Albany: Integrating Algorithmic Components to Build Advanced Applications

FASTMATH

Sandia National Laboratories

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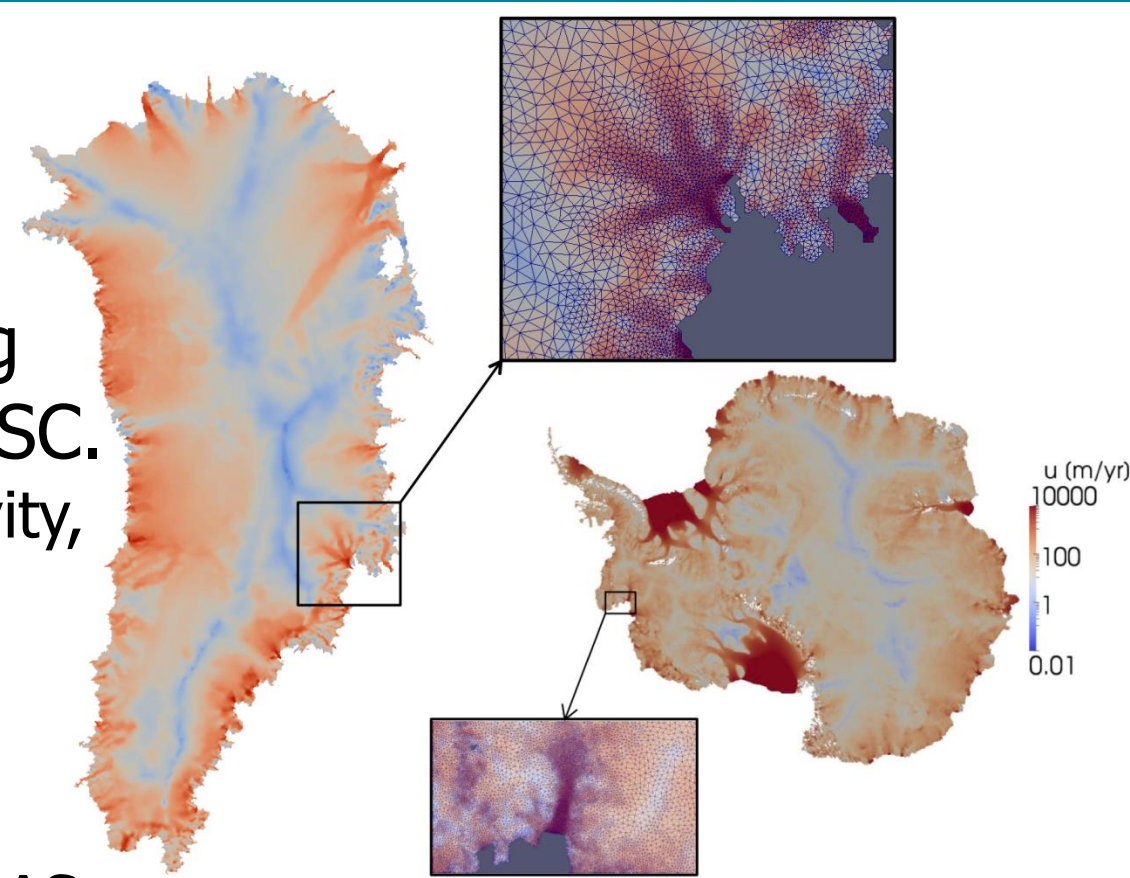
Albany is a finite element application code base that is an early adopter of new algorithmic capabilities from the Trilinos, Dakota, and PUMI suites. FASTMath and other SciDAC funding sources play a key role in bridging the valley of death between algorithms and applications.

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.

