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PDE-Constrained Optimization Framework and Inverse Design of Mechanical Metamaterials for Vibration Control

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Overview

- Motivation & Goals
- Designing structures & materials for vibration control
- New approach to design: Modified Error in Constitutive Equations
  - Transient domain formulation
  - Frequency domain formulation
- Numerical examples

Motivation

- Harsh vibration and shock environments are common in engineering systems.
- We want to design materials and structures to control vibration and and dissipate energy.
  - Steady-state behavior: elastic acoustic metamaterial design, base isolator design, etc
  - Transient behavior: shock absorption, impact response, etc.
- (Elastic) metamaterials are a potential solution!
- Application-specific designs may require complex geometries.

How can we design these materials?

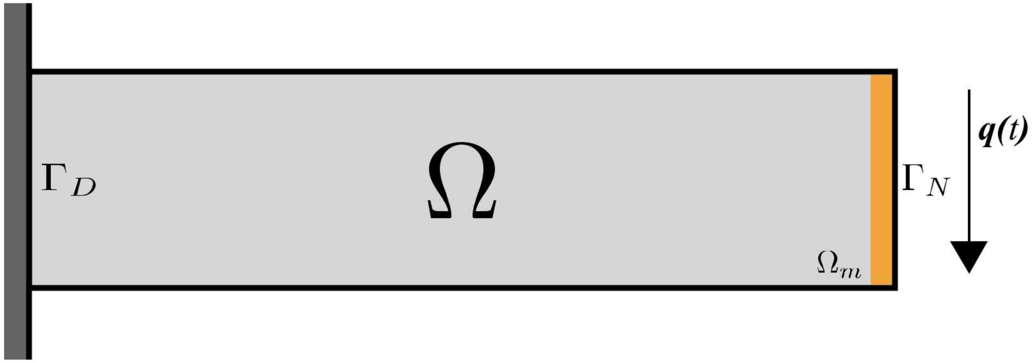
- Topology optimization: Determine the optimal distribution of material within a domain to satisfy structural objective
- Methods to design dynamic materials and structures:
  - Modal design: study frequency response spectra
  - Band-structure/Bloch Floquet analysis: design for material band gaps
  - Minimize dynamic compliance [1]
  - Direct design: design for specific frequency responses
- Solving the design problem: PDE-constrained optimization
  - Gradient-based methods

Objectives

- Develop method to design structures and materials to match desired dynamic behavior
- Desire design method to be:
  - Robust with respect to initial guess, etc
  - Computationally efficient
- Utilize differentiability of constraints for gradient-based methods
- Leverage benefits of inverse-problem methods to avoid numerical and physical instabilities of direct methods

Governing Equations for Transient Elastodynamics

Elastodynamics conservation of momentum equations govern system behavior and provide constraints for optimization. In transient case:



(1) $$\rho\omega^2\ddot{\boldsymbol{u}} = \nabla\cdot\boldsymbol{\sigma} + \boldsymbol{b} \text{ in } \Omega\times[0,T]$$ - Conservation of momentum

$$\boldsymbol{u}(\cdot,0) = \mathbf{0} \text{ on } \Gamma_D\times[0,T]$$ - Dirichlet boundary conditions

$$\dot{\boldsymbol{u}}(\cdot,0) = \mathbf{0} \text{ on } \Gamma_D\times[0,T]$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{n} = \boldsymbol{q}(t) \text{ on } \Gamma_N\times[0,T]$$ - Neumann boundary condition

$$\boldsymbol{\sigma} = \mathbb{C}:\epsilon[\boldsymbol{u}]$$ - Constitutive equations

$$\boldsymbol{\epsilon}[u] = \frac{1}{2}\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\right)$$

