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Developing Inverse Capabilities to Support Computational Modeling of Complex Applications

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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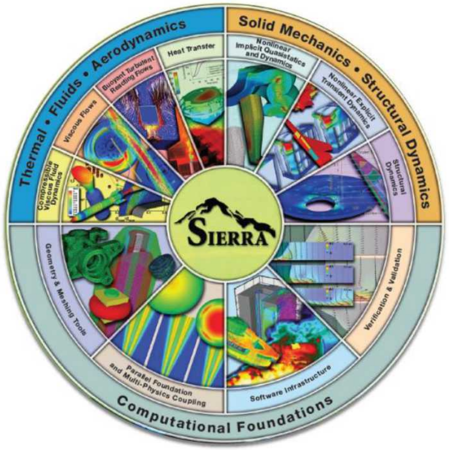

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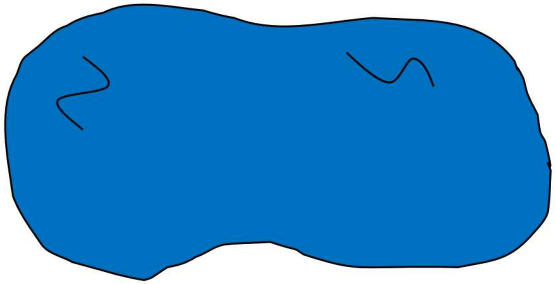
Inverse Problems: Observing the Unobservable

Suppose we have a “black box” system in the *as-manufactured* state that has only partially known parameters

Question: can we *non-destructivel*y interrogate the system to “see what is inside”?



Typical quantities of interest:

- Material properties
- Loads
- Boundary conditions
- Residual stresses
- Size/shape/location of inclusions (e.g. composite materials)

Example applications:

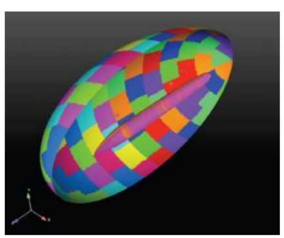
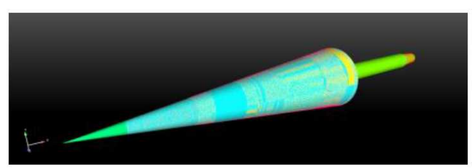
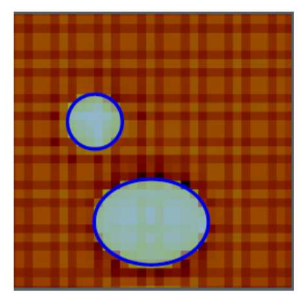
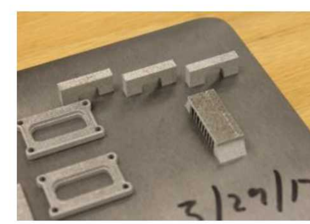
- Seismic imaging
- Medical imaging
- Non-destructive evaluation

Categories of Inverse Problems

- Imaging
  - Medical ultrasound
  - Seismic exploration
- Calibration of material models
  - Structural material properties, circuits, thermal properties, etc.
- Force reconstruction
  - Sub-structuring for mechanical testing of components
- Optimal Experimental Design
  - Best placement of sensors, test fixture setups
- Shape reconstruction
  - E.g. inverse scattering

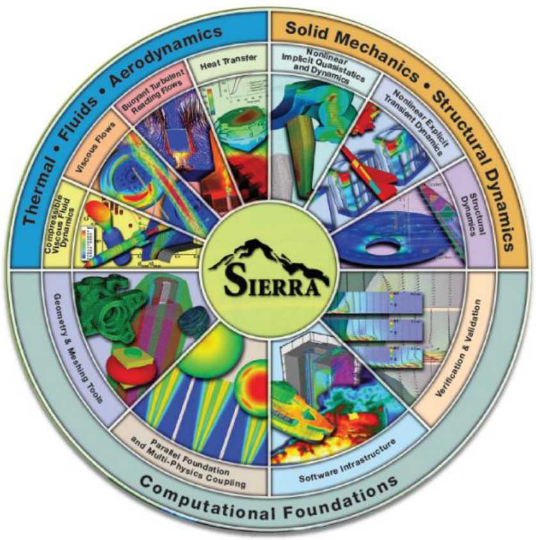
Research Challenges in Inverse Problems: Sandia Applications

