Component-Based Unstructured Mesh Simulation Workflows

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Integration of unstructured mesh technologies with advanced solution methods to impact complex multiphysics applications

Component-Based Unstructured Mesh Simulation

FASTMath components support construction of simulation workflows

- Parallel mesh infrastructure and services
- Dynamic load balancing
- Parallel fields and error estimators
- Parallel mesh optimization/adaptation

Integration with analysis codes to construct adaptive simulation loops

- File-based integration requires no analysis code modification
  - Often first approach implemented
- In-memory methods developed that minimize code modifications
  - Improves efficiency – avoids I/O bottleneck

Integration with component-based analysis code provides increased flexibility and performance opportunities

- Albany FE code based on Agile Component approach
  - Take advantage of Trilinos and Dakota components
  - In-memory integration for adaptivity natural
  - Opportunities for optimization and uncertainty quantification

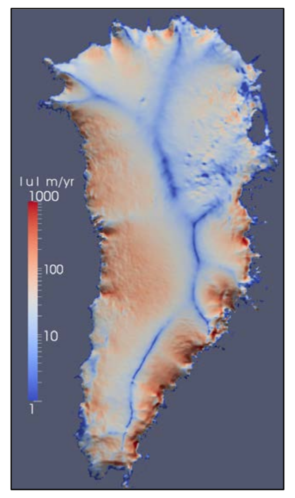
Albany – Agile Components

A parallel, implicit, unstructured mesh finite element code

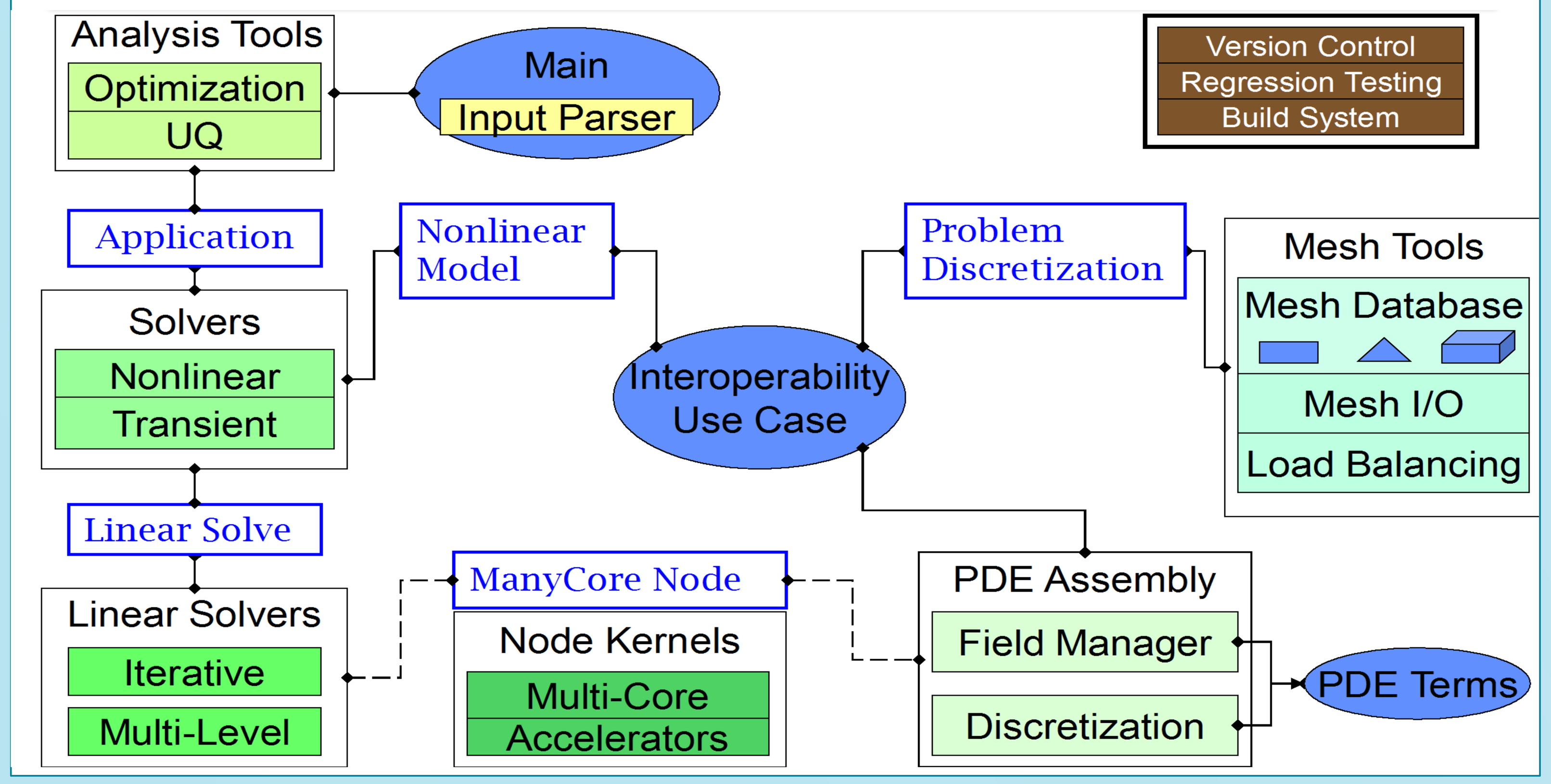
- Being applied to problems from ice sheet modeling to large deformation based structural failures

