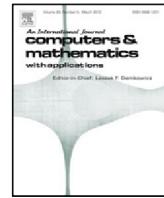




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# The DEAL.II finite element library: Design, features, and insights<sup>☆</sup>

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## ABSTRACT

DEAL.II is a state-of-the-art finite element library focused on generality, dimension-independent programming, parallelism, and extensibility. Herein, we outline its primary design considerations and its sophisticated features such as distributed meshes, *hp*-adaptivity, support for complex geometries, and matrix-free algorithms. But DEAL.II is more than just a software library: It is also a diverse and worldwide community of developers and users, as well as an educational platform. We therefore also discuss some of the technical and social challenges and lessons learned in running a large community software project over the course of two decades.

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## 1. Introduction

Mathematical software has been collected in packages for almost as long as computers have been around. The first of these packages were collections of loosely connected subroutines for specific purposes. In the earliest days, most of these were related to linear algebra problems such as the solution of linear systems, or computing eigenvalues, but also to numerical integration and differentiation. Few of these packages survive to this day, but the BLAS and related LAPACK interfaces [1,2] are still widely used, despite the fact that BLAS was developed and standardized already in the 1970s.

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<sup>1</sup> All authors of the paper are Principal Developers of the deal.II software library. They have all developed substantial pieces of deal.II, participate in patch review, and have participated in the writing of this article.

Since then, mathematical software has seen the emergence of ever more sophisticated and connected libraries. This includes software for sparse linear algebra in the 1980s; support for parallel sparse linear algebra based on MPI [3] in the 1990s; and, since the late 1990s and early 2000s, libraries that provide the tools to build numerical solvers for partial differential equations (PDEs) using finite element, finite difference, or finite volume methods. Many of the libraries in this category are discussed in articles in this issue.

Among the largest of the libraries supporting numerical PDE solvers is **DEAL.II**, whose architecture, feature set, user and developer community, and applications we discuss herein. The origins of this library lie in the Numerical Analysis Group at the University of Heidelberg, Germany, where a predecessor library called **DEAL** (short for the “Differential Equation Analysis Library”) was developed since the mid-1990s. **DEAL.II** is a re-write of **DEAL** using more modern software design principles; it was started in late 1997 by Wolfgang Bangerth, Ralf Hartmann, and Guido Kanschat who, at the time, were all members of the same group in Heidelberg. Since then, **DEAL.II** has grown into a truly worldwide project with more than one million lines of C++ code, to which more than 250 people have contributed, and that is managed by a dedicated group of Principal Developers located at universities, research institutes, and companies across continents.

This paper discusses aspects of the **DEAL.II** project. Specifically, Section 2 is concerned with design considerations that dictate the functionality that **DEAL.II** provides. Section 3 then covers specific functionality provided within this framework. As will become apparent there, our goal is to cover essentially everything that can be provided in a generic way to codes that want to solve specific partial differential equations using the most modern aspects of the finite element method, all while supporting modern hardware. Section 4 discusses some of the lessons we have learned running a large and complex software project, while Section 5 covers how **DEAL.II** supports our views on and activities in education in the Computational Science and Engineering arena. Section 6 briefly outlines some of the complex applications that have been built atop **DEAL.II** over the years and showcases new parallel scalability results. In Section 7 we comment on the vision and future directions of the project. We conclude in Section 8.

We end this introduction by stating that an earlier review of **DEAL.II** was previously published in [4], and that individual releases and new features are discussed in a series of papers of which the most recent ones are [5–8]. Specific features of **DEAL.II**, along with details of their implementation, are discussed in a large number of papers [9–23]. For more details and an updated list, see <https://dealii.org/publications.html> or the summary in [8].

## 2. Design considerations

Any nontrivial software package needs (written or unwritten) design principles to guide its development. Such principles provide a mental backdrop for expectations on how its components are used and interact with each other. Design principles also enable users to learn a software package efficiently, build a foundation for the evolution of the software, and aid developers in gauging an appropriate and idiomatic implementation of new features.

In the following subsections, we outline the design principles upon which **DEAL.II** is built today. Some of these principles were already present at the start in 1997 – as explicit design goals of what we wanted to achieve at the time –, whereas others developed over time: implicitly at first, and explicitly codified as part of our development practices later on.

### 2.1. A complete toolbox for finite element codes

Finite element codes are often large and complex. They use many pieces of functionality, including meshes, geometry descriptions, shape functions, mappings, quadratures, linear algebra representations and algorithms, and more. As a consequence, such codes can run into tens or hundreds of thousands of lines of code when written from scratch.

**DEAL.II** strives to provide all functionality related to the finite element discretization of partial differential equations: an extensive collection of tools that are *generic* with respect to the discretization of any one partial differential equation, while *leaving the decision about how to put these pieces together* to the user who can combine them freely in their application codes.

### 2.2. No hidden magic: **DEAL.II** is a library, not a framework

Computational software packages can roughly be categorized as either libraries or frameworks. A library is a collection of building blocks (data structures and algorithms that work on them) that can be combined in more or less arbitrary ways in a user program that *builds on* the library and that typically provides the overall logic and outer loops. One can think of MATLAB as an exemplar of a library in this sense; BLAS and LAPACK are more traditional examples. On the other hand, frameworks provide the overall logic and let users fill in specific pieces. Many solid mechanics software packages are of this kind: they implement the overall solution algorithms and users only have to describe specifics such as the geometry, boundary conditions, loading forces, and the details of the material constitutive laws. Frameworks are therefore often easy to use but are restricted to specific purposes: It is easy to replace one material description by another, but it might be impossible to implement a dual-weighted error estimator requiring the solution of an adjoint problem since this would require changing the outermost logic, which may not be accessible to users.

**DEAL.II** is a library in this dichotomy. It strives to provide all tools our users may need to write efficient and flexible finite element programs, but it does not dictate the overall structure of the program. As a consequence, users have been able to solve problems far outside the application range originally anticipated by the **DEAL.II** authors, by combining building blocks in unexpected and creative ways. On the other hand, a number of tutorial programs (see Section 2.9) illustrate how the parts of **DEAL.II** can be assembled into typical finite element programs.

### 2.3. Do not reinvent wheels

Building efficient finite element codes requires tools from a remarkably broad range of disciplines, ranging across (i) continuous mathematics, such as in the analysis behind the derivation of error estimators or approximation results; (ii) discrete and combinatorial mathematics, e.g., in the graph algorithms used to partition meshes for parallel computations; (iii) geometry, for example in the description of meshes with curved boundaries or on surfaces; (iv) linear algebra for the formulation and solution of linear systems; (v) computer science concepts related to parallel computing as well as the design of software as a whole. Other areas also show up, for example the visualization of data, along with questions of how to best present data.

No scientific computing project has the manpower and breadth of expertise to address all of these areas with equal attention to the state of the art. Thus, a project has to decide to either use only rudimentary algorithms in some areas, or to use external packages for certain tasks. **DEAL.II** has chosen the second route, relying on other software for pre- and post-processing (i.e., for mesh generation and visualization) and interfacing with a large number of other software libraries for linear algebra operations, parallelization, I/O via XML and HDF5, and many other tasks. The latest **DEAL.II** version (9.1 at the time of writing) lists 26 other packages with which it interfaces [8].

This approach has advantages and disadvantages: It allows providing much more state-of-the-art functionality than we could otherwise. On the other hand, it requires writing wrappers that may not always expose all options an underlying package may offer. Furthermore, dealing with large numbers of dependencies has a substantial cost to both developers and users and is generally not very well liked. We comment on this in Section 4.2.

### 2.4. Dimension-independent programming

The way we write partial differential equations today is generally independent of the dimension we are in. For example, the definition of the bilinear form for the weak formulation of the Laplace equation is commonly written as

$$a(u, v) := (\nabla u, \nabla v)_{\Omega} = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (1)$$

in which the gradient is a  $d$ -dimensional vector, the dot product represents a sum over  $d$  components, and the integral stretches over a  $d$ -dimensional domain  $\Omega \subset \mathbb{R}^d$ . The actual value of  $d$  does not matter.

It would be nice for many reasons if we could reflect this independence in implementations of the finite element method. For example, such a scheme makes it easier to read code because there is a 1:1 relationship with mathematical notation; it also allows writing code only once, so that it can be tested using relatively cheap 2d simulations and then used for production runs in 3d without having to develop and debug a second version. Earlier finite element libraries, such as DiffPack [24], did so by equipping essentially every class with a member variable that represents the dimension. Several modern finite element libraries, such as libMesh [25], implement a hybrid approach where some classes, such as `libMesh::FE`, are templated on the spatial dimension but others, like `libMesh::FEMap`, are not. These approaches work but have two disadvantages: (i) Finite element codes contain an incredible number of loops over  $i = 1, \dots, d$ ,<sup>2</sup> and many of these are in the hot paths of typical execution scenarios; since the dimension  $d$  is a run-time variable in this system, none of these loops can be unrolled by the compiler. (ii) Memory allocation for  $d$ -dimensional vectors (such as the gradients in (1)) must either occur on the heap using dynamic addressing or use a fixed-size array that is large enough for all supported spatial dimensions. Other libraries have made the dimension  $d$  a single global constant selected through the build system to avoid these issues; however, such a system does not allow mixing 2d and 3d simulations, for example for coupled bulk-surface models.