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


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

u (m/yr) 10000 100 0.01

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.
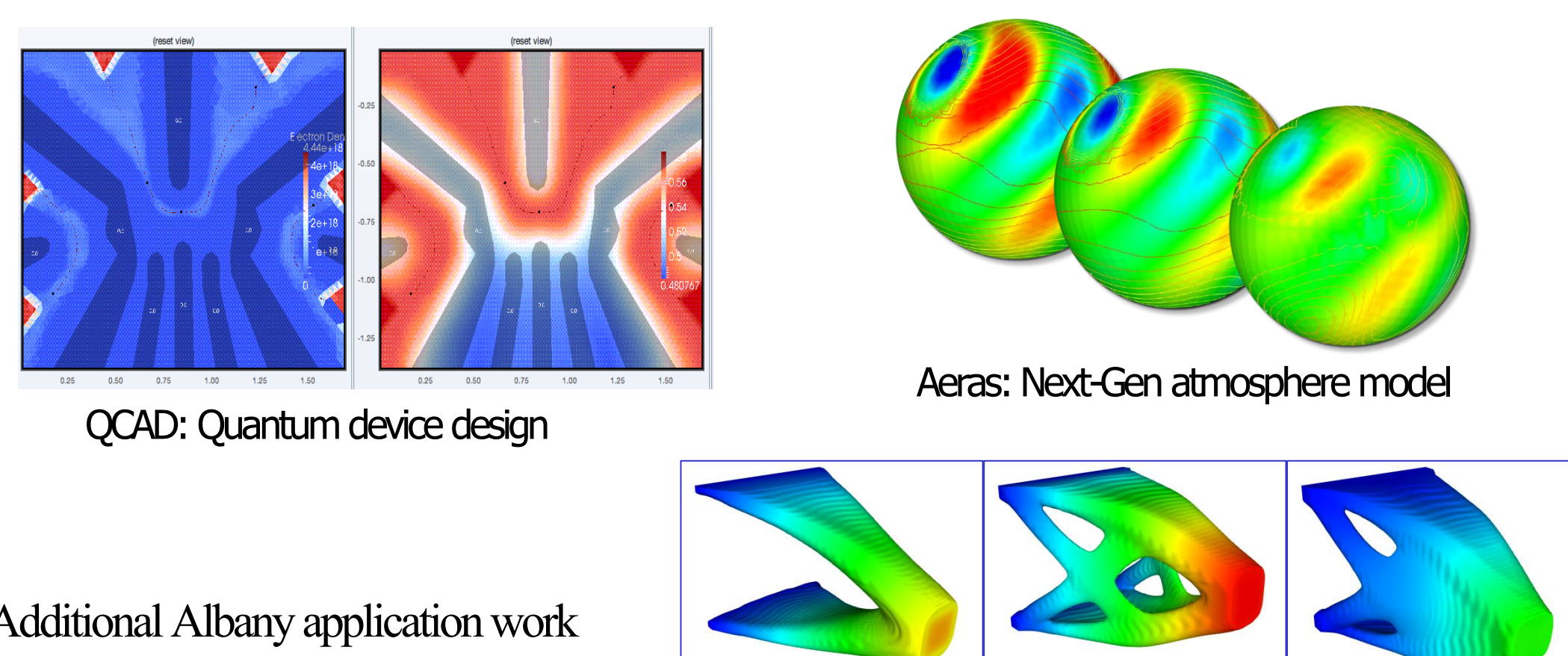
Application Impact: Computational Mechanics

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, detecting scalability issues.
- Research code important for mission customers.

