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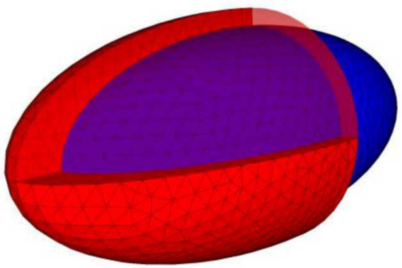

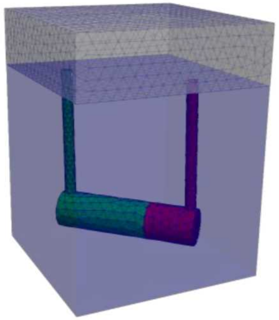

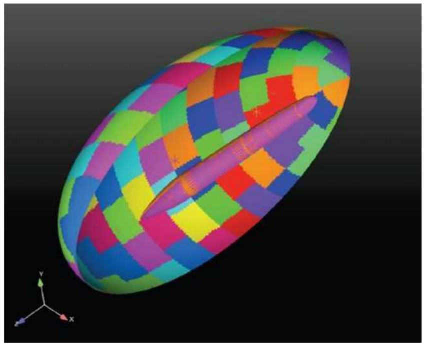

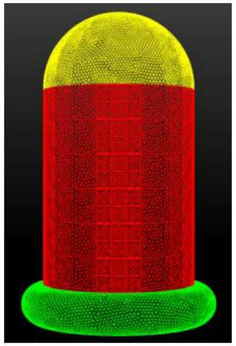

High Performance Computing in Structural Acoustics w/ Applications to Acoustic Metamaterials

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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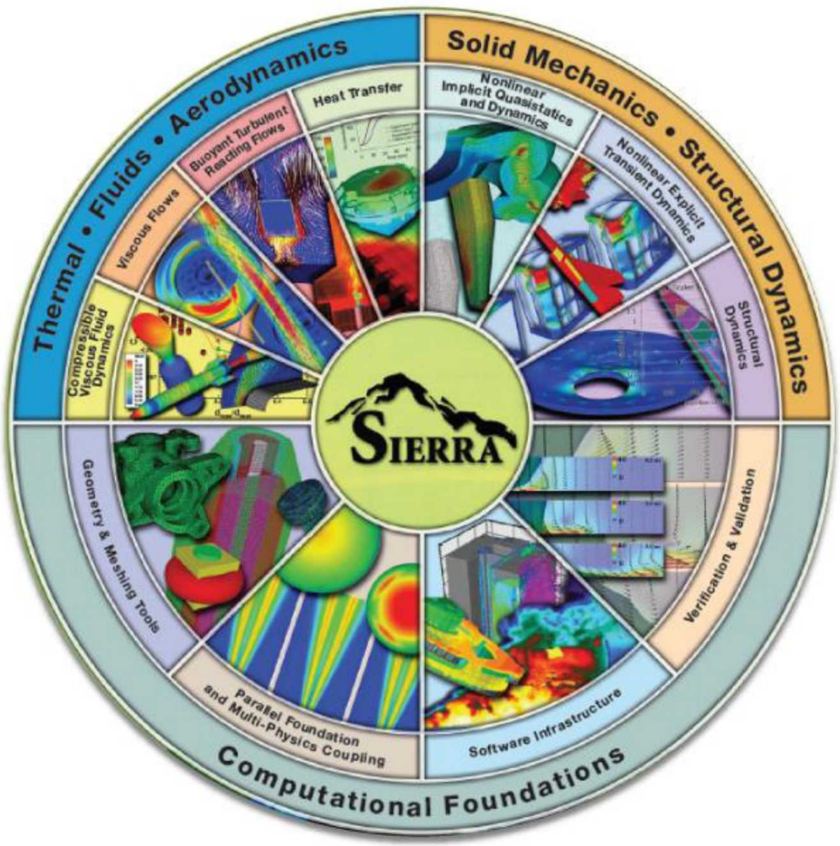
Outline

- Overview of Sierra Mechanics
- Overview of Sierra-SD(Salinas)
  - Current structural acoustic FEM capabilities
- Some new additions to Sierra-SD acoustics
- Example applications of Sierra-SD for acoustics, inverse problems, metamaterials

Overview of Sierra Mechanics

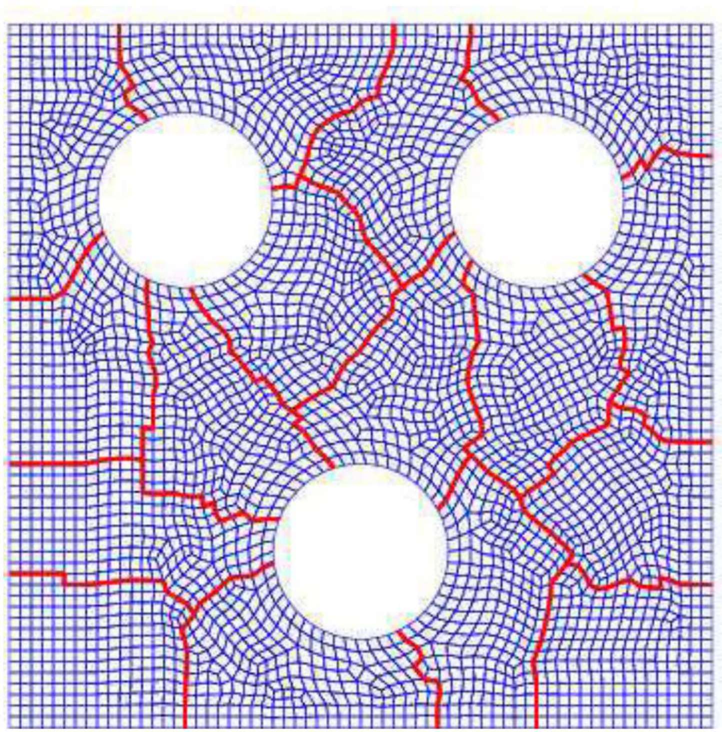
- Goal: massively parallel coupled multiphysics calculations
- Modules for structural dynamics, solid mechanics, fluids, thermal, etc



Sierra-SD: A Brief History

- Sierra-SD (Salinas) was created in the 1990's at Sandia National Laboratories for large-scale structural analysis
- Intended for extremely complex structural and structural acoustics models
  - Routinely used to solve models with 100's of millions of degrees of freedom
  - Recently used to solve (implicit) model with 1 billion degrees of freedom (>10,000 cores)
- Scalability is the key
  - Sierra-SD can solve n-times larger problem using n-times many more compute processors, in nearly constant CPU time
- Typical solution methods: transient dynamics, eigenanalysis, direct frequency response, random vibration, modal superposition, etc.

Domain Decomposition



- Decompose model into smaller subdomains
- Each subdomain is often assigned to one processor
- Two-level methods have “local” subdomain solves and “global” coarse solve
- Solve using preconditioned conjugate gradient or gmres
- POC: Clark Dohrmann (GDSW) , Kendall Pierson (FETI-DP) (Sandia)

Overview of Sierra-SD Structural Acoustic Capabilities

- Massively parallel
- Hex, wedge, tet acoustic elements (up to order p=6), coupled with both 3D and 2D (shell) structural elements
- Linear and nonlinear acoustics
- Allows for mismatched acoustic/solid meshes
  - Mortar or multi-point constraints (MPC)'s
- Infinite elements and Perfectly Matched Layers (PML)
- Solution procedures:
  - Frequency response (frequency-domain)
  - Transient (time-domain)
    - Fully coupled and loosely (staggered) coupled methods
  - Eigenvalue (modal) analysis
    - Linear and quadratic (complex modes)

Recent Development Efforts in Sierra-SD

- Nonlinear acoustics
- Infinite elements and Perfectly Matched Layers (PML)
- High order (‘p’) finite elements
- Cavitating acoustic finite elements
- Coupling with nonlinear solver (Sierra-SM)
- Large-scale (adjoint-based) optimization
  - Inverse problems
  - Source identification, material identification, interface identification
  - Metamaterials design

