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Solving Complex Inverse Problems for Design and Manufacturing Using High-Performance Computing

Timothy Walsh, Sandia National Laboratories

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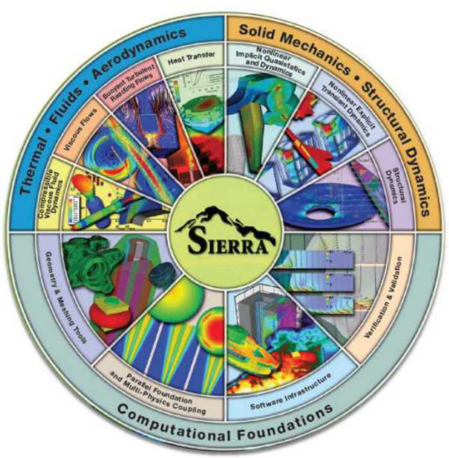
Acknowledgments

- Sierra Teams (SNL)
- Denis Ridzal, Drew Kouri, Rapid Optimization Library (SNL)
- Wilkins Aquino, Duke University
- Murthy Guddati, NC State University



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Environmental Tests and Computational Simulation

Capabilities Required to Design, and Qualify the Stockpile

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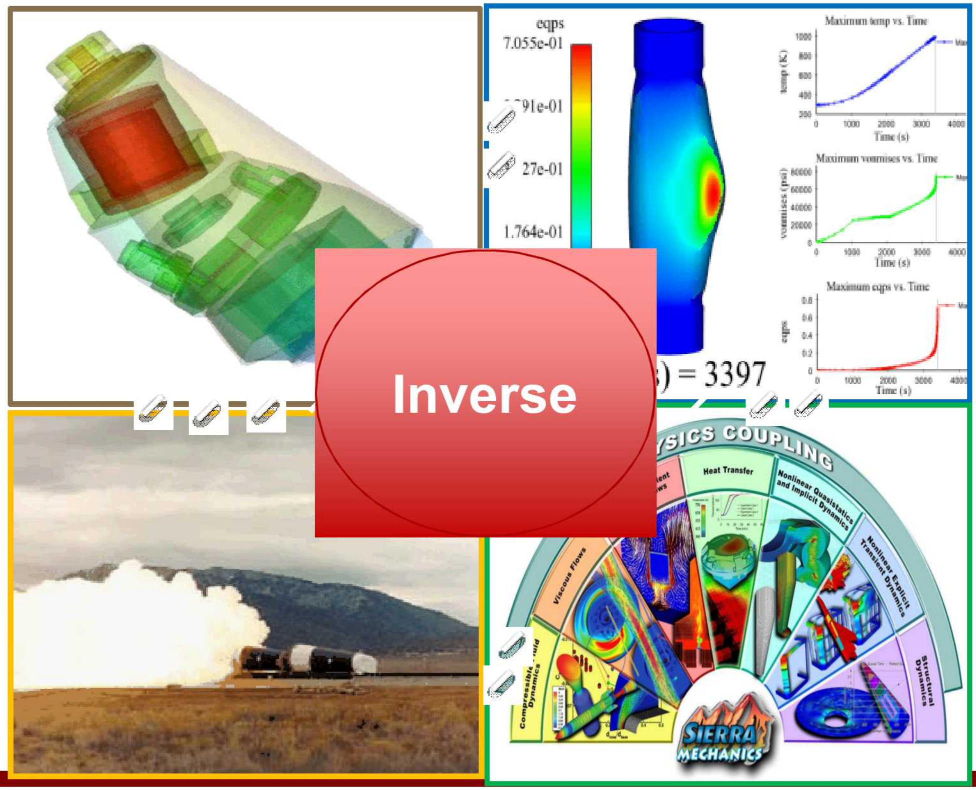
Integrated theory, computational simulation and experimental discovery/validation across length and time scales is critical to develop the technical basis for complex systems.

Engineering Analysis

Environmental Simulation & Test



Engineering Science Physical Phenomena

Computational Simulation Technology

Inverse Problem Strategy in Sierra

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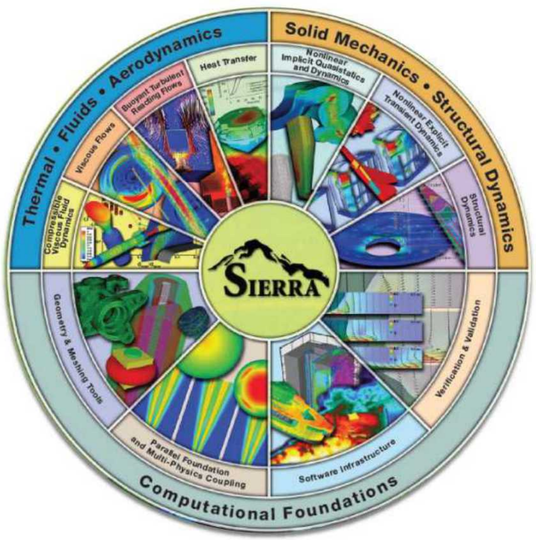
Finite Element and Optimization Codes operate as independent entities



Objective function, derivative operators

Next iterate of design variables

ROL
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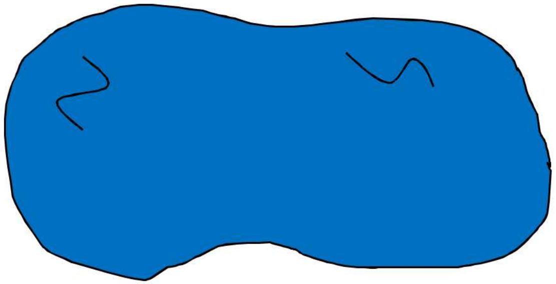
Sierra Mechanics – massively parallel multiphysics simulation

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

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-destructively* 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:

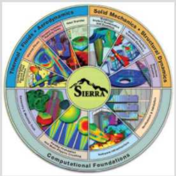
- Seismic imaging
- Medical imaging
- Non-destructive evaluation

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

Use Cases for Inverse Problems

Adjoint-based inversion enables new use cases for Sierra Apps

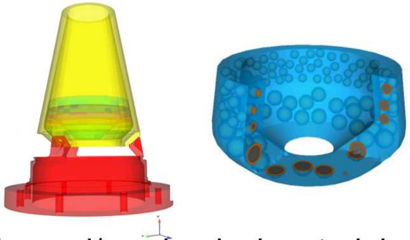


+ RAPID OPTIMIZATION LIBRARY + Experiment + InverseOpt Toolkit

Enables use cases

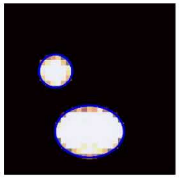
Flux boundary conditions

Source Reconstruction



Thermal/mechanical material reconstruction, residual stress, metamaterial design

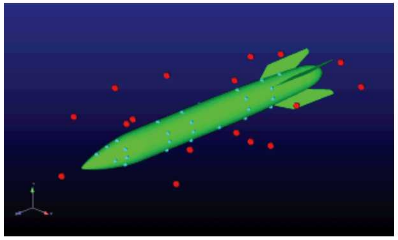
Material/residual stress Reconstruction



Detected debonded regions
(Thresholded plot)