- 3D models required since measurements at several locations
- Large parameter spaces/high-dimensionality of inverse problem
  - Spatially-varying material parameters
  - Temporally-varying functions (boundary conditions, loads, etc)
- Rolling uncertainty quantification into the inverse problem: 2 approaches
  - Stochastic optimization
  - Bayesian methods

Inverse Problem Strategy in Sierra

Finite Element and Optimization Codes operate as independent entities



Objective function, derivative operators

Next iterate of design variables

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Sierra Mechanics – massively parallel multiphysics simulation

Gradient-based optimization (adjoint methods used to compute gradients)

Inverse Capabilities in Sierra

Enabling adjoint-based inversion capabilities across Sierra Mechanics

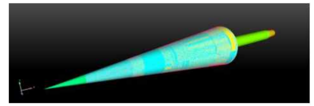
2010

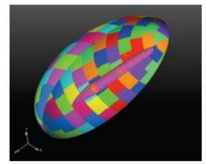
Sierra-SD

Aquino sabbatical

source identification

material identification

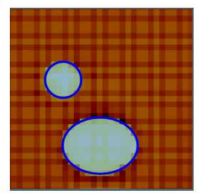




2014

contact identification
- welds, delaminations

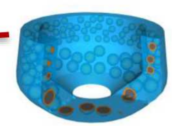
residual stress



2016

Sierra 4.42 release

metamaterial design



InverseOpt toolkit

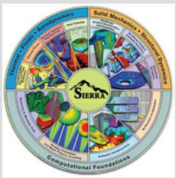
Aria/Fuego thermal conductivity unit tests

today

- Example applications
  - Force/material/contact area reconstruction (structural, acoustic, and thermal)
  - Viscoelastic material parameter identification
  - Thermal flux, conductivity distributions (under development)
  - Additive Manufacturing: residual stress, acoustic metamaterials

Use Cases for Inverse Problems

Adjoint-based inversion enables new use cases for Sierra Apps



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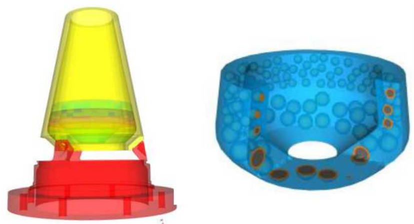
Experiment

InverseOpt Toolkit

Enables use cases

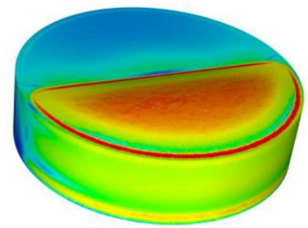
Flux boundary conditions

Source Reconstruction



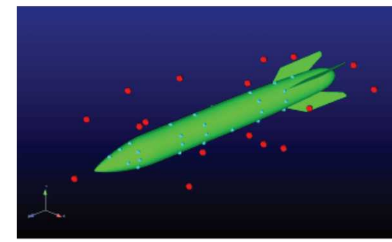
Thermal/mechanical material reconstruction, residual stress, metamaterial design

Material/residual stress Reconstruction



Delamination/weld characterization

Contact surface Reconstruction



Ground-based acoustic/thermal tests

Design of Experiments

Sierra-SD, Sierra-SM, Sierra-TF
with embedded sensitivities (adjoints, etc)

Goal: enable all Sierra apps to reconstruct forces, materials, contact surfaces, and assist in designing experiments

Uniqueness: CompSim-enabled inverse optimization that provides capabilities for the above use cases

PDE-Constrained Optimization Formulation

Abstract optimization formulation

$$\underset{\boldsymbol{u},\boldsymbol{p}}{\text{minimize}} \quad J(\boldsymbol{u},\boldsymbol{p})$$

Objective function

$$\text{subject to} \quad \boldsymbol{g}(\boldsymbol{u},\boldsymbol{p}) = \boldsymbol{0}$$

PDE constraint

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{w}) := J + \boldsymbol{w}^T\boldsymbol{g}$$

Lagrangian

$$\begin{Bmatrix} \mathcal{L}_u \\ \mathcal{L}_p \\ \mathcal{L}_w \end{Bmatrix} = \begin{Bmatrix} J_u + \boldsymbol{g}_u^T\boldsymbol{w} \\ J_p + \boldsymbol{g}_p^T\boldsymbol{w} \\ \boldsymbol{g} \end{Bmatrix} = \{0\}$$

