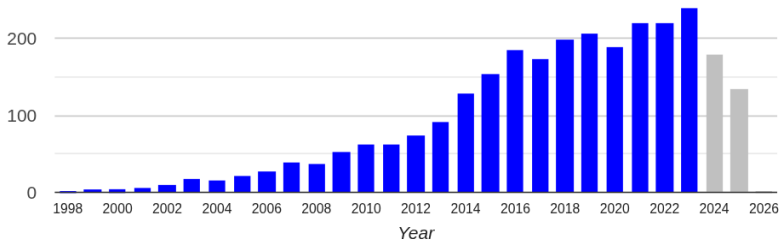
- write applications using deal.II
- use documentation
- potentially start from a tutorial
- interaction via google group



- use application/libraries using deal.II (e.g., ASPECT for geosciences)
- rare interaction
- citation

Publications

Number of publications (total: 2746) gives an indication of number of users:



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Workshops

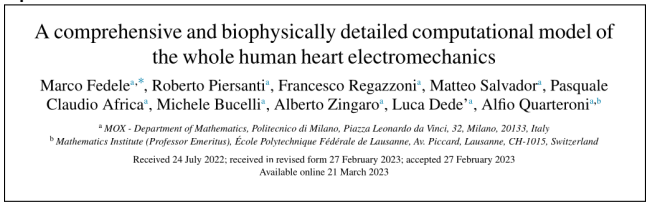
(Yearly) workshops:

Fort Collins, Colorado, USA, 2024

+ get-together at workshops

Workshops (cont.)

Best deal.II-based paper award:



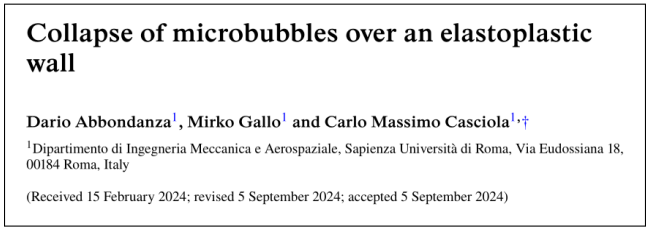
A comprehensive and biophysically detailed computational model of the whole human heart electromechanics

Marco Fedele[a,*], Roberto Piersanti[a], Francesco Regazzoni[a], Matteo Salvador[a], Pasquale Claudio Africa[a], Michele Bucelli[a], Alberto Zingaro[a], Luca Dede'[a], Alfio Quarteroni[a,b]

[a] MOX - Department of Mathematics, Politecnico di Milano, Piazza Leonardo da Vinci, 32, Milano, 20133, Italy
[b] Mathematics Institute (Professor Emeritus), École Polytechnique Fédérale de Lausanne, Av. Piccard, Lausanne, CH-1015, Switzerland

Received 24 July 2022; received in revised form 27 February 2023; accepted 27 February 2023
Available online 21 March 2023

2023: Computer Methods in Applied Mechanics and Engineering



Collapse of microbubbles over an elastoplastic wall

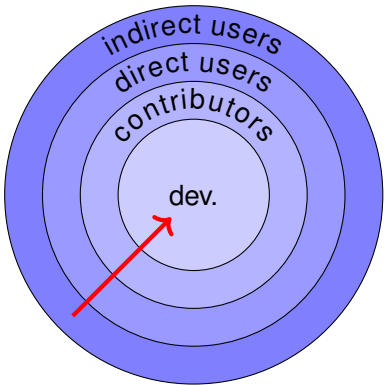
Dario Abbondanza[1], Mirko Gallo[1] and Carlo Massimo Casciola[1],†

[1]Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza Università di Roma, Via Eudossiana 18, 00184 Roma, Italy

(Received 15 February 2024; revised 5 September 2024; accepted 5 September 2024)

2024: Journal of Fluid Mechanics

Becoming more involved



Typical path:

- start to use deal.II (as student)
- contribute a lot
- become co-author of release paper
- contribute much more and be active in the community
- become principal developer

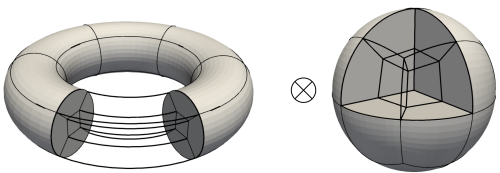
About myself

First project using deal.II (2019, student project): Vlasov equation (comp. plasma physics):

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \boldsymbol{a}(t, f, \boldsymbol{x}, \boldsymbol{v}) \cdot \nabla_{\boldsymbol{v}} f = 0 \quad \text{w.} \quad \boldsymbol{a}(t, f, \boldsymbol{x}, \boldsymbol{v}) = -\boldsymbol{E}(t, \boldsymbol{x}) \quad \text{(Poisson problem)}$$

Derivative in phase ($\boldsymbol{v}$-)space implies high-dimensional nonlinear advection equation.