Delamination/weld characterization

Contact surface Reconstruction



Ground-based acoustic/thermal tests

Design of Experiments

Sierra apps with embedded sensitivities (adjoints, etc)

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

Uniqueness: Massively parallel inverse optimization framework that leverages Sierra Mechanics

PDE-Constrained Optimization Formulation

Abstract optimization formulation

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

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

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

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

First order optimality conditions

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

Newton iteration

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

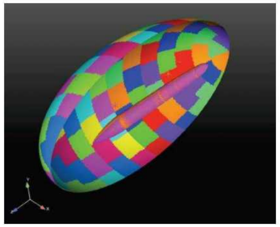
$$W = g_p^T g_u^{-T}(\mathcal{L}_{uu} g_u^{-1} g_p - \mathcal{L}_{up}) - \mathcal{L}_{pu} g_u^{-1} g_p + \mathcal{L}_{pp}$$

Hessian calculation

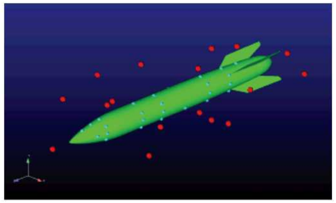
Example: Source Reconstruction

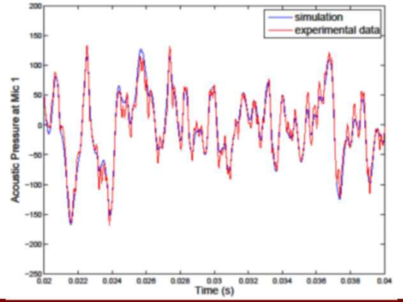
- Goal: reconstruct structural, thermal, and/or acoustic energy sources that produce the given accelerometer/temperature/microphone measurements
- Large parameter space – time histories for pressure functions
- Sensor placement – design of experiments

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



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





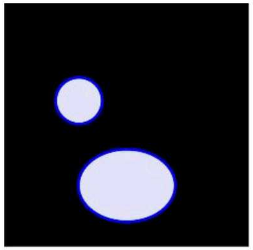
<u>Thermal flux loads</u>
Flux distributions from temperature measurements

Fire flux boundary conditions

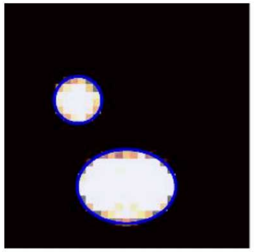
Example: Partially Connected Surfaces

- 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



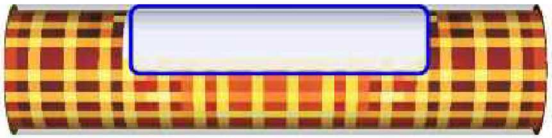
Target debonded regions



Detected debonded regions (Thresholded plot)

Partially bonded plates

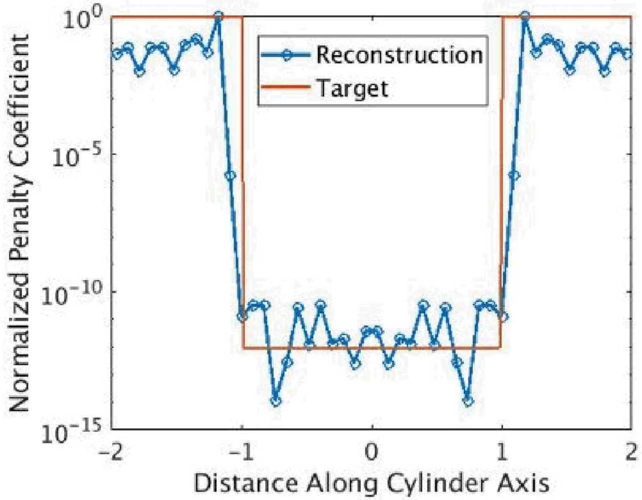
Target Debonded Region



Reconstructed Density Field (β_h)

Detected Debonded Region (Thresholded plot)

Partially bonded cylinders



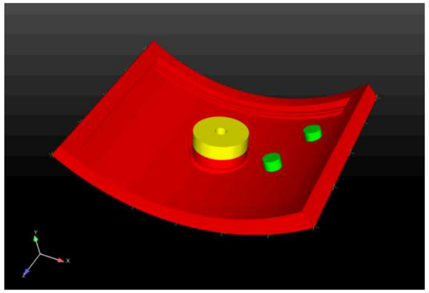
Line plot through delaminated area

Example: Material Parameter Extraction

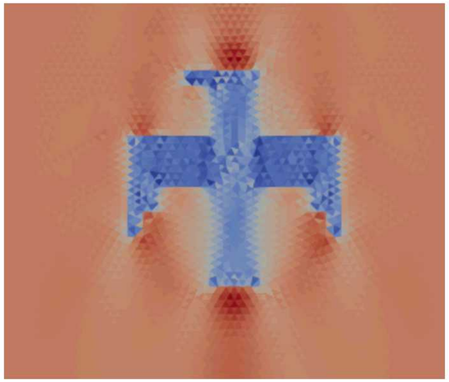
Problem: in-situ material parameters often unknown

- 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



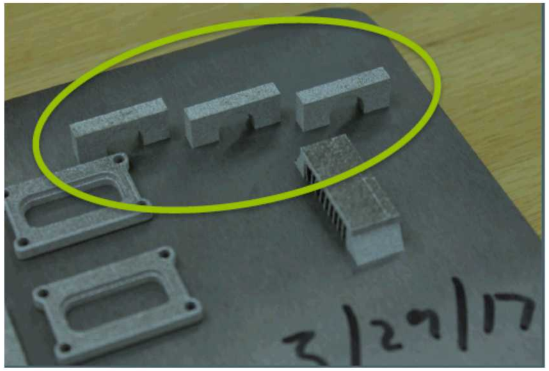
Reconstructed thermal conductivity from Sierra-TF (Aria)

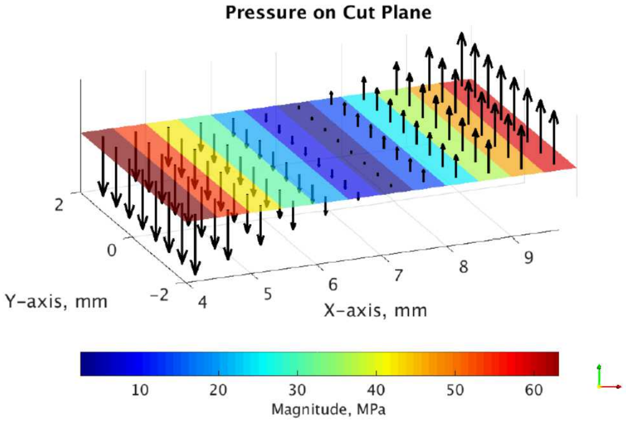
Example: Residual Stress Extraction

Problem: additively manufactured parts suffer from large residual stresses

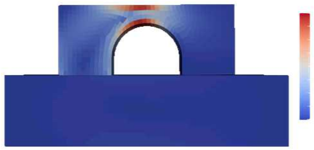
- Compromises part integrity
- FEM modeling needs stresses for initial conditions
- Stress is not a measurable quantity
- Large parameter space – spatially-varying stress fields