**DEAL.II** instead equips many classes with an integer-valued template argument, in a technique called “dimension-independent programming” [26]. For example, points in  $d$ -dimensional space are represented by a class that can be thought of as follows (with many details omitted):

```
template <int dim> class Point {
    private: double coordinates[dim];
    public:  double operator[] (const unsigned int i);
};
```

Here, the dimension of the object is known at compile time, allowing the compiler to unroll and vectorize loops, as well as to allocate the `coordinates` array on the stack without wasting space in lower dimensions. Furthermore, it is possible to use both `Point<2>` and `Point<3>` in the same program.

As most **DEAL.II** classes have such template arguments, it is possible to write code that describes things such as the bilinear form of a partial differential equation in a way that almost exactly resembles mathematical notation, and compiles to the appropriate code in whatever dimension is eventually selected. The following code snippet is taken from the tutorial program `step-4`<sup>3</sup> and assembles the matrix corresponding to  $a(\cdot, \cdot)$  and the vector corresponding to a right-hand side term  $l(v) := \int_{\Omega} v f \, dx$  on one cell:

<sup>2</sup> For example, **DEAL.II** has some 3000 loops that are terminated in some way by a condition that depends on a constant expression involving  $d$ .

<sup>3</sup> [https://www.dealii.org/current/doxygen/deal.II/step\\_4.html](https://www.dealii.org/current/doxygen/deal.II/step_4.html).

```

for (unsigned int q = 0; q < n_q_points; ++q)
  for (unsigned int i = 0; i < dofs_per_cell; ++i)
  {
    for (unsigned int j = 0; j < dofs_per_cell; ++j)
      cell_matrix(i, j) +=
        fe_values.shape_grad(i, q) *
        fe_values.shape_grad(j, q) *
        fe_values.JxW(q);
    const Point<dim> x_q = fe_values.quadrature_point(q);
    cell_rhs(i) += fe_values.shape_value(i, q) *
      right_hand_side.value(x_q) *
      fe_values.JxW(q);
  }
}

```

The code runs in any dimension and is a literal translation of the mathematical notation obtained by substituting  $\varphi_i(\mathbf{x}_q)$  with `fe_values.shape_value(i, q)`,  $\nabla\varphi_i(\mathbf{x}_q)$  with `fe_values.shape_grad(i, q)`, and noting that (with numerical quadrature) `fe_values.JxW(q)` corresponds to the `dx` in the integral. Here,  $\mathbf{x}_q$  denotes the location (in real space) of the  $q$ th quadrature point.

## 2.5. Iterator-based programming

DEAL.II provides access to cells, faces, and vertices via *iterators*. Indeed, iterators are flexible because they do not have to point to an *object* that has member variables (e.g., a cell that stores the indices or coordinates of its vertices, its material and subdomain id, etc.); rather, iterators can point to “accessor” objects that store nothing except whatever information is necessary to *retrieve* pieces of data about a cell or face.

In particular, accessors enable the use of far more complicated data structures than simple arrays of structures. Indeed, the way DEAL.II stores data is generally in the form of structures of arrays, rather than arrays of structures, as this leads to substantially better cache locality [27]: Loops over all cells rarely access *all* of the information that is available for each cell, but typically access the same pieces of data for each cell visited one after the other.

Furthermore, iterators and accessors avoid having to expose the internal data structures used in DEAL.II classes – a benefit in maintaining and optimizing software over the course of many years. As a consequence, DEAL.II also uses iterator- and accessor-based designs for many other classes, including sparsity patterns, matrices, index sets, and others. This design paradigm enables both the now idiomatic use of C++11-style range-based for loops, but also the notion of applying a kernel (often a lambda function) to all elements of a collection.

DEAL.II supports accessing the subobjects of a cell, such as its faces or (in 3d) its lines, by returning iterators with different template parameters:

```

template <int dim, int spacedim>
class CellAccessor : public TriaAccessor<dim, dim, spacedim> {
  public:
  TrialIterator<TriaAccessor<dim-1, dim, spacedim>>
  face(const unsigned int i) const;
};

```

The dimensionality of the current structure (`structdim`, here equal to `dim-1`), the topological dimension of the mesh (`dim`), and the dimension of the space in which the mesh is embedded (`spacedim`) are all described by compile-time constants. One can write `cell->face(0)` to obtain an iterator for accessing the first face of the given cell (so the structure dimension, the first template argument, is decremented by one). This technique provides a dimension-independent way of accessing the faces of an element without the need to construct a proxy element or, in fact, storing any information in a face-based data structure.

## 2.6. Large-scale parallelism

With the demise of the exponential increase of computing speed of individual processor cores in the early 2000s, it has become clear that the numerical solution of complex, three-dimensional PDEs will only ever be possible by using parallel computing. Hence, DEAL.II supports serial computations for prototyping as well as parallelization on both workstations and clusters, and provides an upgrade path between the two.

Many operations inside DEAL.II are parallelized using task-based programming (currently via the Threading Building Blocks library [28]), with higher level abstractions building on these concepts [21]. This approach already makes efficient use of shared-memory systems for many common operations. Beyond this, DEAL.II also provides distributed memory parallelization of essentially all operations, using MPI [3] and libraries built on top of MPI [12,29–34]. This has allowed for the creation of programs that make efficient use of machines with hundreds of thousands of processor cores, see Section 6.

## 2.7. Interoperability of all features

As outlined above, we see **DEAL.II** as a library with flexible and re-usable building blocks. From a practical perspective, these ought to all work together: If a user wants to switch from a sequential to a parallel mesh, they expect that the finite element class used before will continue to be usable.

In practice, providing this kind of interoperability leads to a combinatorial matrix of features that need to be implemented, tested, and documented if, for example, different triangulation classes had different requirements of finite element classes. Other examples include supporting both CPU and GPU computations on both  $h$ - and  $hp$ -refined meshes, and providing every finite element class with the necessary interfaces for  $hp$ -adaptivity. Despite these difficulties, one of our design goals is to allow all combinations of features. We place great emphasis on early design, code review, and finding the right abstractions in the development of new features, as these steps make interoperability substantially easier in the long run.

At the same time, **DEAL.II** does have combinations of features that do not (currently) work together. In most of these cases, poor planning can be attributed to it in retrospect. We will comment on this in Section 4.

## 2.8. Design for extensibility

The object-oriented design of **DEAL.II** enables large features to be added to the library without making invasive changes to existing classes or functions. This permits users to replace fundamental parts of the library with their own implementations.

All finite element classes are ultimately derived from an abstract base class that specifies the public interface required by the rest of the library. This is more general than some other libraries such as **libMesh**, where **libMesh**::**FEFamily** is an enumeration provided by the library and cannot be changed by the user. Indeed, users have contributed new and sophisticated elements, such as a new Nédélec element that supports arbitrary approximation orders [35]. Implementations of mappings and geometry descriptions are done in a similar manner: users can implement these by inheriting from the **Mapping** or **Manifold** classes, respectively.

In other cases, extensibility is provided by template-based generic programming. In addition to its own linear algebra data structures and solvers, **DEAL.II** has wrappers for the linear algebra components of PETSc [32], TRILINOS's Epetra and Tpetra subpackages [29], cuSPARSE [36], and Ginkgo [37]. All of these classes are assumed to conform to a standard interface that permits the use of, e.g., any vector type in the library with any function that takes a vector argument. For example, functions that take a finite element coefficient vector, such as **VectorTools**::**integrate\_difference()**, leave the vector type as a template argument and expect each vector class to implement a member function **extract\_subvector\_to()**.

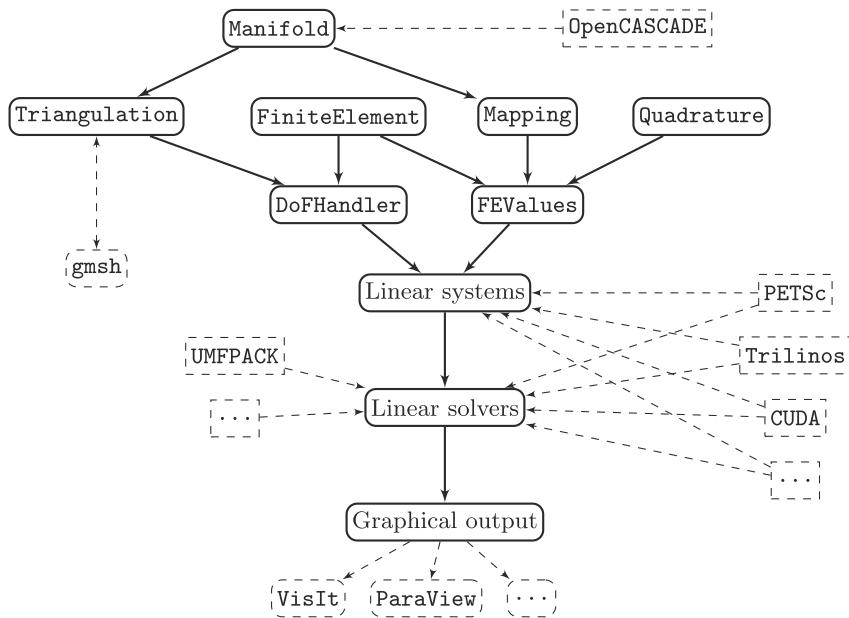
Finally, classes often have nontrivial data dependencies or interdependencies. For example, **GridTools**::**Cache** stores computationally intensive information about a triangulation. A **GridTools**::**Cache** object will register itself with its associated **Triangulation** via a signal/slot mechanism: That is, if the triangulation is changed, it will inform the cache object, which will then invalidate relevant information. This pattern is commonly used in **DEAL.II** and permits users to express new data dependencies without changing the implementation of classes in the library.