Approach: high-order discontinuous Galerkin method up to 6D



$\otimes$

$2\times$ deal.II $\rightarrow$

hyper.deal

Challenges:

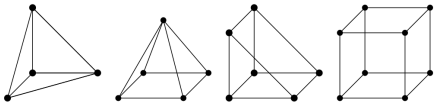
- mesh generation (open-source packages only support 1D-3D)
- performance: large working sets, communication pattern/data *curse of dimensionality* ↯
- Munch, P., Kormann, K. and Kronbichler, M., 2021. hyper. deal: An efficient, matrix-free finite-element library for high-dimensional partial differential equations. ACM TOMS.

About myself (cont.)

Since 2020 (beginning of second year of PhD), one of the principal developers of deal.II

Projects in deal.II:

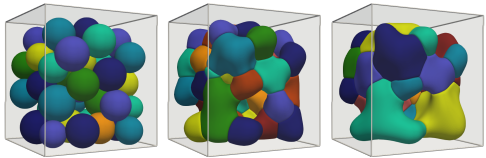
- simplex/mixed-mesh support



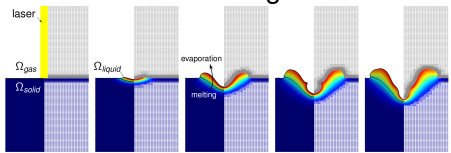
- (global-coarsening) multigrid
- hp-adaptivity, non-matching algorithms
- (fully) distributed triangulation (project 2)
- large-scale computations $\rightarrow$ consensus algorithm (project 1)
- performance optimization, e.g., matrix-free algorithms

Projects using deal.II:

- solid-state sintering

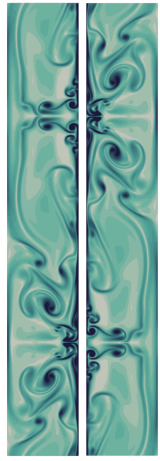


- additive manufacturing



- stage-parallel IRK and space-time FEM
- Galerkin difference methods
- direct solvers

About myself (cont.)

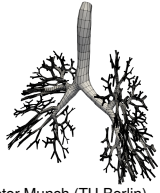


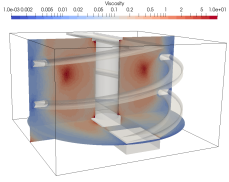
Weak form of (stabilized) incompressible Navier–Stokes equations:

$$
\begin{aligned}
&\left(\partial_t \mathbf{u},\ \mathbf{v}\right) + \left(\mathbf{u}\cdot\nabla\mathbf{u},\ \mathbf{v}\right) - \left(p,\ \nabla\cdot\mathbf{v}\right) + \left(\nu\varepsilon(\mathbf{u}),\ \varepsilon(\mathbf{v})\right) \\
&\qquad + \delta_1\left(\partial_t\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p - \nu\Delta\mathbf{u},\ \mathbf{u}\cdot\nabla\mathbf{v}\right) + \delta_2\left(\nabla\cdot\mathbf{u},\ \nabla\cdot\mathbf{v}\right) = 0, \\
&\left(\nabla\cdot\mathbf{u},\ q\right) + \delta_1\left(\partial_t\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p - \nu\Delta\mathbf{u},\ \nabla q\right) = 0
\end{aligned}
$$

Solve with BDF2/ST and Newton–Krylov method with Jacobian:

$$
J = \begin{bmatrix} A & B^T \\ C & D \end{bmatrix} \quad \rightarrow \quad J' = \begin{bmatrix} A & B^T \\ 0 & S \end{bmatrix} \quad \rightarrow \quad \text{(monolithic) multigrid}
$$





Interests:

– preconditioning
– multiphysics
– performance
– hp-adaptivity
– open-source dev.: deal.II, Lethe

Compressible NS (+reaction, cut)

$$
\boldsymbol{U}_t + \nabla\cdot\left(F_a(\boldsymbol{U}) + F_v(\boldsymbol{U})\right) = G(\boldsymbol{U})
$$

Part 4:

Challenges

① Backwards compatibility

- during development, mistakes are made
- correcting them if they are user-visible is not that easy

Example:

- old interface:

```
template <int dim, int spacedim>
void
extract_locally_active_dofs(const DoFHandler<dim, spacedim> &dof_handler,
                            IndexSet                        &dof_set);
```

- new interface:

```
template <int dim, int spacedim>
IndexSet
extract_locally_active_dofs(const DoFHandler<dim, spacedim> &dof_handler);
```

① Backwards compatibility (cont.)