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



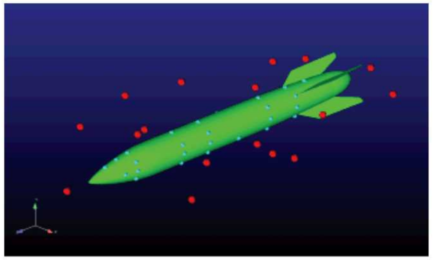


Predicted traction field from inverse solution (Sierra-SD)



Reconstructed stress field from inverse solution (Sierra-SD)

Optimal Experimental Design (OED) in Sierra



Motivation:

- Experiments are expensive and time-consuming
- Would like to use simulation and optimization to accelerate the process
  - Sensor placement optimization
  - Source design/placement for control problems
- Decomposition into two optimization problems
  - Design of experiment
  - Solution of inverse problem from gathered experimental measurements

“Sequential” design of experiments

Example: Optimization for Sensor Placement

$$\bar{s}(\theta) := \arg\min_{s \in \mathcal{Z}} \left(\frac{1}{2} \|T(\theta)s - \hat{u}_o\|_2^2 + \frac{\alpha}{2} \|Ws\|_2^2 \right)$$

$$\hat{u}_o = T(\theta)s + \epsilon$$

$$\bar{\theta} := \arg\min_{\theta \in \mathcal{Q}} \phi(C(\theta))$$

$$\bar{\theta} := \arg\min_{\theta \in \mathbb{R}^M} \phi(C(\theta))$$

$$\text{such that } \sum_i \theta_i = 1,\ 0 \leq \theta_i \leq 1$$

Sparsification constraint

Inverse problem of interest

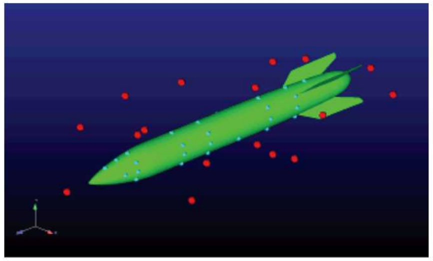
Additive noise model

Form covariance matrix

Choose optimality criteria

$\phi(C)$	Denomination
trace(C)	A-Optimal
$\det(C)$	D-Optimal
$\lambda_{\max}(C)$	E-Optimal

Data from experiment



Conclusions

- Adjoint-based optimization enables inversions with large parameter spaces and/or high dimensionality of interest to Sandia
- Sandia's Sierra Mechanics suite ported to NGP platforms
- 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

Design, Optimization, and Fabrication of Mechanical Metamaterials for Vibration Isolation

Timothy Walsh, Sandia National Laboratories

Ackowledgements

- Harlan Brown-Shaklee, Mike Sinclair, Bradley Jared, Sandia – 3D printing
- Ryan Schultz, Sandia (vibration testing)
- Chris Hammeter, Sandia (finite element simulations)
- Prof. Fabio Semperlotti et al, Purdue (metasurface collaboration)
- Wilkins Aquino, Clay Sanders Duke University (MECE-based optimization)
- Rapid Optimization Library (ROL) team, Sandia

Outline

- The need for large-scale optimization in mechanical metamaterials
  - Optimization strategy – Sierra + ROL
  - Parameter estimation and optimization of unit cells
  - joint work with Aquino et al, Duke University
- 3D printing of mechanical metamaterials
  - Single material
  - Multi-material
  - Optimization of multi-material metamaterials
- Comparison of vibration test results and FEM simulations
- Metasurfaces for vibration control (joint work with Semperlotti et al, Purdue)
  - Total internal reflection (TIR) elastic metasurfaces
  - Achieves filtering with extremely thin material layer

The Need for Large-Scale Optimization in Metamaterial Design

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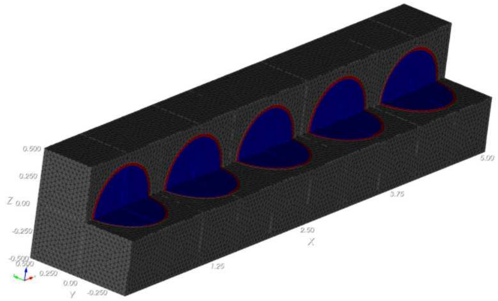
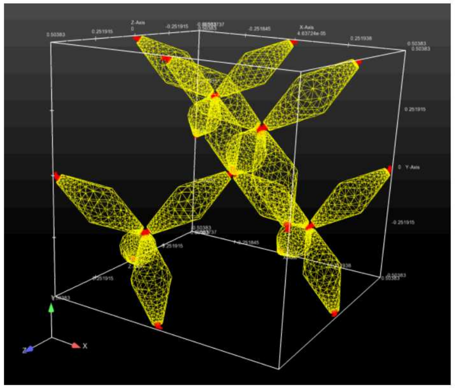
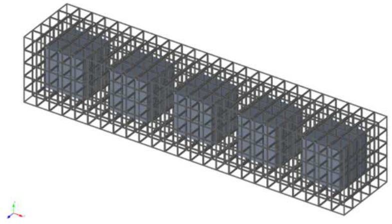
- Acoustic metamaterials: large number of parameters (>1000's to millions) poses challenge for global search-based optimization
- Adjoint (gradient) based optimization allows for sensitivity computations that are independent of number of design variables

Multiphase composite



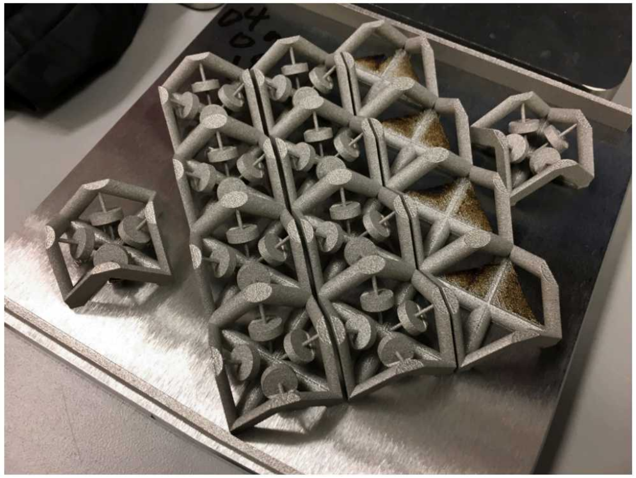
Pentamode lattice





Lattice with embedded masses

Large number of tunable parameters



Single-material print (steel)

