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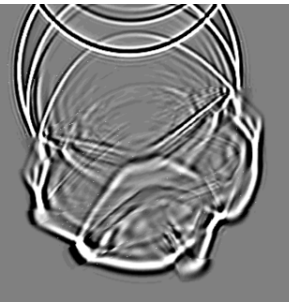

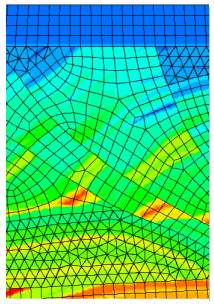

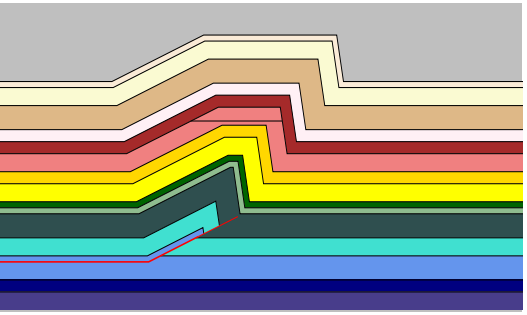

Capability and Application Highlights for HPC in the Center for Computing Research

Curtis C. Ober
Principal Member of the Technical Staff
Multiphysics Applications

Pioneer Natural Resources, Oak Ridge National Laboratories, and Sandia National Laboratories Workshop

Time: 2/21/2017 11:45am - 1:00 PM
Location: 823/4304

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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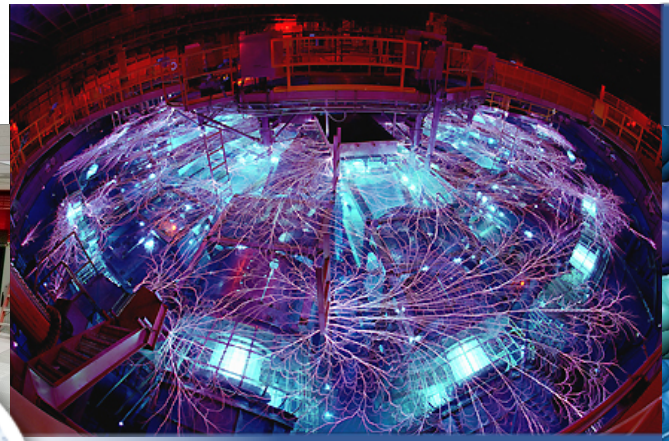
Sandia's Research Framework

Research foundations drive capability development

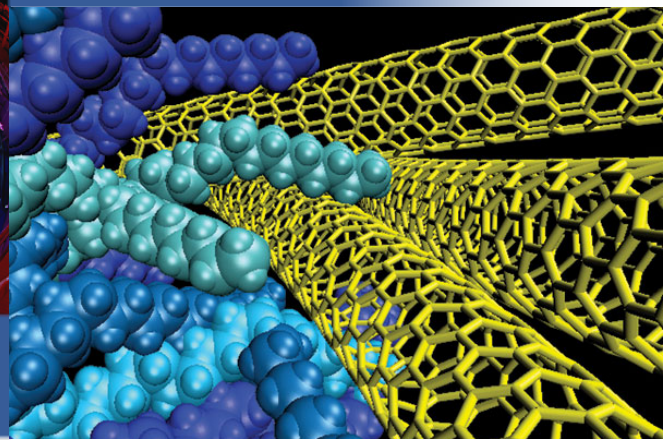
Sandia National Laboratories

Computing & Information Sciences

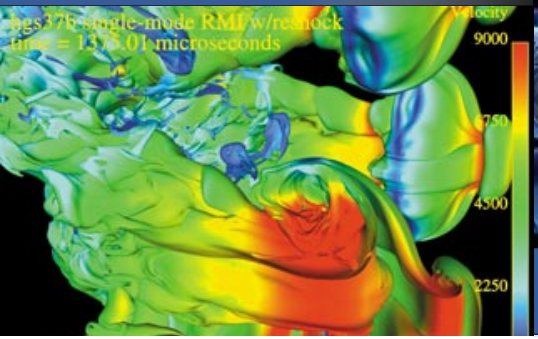
Radiation Effects & High Energy Density Science