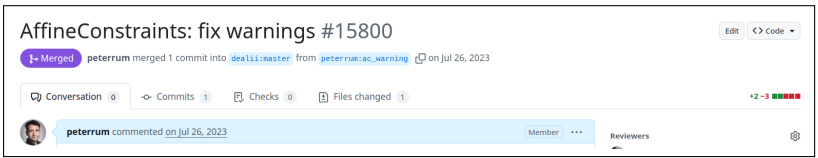
Solution: deprecation warnings

```
template <int dim, int spacedim>
DEAL_II_DEPRECATED void
extract_locally_active_dofs(const DoFHandler<dim, spacedim> &dof_handler,
                            IndexSet                        &dof_set);
```

- preprocessing macro
- deprecation takes 2 years: *early deprecation* $\rightarrow$ *deprecation*
- macros can be disabled
- user experience: “New warning/incompatibility after each update of deal.II!”

② Keeping up to date: new compilers

- support newest versions of GCC, ICC, Clang
- keep supporting old versions since not everyone has access to the newest versions
- tested versions
  - GCC: 9.4.0 (Ubuntu 20.04 LTS), 10.2.1, 10.4.1, 11.3.1, 11.4.0, 12.2.0, 12.2.1, 13.1.1, 13.3.0, 14.2.0, 14.2.1, 15.1.0, ...
  - Clang: 13.0.1, 14.0.6, 15.0.6, 16.0.6, 17.0.6, 18.1.8, 19.1.6, 19.1.7, 20.1.7, 21.1.7, ...
- goal: no warnings!



② Keeping up to date: new versions of C++

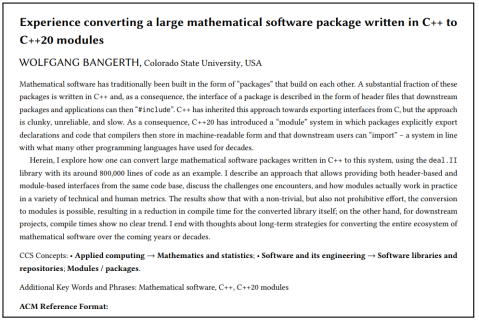
- we want to use/support newest versions of the C++ standard
- however, many used compilers do not support current features; requirement: C++17

Solutions:

- check C++ version during configuration
- provide own implementations

```
#ifndef DEAL_II_HAVE_CXX20
  template <typename T, typename B>
  using iota_view = boost::integer_range<T>;
#else
  using std::ranges::iota_view;
#endif
```

- modules (C++20) supported!



Experience converting a large mathematical software package written in C++ to C++20 modules

WOLFGANG BANGERTH, Colorado State University, USA

Mathematical software has traditionally been built in the form of "packages" that build on each other. A substantial fraction of these packages is written in C++ and, as a consequence, the interface of a package is described in the form of header files that downstream packages and applications can then "`#include`". C++ has inherited this approach towards exporting interfaces from C, but the approach is clunky, unreliable, and slow. As a consequence, C++20 has introduced a "module" system in which packages explicitly export declarations and code that compilers then store in machine-readable form and that downstream users can "import" – a system in line with what many other programming languages have used for decades.

Herein, I explore how one can convert large mathematical software packages written in C++ to this system, using the `deal.II` library with its around 800,000 lines of code as an example. I describe an approach that allows providing both header-based and module-based interfaces from the same code base, discuss the challenges one encounters, and how modules actually work in practice in a variety of technical and human metrics. The results show that with a non-trivial, but also not prohibitive effort, the conversion to modules is possible, resulting in a reduction in compile time for the converted library itself; on the other hand, for downstream projects, compile times show no clear trend. I end with thoughts about long-term strategies for converting the entire ecosystem of mathematical software over the coming years or decades.

CCS Concepts: • **Applied computing** → **Mathematics and statistics.** • **Software and its engineering** → **Software libraries and repositories**; **Modules / packages**.