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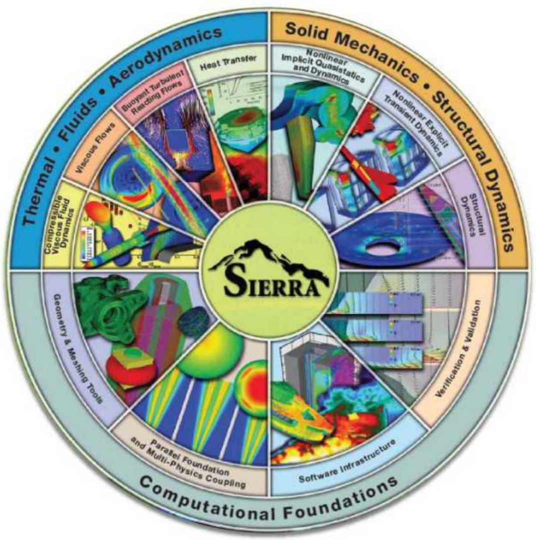
Design Optimization for Metamaterials

Finite Element and Optimization Codes operate as independent entities



Objective function, derivative operators

Next iterate of design variables

R L

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Sierra Mechanics – massively parallel multiphysics simulation

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

PDE-Constrained Optimization Formulation for Material Design

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

Objective Functions for Inverse Problem

Time Domain objective function

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

Mode Shape/Frequency objective function

$$J(\{\lambda_i\},\{\boldsymbol{u}_i\},\boldsymbol{p}) := \frac{\beta_i}{2}\|\{r_i\}\|^2+\frac{\kappa_i}{2}\mathscr{G}(\{\boldsymbol{u}_i\},\{\boldsymbol{u}_{mi}\})+\mathscr{R}(\boldsymbol{p})$$

$$r_i = \frac{\lambda_i-\lambda_{mi}}{\lambda_{mi}}$$

Frequency Domain objective function

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

Discrete Equations for Inverse Problem

Time-domain

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

Frequency-domain

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

Eigenvalue (modal)

$$\boldsymbol{g}_i = \boldsymbol{g}(\boldsymbol{u}_i, \lambda_i, \boldsymbol{p}) = \boldsymbol{K}(\boldsymbol{p})\boldsymbol{u}_i - \lambda_i\boldsymbol{M}\boldsymbol{u}_i = \boldsymbol{0}$$

Optimization Results

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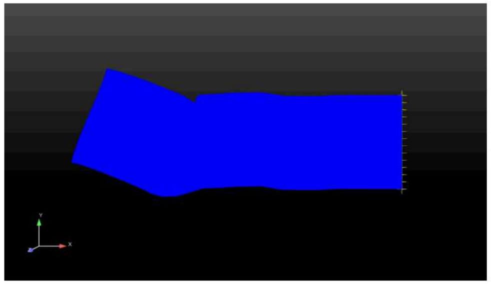
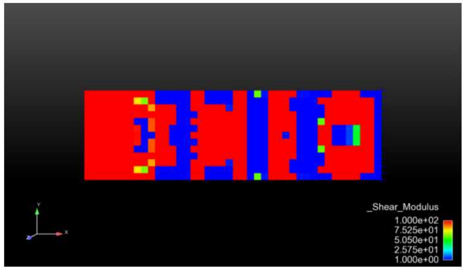
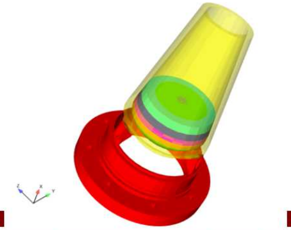
Structural Isolation: Material distribution

Frequency-domain objective: Two-phase material distribution

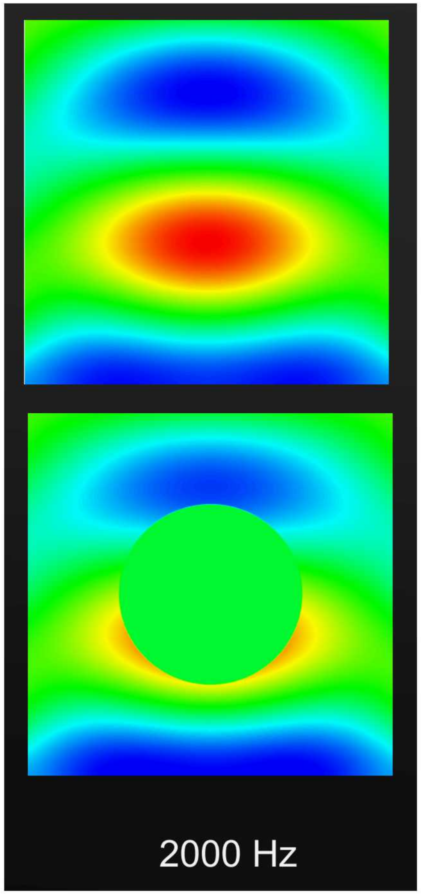




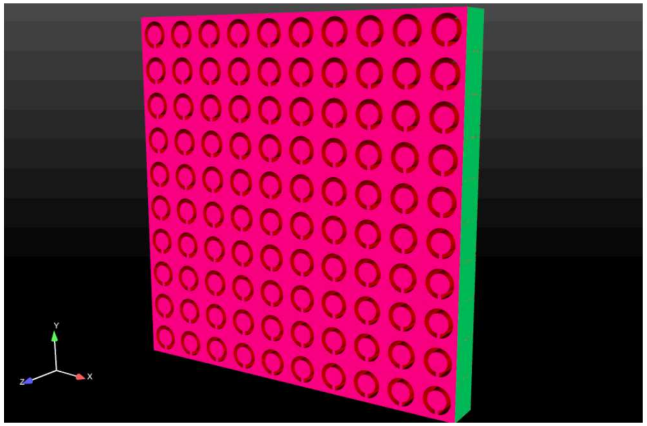
Viscoelastic foam optimization

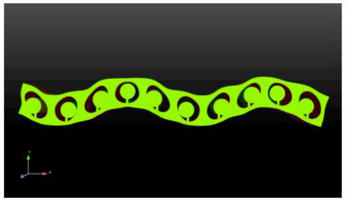


Acoustic cloaking: Viscoelastic foam optimization

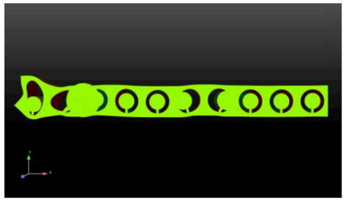


Split-Ring Resonators: resonator radius and beam thickness optimization

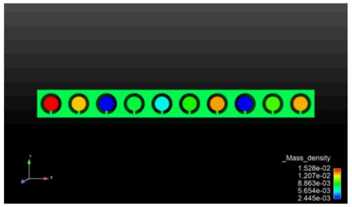




Initial guess



Optimized Structure



Optimized mass distribution

2 strategies: optimize continuum material vs optimize distribution of discrete parameters

