Albany: Integrating Algorithmic Components to Build Advanced Applications


Albany is a finite element application code base that is an early adopter of new algorithmic capabilities from the Trilinos, Dakota, and PUMI suites. FASTMath and other SciDAC funding sources play a key role in bridging the valley of death between algorithms and applications.

**Application Impact: Ice Sheets**

Under PISCEES, the FELIX-FO unstructured-grid finite element flow solver has been developed in Albany. This work leverages numerous enabling technologies supported by ASCR and ASC.

- Nonlinear solvers, linear solves, UQ, adaptivity, and performance portability [details below]
- Automatic differentiation, discretizations, software engineering tools & processes, partitioning, mesh database and 1/0
- Albany/FELIX is being deployed within the MPAS Land Ice component in the ACME climate model.
- Ice Sheet work in Albany has been funded by PISCEES and FASTMath.

**Nonlinear Solvers and Inversion**

Under FASTMath, we have impacted applications with the development of Homotopy and Anderson Acceleration in Trilinos::NOX.

- New general-purpose Adjoint-Based Inversion capability implemented in Albany
- Uses Automatic Differentiation, Preconditioning, Optimization algorithms from Trilinos
- Driven by PISCEES project, for ice sheet initialization
- On critical path of ACME climate simulations
- Impacting NNSA application as well

Nonlinear Solver Inversion work in Albany leverages FASTMath, QUEST, PISCEES, and ASC/ATDM projects (Objective functional: \( \int_{\Omega} \frac{1}{2} \nabla u \cdot \nabla u + a \int_{\Omega} f u \, \, dx \)).

**Embedded UQ**

Embedding ensembles move them to an inner loop instead of an outer loop, executing them concurrently.

- The Sacado library in Trilinos has an Ensemble type
- Operations (e.g. +, -, exp, sqrt, cos) are implemented on an arrays of data
- Performance gains are realized by:
  - Amortizing costs for mesh-dependent calculations
  - Easy compiler vectorization of kernels over ensembles
  - Amortizing latency over larger MPI messages
  - Contiguous memory access for arrays of data

UQ work in Albany leverages efforts in the QUEST, Equinox, PISCEES, LDRED, and ATDM projects.

**Additional Application Impact**

- Additional Albany application work has been funded by LDRED, ASC, and WFD, and is impacted by FASTMath investments.

**Scalable Linear Algebra**

Scalability of Albany simulations hinge largely on the preconditioning. Multi-level solves are essential for the largest problems:

- A new semi-coarsening multi-level algorithm was implemented for thin, extruded domains, motivated by Ice Sheet application.
- Algorithm has impacted NNSA application
- Implementations for architectures with high degrees of on-node parallelism are underway
- Albany/Trilinos has been funded by PISCEES, ASC/ATDM, ASC Projects, and FASTMath projects.

**Application Impact: Computational Mechanics**

The LCM computational mechanics research code has been developed in Albany. This challenging application has been a driver for many enabling technologies:

- Primary driver for mesh adaptivity collaboration under FASTMath between SNL and SCOREC.
- Generated largest implicit problem solved in Albany of 1.7B degrees of freedom, detecting scalability issues.
- Research code important for mission customers.

Computational Mechanics work in Albany has been funded by the ASC program, LDRED, WFD, and FASTMath.

**Mesh Adaptivity**

Mesh adaptation can be essential for efficiency and robustness.

- Under FASTMath, parallel adaptive loop simulations involving PUMI and Albany/Trilinos have been developed.
  - Targeting computational mechanics applications.
    - Remeshing is crucial for large-deformation problems
  - Adaptive solution loop work in Albany leverages efforts in FASTMath and ASC/ATDM projects.

**Performance Portability**

The Kokkos programming model enables performance portability of kernels.

Kokkos has abstraction layer so code can be tailored for specific devices:

- Memory layout for the MultiDimVector. Accessor syntax \( \text{ Kokkos::Real } \) unchanged.
- Parallel kernel launch directives under the kokkos::Parallel_for() call.

Performance Portability work in Albany leverages efforts in FASTMath, LDRED, and ASC/ATDM projects. Portable execution of finite element assembly of Ice Sheet PDEs with a single Kokkos implementation.