Additional Key Words and Phrases: Mathematical software, C++, C++20 modules

ACM Reference Format:

```
template <int dim, int spacedim>
DEAL_II_CXX20_REQUIRES((concepts::is_valid_dim_spacedim<dim, spacedim>))
class Triangulation;
```

② Keeping up to date: external libraries

The interfaces of external libraries change over time, and features are added/removed.

Solution: check version during configuration and use preprocessing macros.

Example:

```
# DEAL_II_WITH_PETSC set up with external dependencies
#     PETSC_VERSION = 3.18.6.
#     PETSC_DIR = /homes/numerik/muench/store/sw-candi/petsc-3.18.6
```

```
#if DEAL_II_PETSC_VERSION_LT(3, 8, 0)
  ierr = MatTranspose(tmp, MAT_REUSE_MATRIX, &tmp);
#else
  ierr = MatTranspose(tmp, MAT_INPLACE_MATRIX, &tmp);
#endif
```

② Keeping up to date: new hardware architecture

To support different CPU architectures, large part of the library does not use double/float directly but wraps them in structs:

double	**float**	**ISA**
VectorizedArray<double, 1>	VectorizedArray<float, 1>	(auto-vectorization)
VectorizedArray<double, 2>	VectorizedArray<float, 4>	SSE2/AltiVec/ARM NEON
VectorizedArray<double, 4>	VectorizedArray<float, 8>	AVX/AVX2
VectorizedArray<double, 8>	VectorizedArray<float, 16>	AVX-512

Use cases: vectorization over cells and quadrature points

With C++23, we will be able to replace (hopefully) our own implementation!

VectorizedArray (`deal.II`)	**std::simd (C++23)**
VectorizedArray<Number>	std::experimental::native_simd<Number>
VectorizedArray<Number, size>	std::experimental::fixed_size_simd<Number, size>

Support of mixed precision, e.g., double-float in geometric multigrid.

What about GPUs?

③ Development by PhD students

Many features of deal.II are developed by PhD students/early-carrier researchers:

- distributed meshes → Timo Heister (2011, Göttingen)
- matrix-free operator evaluation → Martin Kronbichler (2012, Uppsala)
- matrix-free operator evaluation on the GPU → Karl Ljungkvist (2014, Uppsala)
- distributed hp-adaptive computation → Marc Fehling (2019, Jülich)
- simplex/mixed-mesh support → Peter Munch (2021, Geesthacht)

Observations:

- projects are continued as postdoctoral researchers/professors
- projects are continued by new PhD students
- maintenance by others
- but ...

③ Development by PhD students (cont.)

Karl Ljungkvist (Uppsala University) has implemented matrix-free operator evaluation on the GPU during his PhD. At that time, state-of-the-art implementation.

- **Ljungkvist**, K., 2014. Matrix-free finite-element operator application on graphics processing units. In European Conference on Parallel Processing (pp. 450-461). Cham: Springer International Publishing. **16 citations.**
- **Ljungkvist, K.**, 2017. Matrix-free finite-element computations on graphics processors with adaptively refined unstructured meshes. In Proceedings of the 25th High Performance Computing Symposium (pp. 1-12). **38 citations.**
- **Ljungkvist**, K. and Kronbichler, M., 2017. Multigrid for matrix-free finite element computations on graphics processors. **11 citations.**
- Kronbichler, M. and **Ljungkvist, K.**, 2019. Multigrid for matrix-free high-order finite element computations on graphics processors. ACM TOPC. **97 citations.**
- Munch, P., **Ljungkvist, K.** and Kronbichler, M., 2022. Efficient application of hanging-node constraints for matrix-free high-order FEM computations on CPU and GPU. ISC. **7 citations.**

③ Development by PhD students (cont.)

After the PhD was concluded, the development of GPU features in deal.II stalled. Others group have not rested, e.g., NEKO, libCEED, MFEM, NekRK, GALÆXI, ...

Developments:

- port Karl Ljungkvist's code to master
- new tutorial: step-64
- replacing CUDA backend by Kokkos
- overintegration and vectorial elements
- example codes deal.II + libCEED (BP1–BP6 supported)[2]

[2] `https://github.com/CEED/libCEED/tree/main/examples/deal.II`

④ Feature requests

Most requested features of deal.II:

- simplex/mixed-mesh support
- Python wrappers

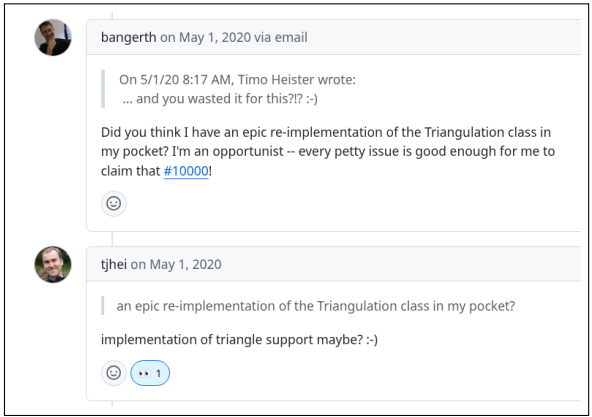
④ Feature requests (cont.)

