THE deal.II LIBRARY, VERSION 8.1

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Abstract. This paper provides an overview of the new features of the finite element library deal.II version 8.1.

1. Overview. deal.II version 8.1 was released December 24, 2013. This paper provides an overview of the new features of this release and serves as a citable reference for the deal.II software library version 8.1. deal.II is an object-oriented finite element library used around the world in the development of finite element solvers. It is available for free under the GNU Lesser General Public License (LGPL) from the deal.II homepage at http://www.dealii.org/.

Version 8.1 contains, along with the usual set of bug fixes and documentation updates, the following noteworthy changes:

- Three new tutorial programs (see Section 3.3, 3.1, and 3.2);
- Improved support for multicore parallelization on shared memory machines (Section 3.4);
- The testsuite was ported to CTest/CDash (Section 3.5);
- Post-install tests (see Section 3.6).

Information on how to cite deal.II is provided in Section 4.

2. Changes to the governance structure. deal.II has been a project with contributors from around the world for a long time already. However, there has never been a formalized way to recognize contributions other than by listing the authors in a file that is part of the documentation.

Starting with this release, deal.II now has a more open governance structure that we hope will more accurately reflect the extensive contributions of many participants in this project: in addition to listing all contributors as before, deal.II is now governed by a council of *developers* – currently Luca Heltai, Martin Kronbichler, Matthias Maier, Bruno Turcksin, and Toby Young – along with principal developers who are responsible for running the technical infrastructure – currently Wolfgang Bangerth, Timo Heister, and Guido Kanschat. It is our hope that this new structure is a more adequate representation of many contributors' long-term effort for this

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project. It is our intention that this structure remains open to others and that this serves as motivation for others to participate!

3. Changes to the library.

3.1. A new tutorial: Elasto-plastic contact problem (step-42). The first of the three new tutorial programs, step-42 (written by Jörg Frohne, Timo Heister, and Wolfgang Bangerth), shows how to solve an elasto-plastic contact problem. The program is an extension of step-41 to a much more complex equation (nonlinear elasto-plasticity) and also demonstrates how to compute solutions for such problems in parallel.

The example shows how to solve a 3d, non-linear problem with a semi-smooth Newton method coupled with an active set strategy on adaptively refined meshes and scales well up to at least 1024 cores and 1 billion unknowns. An accompanying paper [6] explains the details and design of the algorithms behind this tutorial. It also shows scalability results for parallel computations.

3.2. A new tutorial: A hybridizable discontinuous Galerkin method (step-51). Step-51, written by Martin Kronbichler and Scott Miller, shows how to implement a hybridizable discontinuous Galerkin method (HDG) in deal.II. An HDG method is a special DG method which features a reduced number of globally coupled degrees of freedom compared to other DG schemes for implicit systems. This is achieved by introducing a new variable for the numerical trace, i.e., the operator that connects the solution of the subproblems on each element. The linear system to be solved globally then only consists of degrees of freedom in the trace variable, whereas the DG contributions interior to cells are eliminated during assembly by static condensation. The tutorial program shows how to implement this concept in deal.II, where the class FE_FaceQ represents the trace element for the usual DG element FE_DGQ applied to the scalar convection-diffusion equation written as a first order system.

The tutorial program includes a few practical aspects of an HDG implementation, namely the realization of superconvergent post-processing and the utilization of the parallel character of the assembly and static condensation process with the WorkStream class. The tutorial also contains an extensive discussion of efficiency of this approach compared to standard continuous finite elements. The results show that the HDG method is competitive to continuous elements for medium order between about 3 and 6 in terms of solution time on diffusion-dominated systems. For convection-dominated problems, the method inherits the superior stability properties of low to medium order DG methods, which allows for good solution quality already on coarser meshes.

Furthermore, a new element FE_FaceP has been added to the deal.II library that can used for hybridization of the discontinuous elements of complete degree p, FE_DGP. FE_DGP and FE_FaceP of degree p have fewer degrees of freedom per cell compared to the elements FE_DGQ and FE_FaceQ of tensor product degree p.

3.3. A new tutorial: An adaptive mesh solver for the heat equation (step-26). deal.II has long had tutorial programs for the wave equation, but none for the conceptually simpler heat equation. Furthermore, there was no simple tutorial program that showed how one can solve time dependent problems where the mesh changes every few time steps.

The new step-26 tutorial program closes this gap. It is a rather simple program – the program has just 151 lines with a semicolon – and as such serves as a gentle

introduction to these topics.

3.4. Improved WorkStream implementation. The WorkStream namespace has already in the past contained the functions that are used to parallelize (using multithreading) many of the loops over all cells or faces that one encounters in finite element computations. Extensive documentation on how to use this class and the rationale behind it is provided in the "Parallel computing with multiple processors accessing shared memory" module.

This class has been significantly revamped in an effort to improve scaling to large multicore workstations. In particular, we now use thread-local variables in some places to improve cache performance. In addition, the namespace has obtained another implementation of WorkStream::run that does not just take a sequence of cells (or other objects to work on), but such a sequence that has been colored in a way to indicate which cells will conflict with others when writing into the global matrix, right hand side, or other object. Using this function instead of the previously existing one obviously requires changes to existing code bases, but can provide significant speedups in some circumstances when using significant numbers of threads (say, above 16 or 32). The details of these algorithms have been documented in [10].

As part of the changes necessary to allow this, deal.II has also gained a set of generic functions that provide graph coloring algorithms. The are located in namespace GraphColoring.