First order optimality conditions

$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{up} & \boldsymbol{g}_u^T \\ \mathcal{L}_{pu} & \mathcal{L}_{pp} & \boldsymbol{g}_p^T \\ \boldsymbol{g}_u & \boldsymbol{g}_p & 0 \end{bmatrix} \begin{Bmatrix} \delta\boldsymbol{u} \\ \delta\boldsymbol{p} \\ \boldsymbol{w}^\star \end{Bmatrix} = -\begin{Bmatrix} J_u \\ J_p \\ \boldsymbol{g} \end{Bmatrix}$$

Newton iteration

$$\boldsymbol{W}\Delta\boldsymbol{p} = -\hat{J}',$$

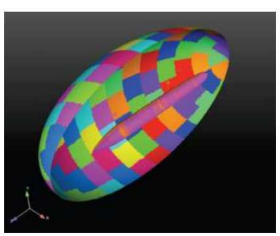
$$\boldsymbol{W} = \boldsymbol{g}_p^T\boldsymbol{g}_u^{-T}(\mathcal{L}_{uu}\boldsymbol{g}_u^{-1}\boldsymbol{g}_p - \mathcal{L}_{up}) - \mathcal{L}_{pu}\boldsymbol{g}_u^{-1}\boldsymbol{g}_p + \mathcal{L}_{pp}$$

Hessian calculation

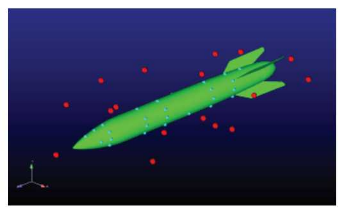
Example: Source Reconstruction

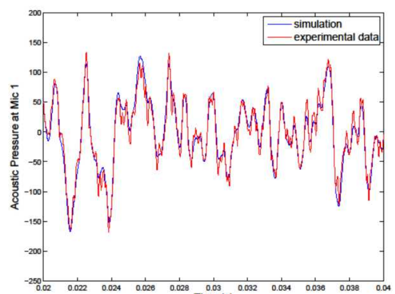
- Goal: reconstruct structural, thermal, and/or acoustic energy sources that produce the given accelerometer/temperature/microphone measurements
- Large parameter space – time histories for pressure functions
- Sensor placement – design of experiments

<u>Structural loads</u>
Attachment forces from accelerometer measurements



<u>Acoustic loads</u>
- Pressure distributions from microphone measurements





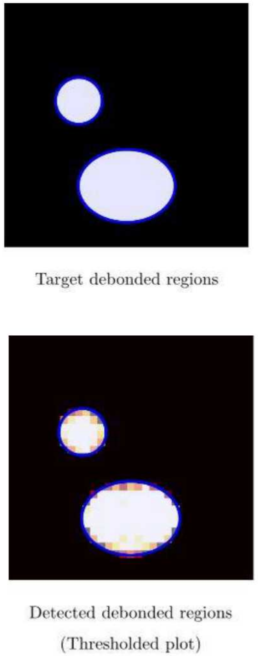
<u>Thermal flux loads</u>
Flux distributions from temperature measurements

Fire flux boundary conditions

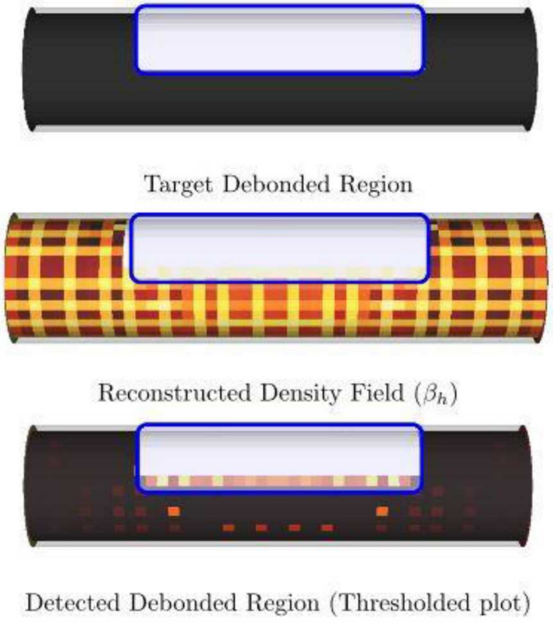
Example: Partially Connected Surfaces

- Partially-bonded plates/cylinders – can we invert for the bonded/debonded regions?
- Large parameter space – number of FEM modes on surfaces