Most requested features of deal.II:

- simplex/mixed-mesh support ✓
- Python wrappers

Addition simplex/mixed mesh support:

- running gag for a long time



- available since 2021
- added by PM, financially backed by Helmholtz-Zentrum Hereon, Germany
- hesitation: long-time maintenance & incomplete feature

④ Feature requests (cont.)

Most requested features of deal.II:

- simplex/mixed-mesh support
- Python wrappers ✗

Python wrappers:

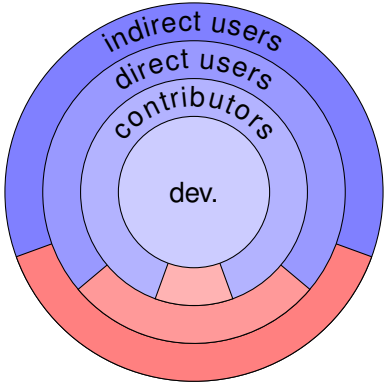
- basic implementation of Python bindings for geometry generation/manipulation

```
import PyDealII.Release as dealii
triangulation = dealii.Triangulation(dim = '2D')
triangulation.read(filename = 'example.msh', format = 'msh')
```

- no bindings for the rest of the library; challenge template arguments?
- observation: C++ difficult for starting when you are used to Python/MATLAB
- in contrast to: FEniCS, Firedrake, Dune, MFEM, libCEED, ...
- no interest/no financial support/no (scientific) motivation since no new innovation

⑤ Diversity

Visualization of men/women distribution:



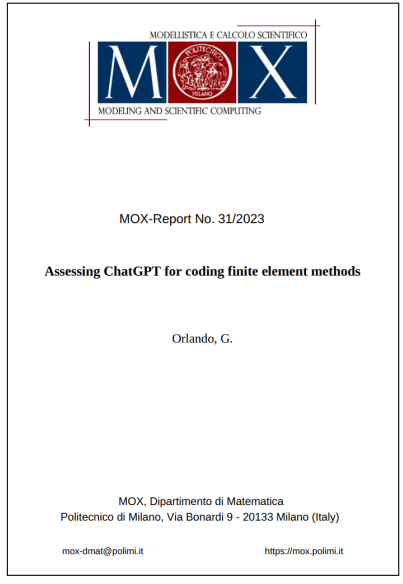
Observation:

- the developer team of deal.II is highly uniform: 13 men!
- however, large fraction of users are women!

Challenge/question: how can we improve?

⑥ Artificial intelligence

- LLMs are trained on open-source code projects
- i.e., can be used to assist in writing code
- an early example (ChatGPT $\leftrightarrow$ deal.II) is given by G. Orlando in 2023


MODELLISTICA E CALCOLO SCIENTIFICO

MODELING AND SCIENTIFIC COMPUTING

MOX-Report No. 31/2023

Assessing ChatGPT for coding finite element methods

Orlando, G.

MOX, Dipartimento di Matematica
Politecnico di Milano, Via Bonardi 9 - 20133 Milano (Italy)

mox-dmat@polimi.it https://mox.polimi.it

⑦ (Under)Appreciation

Is software development (under)appreciated ...

- by the community? which community?
- by funding agencies?
- by journal publishers?
- by hiring committees?

How much time/effort can we spent on developing software?

Part 5:

Opportunities

For users

- rely on maintained, optimized, well-documented code
- one can concentrate on scientific questions without having to reimplement FEM
- benchmark codes can be published to allow reproducibility

For contributors/developers

- good for the CV (contribution to a big open-source project, visible)
- meet and interact with interesting people
- learn *research software engineering* as a side project
- developed features are tested (+ reviewed and as such have high quality), further developed (also by others), maintained, used (also in contexts where the original developer did not imagine)
- fun

Part 6:

Conclusions

Conclusions

- deal.II is an open-source finite-element library written in C++
- well-documented and public development on GitHub
- developer team and active user community
- opportunities overweigh challenges (e.g., maintenance burden)