Complex simulations with the deal.II open source software, and how we use Trilinos for that

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With the help of many other deal.II contributors
A “typical” application in CS&E

What we generally need:
• Non-trivial 2d/3d geometry
• Interfaces to CAD and meshers
• Coupled systems of nonlinear PDEs
• Efficient non-linear iteration strategy
• Efficient linear solver
• Ways to visualize the solution

What we may need:
• Parallel execution on small and large systems
• Mixed or higher order finite elements
• …
A library for finite element computations that supports...

...a large variety of PDE applications tailored to non-experts.
Fundamental premise:
Provide building blocks that can be used in many different ways, not a rigid framework.
deal.II provides:

- Adaptive meshes in 1d, 2d, and 3d
- Tri/quad (2d) and tet/hex meshes (3d)
- Interfaces to all major graphics programs
- Standard refinement indicators
- Most standard finite element types (continuous, discontinuous, low and high order)
- Support for multi-component problems
- Its own sub-library for dense + sparse linear algebra
- Interfaces to PETSC, Trilinos, UMFPACK, ARPACK, OpenCASCADE, ...
- Supports multicore + cluster systems
deal.II

Status today:

- ~1000 downloads per month
- 1.4M lines of C++ code
- 10,000+ pages of documentation
- Portable build environment
- Used in teaching at many universities

- ~300 people have contributed to it
- ~40 people contribute to each release
- ~10 pull requests merged each day
- ~1 new publication per day that uses it
### Examples

Examples of what can be done with deal.II (2013 only):

- Biomedical imaging
- Brain biomechanics
- E-M brain stimulation
- Microfluidics
- Oil reservoir flow
- Fuel cells
- Transonic aerodynamics
- Foam modeling
- Fluid-structure interactions
- Atmospheric sciences
- Quantum mechanics
- Neutron transport
- Nuclear reactor modeling
- Numerical methods research

- Fracture mechanics
- Damage models
- Solidification of alloys
- Laser hardening of steel
- Glacier mechanics
- Plasticity
- Contact/lubrication models
- Electronic structure
- Photonic crystals
- Financial modeling
- Chemically reactive flow
- Flow in the Earth mantle
Example applications: Electromechanics

Electrophysiology of heart muscle fibers (Piersanti et al., 2020)
Example applications: Complex models

Patient-specific fluid-structure interaction with realistic material models for vascular modeling
(de Villiers, McBride, Reddy, Franz, Spottiswoode, 2018)
Example applications: Complex models

Homogenization of models for plasmonic crystals
(Maier et al., 2019)
Parallelization on parallel machines

Scaling of a multigrid solver on up to $2 \times 10^{12}$ unknowns on up to 300,000 processor cores.
Example applications: Complex models

Flow in the earth interior
(Advanced Solver for Problems in Earth Convection, ASPECT)
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Interfacing with other software

We have learned that it is best if deal.II focused on finite element methods.

Other functionality is obtained by interfacing with other software:

- Preprocessing:
  - Assimp
  - CGAL
  - Gmsh
  - OpenCASCADE

- Postprocessing:
  - HDF5
  - VTK-based visualization software
Interfacing with other software

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Other functionality is obtained by interfacing with other software:

- General algorithm support:
  - AdolC
  - ArborX
  - BOOST
  - GSL
  - HDF5
  - Metis
  - MPI
  - muparser
  - p4est
  - SUNDIALS
  - Symengine
  - TBB
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Other functionality is obtained by interfacing with other software:

- Linear algebra:
  - ARPACK
  - BLAS/LAPACK
  - cuSolver/cuSparse
  - Gingko
  - MUMPS
  - PETSc (Vec, Mat, KSP functionality)
  - Scalapack
  - Trilinos (various packages)
  - UMFPACK
deal.II’s Trilinos interfaces were originally written in the late 2000s.

At the time intended to complement our PETSc interfaces.