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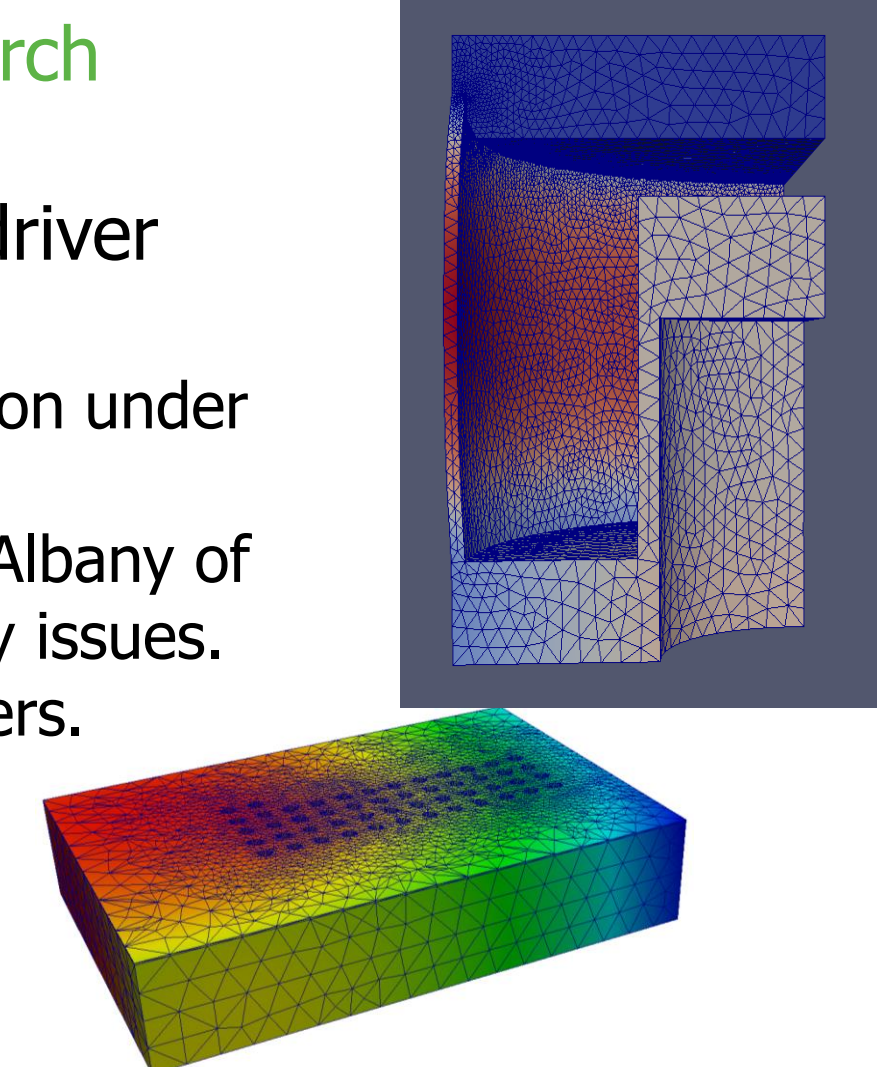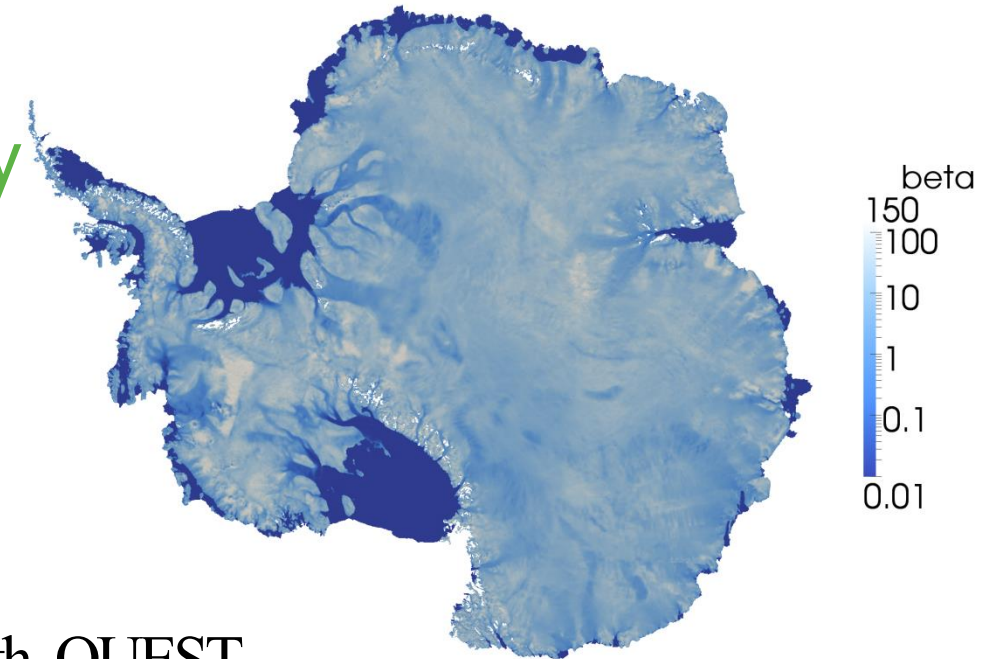

Nonlinear Solvers and Inversion

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

$$\frac{dg}{dp} = \frac{\partial g}{\partial x}^T \frac{\partial f}{\partial x}^{-1} \frac{\partial f}{\partial p} + \frac{\partial g}{\partial p}$$