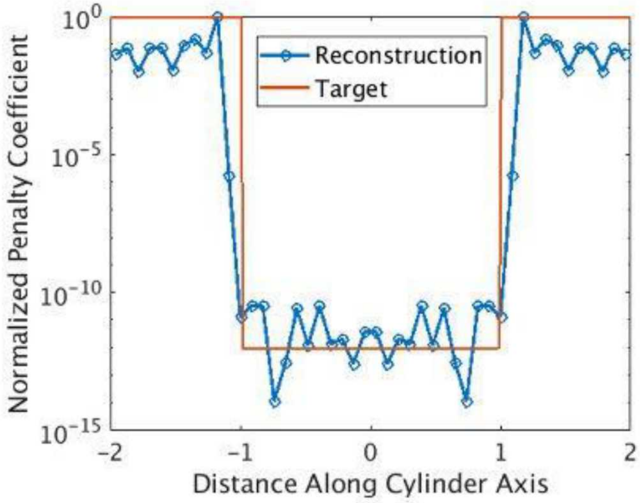
Frequency-domain pressure load at 2000Hz



Partially bonded plates



Partially bonded cylinders



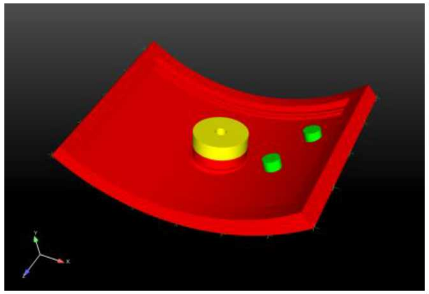
Line plot through delaminated area

Example: Material Parameter Extraction

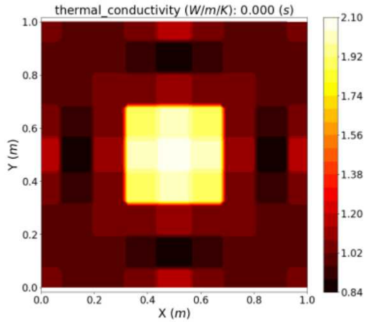
Problem: in-situ material parameters often unknown

- Parameters not measurable without destroying structure
- Interrogate material with mechanical/thermal inputs
- Measure response, infer missing in-situ properties
- Large parameter space – spatially-varying parameters

Viscoelastic material and joint stiffness extraction using Sierra-SD



Orthotropic material extraction for composite panel using Sierra-SD



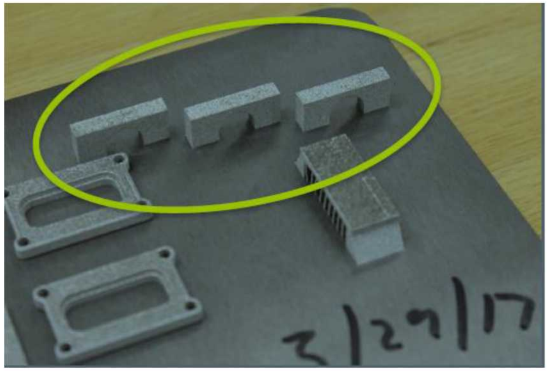
Reconstructed thermal conductivity from Sierra-TF (Fuego)

