DOE has supported computing technologies that have made a difference

Barry Smith
Argonne National Laboratory

- Mathematical libraries
  - reusable encapsulations of mathematical algorithms that can support a large, diverse user base, including scientists, engineers without requiring them to become experts in all the supporting mathematics. Shield users from architectural details of the hardware and provide portability.

Early Years of “DOE” Numerical Libraries

- EISPACK, 1973, eigenanalysis for dense/banded matrices
- LINPACK, 1977, linear solvers for dense/banded matrices
- EPISODE…Vode, 1976--, ODE solver package
- Minpack, 1980, general purpose optimization software
- ….
- LAPACK, 1992, Eispack+Linpack for vector machines
- Massively parallel computing begins to disrupt everything
- MPI, 1994
- A new opportunity for numerical libraries

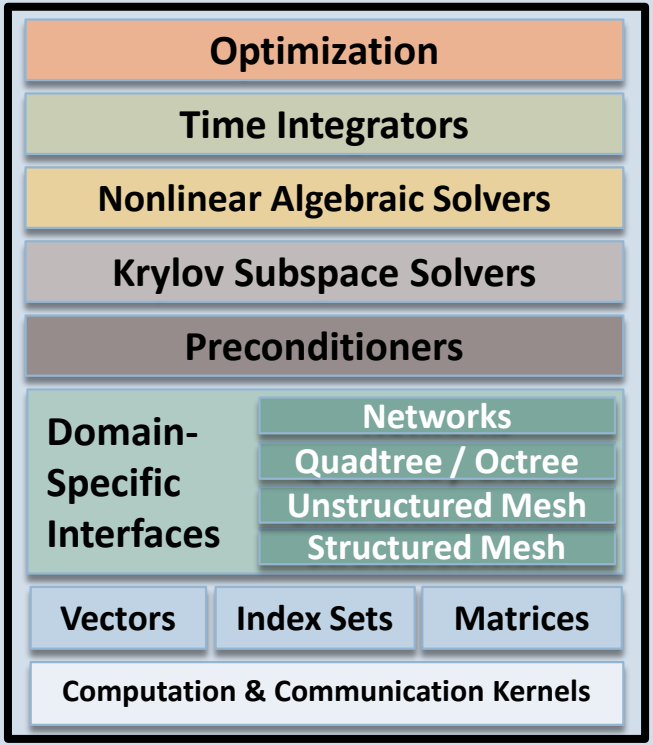
Post MPI Years of DOE Numerical Libraries

- Libraries
  - SuperLU (LBL)
  - hypre (LLNL)
  - Sundials (LLNL)
  - …
- Bundling libraries (frameworks)
  - Trilinos (SNL)
  - PETSc/Tao (ANL)
  - MOOSE (INL)
  - … These leverage many libraries and even other bundled libraries

PETSc/TAO:

Portable, Extensible Toolkit for Scientific Computation / Toolkit for Advanced Optimization

Scalable algebraic solvers for PDEs. Encapsulate parallelism in high-level objects. Active & supported user community. Full API from Fortran, C/C++, Python.



- **Easy customization and composability of solvers <u>at runtime</u>**
  - Enables optimality via flexible combinations of physics, algorithmics, architectures
  - Try new algorithms by composing new/existing algorithms (multilevel, domain decomposition, splitting, etc.)
- **Portability & performance**
  - Largest DOE machines, also clusters, laptops
  - Thousands of users worldwide

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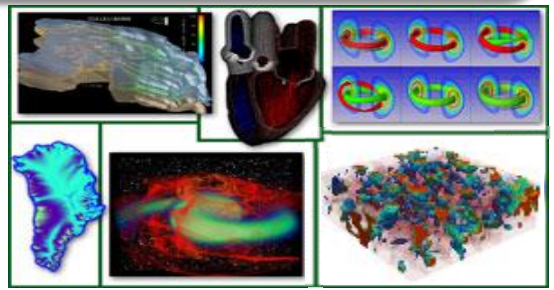

PETSc provides the backbone of diverse scientific applications. clockwise from upper left: hydrology, cardiology, fusion, multiphase steel, relativistic matter, ice sheet modeling

ECP xSDK FASTMATH R&D 100

https://www.mcs.anl.gov/petsc

Future Directions of DOE Numerical Libraries

- Coordination of designs and interfaces among groups and labs
  - e.g., xSDK and IDEAS work (began with ASCR/BER, now funded under ECP)
  - Makes it easier to combine functionality of multiple libraries
- Focus on using large-scale simulations in decision making
  - Requires coordination between simulation-oriented mathematics libraries and optimization libraries
  - Requires propagating uncertainty, statistics, and error estimates around the algorithm stack
    - For example, using the error estimates from spatial and time discretization in producing error estimates on the computed optimal solution