## 2.9. A tool for a large community

**DEAL.II** started in 1997 as a tool for one, and shortly after that for three user-developers, but now serves as the basis for the work of hundreds, maybe thousands of scientists, producing more than 200 publications per year [38], in almost any area of science and engineering one can think of (see also Section 6). It also has far more developers: 30–50 people have contributed in each of the most recent releases, and generate 5–10 pull requests per day. To ensure quality, we require every change to pass various continuous integration steps and to undergo rigorous peer review by at least one of the principal developers.

The sizes of these communities imply very different requirements than those that were applied in the early years. For example, we place great emphasis on compatibility between releases. Likewise, we have built a test suite with more than 12,000 tests that is run many times a day. Development versions are almost universally as stable as releases, and the number of bugs reported on mailing lists and forums is quite small for a project of this size.

A large user community has many other, often more important, consequences for a project. In particular, we have long lost the ability to answer everyone's questions if even a small subset of our user community does not understand certain concepts or features: If every user had only five questions per year, we would have a dozen or more questions each day, consuming resources no volunteer open source project can provide. Rather, we have placed great emphasis on documentation that guides users through the process of learning such a tool. This includes the obvious function and class documentation processed by doxygen [39]. But, it is also important to explain higher level concepts, and so **DEAL.II** also uses doxygen "modules" discussing related groups of classes, as well as a "tutorial" of currently more than 60 programs [40] that show how the different parts of the library can be combined in typical finite element codes. The tutorial is also a *teaching tool* that illustrates many numerical techniques: Each tutorial program consists of an extensive introduction that discusses the theoretical background and motivation for the methods used, along with a thoroughly documented



**Fig. 1.** Core components of DEAL.II and interplay with some external libraries.

implementation. In the same spirit, we have also recorded more than 40 h of video lectures<sup>4</sup> (see also Section 5) that provide a complementary perspective as well as interactive demonstrations.

Finally, the “code gallery” [41] provides a repository of codes contributed by the user community. They are typically not as well documented as tutorial programs, but nevertheless can serve as starting points for others’ research. A curated list of publications based on DEAL.II [38] serves a similar purpose: To showcase what kinds of applications can be solved using the library.

### 2.10. A way to build a community itself

Indeed, our approaches to managing a user community can also be seen as an attempt at *building* a community of learners, users, and developers. Computational Science and Engineering (CS & E) is not an established discipline with a broad base of degree programs, books, tools, and methods that newcomers to the field can rely on – rather, it is a dynamic and new field [42] in which many are recent entries and most are self-taught. Providing concrete, well-documented use cases for others to learn from, as well as nuclei for learning communities (for example through forums where people can ask questions of their own and find answers to others’) are important tools to broaden the knowledge base of CS & E practitioners.

## 3. Features

Having discussed what we want to achieve with DEAL.II, let us now turn to a discussion of the features the library offers. Fig. 1 provides an overview of the biggest building blocks of DEAL.II and their interplay. Each box references a concept that is, in most cases, implemented in several different ways – either as classes derived from a common base class (e.g., in the case of the finite elements, mappings, and quadrature classes), as independent classes using a generic interface (as is the case for the DoFHandler and linear algebra concepts), or a combination thereof. The figure also references a few of the external libraries DEAL.II can interface with.

Rather than discussing each of the components of this graph in detail (this is done in the technical documentation of DEAL.II), we focus instead on several overarching themes and considerations.

### 3.1. Sequential, shared, and distributed triangulations

A key concept in all finite element codes is the mesh, i.e., a collection of cells that cover the domain in question. For historical reasons, meshes are often called “triangulations”, even if – as is the case in DEAL.II – they consist of line segments (in 1d), quadrilaterals (in 2d), or hexahedra (in 3d).

<sup>4</sup> <https://www.math.colostate.edu/~bangerth/videos.html>.

DEAL.II's restriction to quadrilaterals and hexahedra was originally motivated by the observation that, for equal numbers of degrees of freedom, finite element solutions with tensor product elements tend to be more accurate than those using the same approximation order spaces on triangles or tetrahedra (the additional accuracy comes from the extra cross terms, e.g., the  $xy$  basis function in a 2d  $Q_1$  element).

This limitation simplifies a large number of algorithms: For example, many common elements and quadrature formulas can be implemented in a dimension-independent way with arbitrary approximation order by exploiting a tensor-product structure. Similarly, (isotropic)  $h$ -adaptive mesh refinement is executed in essentially the same way in 2d and 3d by splitting parent cells into  $2^{\text{dim}}$  child cells. This kind of adaptive mesh refinement in turn provides a convenient setting for implementing geometric multigrid algorithms: the construction of prolongation and restriction operators (as well as level construction) is greatly simplified in the case of hierarchical mesh refinement. Finally, a large number of topological quantities become compile-time constants: The number of faces, edges, and vertices of cells are all fixed and known if all cells with spatial dimension  $\text{dim}$  are the same shape. At the same time, it is true that it is often difficult to generate good quadrilateral or hexahedral meshes (other than the trivial subdivision of a triangle or tetrahedron into 3 or 4 quadrilaterals or hexahedra, using a tool such as `tethex`). This clearly limits the applicability of DEAL.II in some applications, though our experience is that this really only significantly affects the use of complex, 3d geometries. In many other, practical situations, relatively coarse meshes can either be generated by hand or by mesh generators and then refined automatically to fit the geometry of the object using the techniques described in Section 3.2.

DEAL.II currently has three triangulation classes: sequential, (parallel) shared, and (parallel) distributed. The latter two partition the mesh among MPI processes, making the parallel solution of partial differential equations possible. The difference between the shared and the distributed triangulation is what each process stores: In the shared case, each process stores the entire triangulation – wasteful in terms of memory and only scalable to around 100 processes, but useful when dealing with problems that require knowledge of the entire mesh on each process (as in boundary element methods). In contrast, the distributed triangulation stores the coarse mesh everywhere, which is then refined hierarchically, and each process only stores the subset of locally owned cells of this refined mesh, along with ghost cells surrounding the locally owned cells.

The parallel distributed mesh implementation in DEAL.II is algorithmically much more involved than the parallel shared mesh [12]. On the other hand, it provides a distributed data structure that has been shown to scale to very large numbers of MPI processes and unknowns: We have demonstrated computations on up to 304,128 processes and up to  $2 \times 10^{12}$  [43] unknowns, far beyond what is necessary to solve most problems in practice today.

For all three of the triangulations mentioned above, the dimensionality of the mesh may differ from the dimensionality of the space in which it lives. This allows for the solution of equations on surfaces embedded in higher-dimensional spaces. Examples where this is useful are the use of boundary element methods, but also modeling surface processes on solids and fluids (possibly coupled to models of the enclosed bulk medium) such as surface tension, erosion, or diffusion on membranes.

### 3.2. Geometry abstractions

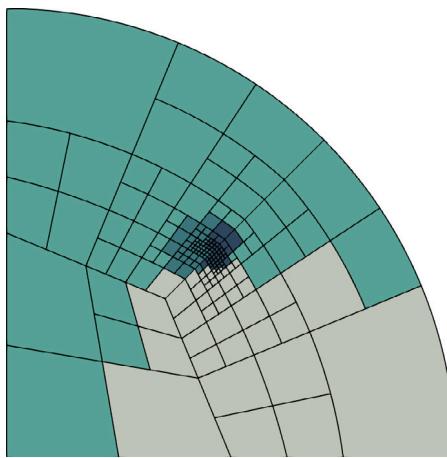
A key feature of DEAL.II is support for adaptive mesh refinement and coarsening. Refining cells in highly distorted or curved domains is a challenging problem that requires both a description of the underlying geometry and algorithms for using this information to create child cells that are no more distorted than their parent cell. It is also often necessary to propagate information from a curved boundary into the interior of a triangulation to achieve a well-conditioned discretization. These problems are especially important when computing solutions on surfaces embedded in higher dimensional surfaces since, in this context, all cells will usually be curved. Accurate geometry descriptions are also critical for higher-order discretizations because they enable one to use a boundary description whose order of accuracy matches that of the finite element space (e.g., isoparametric and isogeometric finite elements).