Materials Sciences

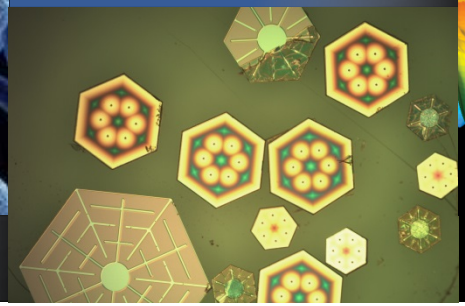


Engineering Sciences

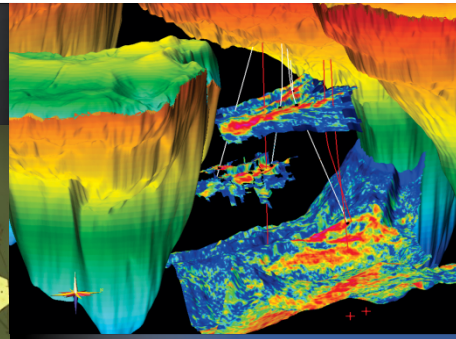


Bioscience

Nanodevices & Microsystems

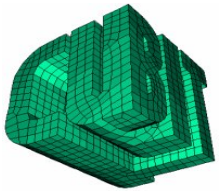


Geoscience



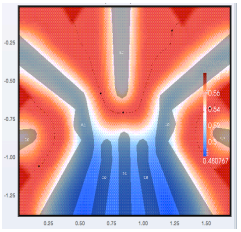
Multidisciplinary Collaborative Research

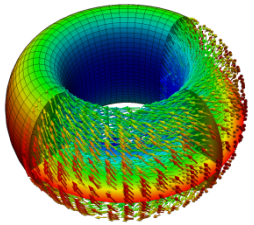
Sandia National Laboratories

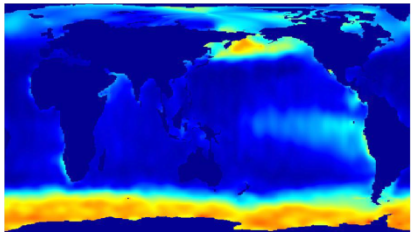


Trilinos

DAKOTA

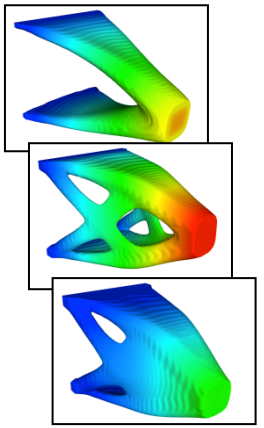






Leading Edge Algorithms and Enabling Technologies

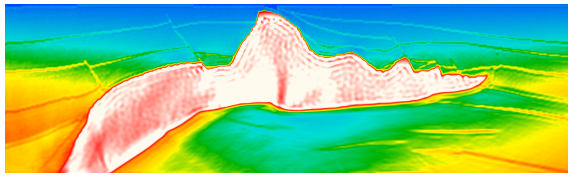
State-of-the-art Computational Science Applications