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
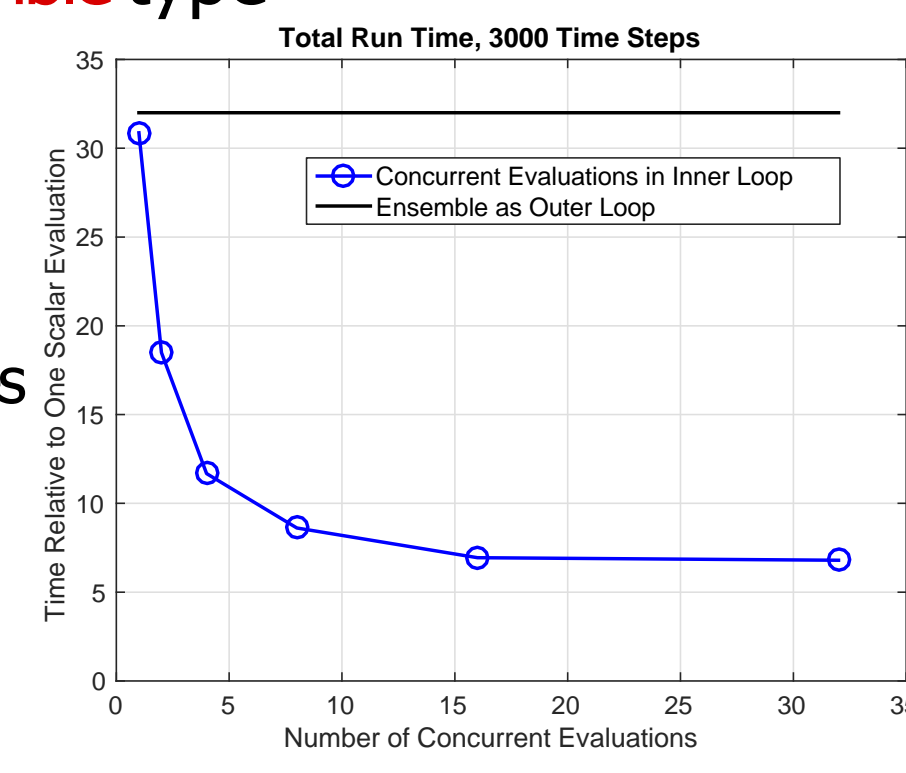 - Impacting NNSA application as well

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

Objective functional: $\mathcal{J}(\mathbf{u}(\beta),\ \beta) = \int_{\Sigma} \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2\, ds + \alpha \int_{\Sigma} |\nabla \beta|^2\, ds$

beta 150 100 10 1 0.1 0.01

Application Code
Albany

Enabling Technologies
DAKOTA   Trilinos   PUMI Parallel Unstructured Mesh Infrastructure

Mesh Adaptivity

Mesh adaptation 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.
  - Remeshing is crucial for large-deformation problems

Adaptive solution loop work in Albany leverages efforts in FASTMath and ASC/ATDM projects.
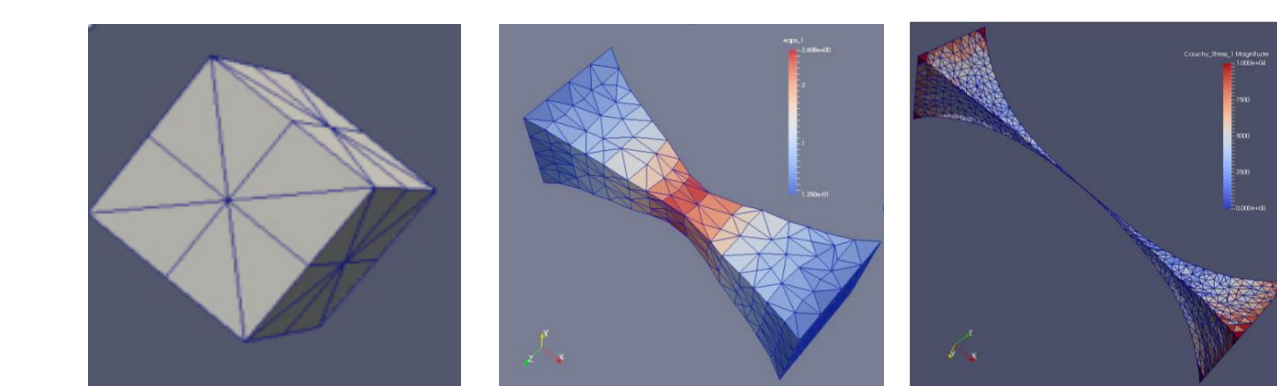
Remeshing of a cube geometry being driven to large deformation by the LCM elasticity and J2 plasticity models.