The implementation of this functionality in DEAL.II is based on the language of differential geometry and resides in classes inheriting from `Manifold`. These manifold descriptions are used in (i) placing new vertices upon mesh refinement, (ii) computing normal and tangential vectors to the boundary, and (iii) defining the mapping from the reference cell to a concrete cell of the mesh; they also appear in a number of other operations. Isoparametric finite elements use `Manifold` objects to compute the coordinates of support points that lie along curved faces as well as support points on the interior of the cell (through the `MappingQ` and `MappingFEField` classes). Similarly, the abstraction provided by manifolds enables the use of isogeometric mappings (through the `MappingManifold` class), where the exact geometry is used directly to define the mapping from the reference cell to a concrete cell of the mesh.

When a volumetric description of the geometry is not available, CAD models can be used to represent the geometry of the boundaries, and transfinite interpolation [44] may be used to extend surface geometry descriptions into the interior of the domain. A complete discussion of these issues is provided in [23]; an example is shown in Fig. 2.

### 3.3. $h$ and $hp$ adaptivity

DEAL.II was originally designed as a library supporting adaptive mesh refinement, i.e.,  $h$ -adaptivity, using hanging nodes as a means to deal with differing cells sizes. It was later extended to also support  $hp$ -adaptivity whereby one can also



**Fig. 2.** A mesh adaptively refined from 3 coarse cells with hanging nodes and curved faces. The geometry description represents the boundary as an exact circle. This geometry is extended into the interior using transfinite interpolation. Cells are colored based on a partitioning onto four processes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

individually select the finite element, and therefore the polynomial degree, on each cell [13]. While technically difficult to implement – in particular for continuous elements, in 3d, and in parallel – supporting *hp*-adaptivity has also enabled a host of other, unexpected applications if one allows for different cells to use entirely different kinds of finite elements. In particular, the introduction of the `FE_Nothing` element that represents a space with no degrees of freedom (i.e., only consisting of the zero function), has allowed representing multiphysics applications in which some equations are only posed on parts of the domain.

### 3.4. Finite elements, mappings, and evaluating them

Over the past few decades, an entire zoo of finite element spaces has been described in the literature. The publication by Arnold and Logg in [45] and references therein summarizes the most commonly used ones, but there are many others (a subset illustrating the breadth of elements can be found in [46–50]). `DEAL.II` implements a substantial fraction of these, starting with the common continuous and discontinuous Lagrange elements, but also the Nédélec, Raviart–Thomas, Arnold–Boffi–Falk, Brezzi–Douglas–Marini, Bernardi–Raugel, Bernstein, P1-nonconforming, Rannacher–Turek, and other spaces. There are also implementations of more specialized cases: Finite element spaces enriched by bubble functions or using additional weights (as necessary for the XFEM approach); monomial bases; unmapped non-parametric bases; and finite element spaces defined only on the faces of cells. Almost all of these are available with arbitrary polynomial degree.

Most of these spaces are defined on the reference cell  $[0, 1]^d$  and need to be mapped to each cell of the triangulation. This is done using one of several implementations of the `Mapping` base class: The usual polynomial mappings based on Lagrange interpolation points; a specialized mapping that can be used in case all cells are rectangles/boxes with axes parallel to a Cartesian coordinate system; and mappings that are “exact” in the sense that they respect the underlying manifold description of the domain’s geometry.

An important realization, explored in more detail in [4, Section 3.3], is that while finite element spaces and mappings describe *functions*, in practice they only need to be *evaluated at individual points* because the integrals used in the finite element method are approximated by quadrature. The `FEValues` class provides an interface that allows querying shape functions, transformed to the current cell, at a set of evaluation points. Furthermore, because the quadrature points (in reference coordinates) are typically the same for a loop over all cells, `FEValues` pre-computes and caches as much information as possible, substantially accelerating the computation on a sequence of cells in a transparent manner. Similar classes exist for evaluating shape functions and derivatives on faces.

For problems with multiple solution components – say, a flow problem whose solution consists of  $d$  vector components for a velocity plus one for the pressure – it is often convenient to either consider the combined finite element space of all components (e.g., to correctly size the linear system); or to only consider its restriction to a scalar component, the  $d$  components of a vector, or the  $d^2$  (or  $d(d+1)/2$ ) components of a (symmetric) tensor (e.g., when assembling the bilinear form). In `DEAL.II`, the latter is facilitated by “extractor” objects that, when applied to an `FEValues` object, yield a “view” of the selected finite element space.

### 3.5. Geometric multigrid

The ability to solve large linear systems stemming from finite element discretizations requires solvers that are both optimal in complexity (i.e.,  $O(N)$  where  $N$  is the number of unknowns) and scale well in parallel. Only multigrid methods, either algebraic or geometric, are known to fulfill this requirement for elliptic problems.

DEAL.II has long supported and successfully used algebraic multigrid (AMG) methods as a preconditioner through Trilinos' ML/MueLu packages and PETSc's hypre interfaces; for examples, see [12,51]. However, AMG setup costs become prohibitive for very large problems and core counts [52]. Consequently, DEAL.II also supports geometric multigrid methods; originally written for sequential computations on adaptive meshes in 1999, it now also supports parallelization via multithreading and MPI [11].

While algebraic multigrid methods can often be treated as black-box preconditioners, the implementation of the geometric multigrid algorithm consists of a flexible framework with various options and customization points: First, it integrates seamlessly with existing linear algebra classes (PETSc, TRILINOS) or matrix-free smoothers and transfer operators (see Section 3.6). Second, there is a large collection of smoothers that can be used, from matrix-based operations (e.g., Jacobi or SSOR, including various parallel variants), to Schwarz smoothers that allow local smoothers on cells or patches of cells. Similarly, coarse solvers can be provided through various means, including switching to algebraic multigrid.

This framework has been shown to scale to extremely large problems, see Section 6. Customization points and block composition of solvers allows using the multigrid framework for a wide variety of PDEs.

### 3.6. Matrix-free operators

It is well-understood that matrix-based linear solvers can no longer adequately use the computational power of modern CPUs or GPUs because of the disparity between the high cost of transferring data from memory and the speed of floating point operations. Consequently, for computational efficiency, linear solvers need to find a better balance between precomputing and storing data, versus computing more information on the fly.

To this end, DEAL.II contains functionality for matrix-free computations that merges the assembly and solver steps. In this paradigm, a global sparse matrix is never built and linear systems are only solved by the action of the underlying linear operator on a vector via the integrals in the weak form, such as  $(\nabla v, \nabla u)_\Omega$  from Eq. (1). Since the information needed to compute the integrals in terms of the geometry and possibly some coefficients is much smaller in memory than a sparse matrix that encodes the coupling of every unknown to the others, a matrix-free approach has the potential to avoid the limitations of slow memory access. It also often allows one to fit bigger problems into memory. Matrix-free setups offer more optimization possibilities than sparse matrices because one can choose what should be pre-computed and stored; the fundamental question being whether any increase in arithmetic operations costs less than what one can win from the reduced memory transfer. On today's hardware, it turns out to be particular useful if one can exploit the tensor-product form of shape functions [15,16]. In DEAL.II, we provide matrix-free capabilities on a subset of element types; currently, these are in particular the tensor-product continuous and discontinuous elements.

To map these arithmetically intensive operations efficiently onto modern hardware, DEAL.II supports single-instruction/multiple data (SIMD) instructions, such as SSE, AVX, and AVX-512 on x86 hardware or AltiVec on IBM's Power. Given that the compilers' auto-vectorization is typically only applicable to operations in the innermost loops, which are often operations over the components of a tensor in  $d$  spatial dimension, loop reorganization towards array-of-struct-of-array data layouts promise much better performance [16]. In DEAL.II we provide such layouts by a single class called `VectorizedArray` that internally applies intrinsics for the various instruction set extensions. To the user code, the usual operator overloading infrastructure makes it behave similarly to the built-in types `double` or `float`, while abstracting away the detail of the innermost array dimension. All use cases can transparently invoke the most beneficial SIMD array width for the hardware, without compromising code portability among CPU architectures.

### 3.7. Support for graphics processing units

Similarly, DEAL.II also supports operations on Graphics Processing Units (GPUs), due to their superior floating point capabilities and memory bandwidth for a given power consumption. Multiple programming models are available for running code on a GPU, e.g., CUDA [53], Kokkos [54], RAJA [55,56], OCCA [57], and OpenMP [58]. DEAL.II builds on CUDA, due to the maturity of the language; while this limits the use of these features to Nvidia GPUs, the extension to AMD GPUs using `hipify` [59] is underway. GPU capabilities in DEAL.II consist of matrix-based classes wrapping functionality of the cuSPARSE and cuSOLVER libraries [36,60], and matrix-free support.