3D Printing Optimized Internal Mass Resonators

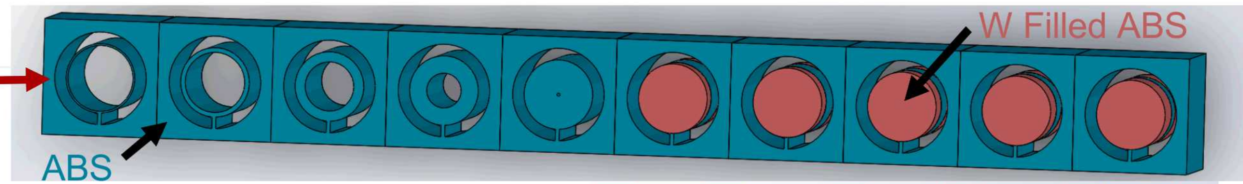
Multi-material additive manufacturing enables optimized mass distributions

1. Input optimized resonator mass values

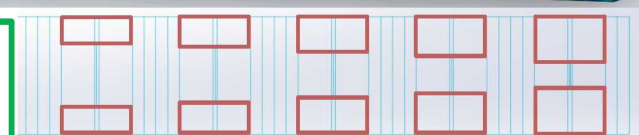
GlobalVariables.txt - Notepad

File Edit Format View Help

```
"m1"=0.1
"m2"=0.25
"m3"=0.5
"m4"=0.75
"m5"=1
"m6"=1.25
"m7"=2
"m8"=3
"m9"=4
"m10"=5
"rho_abs"=1.05
"rho_Wf"=8
"t"=1.5
"D1"=0.9
```

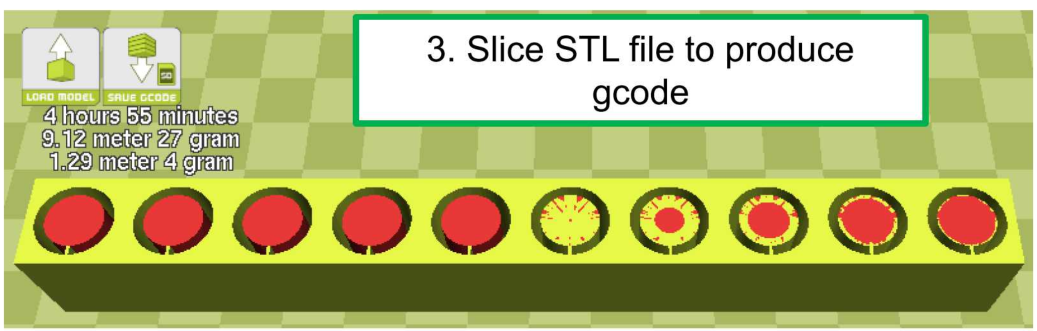


2. Global variables modify resonator geometry in SolidWorks



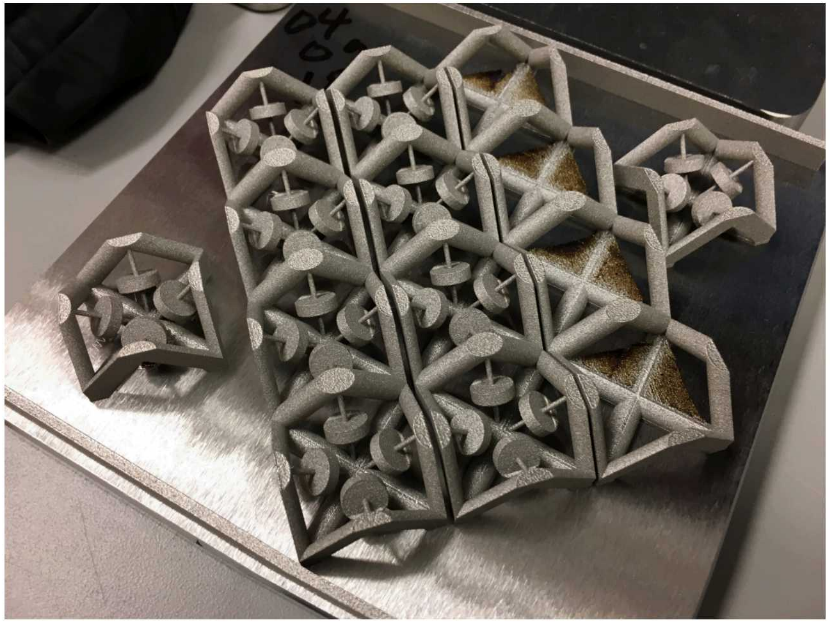
4. 3D print optimized resonator masses up to 7.3 g

3. Slice STL file to produce gcode

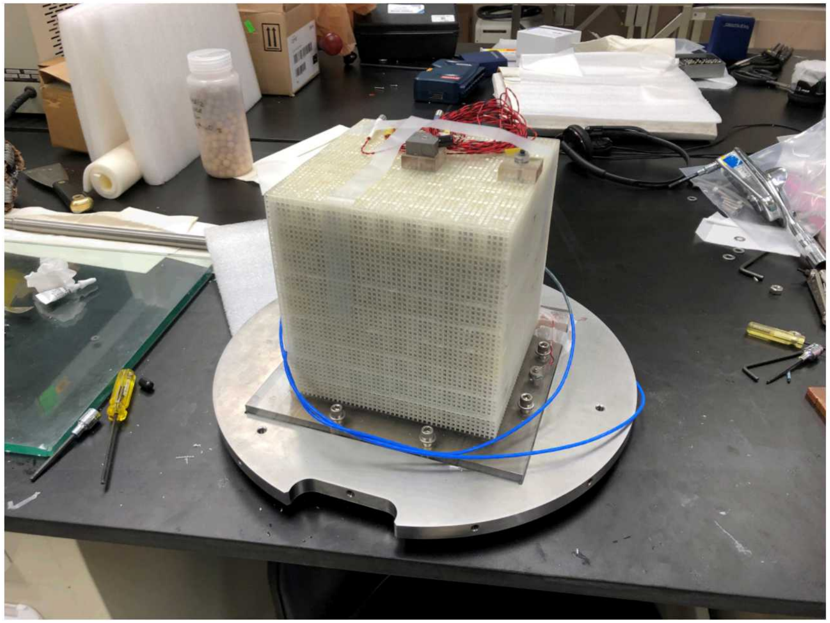


3D Printed Lattices with Embedded Resonators

3D vibration control applications require additively manufactured materials that filter in kHz regime