Structural Acoustic Equations of Motion

acoustics

$$\nabla^2 \phi = \frac{1}{c^2}\ddot{\phi}, \text{ in } \Omega_f \times (0,T)$$

$$\nabla \phi \cdot \boldsymbol{n}_f = -\rho_f \ddot{u}_n, \text{ on } \partial\Omega_f^N \times [0,T]$$

$$\phi = 0, \text{ on } \partial\Omega_f^D \times [0,T]$$

$$\phi(0,T) = 0, \text{ in } \Omega_f$$

$$\dot{\phi}(0,T) = 0, \text{ in } \Omega_f$$

solid mechanics

$$\nabla \cdot \boldsymbol{\sigma} = \rho \ddot{\boldsymbol{u}}, \text{ in } \Omega \times (0,T)$$

$$\boldsymbol{\sigma n} = \boldsymbol{h}, \text{ on } \partial\Omega^N \times [0,T]$$

$$\boldsymbol{\sigma} = \boldsymbol{D} : \boldsymbol{\nabla u}, \text{ in } \Omega \times [0,T]$$

$$\boldsymbol{u} = \boldsymbol{0}, \text{ on } \partial\Omega^D \times [0,T]$$

$$\boldsymbol{u}(0,T) = \boldsymbol{0}, \text{ in } \Omega$$

$$\dot{\boldsymbol{u}}(0,T) = \boldsymbol{0}, \text{ in } \Omega$$

Time domain

$$[M]\boldsymbol{a}(t) + [C]\boldsymbol{v}(t) + [K]\boldsymbol{u}(t) = \boldsymbol{f}(t)$$

Frequency domain (Helmholtz)

$$[H(\omega)]\boldsymbol{z}(\omega) = \boldsymbol{F}(\omega)$$

$$[H(\omega)] = -\omega^2[M] + i\omega[C] + [K]$$

Discretized Equations of Motion

- Fully coupled time domain formulation

$$\begin{bmatrix} M_s & 0 \\ 0 & -M_a \end{bmatrix} \begin{bmatrix} \ddot{u} \\ \ddot{\phi} \end{bmatrix} + \begin{bmatrix} C_s & L^T \\ L & -C_a \end{bmatrix} \begin{bmatrix} \dot{u} \\ \dot{\phi} \end{bmatrix} + \begin{bmatrix} K_s & 0 \\ 0 & -K_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} = \begin{bmatrix} f_s \\ -f_a \end{bmatrix}$$

- Fully coupled eigenanalysis formulation

$$\lambda^2 \begin{bmatrix} M_s & 0 \\ 0 & -M_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} + \lambda \begin{bmatrix} C_s & L^T \\ L & -C_a \end{bmatrix} \begin{bmatrix} u \\ \dot{\phi} \end{bmatrix} + \begin{bmatrix} K_s & 0 \\ 0 & -K_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

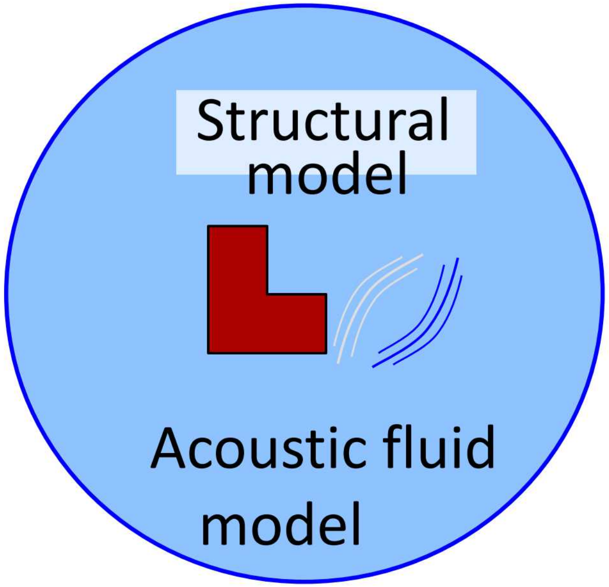
- Fully coupled frequency-domain formulation

$$-\omega^2 \begin{bmatrix} M_s & 0 \\ 0 & -M_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} + i\omega \begin{bmatrix} C_s & L^T \\ L & -C_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} + \begin{bmatrix} K_s & 0 \\ 0 & -K_a \end{bmatrix} \begin{bmatrix} u \\ \phi \end{bmatrix} = \begin{bmatrix} f_s \\ -f_a \end{bmatrix}$$

Why Nonlinear Acoustics?

Linear acoustics is inadequate for many applications

- **Resonating cavities**
- **Large-amplitude sources**
- **Far-field of explosions**
- **Aeroacoustic noise**



<u>Assumptions of Linear Acoustic Theory</u>

- Small amplitude waves
- Linear constitutive fluid model
- No fluid convection

<u>Consequences</u>

- Resonance leads to infinite amplitude waves
- "Sine wave remains a sine wave"
- No wave distortion
- Wavespeed independent of stress state in fluid

Eulerian Formulations for Nonlinear Acoustics

- The linear acoustic wave equation

$$\frac{1}{c^2}\phi_{tt} - \Delta\phi = 0$$

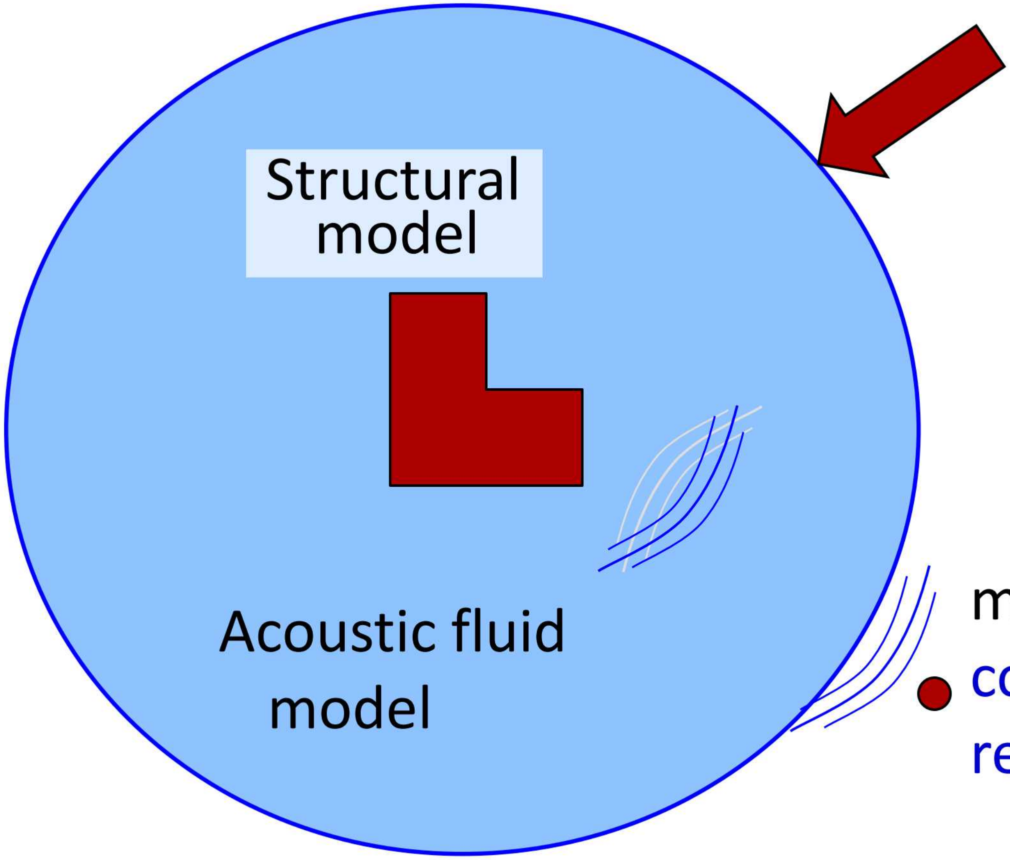
- The 2nd order Kuznetsov Equation

$$\frac{1}{c^2}\phi_{tt} - \Delta\phi + \frac{1}{c^2}\frac{\partial}{\partial t}\left[(\nabla\phi)^2 + \frac{B/A}{2c^2}\left(\frac{\partial\phi}{\partial t}\right)^2 + b\nabla^2\phi\right] = 0$$