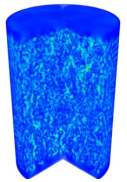


Albany

Multigrid Framework MueLu

ROL

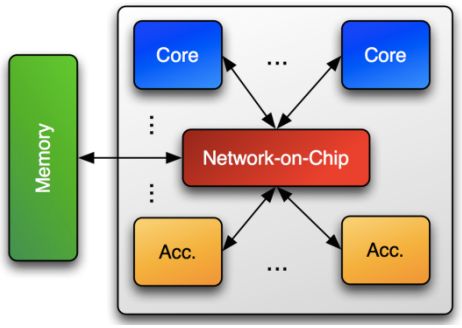




Scalable HPC Architecture and Systems Research

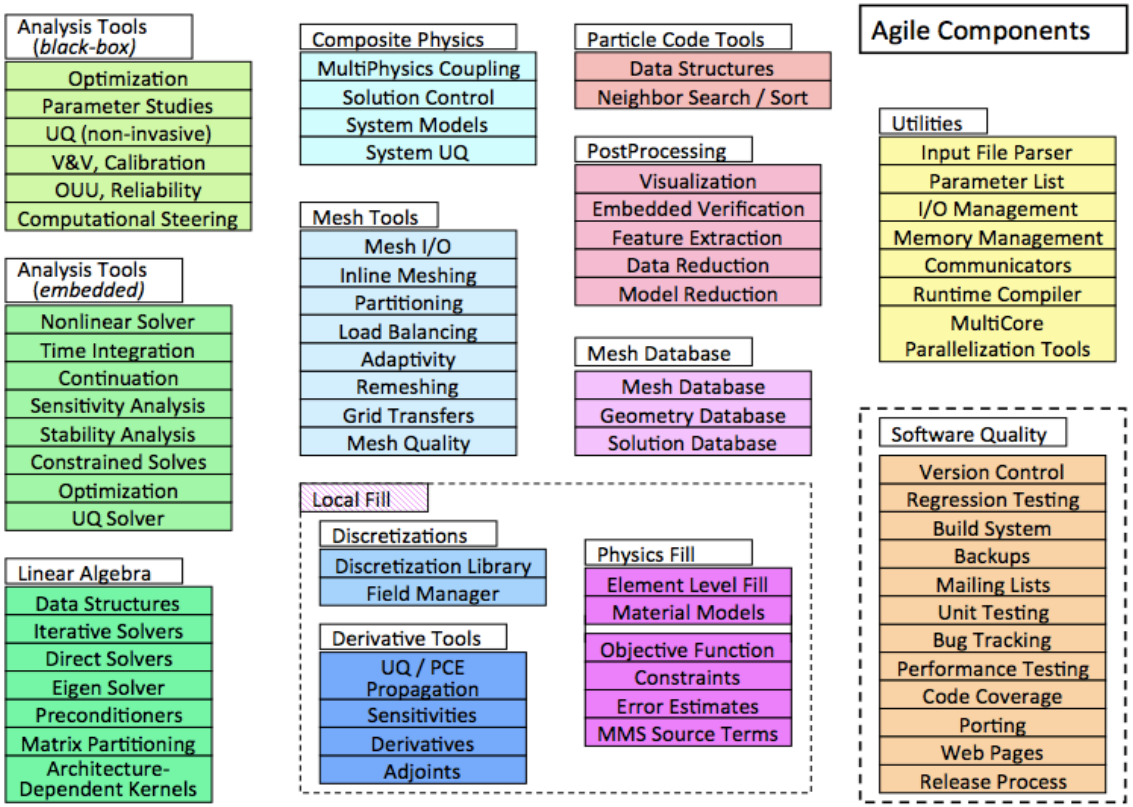
Strong External Collaborations

CENTER FOR COMPUTING RESEARCH



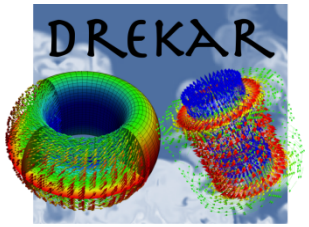
Trilinos & Agile Components

- Future flexibility for application codes relies on integrated component-based software – ***Agile Components***
- Object-oriented software framework for solving large complex science & engineering problems.
- Trilinos is made of packages (not monolithic). Use the set of packages you choose.
- Each package developed by domain experts – Substantial algorithms R&D foundation.
- Many Trilinos-based codes.

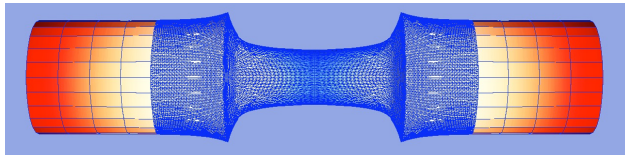


Algorithm Capabilities

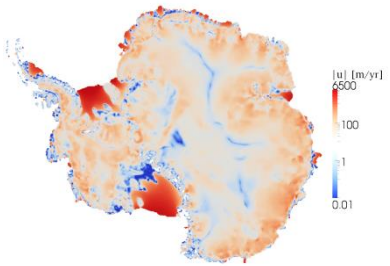
- Trilinos provides the foundational capabilities, but they must still be integrated into functioning applications. Here are a few:
- Drekar – Extreme scale magneto-hydrodynamics

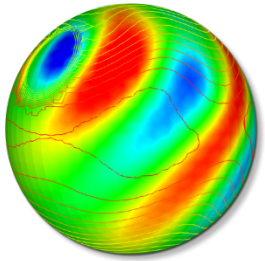


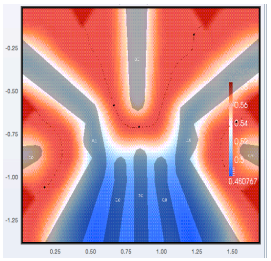
- Albany – Open-source framework for multiphysics application codes