For matrix-based computations, the linear system needs to be assembled on the host first. The data is then moved to the device, converted to a format usable with cuSPARSE, and finally handed to the preconditioners and direct solvers from cuSOLVER. DEAL.II's own iterative solvers can also be used, with all linear algebra operations performed on the GPU.

In contrast, DEAL.II's CUDA matrix-free framework evaluates the finite element integrals directly on the device. This implies that users will need to write part of their code in CUDA. Given most users' lack of CUDA experience, we have minimized the amount of necessary CUDA code by only requiring a user interface with a single functor that can be implemented using code close to what the user would write when doing matrix-free implementations on the host. While we have striven to have the interface for GPU matrix-free framework to be as close as possible to the CPU matrix-free framework, they are not identical. Aside from the obvious difference of having the user writing a functor annotated with `__device__`, the more fundamental difference is due to the way the parallelization is done. On the CPU, each thread works on a separate chunk of cells while on the GPU, each thread works on a different degree-of-freedom. This is due to the

fact that the GPU has much more parallelism available but not as much memory per thread. Details of the implementation are discussed in [61].

The matrix-free framework can also take advantage of multiple GPUs through the use of MPI via DEAL.II's own data structures and solvers. Data can be transferred between different GPUs on different systems either via the host's memory or, if an implementation supports it, without this detour.

### 3.8. Assisted differentiation and linearization

Many realistic applications use formulations derived from complicated energy functionals or residuals. Examples are large deformation formulations of materials with nonlinear constitutive laws, fluid-structure interaction problems, or chemically reacting flows. In such cases, deriving and consistently implementing the bilinear forms and right hand sides that characterize each nonlinear step is often fraught with opportunities for error. Additionally, validating an implementation with no analytical solution or verifying that the convergence rate of a nonlinear solution scheme is optimal also becomes extremely challenging.

In many such cases, workflows can be substantially simplified by integrating tools for automatic differentiation (AD). To this end, DEAL.II leverages ADOL-C [62,63] and Sacado [64–66] to automatically compute first and second derivatives. On the finite element level, this approach allows computing the Newton matrix from a residual ("linearization"), or both the residual and its linearization can be determined from an energy functional. The same can analogously be done on the quadrature point level. This framework abstracts away the specialized function calls and operations that each of the supported automatic differentiation (AD) libraries (and the underlying number types) requires and offers a clear and unified interface to the users.

Complementing the AD framework is an interface to the high performance Computer Algebra System (CAS) and symbolic toolbox SymEngine [67] that performs symbolic calculations on scalar types using common C++ syntax through operator overloading. Valid operations not only include standard mathematical operations and symbolic differentiation, but also comparison, logical, and conditional operations. Having integrated the scalar SymEngine wrapper class, called `Expression`, into the pre-existing `Tensor` and `SymmetricTensor` classes, we have also equipped the framework to perform tensorial computations and, subsequently, symbolic tensor differentiation as tensors are commonly used in the definition of residuals and energy functionals. Its flexibility makes the symbolic framework well suited to perform specialized tasks that have a complex code path and require either partial or total derivatives to be computed.

The framework above lays the foundation to include other exciting features in the future. In particular, opportunities include offloading symbolic computations to a just-in-time compiler for more rapid execution of computed operations, and symbolic finite element level assembly and linearization in a similar spirit to that previously described for the AD framework.

## 4. Lessons learned from the development of complex software

Having discussed design goals and available functionality in the previous two sections, it may be interesting to also put all of this development into perspective: What have we learned about the development of a complex scientific software library intended for a large user community?

In [68], we have previously given some answers on what we think makes scientific software libraries successful. Let us here summarize some of the points made there and explain how they relate to DEAL.II specifically, but also – and in particular – discuss a few of the things we know are difficult or for which we do not know how to do them well.

### 4.1. A success: Testing

As mentioned in Section 2.9, having an extensive testsuite is essential to providing stable functionality. This is in particular true in view of the continuous growth in the number of possibilities to configure the library, using different compilers, different dependencies, and hardware platforms. To this end, DEAL.II's test suite with more than 12,000 tests is run continuously with a wide cross-section of all configuration combinations. Compiling and running a substantial fraction of the test suite is part of the continuous integration hook for each patch, and success is required before a patch can be merged.

### 4.2. A challenge: Dependency hell and installation support

A consequence of the design decision to not implement functionality for which specialized external libraries exist (see Section 2.3), is that DEAL.II relies on *many* other packages. Almost all of these (and their corresponding wrappers) are optional, but most advanced DEAL.II-based projects likely still depend on some. Thus, users are required to install these external projects by hand, rely on pre-installed versions made available by their system administrators, or use tools that facilitate building scientific software such as Spack [69].

Configuration management is notoriously complicated. Many scientific packages, to this day, use installation procedures based on Makefile snippets or autoconf, neither of which export the details of their installation for downstream

packages. Many also have broken installations in which, for example, shared libraries do not record which other shared libraries they depend upon, leaving it to downstream projects to figure out what to link with. Furthermore, every system seems to be different: Not just between Linux, macOS, and Windows, but even within each of these operating systems, there are substantial differences in what is available, where, and how. Finally, the projects DEAL.II can interface with make incompatible changes between versions, either requiring supporting multiple versions at once, or requiring users to use a specific version.

All other scientific software projects we know of struggle with this “dependency hell” and “version hell”; no particular good and widely usable solutions appear to exist. We try to address these issues by providing installation scripts that automatically download optional dependencies, such as candi [70], and by working through package managers (of package repositories such as Debian or Ubuntu, or source based installers such as Spack [69] and the xSDK [71] environment that builds on it).

#### 4.3. A success: Backward compatibility issues

Just like other packages, DEAL.II carries legacy functionality for which we have found better solutions over time. This is particularly relevant because libraries such as DEAL.II expose such large interfaces to users: hundreds of classes and thousands of functions are accessible to users. Replacing or changing any of them would break downstream codes, and prevent upgrade paths for our users from one version to the next.

We have always tried to minimize incompatible changes that would impact users. Where this cannot be avoided, we deprecate functionality in one version and remove it in the next. Using compiler features, the use of deprecated functionality is possible, but triggers a compiler warning alerting users to the need to eventually update their code. This appears to be working: We very rarely hear complaints about lack of backward compatibility.

#### 4.4. A challenge: Support for changing architectures

Computer architectures are changing and, with the advent of GPUs and Xeon Phis, also more diverse. Some architectures have multiple levels of heterogeneity: Nvidia’s Volta GPU architecture is itself accelerated by “tensor” cores. Any open source project will struggle with natively supporting all of them. DEAL.II does support a limited number of architectures (x86, POWER, and Nvidia GPUs) natively. For other architectures, DEAL.II will need to rely on third-party libraries such as the Tpetra package of TRILINOS [29] that uses Kokkos [54] for performance portability.

#### 4.5. A challenge: Supporting “different” discretizations

Not all discretizations considered widely useful are as simple as standard isoparametric Lagrange finite elements mapped to each element via a polynomial mapping. Isogeometric analysis (IGA), finite elements based on Catmull–Clark’s subdivision surfaces, the extended finite element method (XFEM), and certain types of enriched finite elements all do not fit into this scheme. In those cases, the degrees of freedom cannot be thought of as being associated with a specific mesh object, but rather a collection of such objects (for example, a patch of cells). For these, shape functions may not be defined based on some “reference cell”, they may extend beyond just one cell and its immediate neighbors, and the number of shape functions supported on a given cell may depend on the topology of the mesh around that element (as is the case for Catmull–Clark’s finite elements).

Some of these schemes are difficult to press into the current design of the `FiniteElement` class, and of the `FEValues` class that provides point values and derivatives (see Section 3.4). Similarly, enumeration of degrees of freedom (DoFs) poses challenges. To address these issues, the description of the finite element space, represented by the `FiniteElement` class, will have to learn to provide information on how many of those “non-local” DoFs there are on a given mesh. This information will then need to be used by the `DoFHandler` class responsible for globally enumerating DoFs. Additional complications arise in the MPI-parallel context where ownership of a non-local DoF can no longer be determined based on which cells each process owns because these degrees of freedom are no longer associated with a particular cell. One might also need to have a ghost layer thicker than a single cell.

No library can support everything, but there is an ongoing effort to add basic support for such “non-local” DoFs to the DEAL.II library.

#### 4.6. A challenge and a success: Interoperability of “single-use” features

Some of DEAL.II’s features have turned out to not to be interoperable with other parts of the library. They were typically written for a single use case, and often only implemented or understood by a single person. Their focus on specific topics hinders adoption by a larger number of users; those who do use them find themselves frustrated by lack of support for these features in other parts of the library. These features are also often poorly documented, and are overrepresented among questions on the online forums.

In hindsight, these features were contributed with good intentions, but became a maintenance problem especially if the contributor later walked away from the project. We have learned from this: The modules in question predate the time when every patch had to pass peer review, and large patches are now often extensively discussed for design choices and interoperability before they are accepted. Our standards for documentation are also far higher today than they were before every patch was reviewed.