Build on over 100 component pieces

- Components include
  - Libraries – solvers, UQ, Optimization
  - Interfaces – parallel meshes
  - Software quality control tools
  - Demonstration applications



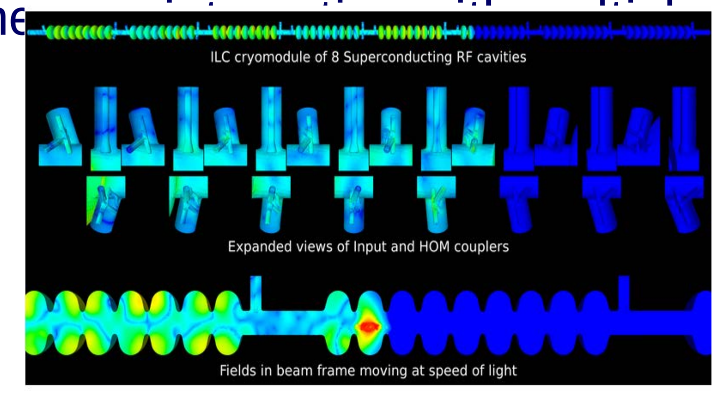
Greenland Ice Sheet Surface Velocities (constant friction model)



Component-Based Adaptive Simulation

Goal is to execute massively parallel, automated, adaptive simulations

- Employ a component-based approach using FASTMath unstructured mesh components – PUMI, APF, Zoltan, ParMA, MeshAdapt
- Support direct geometry interfaces design data
- Integrated with automatic meshing technologies
- Support both file-based and/or in-memory integration with multiple analysis codes