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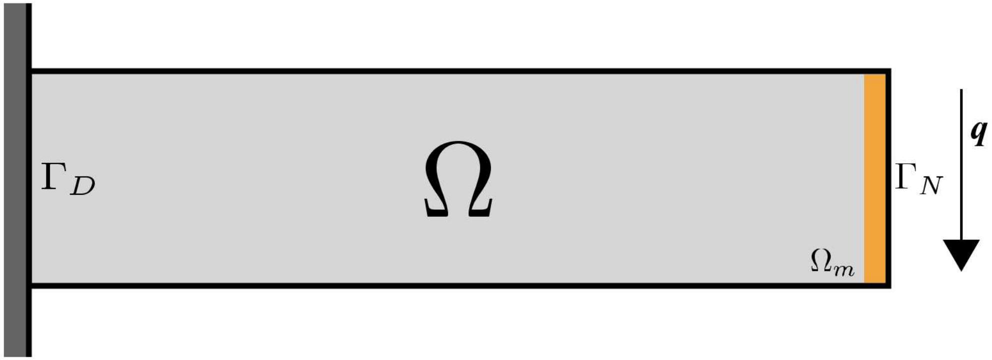
Governing Equations for Frequency-Domain Elastodynamics

In steady-state dynamics, the equations of motion may be expressed:



(1)
$$-\nabla \cdot \boldsymbol{\sigma} - \rho\omega^2 \boldsymbol{u} = \boldsymbol{b} \text{ in } \Omega$$
- Conservation of momentum

$$\boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_D$$
- Dirichlet boundary conditions

$$\boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{q} \text{ on } \Gamma_N$$
- Neumann boundary condition

$$\boldsymbol{\sigma} = \mathbb{C} : \epsilon[\boldsymbol{u}]$$
- Constitutive equations

$$\boldsymbol{\epsilon}[u] = \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)$$

Material Modeling and Design Variables

- Linear elastic materials, with strictly enforced constitutive equation, parameterized by bulk and shear modulus:

$$\boldsymbol{\sigma} = \mathbb{C} : \epsilon[\boldsymbol{u}] = (G\boldsymbol{D}_G + b\boldsymbol{D}_b) : \epsilon[\boldsymbol{u}] \qquad \textbf{(2)}$$

- Solid Isotropic Material Penalization (SIMP) scheme for multi-phase material interpolation [2]
  - Penalization parameter $p \geq 1$ discourages intermediate values.
  - Material phases characterized by set of bulk modulus, shear modulus, and mass density:

$$G(\boldsymbol{\beta}; p) := G^0 + (G^1 - G^0)\beta^p$$

$$b(\boldsymbol{\beta}; p) := b^0 + (b^1 - b^0)\beta^p$$

$$\rho(\boldsymbol{\beta}; p) := \rho^0 + (\rho^1 - \rho^0)\beta^p$$

$$\beta_i \in [0, 1], i = 1..d$$

$$p \in \mathbb{Z}^+$$

Least-squares Design Problem

- Define the minimization problem: Find displacements $\boldsymbol{u}$ and design $\boldsymbol{\beta}$ which minimize the least-squares misfit of the target displacement response

$$\begin{aligned} &\underset{\boldsymbol{u},\boldsymbol{\beta}}{\arg\min}\ \mathcal{J}(\boldsymbol{u},\boldsymbol{\beta}) \\ &\text{subject to: Eqn. [1] \& Eqn. [2]} \\ &\beta_i \leq 1, i = 1...d \\ &\beta_i \geq 0, i = 1...d \end{aligned} \quad \textbf{(L2)}$$

Can we solve this problem robustly?

- Least-squares problem can be unstable.

- In frequency domain, resonances different designs' responses within searchable design space cause non-convexity in objective function
  - Inferior local minima may inhibit progress of gradient-based methods
  - Ideally, we want to design for multiple frequencies (difficult, given this phenomenon)

A different approach…

We can allow violation of the constitutive equations, which improves the convexity of the objective function.

Modified Error in Constitutive Equations (MECE): penalty method which weights competing objectives of matching response exactly and explicitly enforcing constitutive equations.

$$\Lambda(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{\beta}; \kappa) = \mathcal{E}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{\beta}) + \frac{\kappa}{2}\mathcal{J}(\boldsymbol{u}, \boldsymbol{\beta})$$

Penalty parameter κ weights the two objectives.

MECE has been successfully utilized **in material identification inverse problems** in frequency and transient scenarios [3,4].

MECE in Transient Problems

In a transient problem, we strive to design a structure such that its dynamic response matches target displacement time histories.