#### 4.7. A success and a challenge: Organizing large volunteer projects

A scientific project with hundreds or thousands of users, and dozens of contributors to each release, can be considered a success. We also know of some 1500 publications from essentially all areas in the sciences and engineering that use DEAL.II [38]; only a small fraction of these was authored by the principal developers of the project.

Getting to these numbers required a lot of deliberate work and thinking about how best to use our human resources: A substantial fraction of our effort is spent on supporting users via online forums,<sup>5</sup> but importantly also on providing extensive documentation and other supports to avoid having to answer everyone's questions on the public forums. It also includes taking the perspective of users into consideration during the development process. Finally, we consciously focus on growing users into developers, by encouraging them to contribute and providing them with mentoring on their patches.

At the same time, there are also challenges when dealing with actual humans. These include dealing with "difficult" community members, not burning any one person in the project out by overloading them with answering forum questions, giving newer project members space to find a niche, and not expecting new contributors to write perfect patches with extensive documentation or tests before a pull request can be merged. An important distinction from other projects appears to be that among the DEAL.II principal developers, none seem to be particularly territorial about their code and all are quite happy to let others reshape the code they wrote. This enables newcomers to contribute without having to fear that they step on old-timers' feet, and has allowed us to avoid the tendency of projects to balkanize into individual developers' territories that only they are allowed to touch.

### 5. Education

As already mentioned in Sections 2.9 and 2.10, libraries such as DEAL.II do not exist in a vacuum. Rather, they are surrounded by user communities requiring education: Help and documentation resources at varying levels, and basic training in the underlying numerical methods and software development. But, a project such as DEAL.II also enables educational opportunities: It is a tool to reach communities who may be interested in computational science. Finally, it is also a tool to research *how best to teach CS&E*.

Indeed, many of us have leveraged DEAL.II for educational purposes: We know that it is used in teaching finite element courses at many universities around the world, and several of us have taught short courses based on it on many continents. Even more broadly used is a collection of currently 67 video lectures that one of us has recorded at KAMU, a professional television studio. These videos – hosted on YouTube<sup>6</sup> as well as the Chinese bilibili video hosting platform<sup>7</sup> – have collectively received more than 140,000 views, indicating robust user-community interest in learning about the computational science concepts discussed, as well as in the interactive demonstrations showing how to build, use, and develop software based on DEAL.II.

The original purpose of the video lectures was to facilitate flipped classroom teaching in which students learn the material before class, allowing the instructor more time for interaction with students. We have found that this approach works well, both anecdotally from the perspective of those who have used this approach in their own teaching, but also backed up by rigorous educational research [72,73].

### 6. Applications

DEAL.II is used by hundreds or thousands of researchers in essentially every field of the sciences and engineering, as shown by the large number of publications that build on it [38] – too many to even try and summarize. Most of these publications use codes written for a specific purpose but not publicly available. However, the project website at <https://www.dealii.org> also links to a number of large projects built on DEAL.II in the geosciences, radiation transport, the material sciences, fuel cell modeling, wave propagation, and multiphysics modeling, that have themselves grown substantial user communities – in some cases with hundreds of users of their own. Finally, we are aware of on the order of 10–20 industry projects that build on DEAL.II, and believe that this is likely a substantial underestimate. Several of the principal developers have industry projects themselves, ranging from the simulation of ship hulls, wave propagation in the aerospace field, resonances of industrial membranes, to 3d printing.

Many of the papers referenced in the list of papers that use DEAL.II [38] provide excellent examples of the breadth and depth of applicability of DEAL.II. Furthermore, the publications mentioned at the end of the Introduction also discuss in great detail individual features. Rather than duplicate this information, let us here only summarize one example of large-scale computations in the following sub-section.

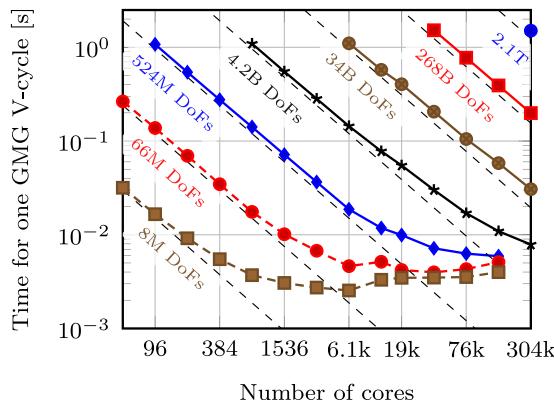
#### 6.1. Large-scale computations

The computations shown in this section are based on [43,74]. Fig. 3 shows a scaling experiment of a geometric multigrid V-cycle on the SuperMUC-NG machine in Garching, Germany, with up to 304,128 Intel Xeon Platinum 8174 cores. The

<sup>5</sup> An overview of resources for help is available at <https://www.dealii.org/participate.html>, including links to the help forum, issue tracker, and the project's GitHub repository.

<sup>6</sup> <https://www.youtube.com/playlist?list=PLdy04DoEepEwRGMbwmPTmNBD5jFvhIZM>.

<sup>7</sup> <https://www.bilibili.com/video/av57103047/>.



**Fig. 3.** Parallel scaling of a GMG V-cycle on up to 304,128 cores and up to  $2 \times 10^{12}$  unknowns. Dashed lines show ideal scaling.

equation being solved here is the three-dimensional Laplace equation; however, solving this or related equations also serves as the basis for block preconditioners for more complicated equations such as the Stokes and Navier–Stokes equations, as well as for elastic and plastic models, and the performance shown here is therefore indicative also of solvers for more complex problems. The example shown uses a symmetric interior penalty discontinuous Galerkin discretization with polynomial degree  $p = 4$  on a hyper-rectangle. The multigrid hierarchy involves a switch from the discontinuous space to the associated continuous finite element space with  $p = 4$  on the same mesh [75] and then progresses to coarser mesh levels until a coarse solver is invoked on a  $2 \times 1 \times 1$  mesh. Chebyshev smoothing of degree 6 for pre- and post-smoothing is used on all levels. For operator evaluation, the matrix-free infrastructure (Section 3.6) with AVX-512 vectorization is used. The multigrid V-cycle is run in single precision to increase throughput, which is the typical usage setting when combined with some double-precision correction [76].

This setup achieves a multigrid convergence rate of about 0.03, i.e., the residual is reduced by 3 orders of magnitude with just two V-cycle applications. The largest problem with  $2.15 \times 10^{12}$  unknowns runs with (single-precision) arithmetic throughput of 5.9 PFlop/s and a memory throughput of 1.2 PB/s (187 GB/s per node), and is primarily limited by the memory bandwidth. The combination of these features then leads to a solver for the Laplace equation that can solve a problem with trillions of unknowns in just a few seconds — opening the door for solving much more complex problems that use the Laplace equation as one block in the preconditioner.

## 7. Vision and future directions

Like many volunteer projects, DEAL.II does not have a formal roadmap that drives development. Rather, most new features stem from individuals' need that arise in their research. That said, we have the following aspirational goals:

- To provide state-of-the-art tools for a broad variety of PDEs.
- To have excellent documentation to enable anyone to use the library.
- To enable fast and scalable algorithms from laptops to the largest supercomputers, including new architectures.
- To create an open, inclusive, participatory community providing users and developers with the resources they need.

In support of these goals, there are a number of technical areas in which concrete work is currently ongoing and that we will discuss briefly in the following.

*Efficient computations on the largest machines.* As the results of the previous section show, DEAL.II-based codes have been used on the full scale of some of the biggest machines available today, with more than  $10^{12}$  degrees of freedom. Another example, among several others, is the code discussed in detail in [77]; in both of these cases, computations are run on more than 100,000 cores. Yet, experience shows that every time one goes to larger numbers of cores or more degrees of freedom, one encounters new bottlenecks. We continue to address these by carefully timing parts of our code base, but also by addressing algorithms that we know cannot scale indefinitely. An example is the implementation and optimization of matrix-free methods, and their current incorporation into multigrid methods that scale to very large problems [11].

*GPU support.* Similarly, we know that for the foreseeable future, the largest compute clusters will draw the majority of their compute power from GPUs and similar devices. Yet, supporting this very different programming model is difficult, and needs to be hidden from user code wherever possible. DEAL.II has supports for GPUs, and strives to make it available more broadly.

*Parallel hp adaptivity.* *hp* refinement has been part of **DEAL.II** for the past 15 years, and parallel distributed meshes for more than 10. Yet, the combination of these two features has only been available for the last year or so. We continue to work on making the necessary connections, and in particular devising practical strategies for ensuring that the resulting computations are well load-balanced.

*Tutorials and other pieces of the documentation.* Providing users with adequate documentation is a continual challenge. There are never enough tutorial programs to cover all of the applications our users have in mind, nor do the existing ones cover the changing programming models we use in view of large-scale parallelism, GPUs, or evolving discretization methods. Likewise, despite 20 years of work, function and class documentation never seems to be adequate to answer all user questions. As a consequence, a substantial fraction of commits over the years has always been to improve the documentation, and there are 2–4 new tutorial programs every year. This trend will surely continue indefinitely.