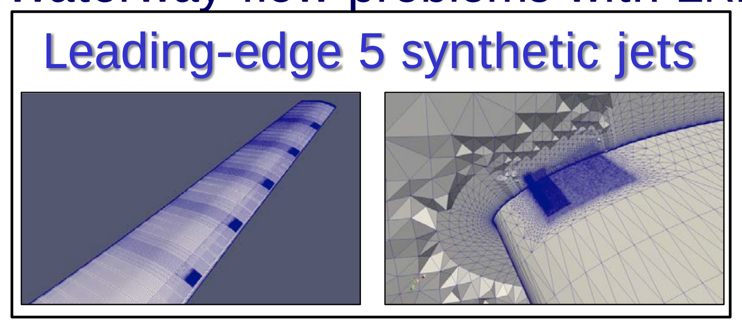


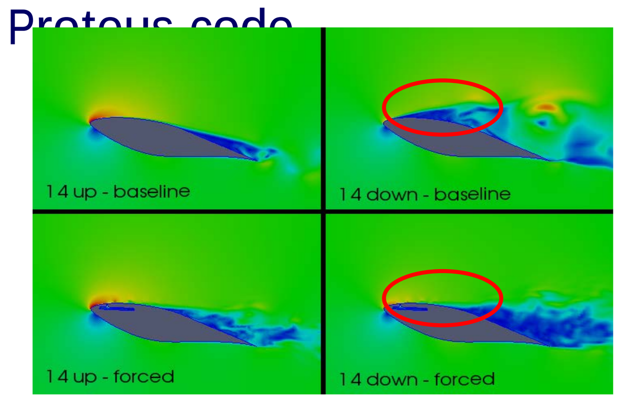
Key current development efforts

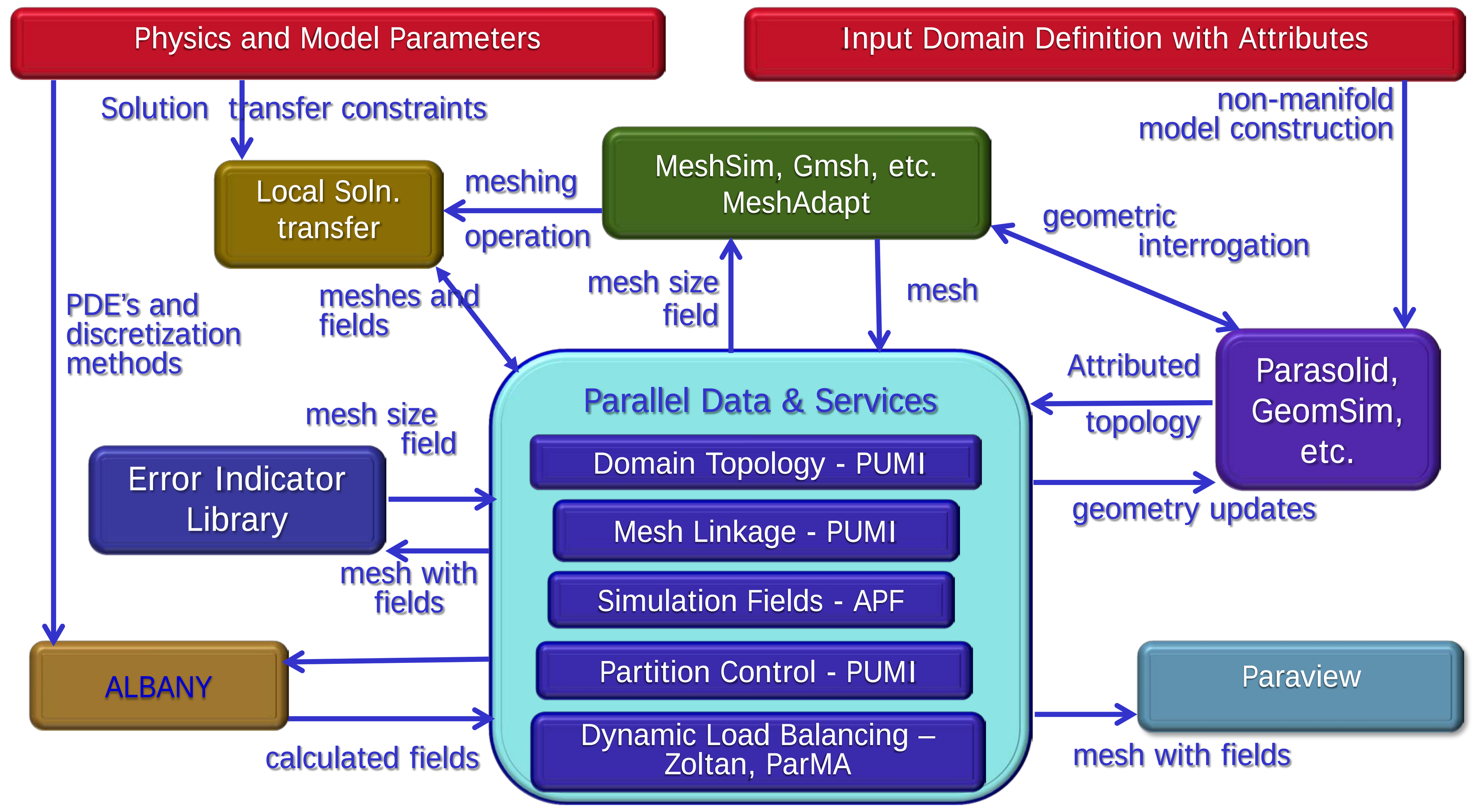
- Parallel fields
- Generalized error estimation library
- Multiple load balancing methods to improve parallel efficiency