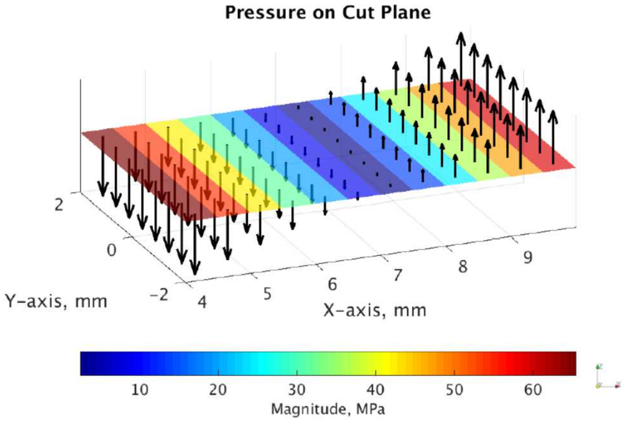
Example: Residual Stress Extraction

Problem: additively manufactured parts suffer from large residual stresses

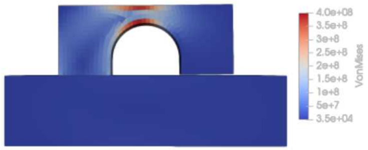
- Compromises part integrity
- FEM modeling needs stresses for initial conditions
- Stress is not a measurable quantity
- Large parameter space – spatially-varying stress fields

Goal: estimate residual stress fields from measured displacement data (digital image correlation)





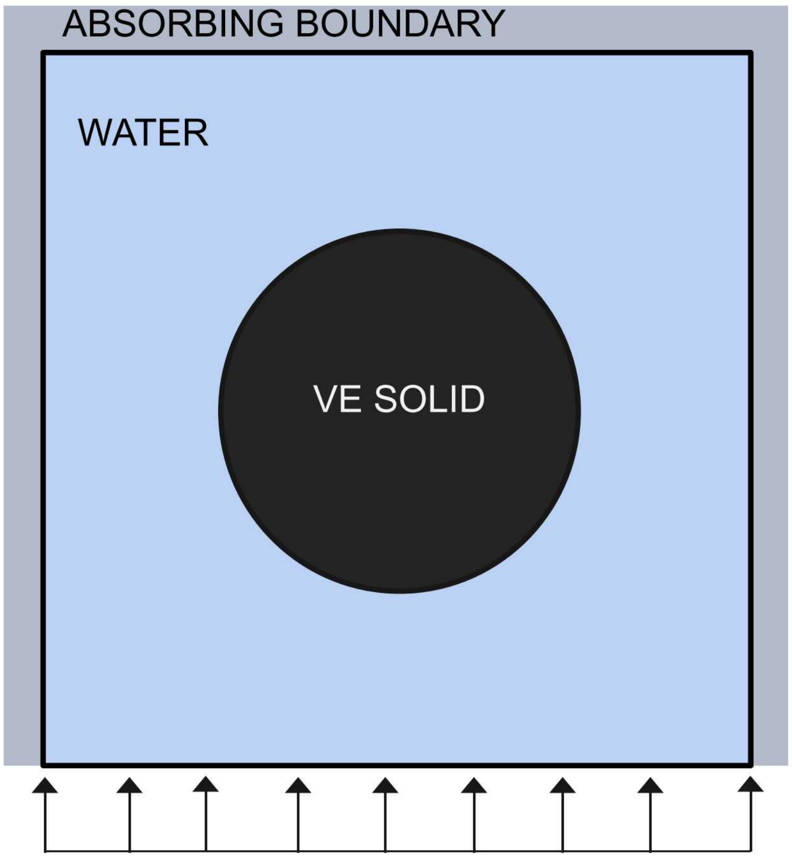
Predicted traction field from inverse solution (Sierra-SD)

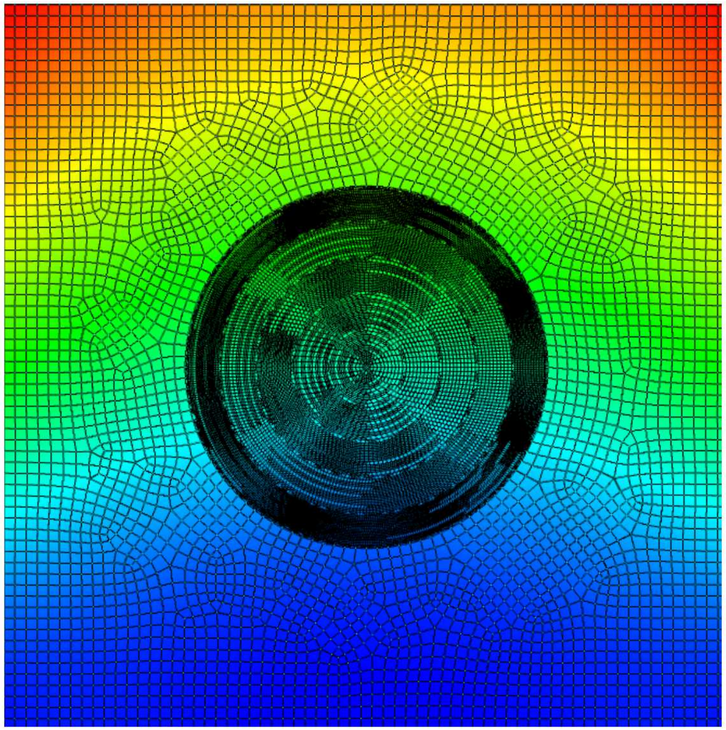


Reconstructed stress field from inverse solution (Sierra-SD)

