Albany: Integrating Algorithmic Components to Build Advanced Applications

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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.

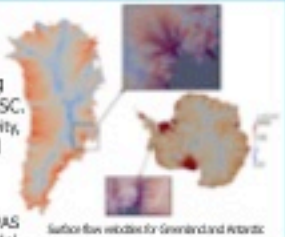
Application Impact: Ice Sheets

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 solves, linear solves, UQ, adaptivity, and performance portability (details below)
- Automatic differentiation, discretizations, software engineering tools & processes, partitioning, mesh database and I/O

Albany/FELIX is being deployed within the MPAS Land Ice component in the ACME climate model.

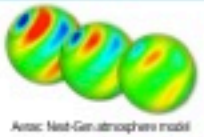


Surface flow velocities for Greenland and Antarctic Ice Sheets, with insets showing unstructured mesh.

Ice Sheet work in Albany has been funded by PISCEES and FASTMath.

Additional Application Impact

QCAD: Quantum device design



Aeras: Next-Gen atmosphere model

ATO: Topology optimization for thermo-mechanical systems

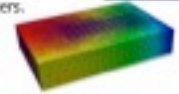
Additional Albany application work has been funded by LDRD, ASC, and WFO, and is impacted by FASTMath investments.

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.
- Research code important for mission customers.



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

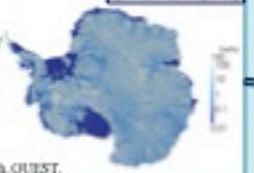
Nonlinear Solvers and Inversion

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

- The robustness of nonlinear solvers are critical when an application is to be called as a sub-component within a larger application code.
- Impacting PISCEES and CASL

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 Solve/Inversion work in Albany leverages FASTMath, QUEST, PISCEES, and ASC/ATDM projects.

Application Code

Albany

Enabling Technologies

DAKOTA · Trilinos · PUMI

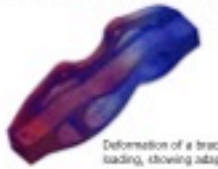
Mesh Adaptivity

Adaptivity can be essential for efficiency and robustness.

Under FASTMath, parallel adaptive loop simulations involving PUMI and Albany/Trilinos has been developed.

- Targeting computational mechanics applications.
  - General mesh modification for evolving geometry (e.g. large deformations, fracture)

Remeshing of a cube geometry being driven to large deformation by the LCM elasticity and J2 plasticity models.



Deformation of a bracket under loading, showing adapted mesh.

Adaptive solution loop work in Albany leverages efforts in FASTMath and ASC/ATDM projects.

Embedded UQ

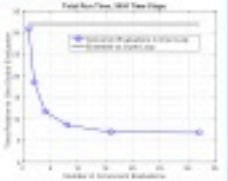
Embedding ensembles move them to an inner loop instead of an outer loop, executing them concurrently.

The Stokhos 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



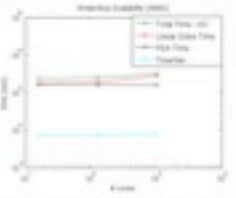
UQ work in Albany leverages efforts in the QUEST, Equinox, PISCEES, LDRD, and ATDM projects.

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.



Weak scaling study of Ice Sheet PDEs for a model of the Antarctic Ice Sheet. Shown to scale well to 1.1B unknowns on 16K procs.

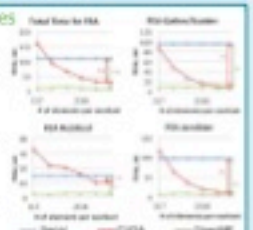
Scalable linear algebra work in Albany leverages efforts in FASTMath, ASCR Base Math (Tominaro), PISCEES, and ASC/ATDM projects.

Performance Portability

The Kokkos programming model enables performance portability of kernels.

Kokkos abstractions allow execution to be tailored to specific devices:

- Memory layout for the MultiDimVector. Accessor syntax v(i,j,k) is unchanged.
- Parallel kernel launch directives under the Kokkos::Parallel_for() call.



Performance Portability work in Albany leverages efforts in FASTMath, LDRD, and ASC/ATDM projects.

Portable execution of finite element assembly of Ice Sheet PDEs with a single Kokkos implementation.

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