## 8. Conclusions

In this contribution, we have outlined the design criteria and functionality of the **DEAL.II** finite element library. Like many other scientific software projects, **DEAL.II** started as a small project within one lab, with no intention of reaching beyond that point; however, it has now grown into a successful and world-wide project that is used in hundreds or thousands of research projects, with nearly a dozen principal developers who spend a substantial fraction of their time on the continued development of the package. This change from a project for a few user-developers to a community project brings with it not only an explosion in functionality (as discussed in Section 3), but also a reckoning on how such software can be developed: It requires an agreement on the design principles that guide continuing development (see Section 2) but also a focus on the technical and social challenges a project of this size brings with it (Section 4). At the same time, it also opens up opportunities as a widely used teaching tool (Section 5).

As this article, and especially Section 6, made clear, **DEAL.II** is no longer a hobbyists' project, but a professionally managed enterprise whose continued development has, over the years, been supported repeatedly by a multitude of funding agencies and that has not only built more than a million lines of C++, but also a vibrant and active user and developer community.

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## References

- [1] C.L. Lawson, R.J. Hanson, D.R. Kincaid, F.T. Krogh, Basic linear algebra subprograms for fortran usage, *ACM Trans. Math. Software* 5 (3) (1979) 308–323.
- [2] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, D. Sorensen, *LAPACK Users' Guide*, third ed., Society for Industrial and Applied Mathematics, Philadelphia, PA, 1999.

- [3] Message Passing Interface Forum, MPI: A Message-Passing Interface Standard Version 3.1, Technical Report, 2015.
- [4] W. Bangerth, R. Hartmann, G. Kanschat, **DEAL.II** – a general purpose object oriented finite element library, *ACM Trans. Math. Software* 33 (4) (2007) 24/1–24/27.
- [5] W. Bangerth, D. Davydov, T. Heister, L. Heltai, G. Kanschat, M. Kronbichler, M. Maier, B. Turcksin, D. Wells, The **DEAL.II** library, version 8.4, *J. Numer. Math.* 24 (2016) 135–141.
- [6] D. Arndt, W. Bangerth, D. Davydov, T. Heister, L. Heltai, M. Kronbichler, M. Maier, J.-P. Pelteret, B. Turcksin, D. Wells, The **DEAL.II** library, version 8.5, *J. Numer. Math.* 25 (3) (2017) 137–146.
- [7] G. Alzetta, D. Arndt, W. Bangerth, V. Boddu, B. Brands, D. Davydov, R. Gassmoeller, T. Heister, L. Heltai, K. Kormann, M. Kronbichler, M. Maier, J.-P. Pelteret, B. Turcksin, D. Wells, The **DEAL.II** library, version 9.0, *J. Numer. Math.* 26 (4) (2018) 173–183.
- [8] D. Arndt, W. Bangerth, T.C. Clevenger, D. Davydov, M. Fehling, D. Garcia-Sanchez, G. Harper, T. Heister, L. Heltai, M. Kronbichler, R.M. Kynch, M. Maier, J.-P. Pelteret, B. Turcksin, D. Wells, The **DEAL.II** library, version 9.1, *J. Numer. Math.* (2019).
- [9] G. Kanschat, Multi-level methods for discontinuous Galerkin FEM on locally refined meshes, *Comput. Struct.* 82 (28) (2004) 2437–2445.
- [10] B. Janssen, G. Kanschat, Adaptive multilevel methods with local smoothing for  $H^1$ - and  $H^{\text{curl}}$ -conforming high order finite element methods, *SIAM J. Sci. Comput.* 33 (4) (2011) 2095–2114.
- [11] T.C. Clevenger, T. Heister, G. Kanschat, M. Kronbichler, A flexible, parallel, adaptive geometric multigrid method for FEM, 2019, <https://arxiv.org/abs/1904.03317>, in press.
- [12] W. Bangerth, C. Burstedde, T. Heister, M. Kronbichler, Algorithms and data structures for massively parallel generic adaptive finite element codes, *ACM Trans. Math. Software* 38 (2011) 14/1–28.
- [13] W. Bangerth, O. Kayser-Herold, Data structures and requirements for  $hp$  finite element software, *ACM Trans. Math. Software* 36 (1) (2009) 4/1–4/31.
- [14] D. Davydov, T. Gerasimov, J.-P. Pelteret, P. Steinmann, Convergence study of the  $h$ -adaptive PUM and the  $hp$ -adaptive FEM applied to eigenvalue problems in quantum mechanics, *Adv. Model. Simul. Eng. Sci.* 4 (1) (2017) 7.
- [15] M. Kronbichler, K. Kormann, A generic interface for parallel cell-based finite element operator application, *Comput. & Fluids* 63 (2012) 135–147.
- [16] M. Kronbichler, K. Kormann, Fast matrix-free evaluation of discontinuous Galerkin finite element operators, *ACM Trans. Math. Software* 45 (3) (2019) 29:1–29:40.
- [17] A. DeSimone, L. Heltai, C. Manigrasso, Tools for the Solution of PDEs Defined on Curved Manifolds with **Deal.II**, Technical Report 42/2009/M, SISSA, 2009.
- [18] N. Giuliani, A. Mola, L. Heltai,  $\pi$ -BEM: A flexible parallel implementation for adaptive, geometry aware, and high order boundary element methods, *Adv. Eng. Softw.* 121 (March) (2018) 39–58.
- [19] M. Maier, M. Bardelloni, L. Heltai, LinearOperator – a generic, high-level expression syntax for linear algebra, *Comput. Math. Appl.* 72 (1) (2016) 1–24.
- [20] M. Maier, M. Bardelloni, L. Heltai, Linearoperator benchmarks, version 1.0.0, 2016.
- [21] B. Turcksin, M. Kronbichler, W. Bangerth, Workstream – a design pattern for multicore-enabled finite element computations, *ACM Trans. Math. Software* 43 (1) (2016) 2/1–2/29.
- [22] A. Sartori, N. Giuliani, M. Bardelloni, L. Heltai, deal2lkit: A toolkit library for high performance programming in **DEAL.II**, *SoftwareX* 7 (2018) 318–327.
- [23] L. Heltai, W. Bangerth, M. Kronbichler, A. Mola, Using exact geometry information in finite element computations, 2019, <https://arxiv.org/abs/1910.09824>, in press.
- [24] H.P. Langtangen, A.M. Bruaset, A comprehensive set of tools for solving partial differential equations; *diffpack*, in: M. Dæhlen, A. Tveito (Eds.), *Numerical Methods and Software Tools in Industrial Mathematics*, Birkhäuser, Boston, MA, 1997, pp. 63–92.
- [25] B.S. Kirk, J.W. Peterson, R.H. Stogner, G.F. Carey, Libmesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations, *Eng. Comput.* 22 (3) (2006) 237–254.
- [26] W. Bangerth, Using modern features of C++ for adaptive finite element methods: dimension-independent programming in **DEAL.II**, in: M. Deville, R. Owens (Eds.), *Proceedings of the 16th IMACS World Congress 2000*, Lausanne, Switzerland, 2000, Document Sessions/118-1, 2000.
- [27] J.L. Henning, Session details: *SPEC CPU2006 analysis*, *ACM SIGARCH Comput. Archit. News* 35 (1) (2007) 63.
- [28] J. Reinders, *Intel Threading Building Blocks: Outfitting C++ for Multi-Core Processor Parallelism*, O'Reilly, 2007.
- [29] M.A. Heroux, R.A. Bartlett, V.E. Howle, R.J. Hoekstra, J.J. Hu, T.G. Kolda, R.B. Lehoucq, K.R. Long, R.P. Pawlowski, E.T. Phipps, A.G. Salinger, H.K. Thornquist, R.S. Tuminaro, J.M. Willenbring, A. Williams, K.S. Stanley, An overview of the Trilinos project, *ACM Trans. Math. Software* 31 (2005) 397–423.
- [30] M.A. Heroux, et al., Trilinos web page, 2018, <http://trilinos.org>.
- [31] S. Balay, S. Abhyankar, M.F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W.D. Gropp, D. Karpeyev, D. Kaushik, M.G. Knepley, D. May, L.C. McInnes, R. Mills, T. Munson, K. Rupp, P.S.B.F. Smith, S. Zampini, H. Zhang, H. Zhang, PETSc web page, 2018, <http://www.mcs.anl.gov/petsc>.
- [32] S. Balay, S. Abhyankar, M.F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W.D. Gropp, D. Karpeyev, D. Kaushik, M.G. Knepley, D. May, L.C. McInnes, R. Mills, T. Munson, K. Rupp, P.S.B.F. Smith, S. Zampini, H. Zhang, H. Zhang, PETSc Users Manual, Technical Report ANL-95/11 – Revision 3.9, Argonne National Laboratory, 2018.
- [33] C. Burstedde, L.C. Wilcox, O. Ghattas, P4est: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees, *SIAM J. Sci. Comput.* 33 (3) (2011) 1103–1133.
- [34] C. Burstedde, Parallel tree algorithms for AMR and non-standard data access, 2018, arXiv e-prints, [arXiv:1803.08432](https://arxiv.org/abs/1803.08432).
- [35] R. Kynch, P. Ledger, Resolving the sign conflict problem for  $hp$ -hexahedral Nédélec elements with application to eddy current problems, *Comp. Struct.* 181 (2016).
- [36] CuSPARSE, 2019, <https://developer.nvidia.com/cusparse>.
- [37] Ginkgo: high-performance linear algebra library for manycore systems, 2019, <https://github.com/ginkgo-project/ginkgo>.
- [38] Publications based on **deal.II**, 2019, <http://www.dealii.org/publications.html>.
- [39] Doxygen, 2019, <http://doxygen.nl>.
- [40] The **DEAL.II** tutorial, 2020, <https://dealii.org/developer/doxygen/deal.II/Tutorial.html>.
- [41] The **DEAL.II** code gallery, 2020, <https://www.dealii.org/code-gallery.html>.
- [42] U. Rüde, K. Willcox, L.C. McInnes, H.D. Sterck, Research and education in computational science and engineering, *SIAM Rev.* 60 (3) (2018) 707–754.
- [43] D. Arndt, N. Fehn, G. Kanschat, K. Kormann, M. Kronbichler, P. Munch, W.A. Wall, J. Witte, ExaDG – high-order discontinuous Galerkin for the exa-scale, in: H.-J. Bungartz, W.E. Nagel, S. Reiz, B. Uekermann, P. Neumann (Eds.), *Software for Exascale Computing – SPPEXA 2016–2019*, Springer International Publishing, Cham, 2020, in press.
- [44] W.J. Gordon, L.C. Thiel, Transfinite mappings and their application to grid generation, *Appl. Math. Comput.* 10 (1982) 171–233.
- [45] D.N. Arnold, A. Logg, Periodic table of the finite elements, *SIAM News* 47 (9) (2014) 212.
- [46] A. Adini, R.W. Clough, Analysis of Plate Bending By the Finite Element Method, Technical Report G.7337, National Science Foundation, 1961.