Inverse Problems: *Acoustic Cloaking*

- 2-D fluid region with circular VE solid inclusion
- Inclusion consists of concentric rings w/ distinct material properties
- Periodic acoustic load applied to end
- Match forward problem pressure distribution by adjusting **VE material parameters**

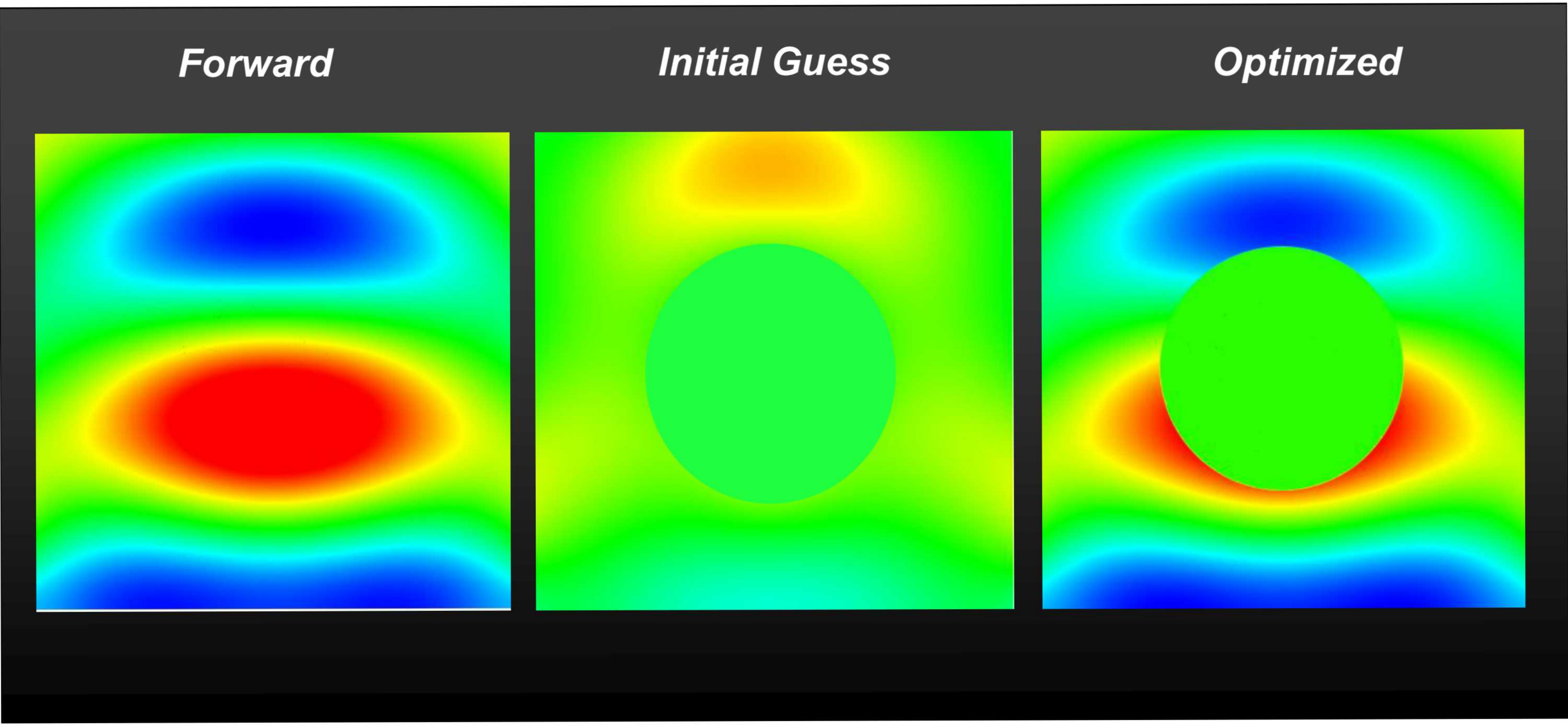




Left: Model Set up
Right: Forward problem pressure distribution (500 Hz loading) in model with 50 layers