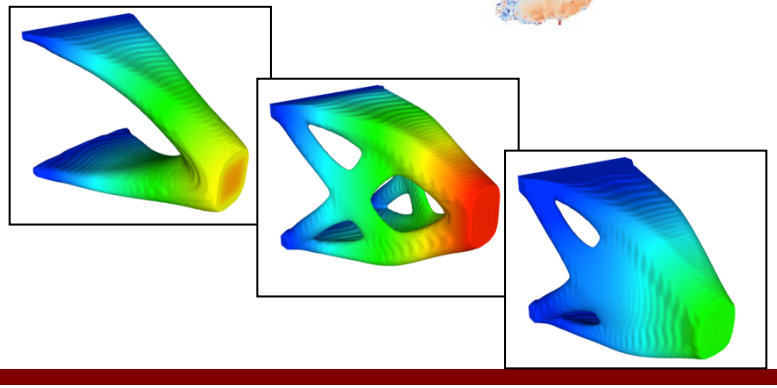


- Albany-based codes include:
  - Laboratory for Computational Mechanics (LCM)
  - Ice Sheet Code (FELIX)
  - Advanced Topology Optimization (ATO)
  - Quantum Dot Computer Aided Design (QCAD)
  - Atmosphere modeling (Aeras)





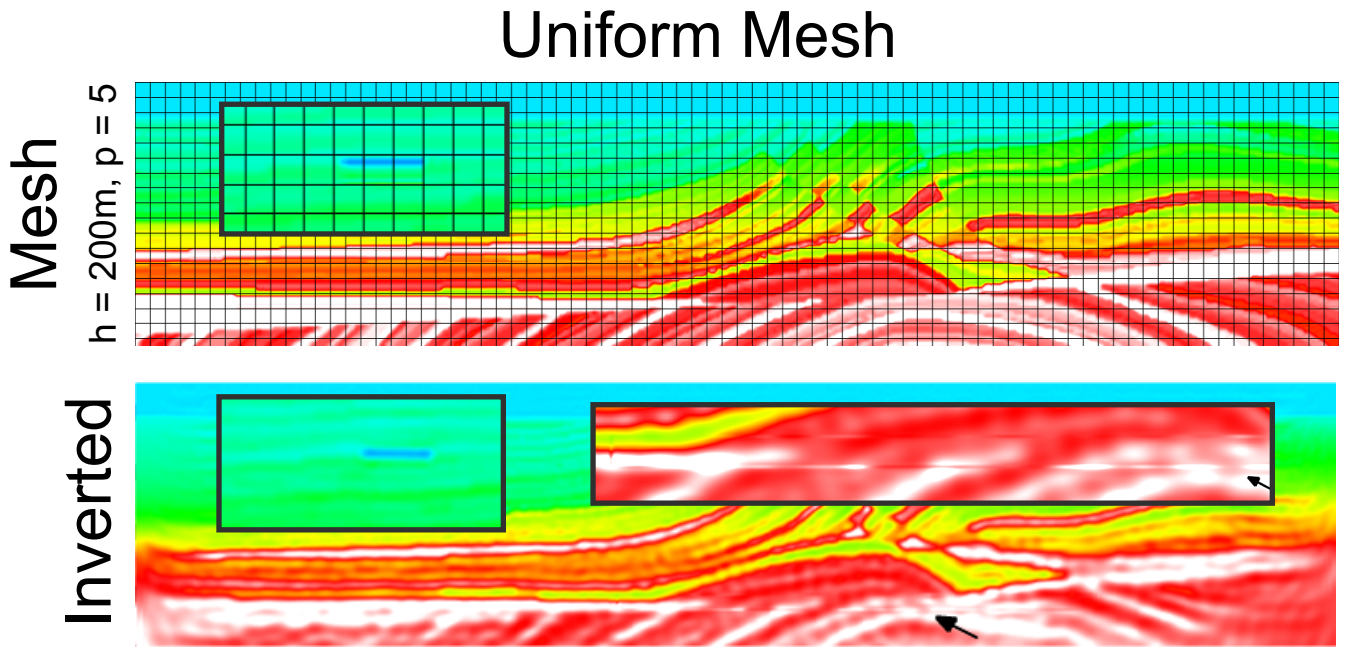




Full-Waveform-Inversion Capability

Sandia National Laboratories

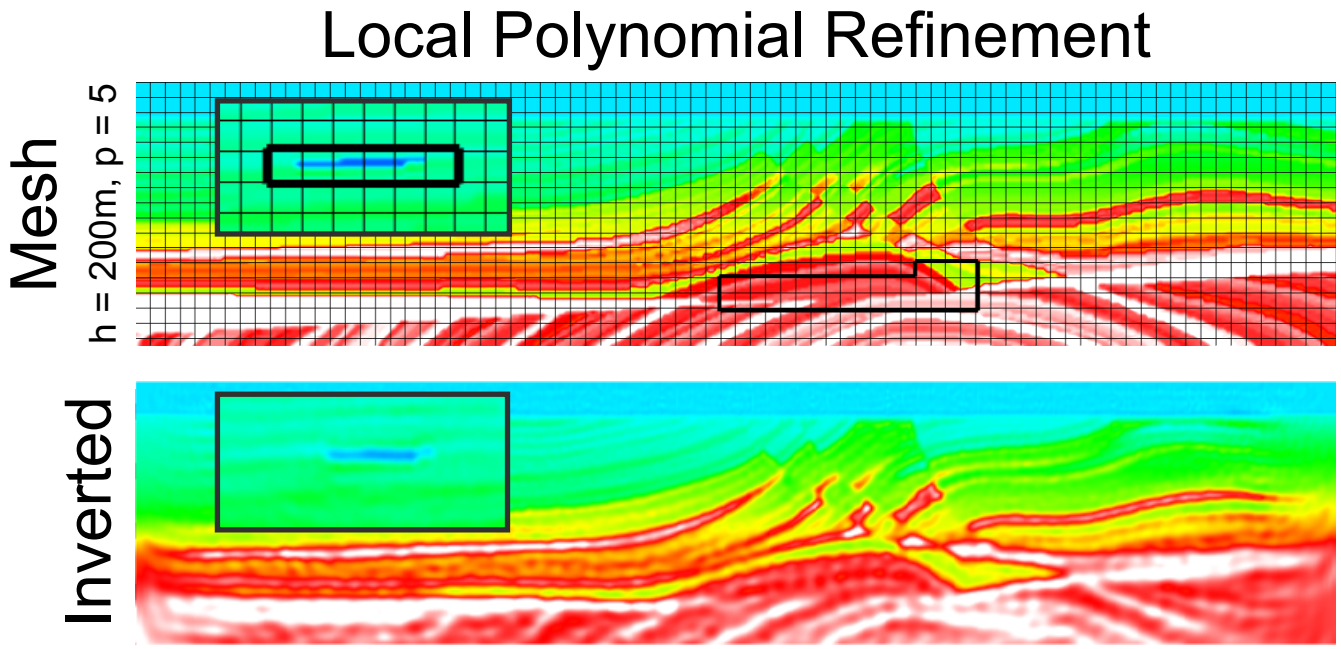
- Discontinuous Galerkin discretization
  - Unstructured meshes
  - Variable-order polynomial representation
    - For both the solution and the media
  - Local polynomial de-/refinement
  - Curved and non-simplicial elements



Full-Waveform-Inversion Capability

Sandia National Laboratories

- Discontinuous Galerkin discretization
  - Local polynomial de-/refinement
    - For both the solution and the media
  - Unstructured hybrid meshes
  - Non-conformal meshing
  - Curved and non-simplicial elements