**Goal:** Scalable data structures, solvers, preconditioners for large linear systems.

→ Built on Epetra

**A good decision:** We are regularly running jobs efficiently on 1000s and occasionally on 10,000s of cores.
Trilinos Epetra interfaces

What we do with Epetra:
We don’t actually need very much:

– Epetra_CrsGraph
– Epetra_FEChrsMatrix
– Epetra_FEVector
+ some custom import/export functionality

– AztecOO solvers (CG, GMRES, …)
– Ifpack preconditioners

– ML
– MueLu via its Epetra interfaces

All of this is wrapped to provide a deal.II-style interface.
Trilinos Epetra interfaces

What we do with Epetra:

We combine these interfaces to build higher-order functionality for block systems.

For example, solve a Stokes system

\[
\begin{pmatrix}
A & B \\
B^T & 0
\end{pmatrix}
\begin{pmatrix}
U \\
P
\end{pmatrix}
=
\begin{pmatrix}
F \\
G
\end{pmatrix}
\]

with a preconditioner of the form

\[
\begin{pmatrix}
A & B \\
0 & S
\end{pmatrix}
^{-1}
\approx
\begin{pmatrix}
A^{-1} & B \\
0 & M^{-1}
\end{pmatrix}
\]

or

\[
\begin{pmatrix}
A^{-1} & B \\
0 & M^{-1}
\end{pmatrix}
\]

- Implemented in deal.II’s “Block*” classes
- Not dissimilar to PETSc’s “field split” approach
- Just better
Problems we have with our Epetra interfaces:

- Epetra has been “end of line” for quite a while
- We have Tpetra wrappers, but they are not used

- We would love to always use Tpetra instead, but:
  - Switch-over has to be atomic
  - We don’t have the manpower
  - Interface stability was not clear for a while
Trilinos Epetra interfaces

Questions about Tpetra:

- We don’t know what functionality we would lose in a conversion.

  For example: Muelu only supports Epetra when Trilinos is not compiled with Tpetra

- Varying coding styles of Trilinos packages don’t make conversions easy

- Documentation is not always sufficient/helpful

But: We are working on switching. There is no alternative.
Interfaces to other packages

Sacado:

• Automatic differentiation package

• Used in a few tutorial programs to compute Jacobians from residuals
  – in fluid dynamics
  – in solid mechanics with complex energy functionals

• More tutorials coming

• Not originally wrapped by deal.II classes

• But there are now wrappers that make uniform whether you use Sacado, AdolC, or SymEngine
Interfaces to other packages

Zoltan:

• Mesh partitioning package

• As an alternative to METIS

• Not widely used because we typically partition meshes based on space-filling curves (via p4est)

• Has become more relevant because we now have mesh classes that do not rely on p4est

• Wrapped via a single deal.II function
Interfaces to other packages

NOX:

- Nonlinear solver package
- Patch is currently pending
- As an alternative to SUNDIAL’s KINSOL package
- Wrapped with deal.II classes that closely mirror our KINSOL interfaces
Interfaces to other packages

ROL:

• Optimization package
• deal.II provides vector adaptors
• Usage unclear
Interfaces to other packages

SEACAS:

- Not actually quite sure what this package is
- We use it to read ExodusII files
- deal.II provides a single function as a wrapper
We have decided to use Kokkos!

- Trilinos requires Kokkos anyway
- deal.II will require it as well, regardless of whether deal.II is configured with Trilinos
- We think that many other applications will sooner or later use Kokkos
- It has functionality that we need but that is just too cumbersome to replicate – specifically how to deal with GPUs.
- We are concerned about Trilinos bundling/using its own Kokkos version, rather than the system one
deal.II is a toolbox to write finite element solvers with.

- Supports nearly every aspect of finite element methods
- Highly scalable to large systems/computations
- Widely used for applications in many engineering and science disciplines.

- Has interfaces to quite a large number of Trilinos packages
- These interfaces have provided us with great functionality for more than 15 years already – thank you!