3.5. Testsuite ported to CTest/CDash. With this minor release deal.II is now fully ported to CMake. The last remaining step was the migration of the testsuite to CTEST as test driver and CDASH as web front end. This involved porting over 3000 tests to a new directory structure. Furthermore, the regression and build tests are no longer independent testsuites, but a combined one; and tests are by default run against both the debug and release versions of the library.

The port of the testsuite was also motivated by the fact that, in order to provide official support for at least three major compiler brands (GCC, CLANG and ICC) on multiple platforms such as Linux, MAC OSX and BSD, it is highly necessary to have regular regression tests available for these platforms. Hence, in addition to the regression tester already present (whose main purpose is to test every single subversion revision) dedicated nightly build tests for a big variety of above compilers and platforms (and external dependencies) have been set up.

The testsuite is set up in the build directory via make setup_tests. After that, tests can be run by invoking the test driver ctest with suitable options. In order to submit test results a CTest script is available that can be passed as an option to the driver, e.g. by ctest -S .../tests/run_testsuite.cmake (or if just the build tests should be run, .../run_buildtest.cmake). The scripts run a configure, build and test stage as necessary and submit the results to a CDash instance. Public, anonymous submission of test results to the CDASH site is possible in order to easily upload and share regression test results.

3.6. Post-install tests. Every installation now ships with a small collection of tests that can be executed by calling make test in the build directory. This is used to identify common configuration problems, bugs in external dependencies, problems in the MPI wrappers, and to check the correct setup of some of the external packages. Running the tests is now part of the installation instructions and we especially recommend to run the tests on new machines.

3.7. Other Changes. The deal.II release 8.1 also includes improvements in the following areas:

- The handling of periodic boundary conditions has been improved and extended to distributed triangulations.
- deal.II's output capabilities have been extended in several aspects. In particular, it is now possible to merge output from vectors belonging to several different DoFHandler objects (a common case when solving multiphysics problems) within a single file instead of forcing the user to join the data in one DoFHandler for output.
- Higher order polynomial boundary descriptions now use support points of the Gauss-Lobatto quadrature formula instead of equidistant ones, which gives much better stability at high orders and more accuracy for some curved boundary shapes due to superconvergence effects.

4. How to cite deal.II. In order to justify the work the developers of deal.II put into this software, we ask that papers using the library reference one of the deal.II papers. This helps us justify the effort we put into it.

There are various ways to reference deal.II. To acknowledge the use of a particular version of the library, reference the present document as follows: @article{dealII81,

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title = {The {\tt deal.{I}{I}} Library, Version 8.1},
author = {W. Bangerth and T. Heister and L. Heltai and G. Kanschat
and M. Kronbichler and M. Maier and B. Turcksin and T. D. Young},
journal = {arXiv preprint \url{http://arxiv.org/abs/1312.2266v4}},
year = {2013},
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}
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The original deal.II paper containing an overview of its architecture is [2]. If you rely on specific features of the library, please consider citing any of the following:

- For geometric multigrid: [7,8];
- For distributed parallel computing: [1];
- For hp adaptivity: [4];
- For matrix-free and fast assembly techniques: [9];
- For computations on lower-dimensional manifolds: [5].

5. Acknowledgements. deal.II is a world-wide project with dozens of contributors around the globe. Other than the authors of this paper, the following people contributed code to this release: Fahad Alrashed, Daniel Arndt, Juan Carlos Araujo Cabarcas, Krzyszof Bzowski, Francesco Cattoglio, Denis Davydov, David Emerson, Armin Ghajar Jazi, Eric Heien, Tobin Isaac, Oleh Krehel, Craig Michoski, Scott Miller, Jean-Paul Pelteret, Andreas Putz, Mayank Sabharwal, Martin Steigemann. Their contributions are much appreciated!

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REFERENCES

- W. Bangerth, C. Burstedde, T. Heister, and M. Kronbichler. Algorithms and data structures for massively parallel generic adaptive finite element codes. ACM Trans. Math. Softw., 38:14/1–28, 2011.
- [2] W. Bangerth, R. Hartmann, and G. Kanschat. deal.II a general purpose object oriented finite element library. ACM Trans. Math. Softw., 33(4), 2007.
- W. Bangerth and G. Kanschat. Concepts for object-oriented finite element software the deal.II library. Preprint 1999-43, SFB 359, Heidelberg, 1999.
- [4] W. Bangerth and O. Kayser-Herold. Data structures and requirements for hp finite element software. ACM Trans. Math. Softw., 36(1):4/1-4/31, 2009.
- [5] A. DeSimone, L. Heltai, and C. Manigrasso. Tools for the solution of PDEs defined on curved manifolds with deal.II. Technical Report 42/2009/M, SISSA, 2009.
- [6] J. Frohne, T. Heister, and W. Bangerth. Efficient numerical methods for the large-scale, parallel solution of elastoplastic contact problems. *submitted*, 2013.
- [7] B. Janssen and G. Kanschat. Adaptive multilevel methods with local smoothing for H¹- and H^{curl}-conforming high order finite element methods. SIAM J. Sci. Comput., 33(4):2095– 2114, 2011.
- [8] G. Kanschat. Multi-level methods for discontinuous Galerkin FEM on locally refined meshes. Comput. & Struct., 82(28):2437-2445, 2004.
- [9] M. Kronbichler and K. Kormann. A generic interface for parallel cell-based finite element operator application. *Comput. Fluids*, 63:135–147, 2012.
- [10] B. Turcksin, M. Kronbichler, and W. Bangerth. WorkStream a design pattern for multicoreenabled finite element computations. submitted, 2013.