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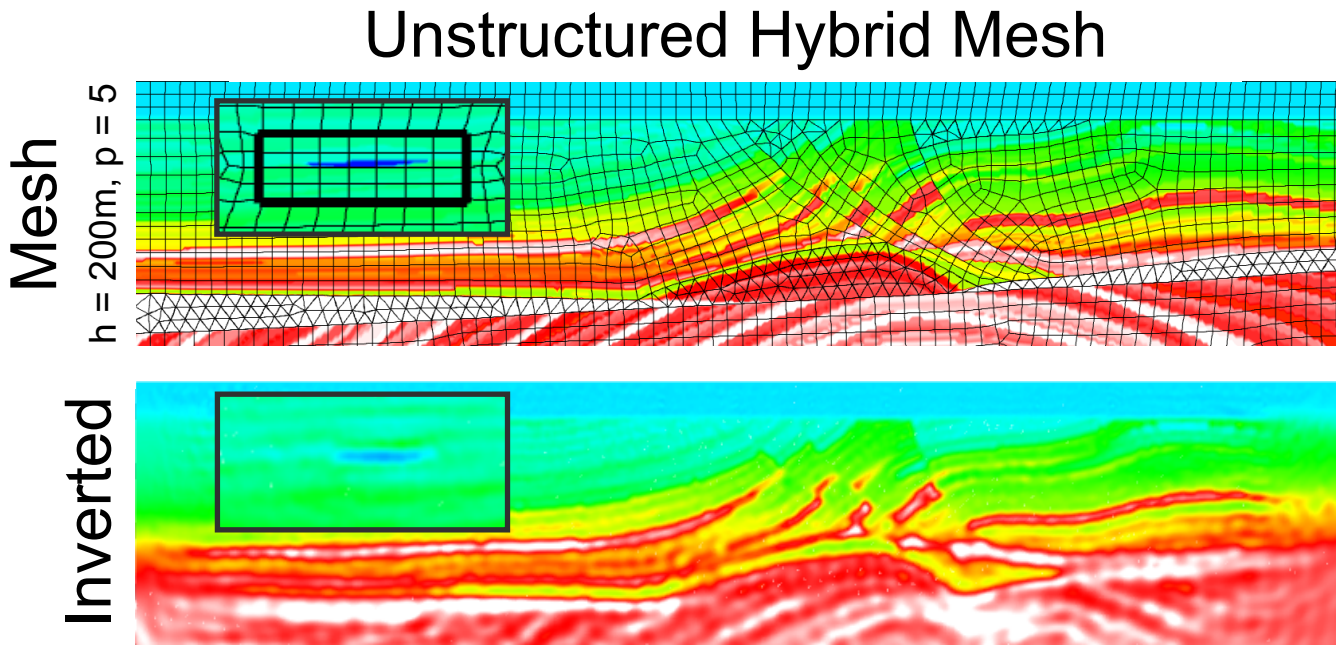

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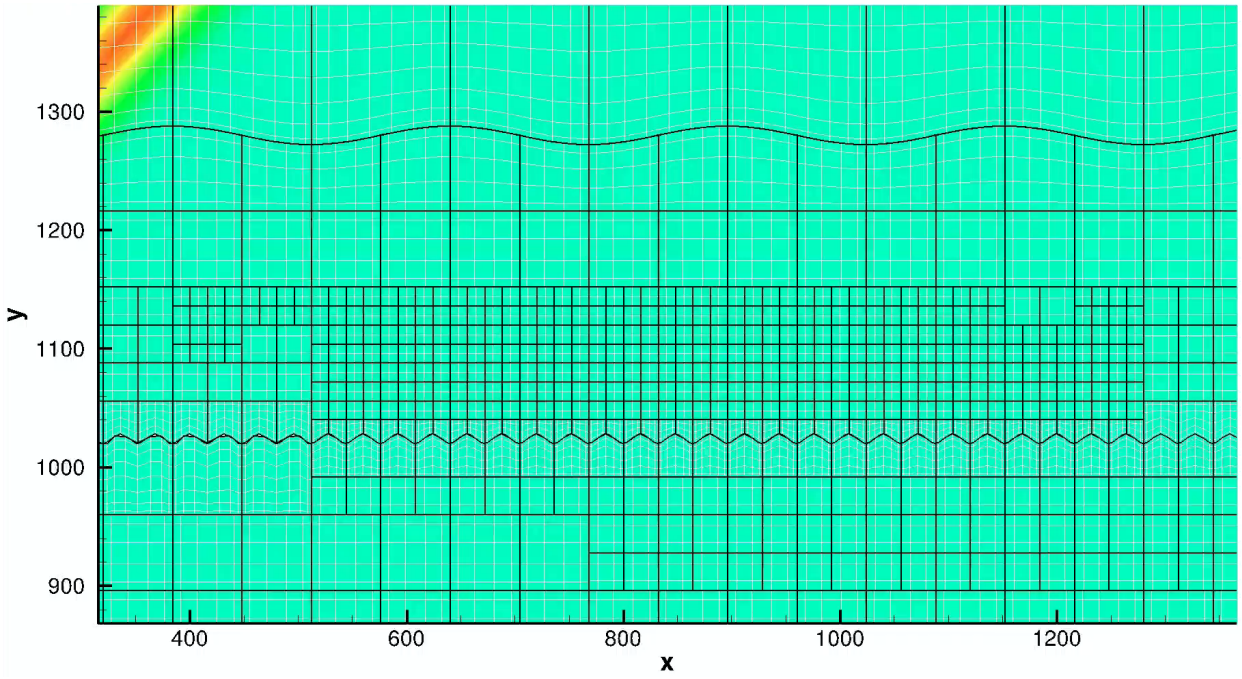
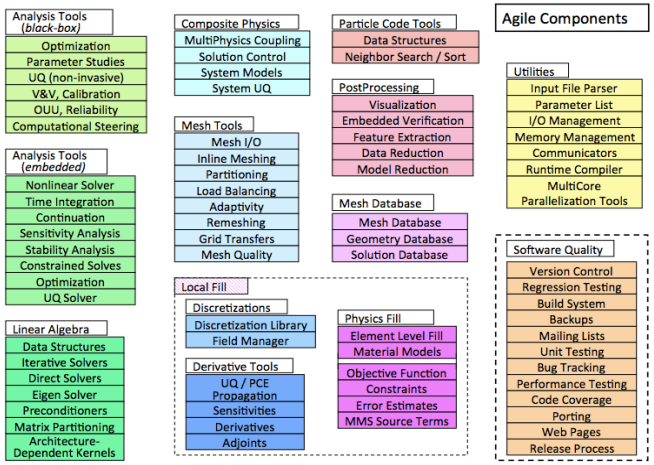