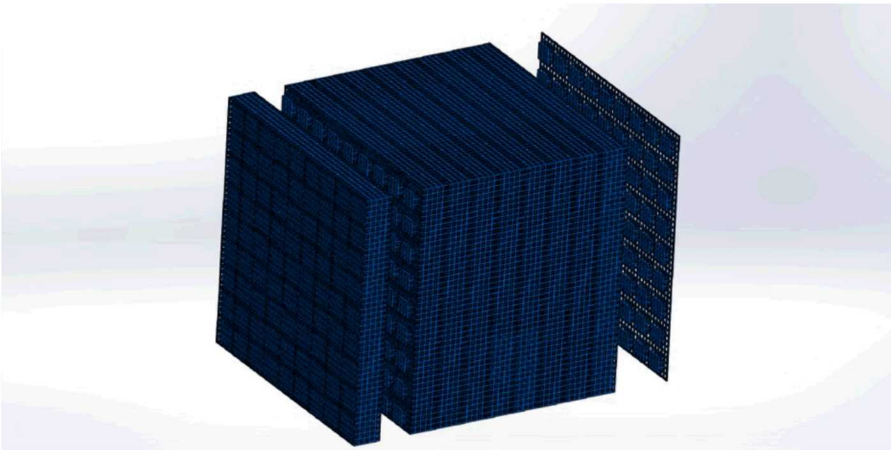


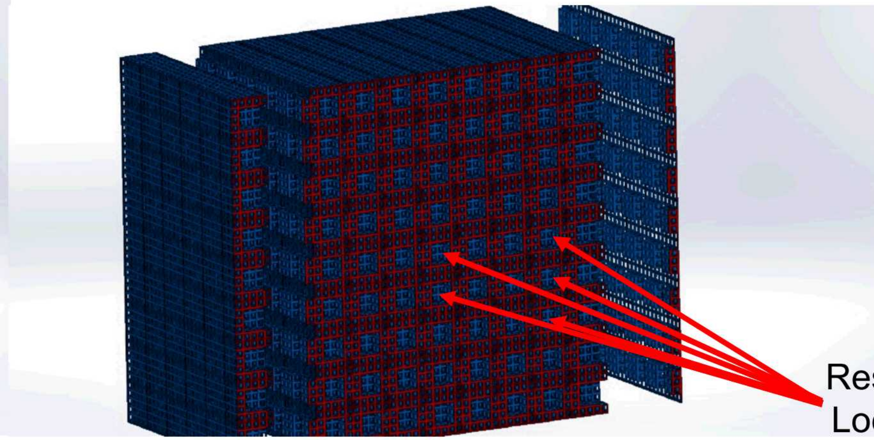
Single material – stainless steel with embedded resonators – filters 6-7kHz

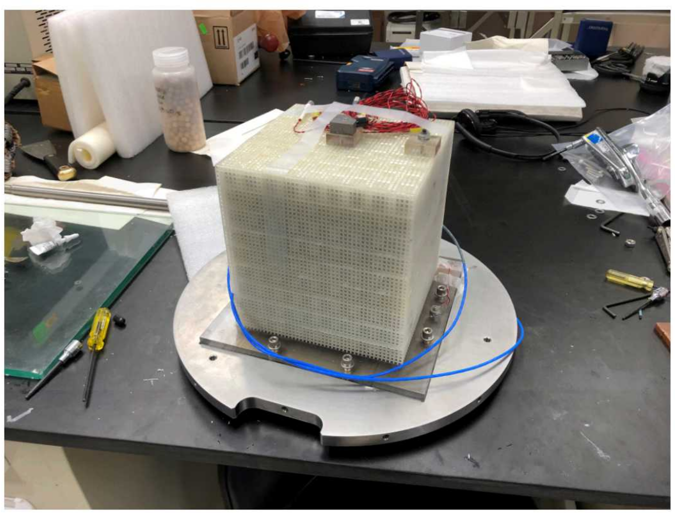


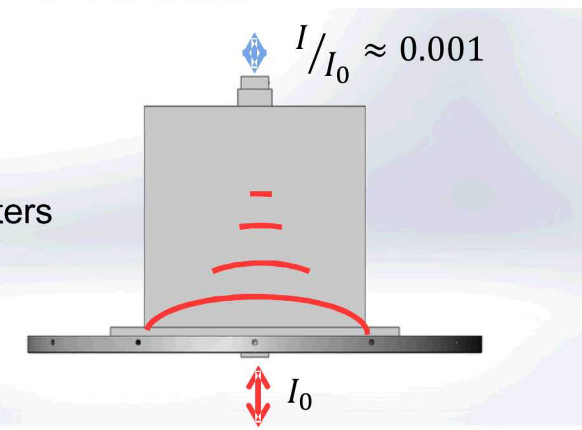
Multi-material – ABS lattice with embedded tungsten cube resonators – filters > 2-5kHz

3D Acoustic Metamaterial: ABS Lattice with Tungsten Resonators



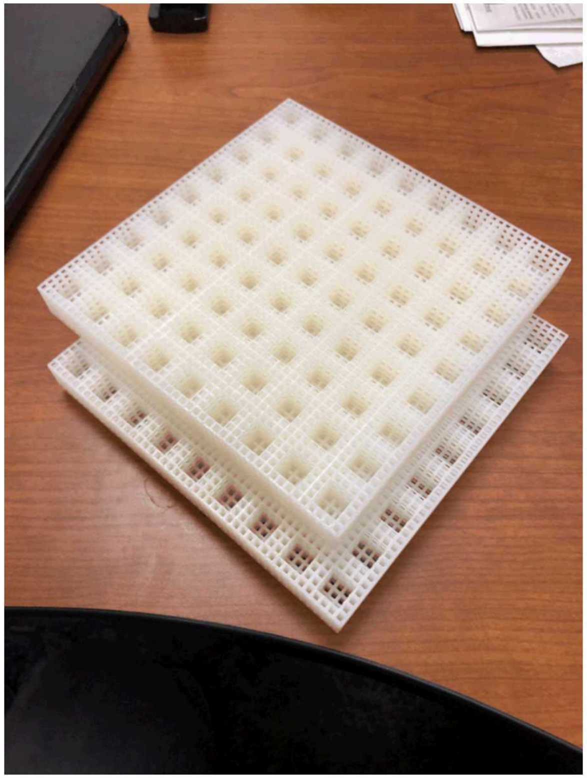




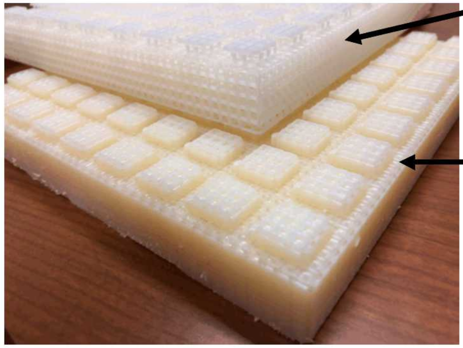


ABS-Tungsten Metamaterials Generated with the Stratasys PolyJet

Multi-material 3D printing still requires some manual assembly



- Print time is ~4 hrs per layer in acrylic "Vero"
  - -36 hr total print time
  - -4.5hr total support removal time
- 729 tungsten cubes
- Structure assembly and bonding
  - -8 hr (estimate)