- High order nonlinear acoustic equation

$$\frac{1}{c^2}\phi_{tt} - \Delta\phi + \frac{1}{c^2}\frac{\partial}{\partial t}\left[(\nabla\phi)^2 + b\nabla^2\phi\right] + \frac{1}{2c^2}\nabla\psi \bullet \nabla(\nabla\phi)^2 + \frac{\gamma - 1}{c^2}\left(\frac{\partial\psi}{\partial t} + \frac{1}{2}(\nabla\phi)^2\right)\Delta\psi = 0$$

Far-Field Acoustics



Common Requirement:
far-field boundary conditions for finite element analysis

- **Infinite Elements**
- **Perfectly Matched Layers (PML)**

microphone:
compute far-field response

Comparison of Infinite Elements and PML

Infinite Elements

- Time and frequency domain formulations are identical (same matrices)
- Restricted to homogeneous media on ellipsoidal domains
- Built-in capability for computing far-field pressures (outside of acoustic mesh)

PML

- Originally restricted to frequency domain solutions
- Works on arbitrarily shaped convex domains (with corners)
- Can also absorb evanescent waves, and in some cases works on heterogeneous domains
- No capability for computing far-field pressure

Infinite Element Formulation

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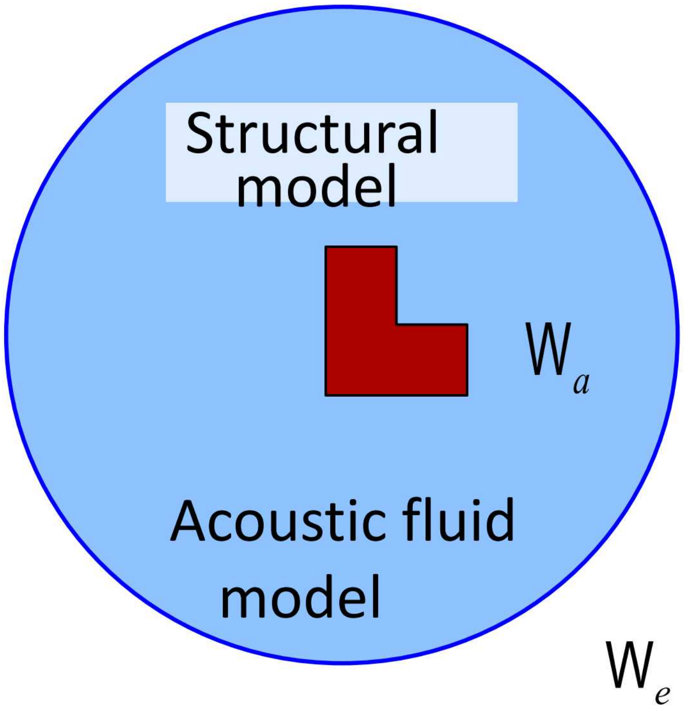


$$\Omega = \Omega_a + \Omega_e$$

Acoustic wave equation for fluid

$$\frac{1}{c^2} p_{tt} - \Delta p = 0 \quad \Omega \times [0, T]$$

$$\frac{\partial p}{\partial n} = g(x,t) \quad \Gamma \times [0, T]$$

Weak formulation on exterior domain

$$\int_{\Omega} \frac{1}{c^2} \ddot{p}\, q\, dV + \int_{\Omega} \nabla p \cdot \nabla q\, dV = \int_{\Gamma} g q\, dS$$

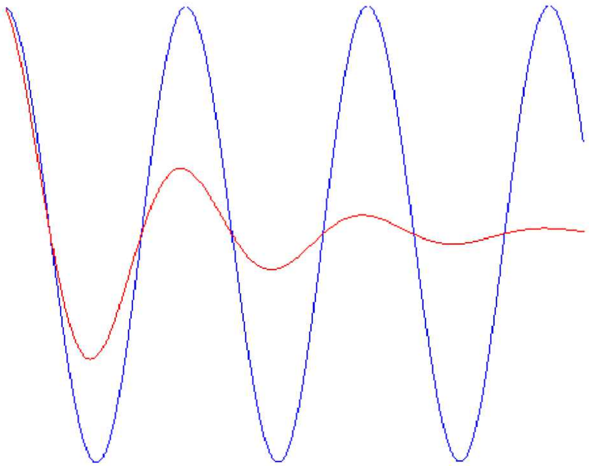
Trial and weight functions

$$\phi(x, \omega) = P(x) e^{-ik\mu(x)} \quad q = D(x) P(x) e^{ik\mu(x)}$$

$$\left(-\omega^2 M + i\omega C + K\right) p = f$$

Overview of PML

- Undamped solution of wave equation: e^{ikx}
  - this wave will propagate indefinitely in the x direction
- Complex Coordinate System:
  - $\tilde{x} = a(x) + ib(x)$
- Wave Equation becomes:
  - $e^{ik\tilde{x}} = e^{i(-ka(x)+ikb(x))} = e^{-kb(x)}e^{ika(x)}$
  - Damped Wave Equation



General Formulation for PML

Complex coordinate stretching $$\tilde{x} = x - \frac{i}{\omega}\int_x^a \sigma(\xi)d\xi \quad a < x < \bar{a}$$

Helmholtz equation over complex coordinates $$-\tilde{\Delta}p - k^2 p = 0$$

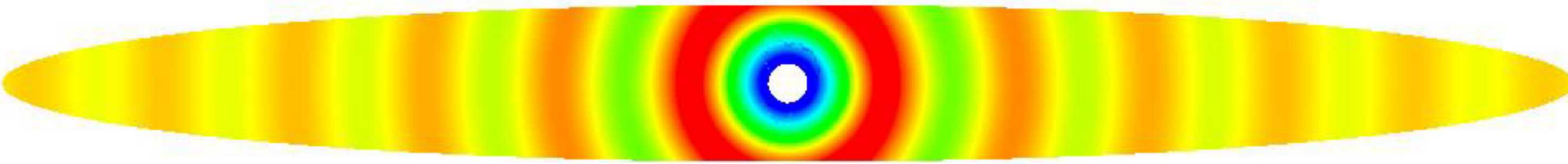
Weak form over complex coordinates $$\int_{\tilde{\Omega}_I} \langle \tilde{\nabla} p, \tilde{\nabla} q \rangle - k^2 pq \; d\Omega_I = \int_{\tilde{\Gamma}_S} gqdS$$

Mapped weak form back to real coordinates $$\int_{\Omega_I} \left[(\boldsymbol{J}^{-1}\nabla p) \cdot (\boldsymbol{J}^{-1}\nabla q) - k^2 pq \right] J(x,y,z) d\Omega_I = \int_{\Gamma_S} gqdS$$

Re-write as Helmholtz equation with variable coefficients $$\int_{\Omega_I} \tilde{\boldsymbol{A}} \langle \nabla p, \nabla \bar{q} \rangle - k^2 \tilde{J} p \bar{q} \; d\Omega_I = \int_{\Gamma_S} g\bar{q} d\Gamma_S$$

$$\tilde{\boldsymbol{A}} = \tilde{J}\tilde{\boldsymbol{J}}^{-1}\tilde{\boldsymbol{J}}^{-T}$$