Full-Waveform-Inversion Capability

Sandia National Laboratories

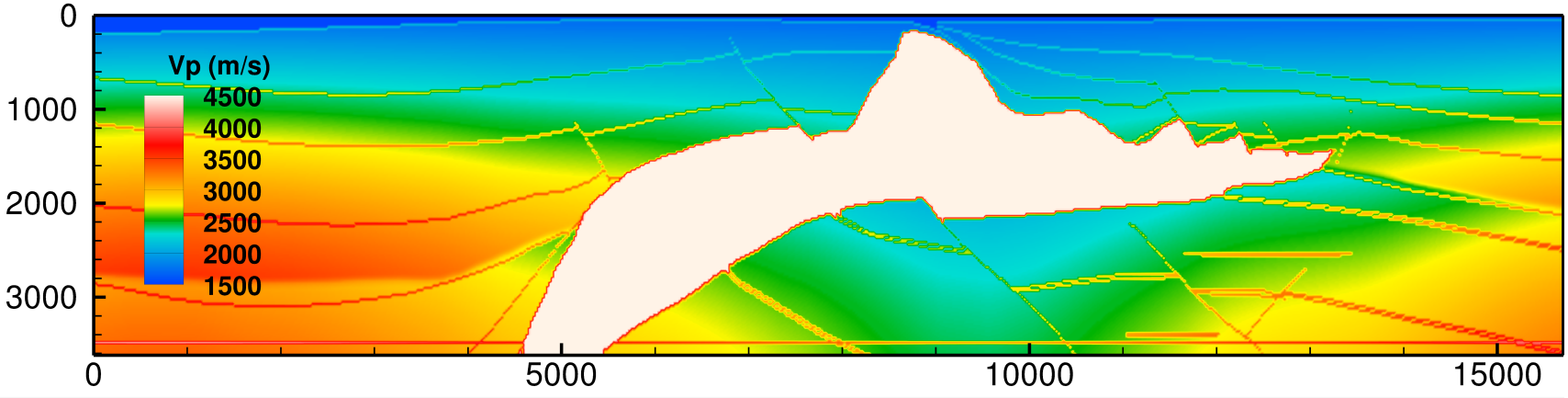
- Discontinuous Galerkin discretization
  - Local polynomial de-/refinement
    - For both the solution and the media
  - Unstructured hybrid meshes
  - Non-conformal meshing
  - Curved and non-simplicial elements
- Component Technology
  - Built on DGM Library (Discontinuous Galerkin Method)
    - Component-based software design for DG
  - Agile Components
    - Access to Trilinos - Zoltan, Rythmos, ROL and Dakota
  - Multiple physics (acoustic, elastic and attenuation)
- Optimization and Inversion
  - Transient optimization
  - Adjoint-based optimization/inversion



SEG 2D Salt Model Inversion

Sandia National Laboratories

True Model



Inverted Model