Acoustic Cloaking

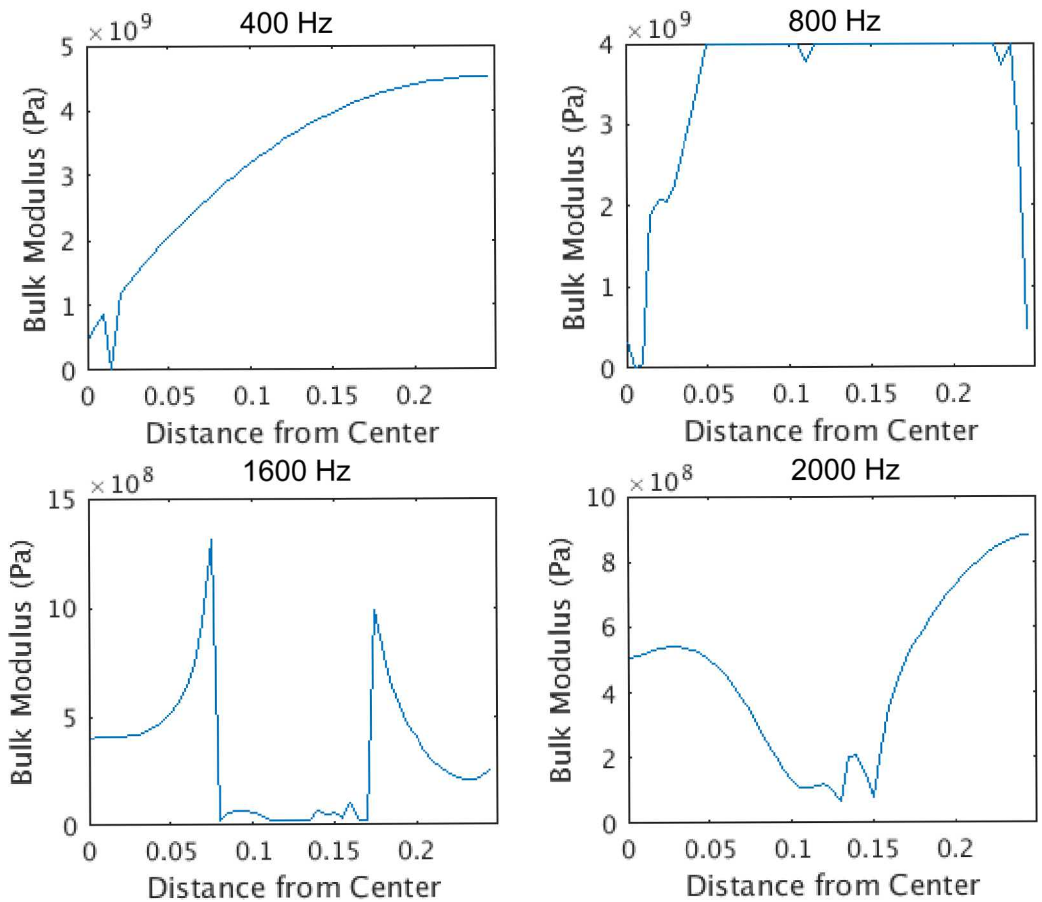
- Optimized VE foams allow recovery of desired pressure distribution



Left: Target acoustic pressure distribution, from forward problem
Center: Acoustic pressure distribution with initial material guess (2000 Hz Loading)
Right: Pressure distribution after convergence to optimized design

Acoustic Cloaking Results: Bulk Modulus

Bulk modulus sensitive to frequency, and varies nontrivially along disk radius



Figures: Real component of bulk modulus along radius, for various frequency

Conclusions

- Adjoint-based optimization enables inversions with large parameter spaces and/or high dimensionality of interest to Sandia
- Leveraging Sandia software components
  - Sierra Mechanics for massively parallel multiphysics forward simulations
  - Rapid Optimization Library (ROL) for gradient-based optimization
- Application spaces at Sandia are broad and continuing to grow