Material with Support Removed

Material Requiring Support Removal

Sierra SD simulation of vibrational energy transfer

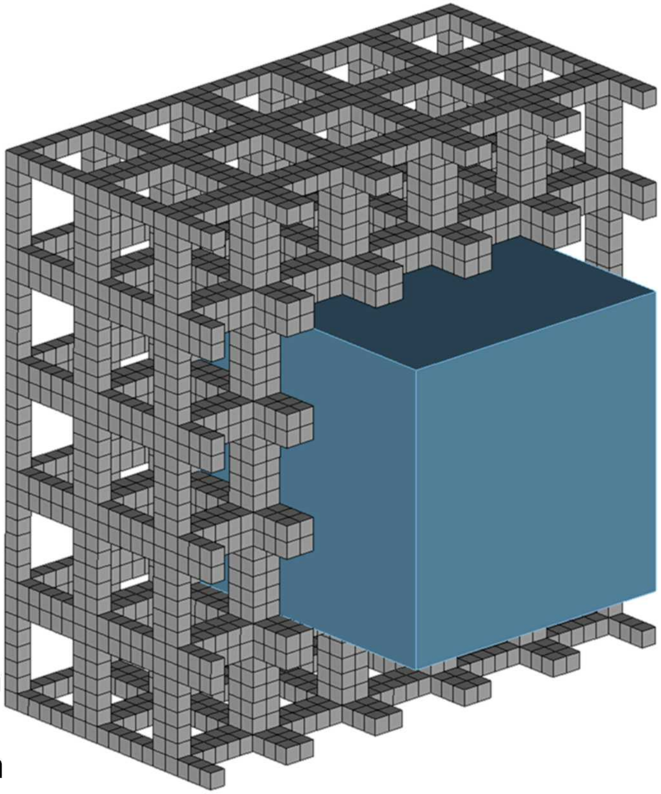
Large-scale FEM for 3D metamaterials with microstructure

-Direct frequency response analysis in Sierra-SD

-5.45 million hex elements
-Ran in 7 hours on 1303 processors
-Mass elements tied to lattice mesh
-Traction applied in negative X-direction on positive X-face of structure. Positive X-face nodes are constrained to remain co-planar.
-Output (transmitted signal) and Input (incident signal) extracted as average displacement/velocity of X-face nodes.

Lattice (Vero Clear) Properties:
G = 1.18 GPa
E = 3.3 GPa
Density = 1.185 g/cm^3

Mass (Tungsten) Properties:
G = 156 GPa
E = 400 GPa
Density = 19.25 g/cm^3

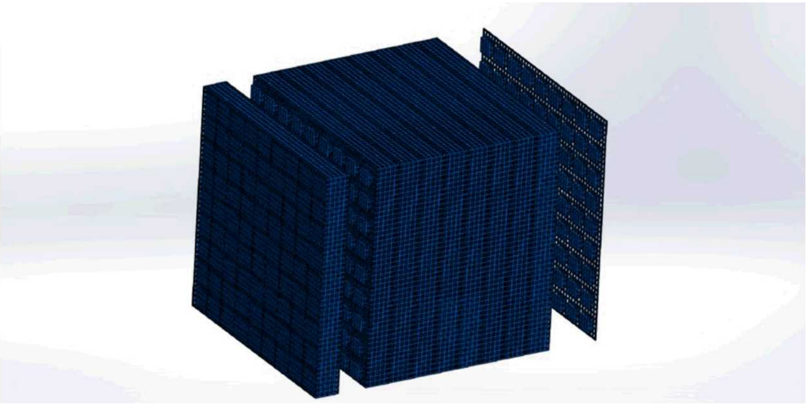


Cut-away of unit cell mesh
Lattice structure meshed with 0.55 mm elements
Masses meshed with a single 9.85 mm element