Parallel adaptive loops developed to date:

- Modeling of nuclear accidents and various flow problems with PHASTA (meshes up-to 92B elements on ¾ cores)
- Accelerator modeling problems with SLAC's ACE3P code
- Fusion MHD with PPPL's M3D-C1 code
- Solid mechanics applications with Albany (see boxes to right)
- Aerodynamics problems with NASA's Fun3D code
- Waterway flow problems with ERDC's Proteus code







Parallel Adaptive Simulations with Albany

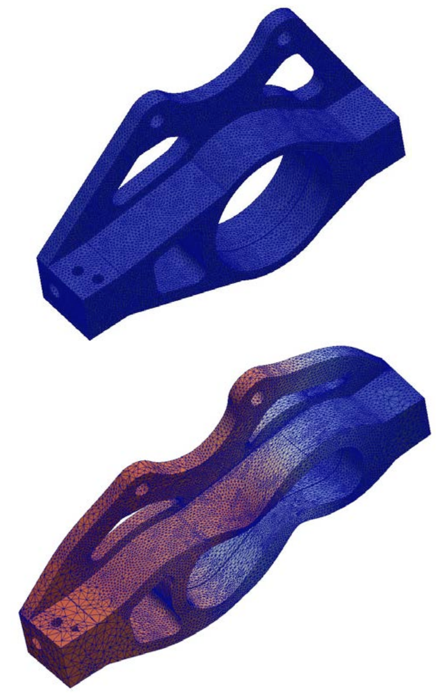
Modeling Large Deformation Structural Failures

Adaptive simulations of finite deformation plasticity with Albany

- Projects include modeling large deformations and weld failures

Efforts to develop adaptive loops that support

- Solution accuracy via error estimation
- High quality element shapes at all load steps
- Accurate solution transfer of state variables
- Predictive load balancing (ParMA, Zoltan) at each adaptive stage



Mechanical Modeling of Integrated Circuits

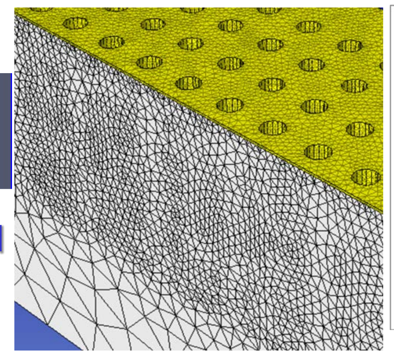
Microelectronics processing is very exacting and mechanical responses impact reliability and manufacturability

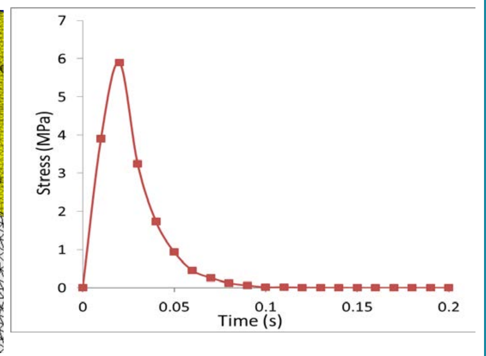
Multi-layer nature of chips interacts with temperature swings, creep, and intrinsic stress of films

- Parallel adaptive simulations of wafer deformation using industry layout formats as inputs to model construction
- Intrinsic stress in film deposited onto surface and into features causes macroscopic deflection of wafer – Interferes with further processing
- Creep occurs in solder joints during use, delamination during cool-down
- Developed combined constitutive model of thermoelastic, plastic, and creep contributions in ALBANY

(below) Displacement vs time curves for combined thermo-elastic, plastic, and creep model.

(right) automatically generated model and mesh from layout file including thin film. (above) Wafer deflection (scaled)





Future Plans

- Tighter integration to geometric model including smooth geometry update for adapting for large deformations, automatic geometry construction, distributed geometry
- Curved mesh adaptation to support higher order methods
- Generalization of the error estimation procedures and move to goal oriented adaptation
- Adjoint calculation component for use in error estimation, optimization and uncertainty quantification

More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130

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