SSI: Open Source Support for Massively Parallel, Generic Finite Element Methods

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Summary

Finite element computations in science and engineering are becoming more complex:

- They incorporate more physics
- They use more advanced numerical methods (adaptive meshes, multigrid preconditioners, coupled or partially coupled nonlinear solvers)
- They use more parallelism, from laptops to supercomputers

There is a clear need for libraries supporting such applications at all levels of complexity and parallelism.

deal.II and *Trilinos* are two widely used, open source libraries providing finite element and linear algebra support. This project aims at broadening support for parallel computations in these libraries for applications built on them:

- For large-scale applications with billions of unknowns on thousands of processors
- For applications running on multicore laptops or workstations
- For applications wanting to use GPU acceleration

Background

There is large demand for generic libraries supporting modern finite element applications. *deal.II* and *Trilinos* both have hundreds or thousands of users and have supported hundreds of projects. But they need to be extended to keep at pace with the size of parallel machines such as those in NSF's XSEDE program.

Furthermore, providing broader support allows wider user groups to use large-scale computing – it democratizes supercomputing and lowers the threshold for entry. Currently, only few groups can make use of even 1000+ cores.

This project aims to do this by extending the parallel computing facilities of the two libraries.

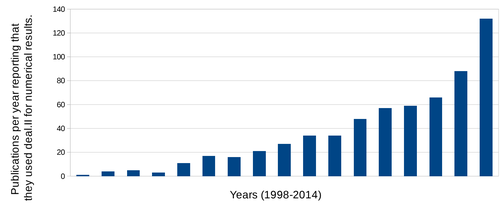

Fig. 1: *deal.II is widely used, with ~450 mailing list members and 120+ known publications in 2014 reporting results obtained with it.*

Achievements 2012-13

64-bit indices: Most finite element software is limited by 32-bit integers to computations with less than 2B unknowns and ~20k processors. We have extended *deal.II* and *Trilinos* to optionally use 64-bit indices instead and verified scalability on model problems up to 27B unknowns. We have also verified scaling on real applications on up to 8,000k cores.

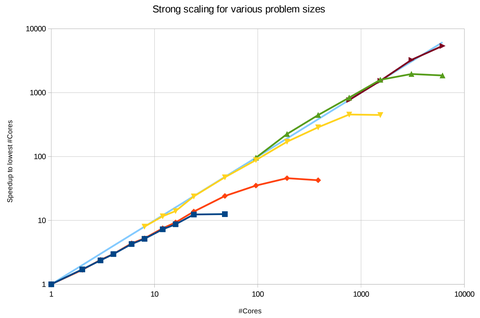

Fig. 2: Scalability results for the ASPECT code, for convection in the Earth mantle, built on deal.II and Trilinos on up to 8000k cores and more than 300M unknowns. (Credit: R. Gassmoeller)

More modern installation support: Supporting more users outside the core CS&E area requires making installation easier. We have switched from Autoconf to CMake to benefit from better external support and to make integration into modern, user-friendly IDEs easier.

Tutorials and online videos: To help new users, we have extended the number of extensively documented tutorials on *deal.II* to now 52. These tutorials as well as many other computational science-related questions are discussed in a sequence of 48 videos by Wolfgang Bangerth posted on YouTube with ~27,000 views so far.

Achievements 2013-14

Better support for multicore machines: Most code is still written and tested on multicore laptops, desktops or workstations. We have extended support for shared memory parallelization within the library and within the user interfaces. Many operations now scale well up to at least 64 cores in a single machine, reaching all the way to current high-end workstations.

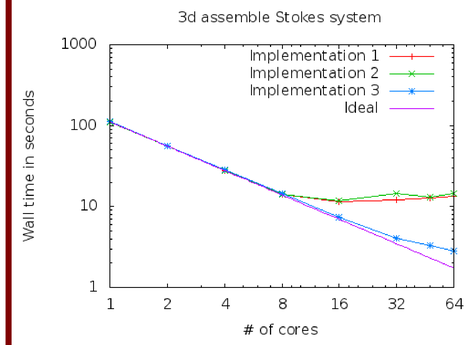

Fig. 3: Scalability of one of the dominant operations of the code shown in Fig. 3, for a single MPI process run on a shared memory multicore machine. The old implementation (implementations 1 and 2) of multicore support only scaled to ~8 cores. The new code (implementation 3) scales at least to 64 cores, allowing for more efficient use of current and future workstations or laptops. (Credit: B. Turcksin, M. Kronbichler and W. Bangerth)

Achievements 2014-15

Support for GPUs and Intel MIC: Support for GPUs is important not only because of the large number of current Top500 supercomputers using them but also because the DOE committed to this architecture with Summit (ORNL) and Sierra (LLNL). Intel MIC is still a relatively new architecture but it has already been adopted by several Top500 supercomputers including Tianhe-2, the fastest supercomputer in the world. Support of these new architectures in *deal.II* is being added using the *Paralution* library and Tpetra of *Trilinos*.

Vectorization: SIMD instructions of modern CPUs work on increasing large data (256 bits on recent x86_64 and 512 bits on future Intel CPUs). Using OpenMP 4.0 SIMD instructions, we have enable the vectorization on most of our vector-vector and vector-matrix operations.

Support MueLu: Add support for the MueLu package of *Trilinos*. This new algebraic multigrid package has been developed to replace ML.

More accurate geometries: *deal.II* can now handle curved and complex geometries much better than before. This includes curved elements in the interior of domains, and interfaces to CAD tools. We have used this in ASPECT to provide better models for the geometry of the Earth, both globally for the spherical shell of the mantle, as well as in local and regional models.

Move to GitHub: We have changed our version control system from svn to git and we now host *deal.II* repository on GitHub.