[47] J.H. Argyris, I. Fried, D.W. Scharpf, The TUBA family of plate elements for the matrix displacement method, *Aeronaut. J.* 72 (692) (1968) 701–709.

[48] R.W. Clough, J.L. Tocher, Finite element stiffness matrices for analysis of plates in bending, in: Proceedings of the Conference on Matrix Methods in Structural Mechanics, AFFDL-TR-68-150, Wright-Patterson A.F.B., Ohio, 1965, pp. 515–545.

[49] J. Douglas Jr, J.E. Santos, D. Sheen, X. Ye, Nonconforming Galerkin methods based on quadrilateral elements for second order elliptic problems, *RAIRO Math. Model. Numer. Anal.* 33 (1999) 747–770.

[50] D.N. Arnold, R.S. Falk, R. Winther, Finite element exterior calculus, homological techniques, and applications, *Acta Numer.* 15 (2006) 1–155.

[51] M. Kronbichler, T. Heister, W. Bangerth, High accuracy mantle convection simulation through modern numerical methods, *Geophys. J. Int.* 191 (2012) 12–29.

[52] T.C. Cleverger, T. Heister, Comparison between algebraic and matrix-free geometric multigrid for a Stokes problem, 2019, <https://arxiv.org/abs/1904.03317>, in press.

[53] CUDA Zone, 2019, <https://developer.nvidia.com/cuda-zone>.

[54] H.C. Edwards, C.R. Trott, D. Sunderland, Kokkos: Enabling manycore performance portability through polymorphic memory access patterns, *J. Parallel Distrib. Comput.* 74 (12) (2014) 3202–3216, <http://www.sciencedirect.com/science/article/pii/S0743731514001257>.

[55] RAJA performance portability layer, 2019, <https://github.com/LLNL/RAJA>.

[56] B. Stiller, T. Bocek, F. Hecht, G. Machado, P. Racz, M. Waldburger, ASC Tri-Lab Co-Design Level 2 Milestone Report 2015, Tech Report, LLNL-TR-677453, Technical Report, Lawrence Livermore National Laboratory, 2015.

[57] D.S. Medina, A. St-Cyr, T. Warburton, OCCA: A unified approach to multi-threading languages, 2014, arXiv preprint <arXiv:1403.0968>.

[58] OpenMP, 2019, <https://www.openmp.org>.

[59] ROCm, a new era in open GPU computing, 2019, <https://rocm.github.io/>.

[60] CuSOLVER, 2019, <https://developer.nvidia.com/cusolver>.

[61] K. Ljungkvist, Matrix-free finite-element computations on graphics processors with adaptively refined unstructured meshes, in: Proceedings of the 25th High Performance Computing Symposium, HPC '17, Society for Computer Simulation International, San Diego, CA, USA, 2017, pp. 1:1–1:12, <http://dl.acm.org/citation.cfm?id=3108096.3108097>.

[62] A. Griewank, D. Juedes, J. Utke, Algorithm 755: ADOL-C: a package for the automatic differentiation of algorithms written in C/C++, *ACM Trans. Math. Software* 22 (2) (1996) 131–167.

[63] A. Walther, A. Griewank, Getting started with ADOL-C, *Combinatorial Scientific Computing*, 2009, pp. 181–202, <https://gitlab.com/adol-c/adol-c/blob/master/ADOL-C/doc/adolc-manual.pdf>.

[64] R.A. Bartlett, D.M. Gay, E.T. Phipps, Automatic differentiation of C++ codes for large-scale scientific computing, in: V. Alexandrov, G. van Albada, P. Sloot, J. Dongarra (Eds.), *Computational Science – ICCS 2006*, Springer, Springer Berlin Heidelberg, 2006, pp. 525–532.

[65] D.M. Gay, Using expression graphs in optimization algorithms, in: J. Lee, S. Leyffer (Eds.), *Mixed Integer Nonlinear Programming*, Springer New York, 2012, pp. 247–262.

[66] E. Phipps, R. Pawłowski, Efficient expression templates for operator overloading-based automatic differentiation, in: S. Forth, P. Hovland, E. Phipps, J. Utke, A. Walther (Eds.), *Recent Advances in Algorithmic Differentiation*, in: *Lecture Notes in Computational Science and Engineering*, vol. 73, Springer Berlin Heidelberg, Berlin, Heidelberg, 2012, pp. 309–319, <arXiv:1205.3506v1>.

[67] O. Čertík, I. Fernando, S. Garg, T. Rathnayake, et al., SymEngine: A fast symbolic manipulation library, 2020, <https://github.com/symengine/symengine>.

[68] W. Bangerth, T. Heister, What makes computational open source software libraries successful? *Comput. Sci. Eng.* 6 (2013) 015010/1–18.

[69] T. Gamblin, M. LeGendre, M.R. Collette, G.L. Lee, A. Moody, B.R. de Supinski, S. Futral, The spack package manager: Bringing order to HPC software chaos, in: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC '15, ACM, New York, NY, USA, 2015, pp. 40:1–40:12, <http://doi.acm.org/10.1145/2807591.2807623>.

[70] Candi - (compile & Install) - downloads, configures, builds and installs DEAL.II, 2019, <https://github.com/dealii/candi>.

[71] R. Bartlett, I. Demeshko, T. Gamblin, G. Hammond, M. Heroux, J. Johnson, A. Klinvex, X. Li, L.C. McInnes, J.D. Moulton, et al., xSDK foundations: Toward an extreme-scale scientific software development kit, *Supercomput. Front. Innov.* 4 (1) (2017).

[72] J. Zarestky, W. Bangerth, Teaching high performance computing: Lessons from a flipped classroom, project-based course on finite element methods, in: *EduHPC '14: Proceedings of the Workshop on Education for High-Performance Computing*, IEEE Press, Piscataway, NJ, USA, 2014, pp. 34–41.

[73] J. Zarestky, M. Bigler, W. Bangerth, Teaching multidisciplinary courses in computational science and engineering, 2020, in press.

[74] M. Kronbichler, W.A. Wall, A performance comparison of continuous and discontinuous Galerkin methods with fast multigrid solvers, *SIAM J. Sci. Comput.* 40 (5) (2018) A3423–A3448.

[75] P.F. Antonietti, M. Sarti, M. Verani, L.T. Zikatanov, A uniform additive Schwarz preconditioner for high-order discontinuous Galerkin approximations of elliptic problems, *J. Sci. Comput.* 70 (2) (2017) 608–630.

[76] M. Kronbichler, K. Ljungkvist, Multigrid for matrix-free high-order finite element computations on graphics processors, *ACM Trans. Parallel Comput.* 6 (1) (2019) 2:1–2:32.

[77] P. Motamarri, S. Das, S. Rudraraju, K. Ghosh, D. Davydov, V. Gavini, DFT-FE – a massively parallel adaptive finite-element code for large-scale density functional theory calculations, *Comput. Phys. Comm.* 246 (2020) 106853.