Results: 10-to-1 Prolate Spheroid



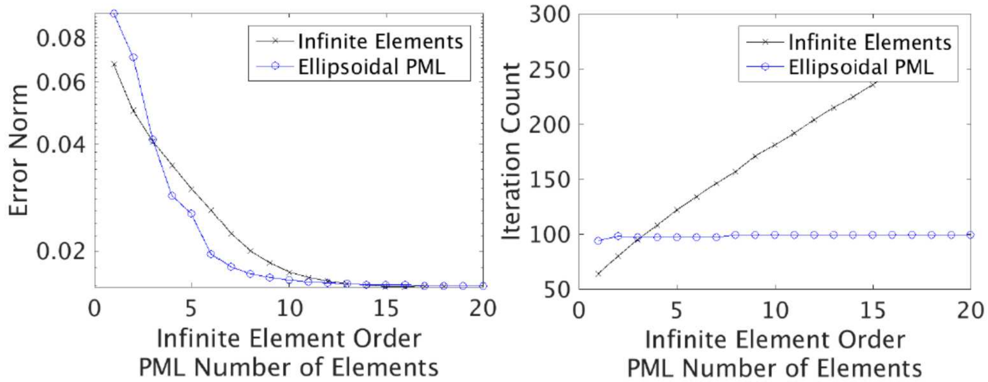
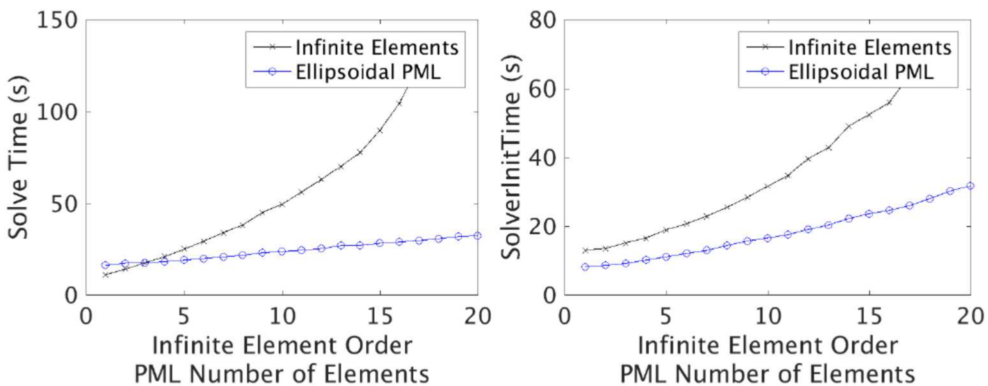


Figure 9: Comparison Between IE and PML (100 Hz)

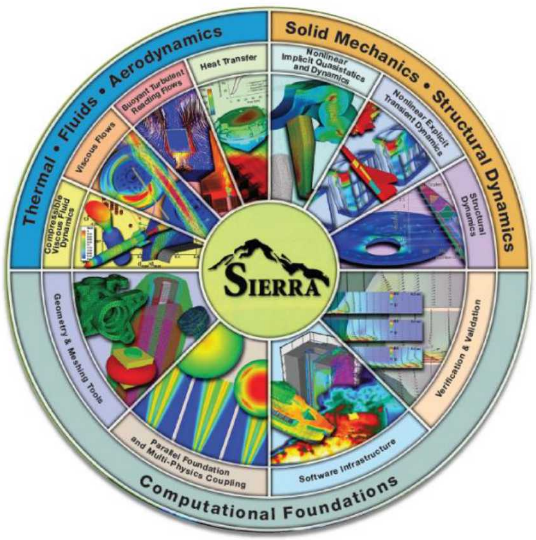


For a fixed level of accuracy

- PML required many less iterations than infinite elements
- PML solution times were much faster
- In frequency domain, PML is clear winner over infinite elements

Large-Scale Optimization in Sierra-SD

Finite Element and Optimization Codes operate as independent entities



Objective function, derivative operators

Next iterate of design variables

ROL
RAPID OPTIMIZATION LIBRARY

- Applications: inverse problems, meta-material design, control problems

Abstract Optimization Formulation

Abstract optimization formulation

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

Objective function

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

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

Inverse Problems

- Inverse problems arise when we have partial information and indirect observations of a system and need to infer (hidden) quantities of interest of the system.
- An inverse problem can be viewed as a quest for information that is not directly available from observations or measurements.
- The pursuit of a solution to an inverse problem calls for a balance synergy between analysis and experimentation.

Inverse Problems - Motivation

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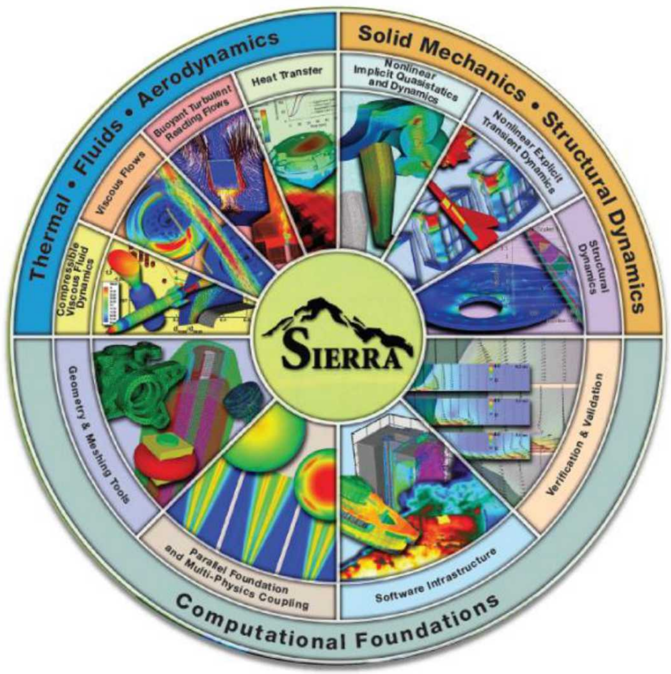
Forward Solver

Material properties
Geometry
Boundary conditions
Loads
Residual stresses
etc



Displacement
Pressure
Temperature
Flow field
etc

State Variables (outputs)

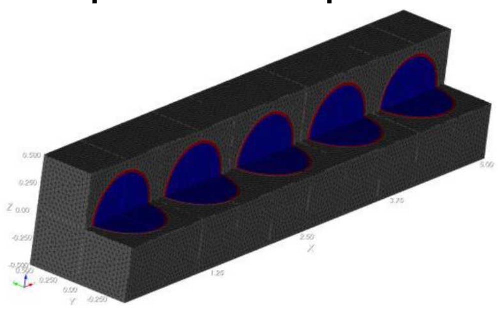
System parameters

Experimental data + inverse solution = missing link!

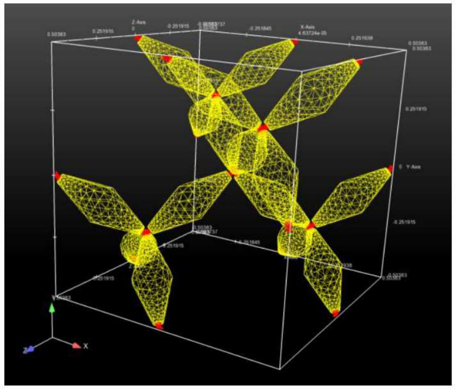
The Need for Large-Scale Optimization in Material Design

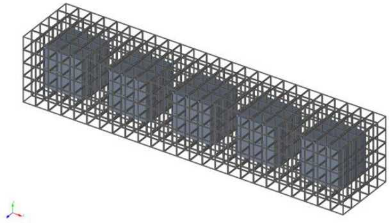
- Acoustic metamaterials: large number of parameters (>1000’s) poses challenge for global search-based optimization (genetic)
- Adjoint (gradient) based optimization allows for sensitivity computations that are independent of number of design variables

Multiphase composite



Pentamode lattice





Lattice with embedded masses

Large number of tunable parameters

$$v = \sqrt{\frac{B}{\rho}} \quad \text{where} \quad B = \text{bulk modulus} = \frac{\Delta P}{-\Delta V / V} = -V\frac{dP}{dV}$$

$$\rho = \text{density}$$

Negative moduli, B, imaginary sound speed (no wave propagation)
Negative density, ρ, imaginary sound speed (no wave propagation)
Negative moduli and density, real sound speed (waves propagate again!)
We can design a mechanical filter by alternating the sign of B and ρ!

