

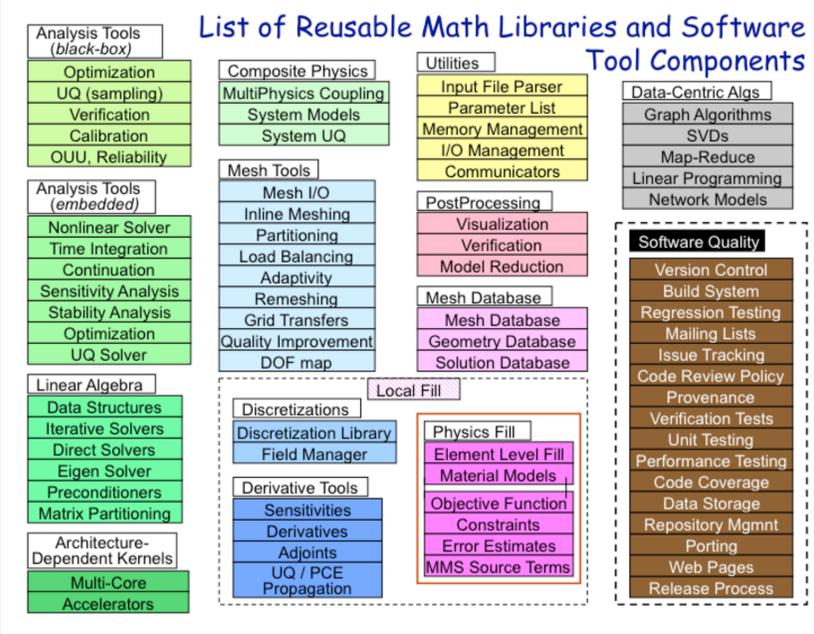
Overview

The goal of this poster is to foster discussions on a collaboration model between Climate Scientists and Computational Scientists.

The Computational Science organization at Sandia has largely adopted a strategy, "AgileComponents" [1], that was designed to maximize the long-term impact to our diverse set of customers. For application codes, this strategy involves leveraging computational mathematics libraries, expertise, and funding streams. A manifestation of the AgileComponents approach is the Albany finite element code, which is now playing a role in DOE climate modeling. Will climate model developers (1) embrace the broad use of components and (2) see real benefits of this leverage?

AgileComponents Strategy: Create, use, and improve a common base of modular, independent-yet-interoperable, software components.

"Components" = Libraries Software Quality Tools
 Interfaces Demonstration Applications



Albany [2] is an application code built primarily from Trilinos [3] math libraries.

Albany plays the Demonstration Application role in the AgileComponents Strategy.

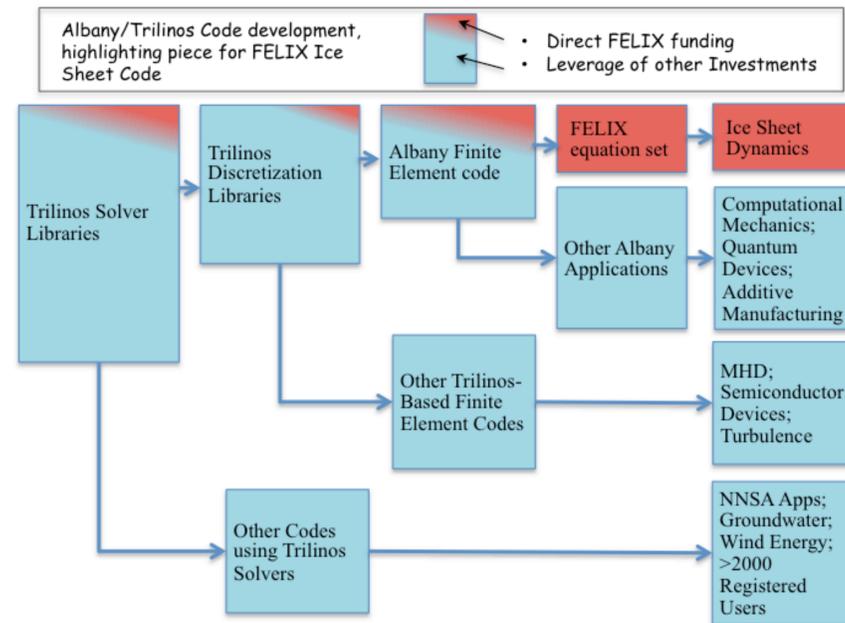
Demonstration Application role:

- Develop abstract interfaces
- Incubator for new libraries
- Demonstrate inter-operability
- Library installation and integration testing
- Library ripening: usability, performance
- Prototype Software Tools, E.g.,
 - git, github, cmake, ctest, cdash
- Research platform for new algorithms
- "Meso-app": step between mini-app and production

Trilinos libraries used in Albany:

- Sacado
- Stokhos
- Intrepid
- Zoltan
- Belos
- Aztec
- ML
- Muelu
- Amesos
- lfpack
- Anasazi
- Epetra
- Tpetra
- NOX
- LOCA
- Piro
- Rythmos
- ROL
- TriKota
- Thyra
- Teuchos
- STK
- Kokkos

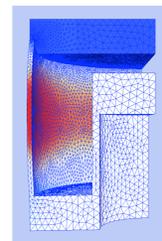
Leveraging of Investments to Develop Albany/FELIX



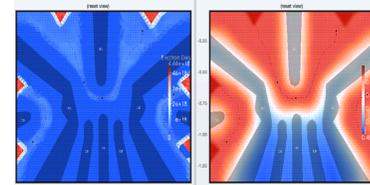
A schematic showing the leverage of the AgileComponents code strategy, highlighting the slice of the code base written specifically for the Albany/FELIX ice sheet application. This figure illustrates how large parts of the code base are also used by other applications -- several of which are listed in the right column -- which all contribute to the development costs, research drivers, and creation of expertise.

Gallery of Rapidly Developed Albany Applications

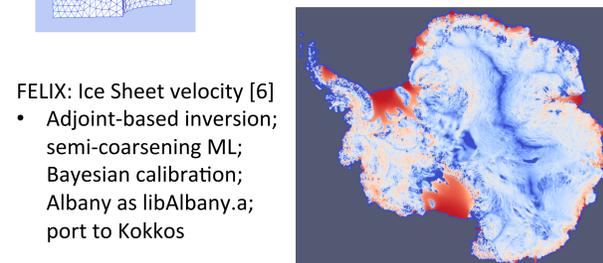
- the Component Development Driven by that App



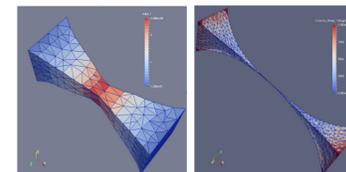
LCM: Computational Mechanics [4]
 • Configure/Build system; mesh database; automatic differentiation; response functions; discretizations



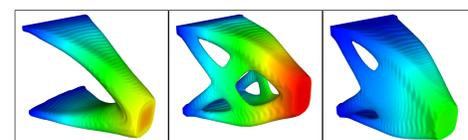
QCAD: Quantum Device Modeling [5]
 • In situ Optimization; Tet elements; Neumann BCs; MultiLevel Prec; Multi-Physics coupling; eigensolver



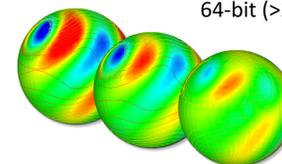
FELIX: Ice Sheet velocity [6]
 • Adjoint-based inversion; semi-coarsening ML; Bayesian calibration; Albany as libAlbany.a; port to Kokkos



PAALS: Mesh Adaptive Loop [7]
 • Adaptivity; github; documentation; 64-bit (>2B) problem size



ATO: Topological Optimization for Additive Manufacturing [8]
 • Multi-physics coupling; level-set equations



Aeras: Next-Gen Atmosphere Model [9]
 • Performance-portable kernels; embedded UQ; explicit integrators; spectral elements

The Value Proposition for Using Component Libraries

- Inclusion of the algorithmic capability into the climate code.
- Access to the algorithmic expert for continued engagement, who can work in his/her own familiar code base.
 - From this foundation, fractional funding streams and even consultations can have large impact.
- Automatic, free upgrades in capability as the library development continues through other funding sources and using developments motivated by other applications.
- A decreased code base that must be supported, and ported to new architectures.
- Encourages more modular code design, for improved agility and maintainability.
- Broadening of the network of people thinking about your application.
- Ability to leverage algorithm and inter-disciplinary funding streams to impact climate science application development.

The Value Proposition for Coding Algorithm Ideas Directly in Climate App

- Inclusion of the algorithmic capability into the climate code.
- Application expert has complete control of code base

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