Deformation of a bracket under loading, showing adapted mesh.

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
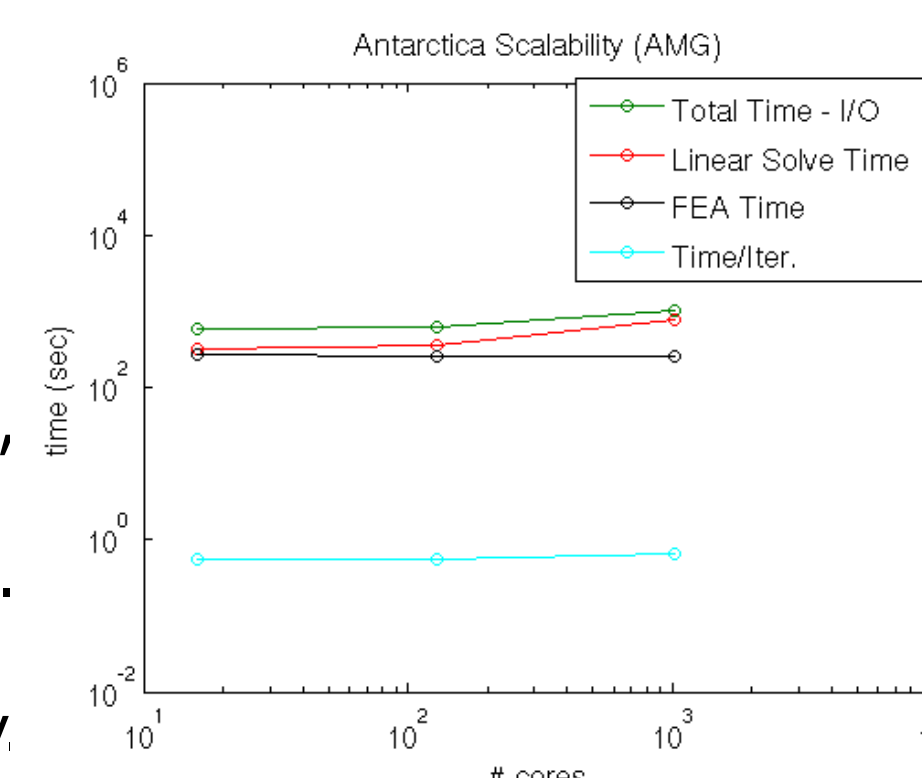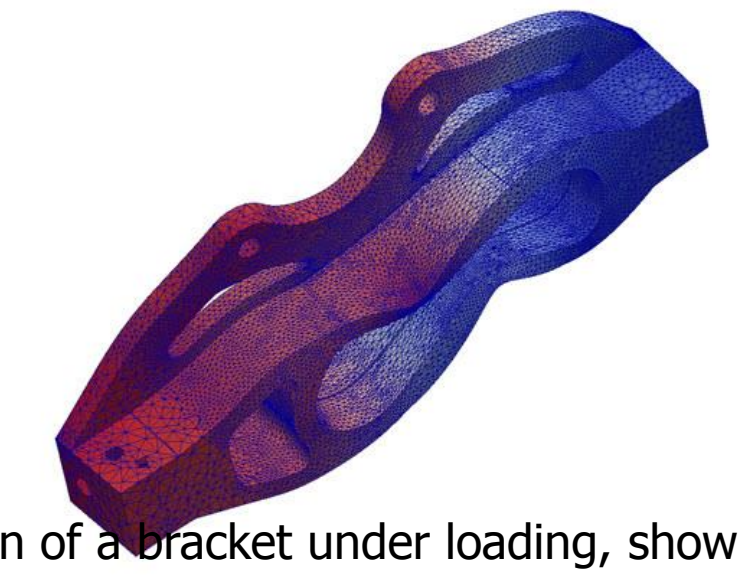- Contiguous memory access for arrays of data

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

Total Run Time, 3000 Time Steps
— Concurrent Evaluations in Inner Loop
— Ensemble as Outer Loop
Time Relative to One Scalar Evaluation / Number of Concurrent Evaluations

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.