Objective Functions for Inverse Problem

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Time Domain objective function

$$J(\{\boldsymbol{u}\},\{\boldsymbol{p}\}) = \frac{\kappa}{2}\Big(\{\boldsymbol{u}\} - \{\boldsymbol{u}_m\}\Big)^{\mathrm{T}}[Q]\Big(\{\boldsymbol{u}\} - \{\boldsymbol{u}_m\}\Big) + \mathscr{R}(\{\boldsymbol{p}\}),$$

- $\{\boldsymbol{u}\}$ State variables (displacement, pressure)
- $\{\boldsymbol{u}_m\}$ Desired values of state variables (displacement, pressure)
- $\{\boldsymbol{p}\}$ Unknown parameters (material parameters)
- $[Q]$ Weight matrix

Frequency Domain objective function

$$\tilde{J}(\{\boldsymbol{p}\}) = \frac{\kappa}{2}\sum_{k=1}^{N}(\mathbf{z}_k - \mathbf{z}_{m_k})^{\mathrm{h}}[Q](\mathbf{z}_k - \mathbf{z}_{m_k}) + \mathscr{R}(\{\boldsymbol{p}\})$$

Discrete Equations for Inverse Problem

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Time-domain

$$g(u, p) = M\ddot{u} + C(p)\dot{u} + K(p)u - f$$

Frequency-domain

$$g(u, p) = \left[K(p) + i\omega C(p) - \omega^2 M\right] u - f$$

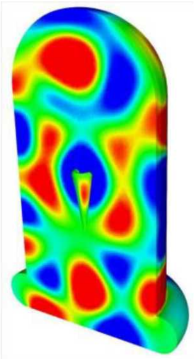
Eigenvalue (modal)

$$g_i = g(u_i, \lambda_i, p) = K(p)u_i - \lambda_i M u_i = 0$$

Applications: Model Validation in Acoustic Environments

- Using ground acoustic tests as validation data for FEM subject to acoustic loads
- Main challenge: What are the loads on the FEM?
- Approaches:
  - Inverse problem: Given test microphone data, generate sources & propagate through acoustic domain to the wetted surface
  - Diffuse Field Synthesis: Given test levels and assumed spatial correlation, create the field at the wetted surface

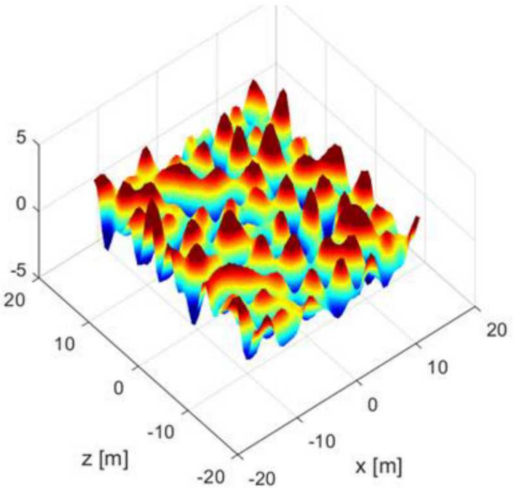
Test



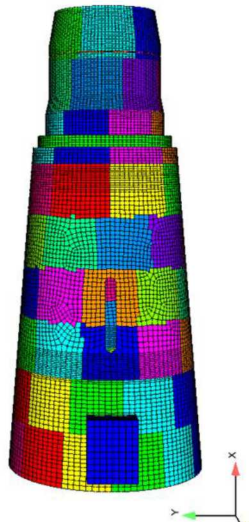
Simulation

Applications: Response Predictions

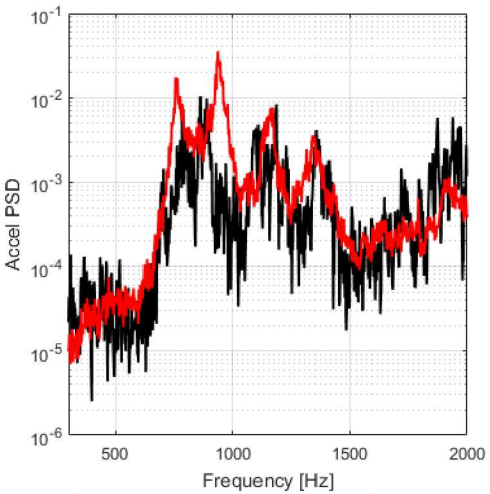
- Synthesizing and applying acoustic loads to FEM structural dynamics models for response predictions
- Approaches:
  - Synthesize acoustic pressures using diffuse field theory
  - Simulate the response/pressure MIMO FRF with Sierra/SD
  - Apply acoustic pressures to patched sections on the wetted surface



Synthesized Field



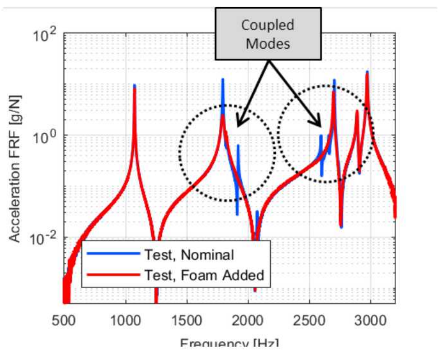
Patched FEM

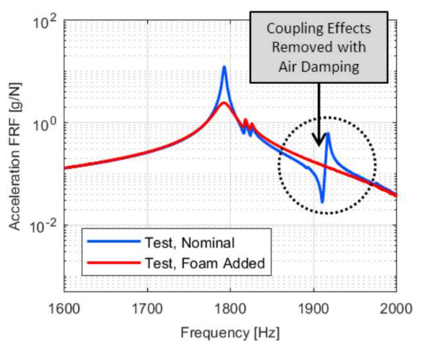


Response Predictions

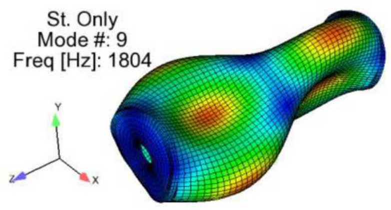
Applications: Acoustoelasticity Simulations

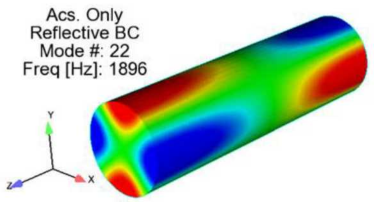
- Coupled structural-acoustic modes can corrupt modal test results
- We can model the effects of the internal acoustic mode coupling
- Objective is to 1) predict if we'll have coupling and 2) correct the coupling issues in test data (subtract off the effects of the air)

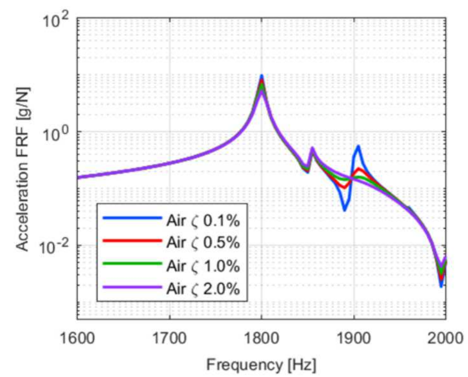




Test Results







Structural-acoustic Simulation

Structural Isolation Example

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Goal: minimize vibration at right end of structure, given steady-state loading at left end of free-free beam