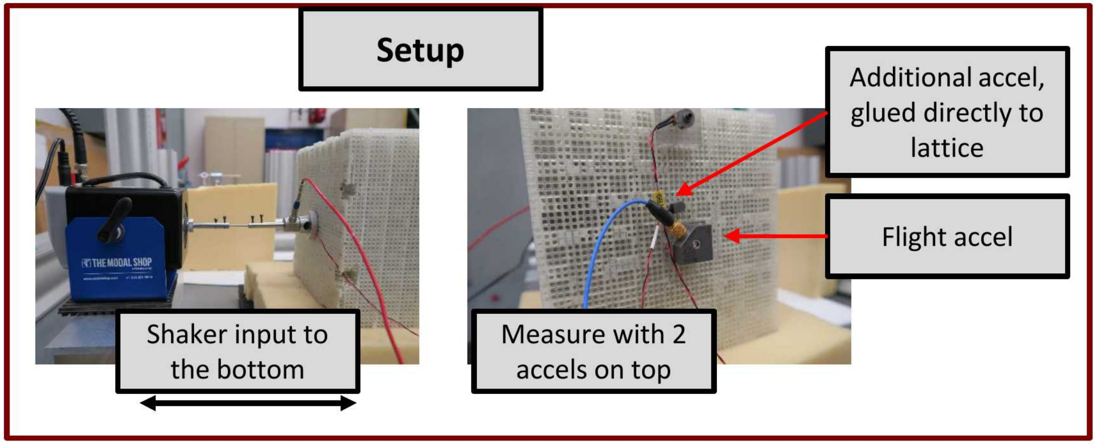
FEM vs. Experiment Comparison

Sandia National Laboratories

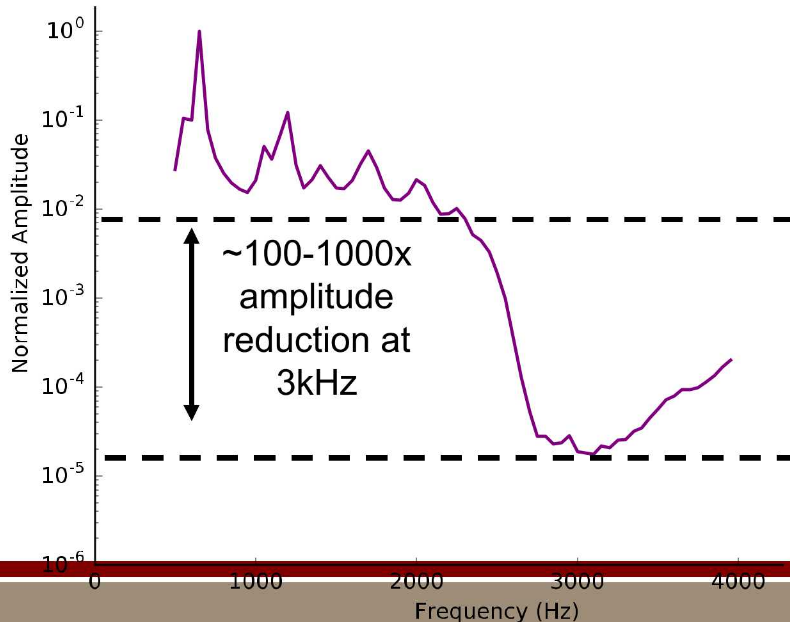
FEM simulation

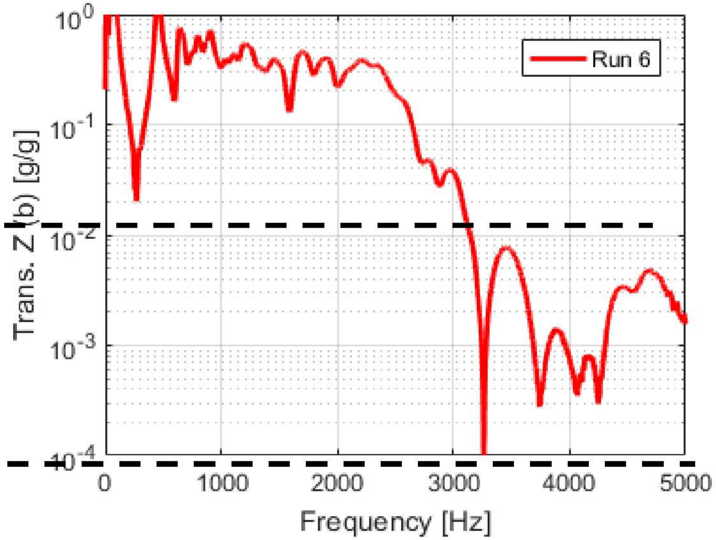


Experiment



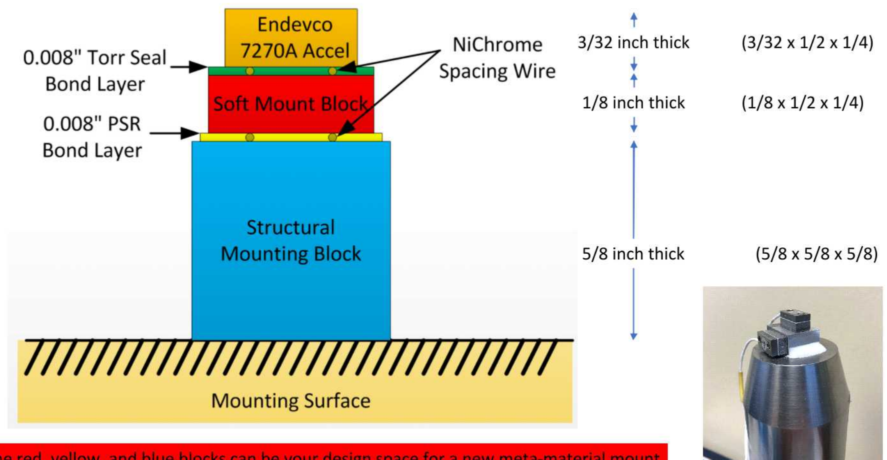
Average transmitted amplitude normalized by the peak amplitude as a function of frequency.



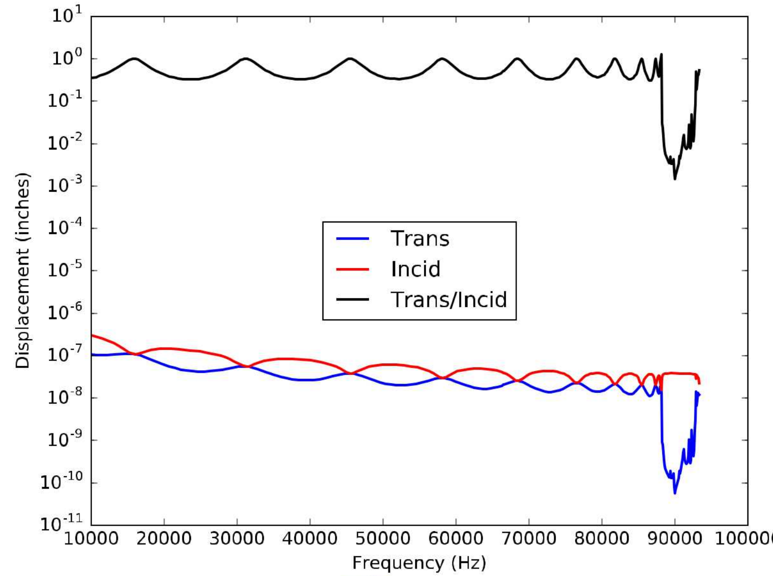


Application: Accelerometer Gauge Frequency Isolation

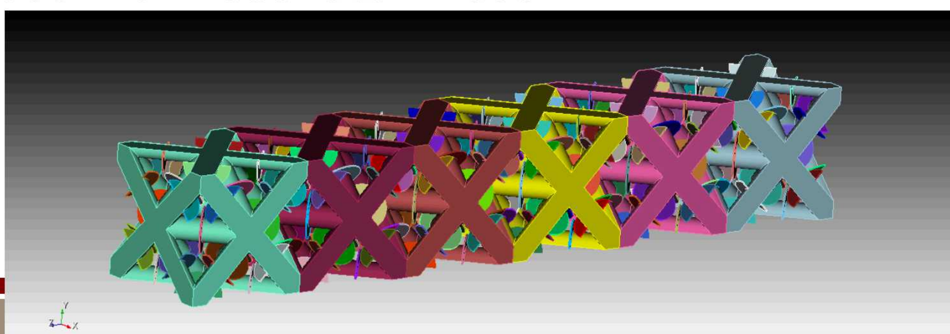
Goal: filter out gauge resonance without altering signal otherwise
Typical gauge resonance (Endevco) 90kHz

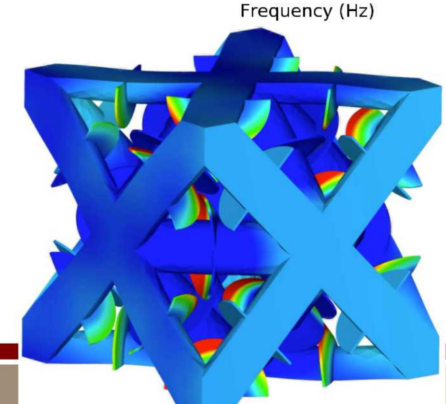


The red, yellow, and blue blocks can be your design space for a new meta-material mount



Lattice with Resonator Discs





Conclusions

- 3D printed, optimized mechanical metamaterials and metasurfaces are practical for kHz filtering
- Inverse optimization framework has been developed in Sierra using Rapid Optimization Library (ROL)
- Spatially-varying mass/stiffness distributions achieved from optimization can be realized with multi-material printing
- 3D metamaterial designs printed on a variety of example applications
- Material samples have been dynamically tested. Initial results demonstrate promising filtering behavior
- Metasurfaces can achieve similar vibration isolation as volumetric metamaterials, but with much thinner layers