Scalable linear algebra work in Albany leverages efforts in FASTMath, ASCR Base Math [Tuminaro], PISCEES, and ASC/ATDM projects.

Antarctica Scalability (AMG)
— Total Time - I/O
— Linear Solve Time
— FEA Time
— Time/Iter.
time (sec) / # cores

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.
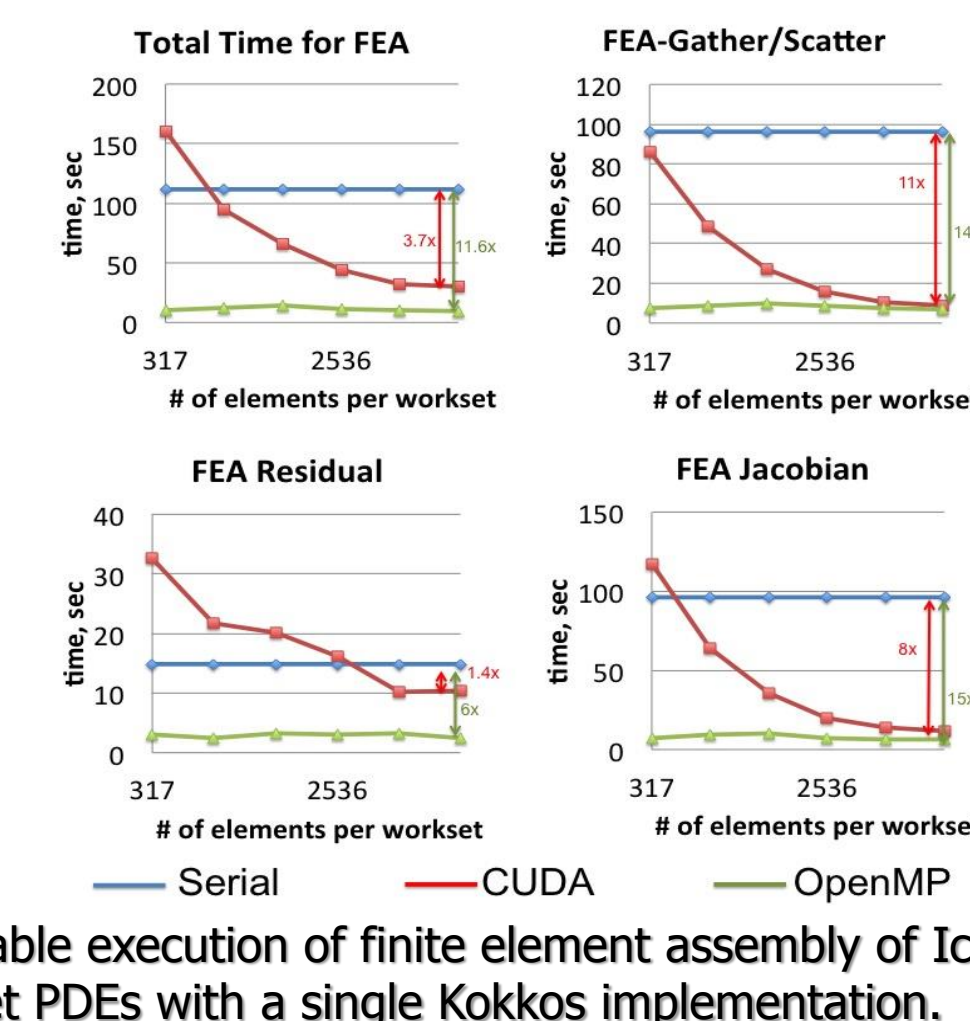
Performance Portability

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 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.

Total Time for FEA   FEA-Gather/Scatter
FEA Residual   FEA Jacobian
— Serial   — CUDA   — OpenMP
# of elements per workset

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

SciDAC Scientific Discovery through Advanced Computing

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