Steady-state traction loading

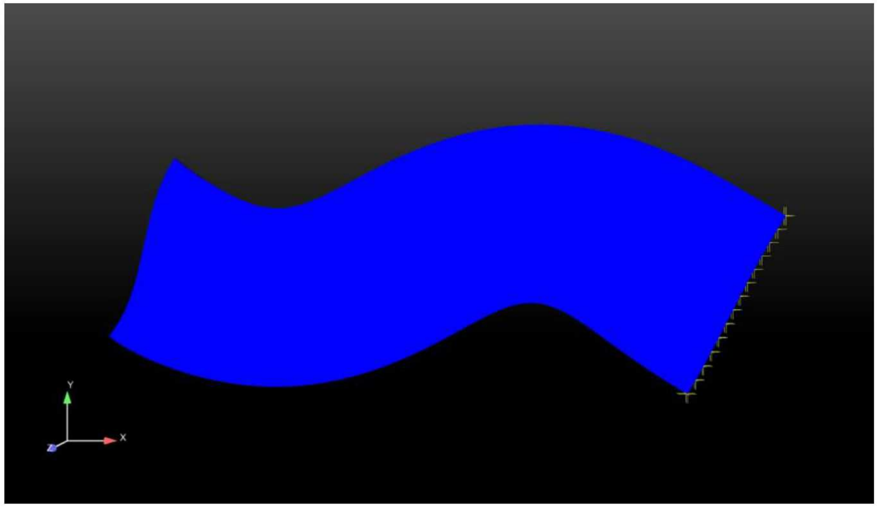
$T = T_0 \sin(\omega t)$

Minimal desired vibration response

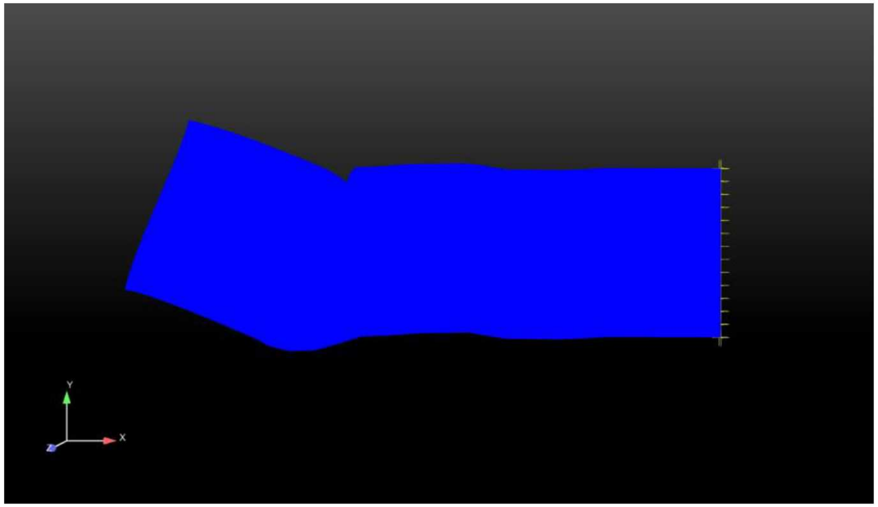
Structural Isolation Example

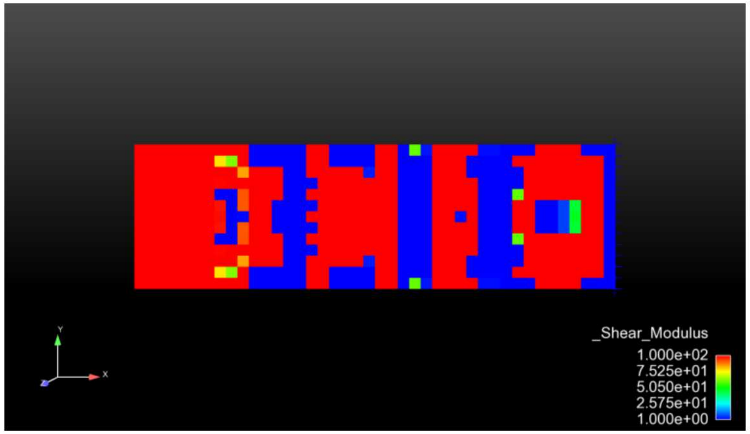
Goal: minimize vibration at right end of structure

Initial beam vibration response



Optimized beam vibration response

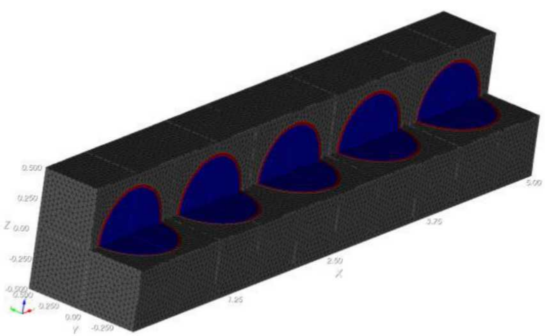




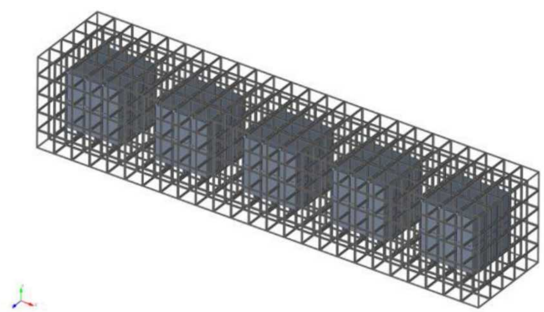
Shear modulus distribution of optimized beam

Tailored Impedance Material Designs

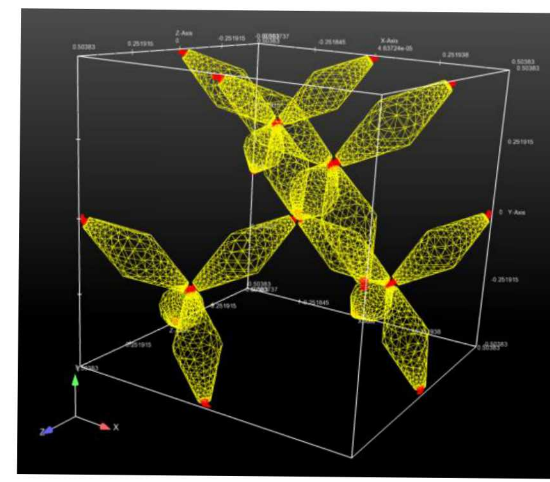
Typical designs for elastic metamaterials



Multiphase composite

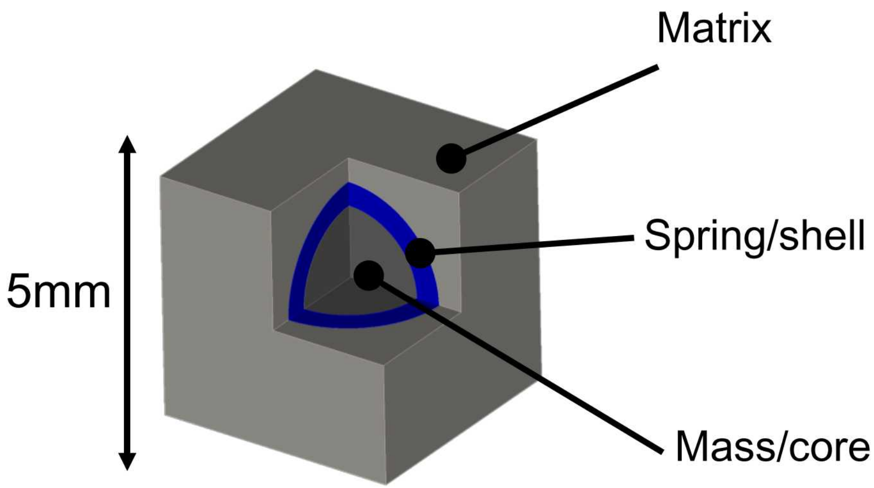


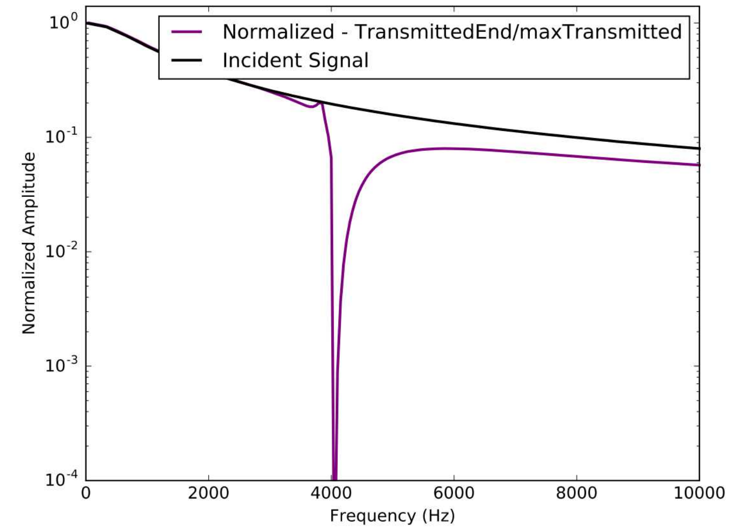
Lattice with embedded masses

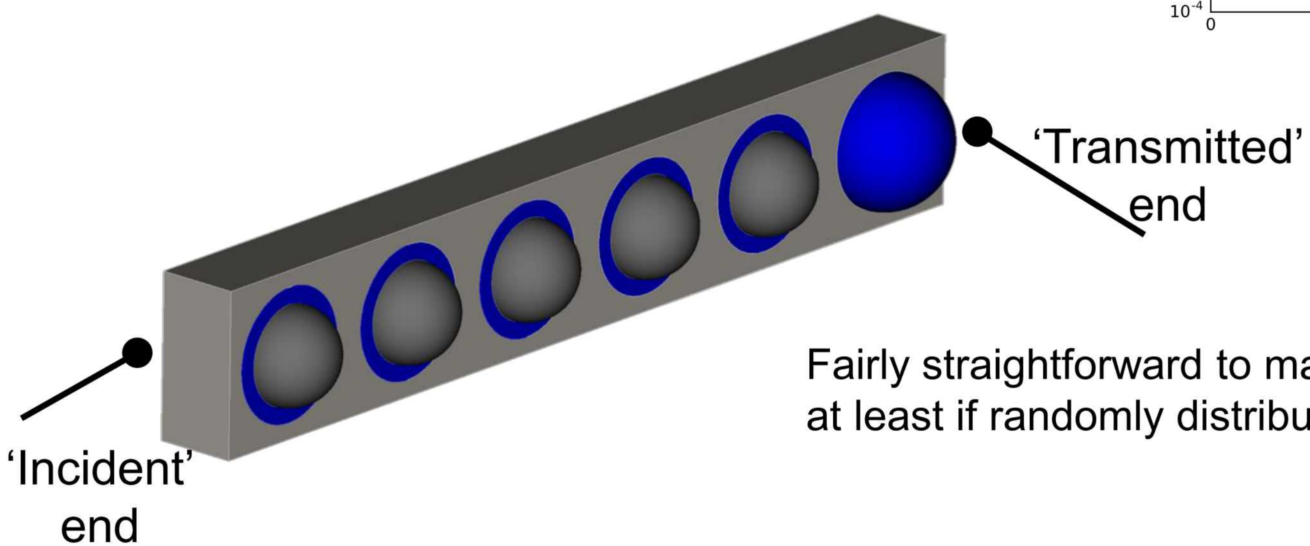


Pentamode lattice

Notch Filter Design



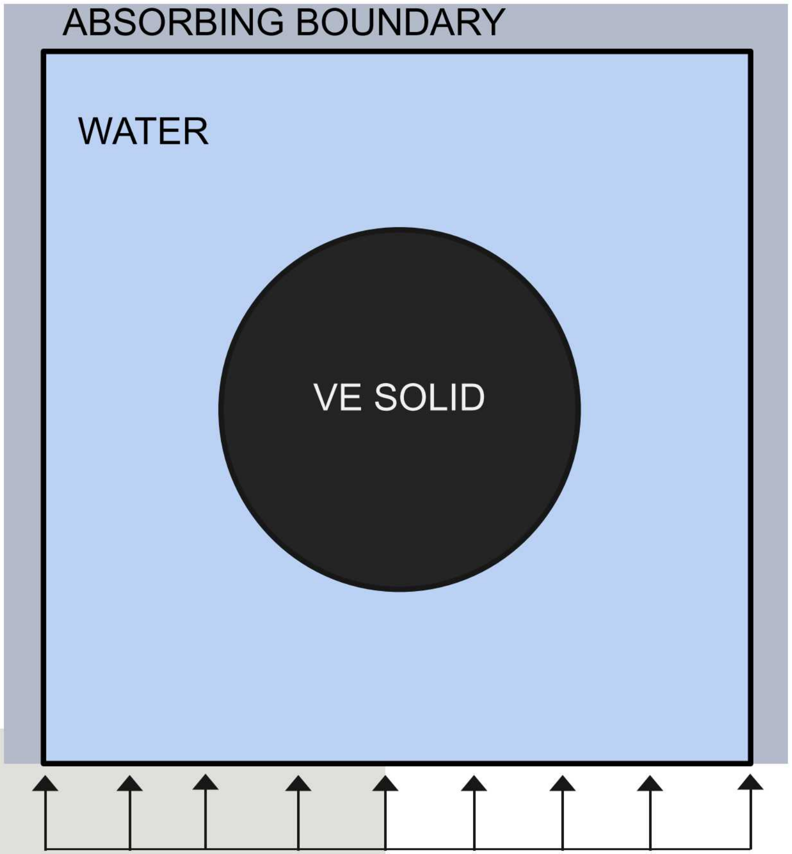


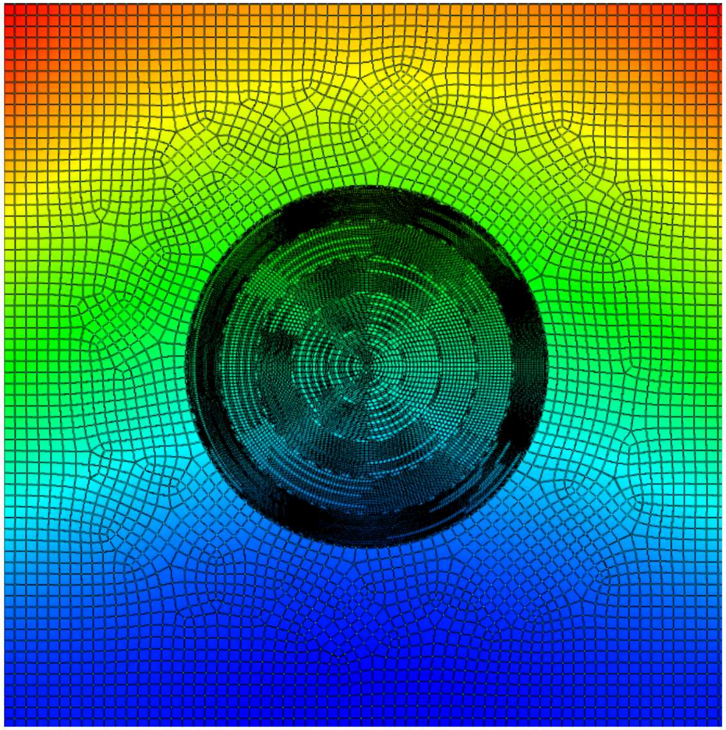


Fairly straightforward to manufacture,
at least if randomly distributed.

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**

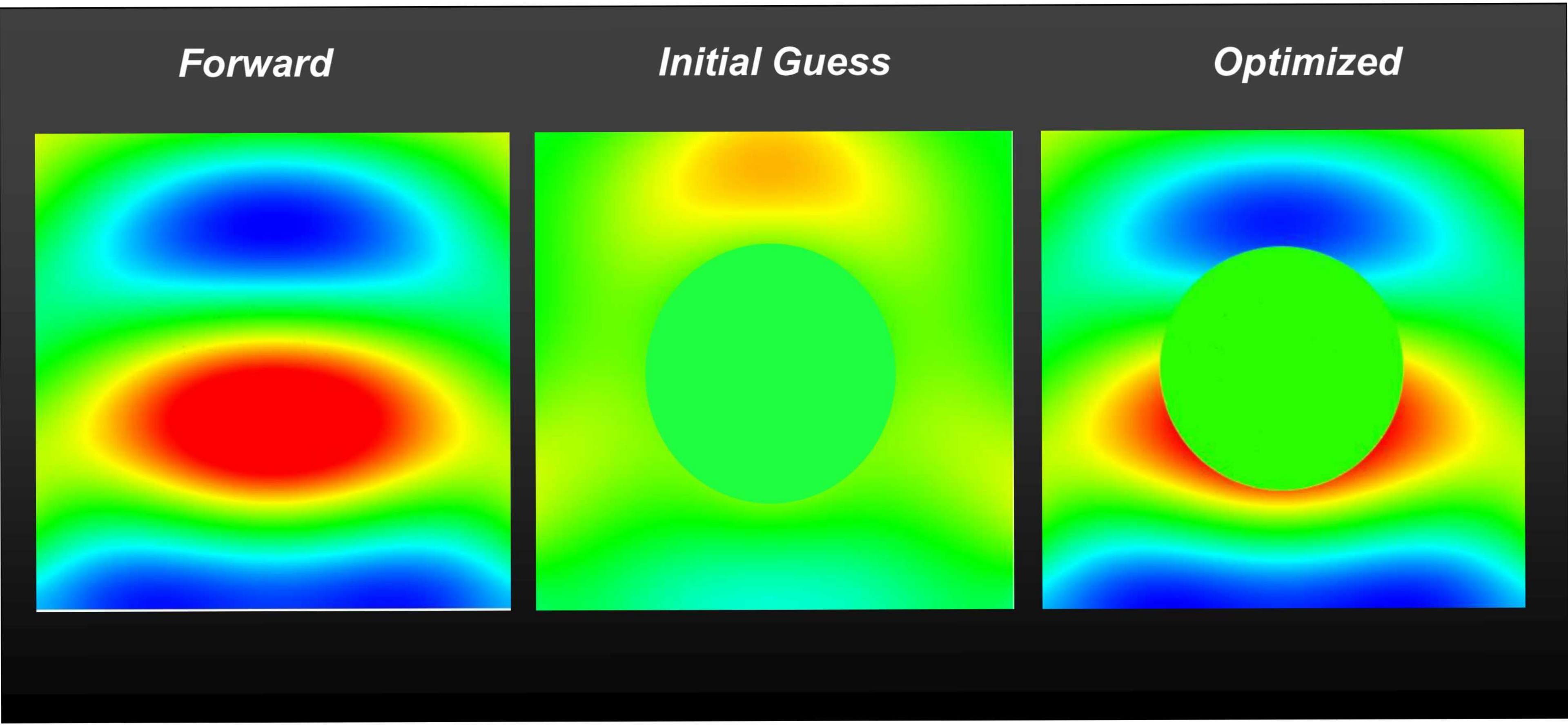




Left: Model Set up
Right: Forward problem pressure distribution (500 Hz loading) in model with 50 layers

Acoustic Cloaking

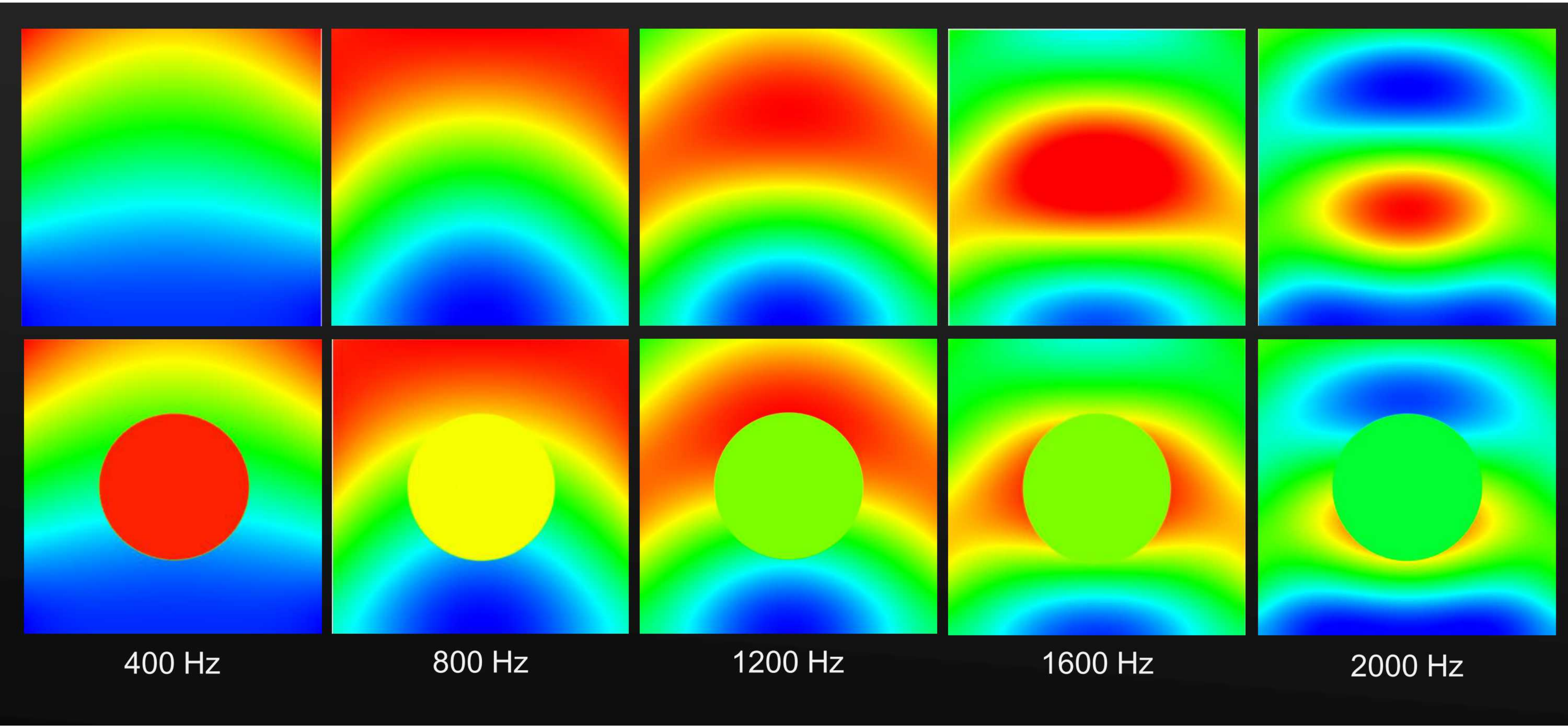
- Optimized VE foams allow recovery of desired pressure distribution



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

- Optimized VE foams allow recovery of desired forward pressure distribution
  - **Top :** Acoustic pressure from forward analysis
  - **Bottom :** Acoustic pressure around optimized solid inclusion



Conclusions

- Massively parallel finite element structural acoustics capability Sierra-SD has been developed for large-scale analysis
- Applicable to large-scale models with many degrees of freedom.
- Sierra-SD and optimization codes have been loosely coupled for the solution of source and material inversion problems.
- Capability has been applied to a variety of problems in structural acoustic modeling and metamaterial design

Backup Slides

Operator-Based Inverse Problems