The objective function components are expressed:

1) **Error in constitutive equations term**: measures violation of constitutive equation relating stresses and strains:

$$\mathcal{E}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{\beta}) = \frac{1}{2} \int_0^T \left((\boldsymbol{\sigma}_t - \mathbb{C}(\boldsymbol{\beta}) : \epsilon[\boldsymbol{u}_t]), \mathbb{C}(\boldsymbol{\beta})^{-1} : (\boldsymbol{\sigma}_t - \mathbb{C}(\boldsymbol{\beta}) : \epsilon[\boldsymbol{u}_t]) \right) dt$$

2) **Least-squares term**: misfit of calculated displacements and target displacement patterns, weighted by penalty parameter

$$\mathcal{J}(\boldsymbol{u}, \boldsymbol{\beta}) = \frac{\kappa}{2} \|\boldsymbol{u} - \boldsymbol{u}^m\|^2_{L_2(\Omega_m)}$$

MECE in Steady-State Problems

We seek to design a structure such that it can match a target vibrational response.

The objective function components are expressed:

1) **Error in constitutive equations term**:

$$\mathcal{E}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\beta}) = \frac{1}{2}\left((\boldsymbol{\sigma} - \mathbb{C} : \epsilon[\boldsymbol{u}]), \mathbb{C}^{-1} : (\boldsymbol{\sigma} - \mathbb{C} : \epsilon[\boldsymbol{u}])\right)_{\Omega}$$

2) **Least-squares term**: misfit of calculated displacements and target displacement patterns

$$\mathcal{J}(\boldsymbol{u},\boldsymbol{\beta}) = \frac{\kappa}{2}\|\boldsymbol{u} - \boldsymbol{u}^{m}\|^{2}_{L_2(\Omega_m)}$$

Optimization for multiple frequencies is represented as sum of objective functions corresponding to individual frequency responses.

MECE Design Problem

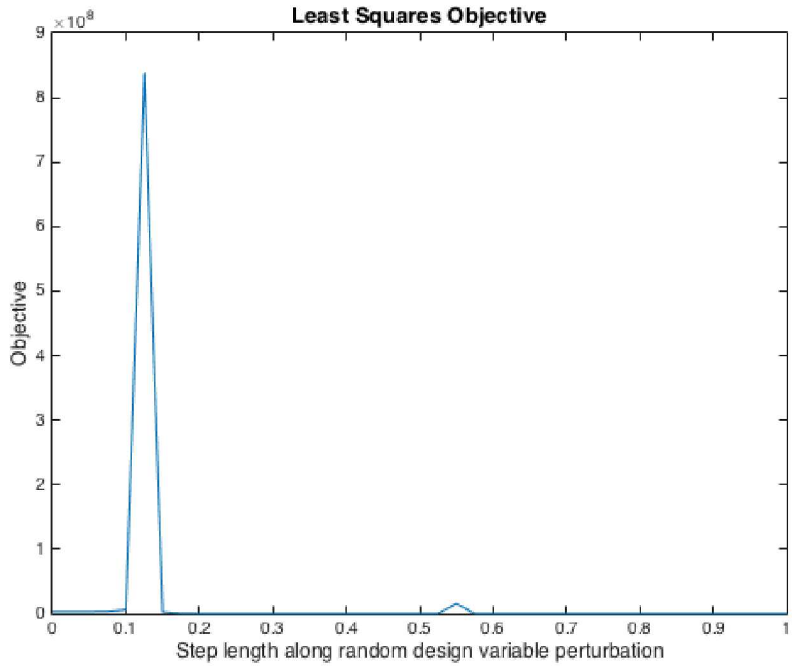
- Define the minimization problem:

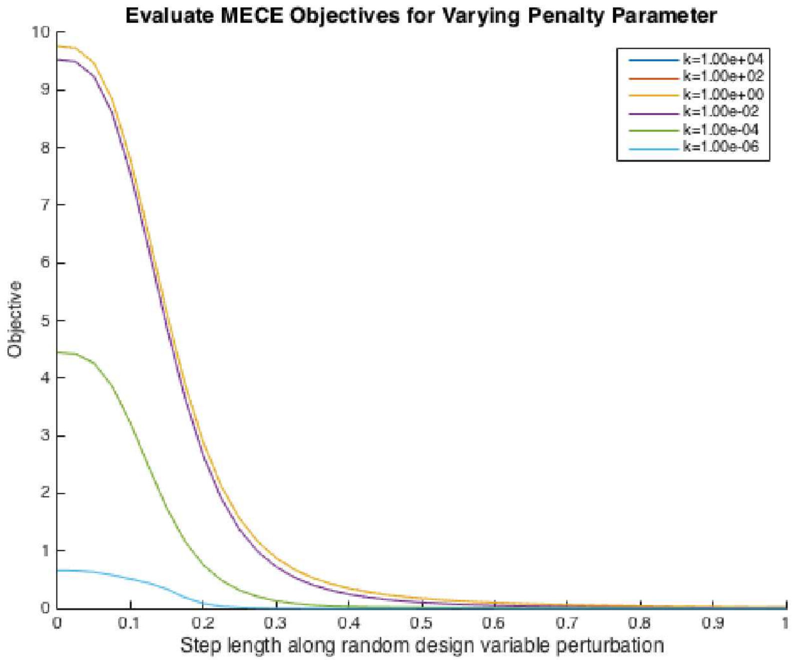
$$\begin{aligned} &\underset{\boldsymbol{u}\in\mathcal{V},\boldsymbol{\sigma}\in\mathcal{S},\boldsymbol{\beta}}{\arg\min}\ \Lambda(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\beta};\kappa) \\ &\text{subject to: Eqn. [1]} \\ &\beta_i \leq 1, i = 1...d \\ &\beta_i \geq 0, i = 1...d \end{aligned} \qquad \textbf{(MECE)}$$

- Constitutive equations now not explicitly enforced as equality constraints

A different approach…

We can compare the objective functions of the L2 and MECE problems.
Objective: minimize the displacement at the end of a vibrating beam.
MECE, with decreasing penalty parameter, converges to Least-squares:





MECE Problem Solution Methods

- Gradient based optimization method
- Form Lagrangian, incorporating objective and PDE-constraints

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\beta},\boldsymbol{w};\kappa) := \Lambda(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\beta};\kappa) + \big((\boldsymbol{\sigma},\epsilon[\boldsymbol{w}]) - \rho(\boldsymbol{\beta})\omega^2(\boldsymbol{u},\boldsymbol{w}) - \boldsymbol{f}(\boldsymbol{w})\big)$$

- KKT first-order optimality conditions lead to:
  - Expression relating stresses to displacement fields $\{u,w\}$:

$$\mathcal{L}'_\sigma[\hat{\boldsymbol{\sigma}}] = 0 \rightarrow \boldsymbol{\sigma} = \mathbb{C} : \epsilon\,[\boldsymbol{u} - \boldsymbol{w}]$$

  - Coupled linear system for forward and adjoint solutions (state variable and Lagrange multipliers)

$$\left\{ \begin{array}{c} \mathcal{L}'_u[\tilde{\boldsymbol{u}}] \\ \mathcal{L}'_w[\tilde{\boldsymbol{w}}] \end{array} \right\} = \left\{ \begin{array}{c} \boldsymbol{0} \\ \boldsymbol{0} \end{array} \right\} \rightarrow \left[\begin{array}{cc} [\boldsymbol{H}](\boldsymbol{\beta}) & \kappa[\boldsymbol{Q}] \\ -[\boldsymbol{K}](\boldsymbol{\beta}) & [\boldsymbol{H}](\boldsymbol{\beta}) \end{array} \right] \left\{ \begin{array}{c} \hat{\boldsymbol{w}}_\beta \\ \hat{\boldsymbol{u}}_\beta \end{array} \right\} = \left\{ \begin{array}{c} [\kappa\boldsymbol{Q}]\hat{\boldsymbol{u}}^t \\ \boldsymbol{F} \end{array} \right\}$$

MECE in Design

In inverse problem approaches, the penalty parameter is selected from criteria based on measurement error (e.g. Morozov discrepancy principle)[3]

How can we interpret the penalty parameter in design?

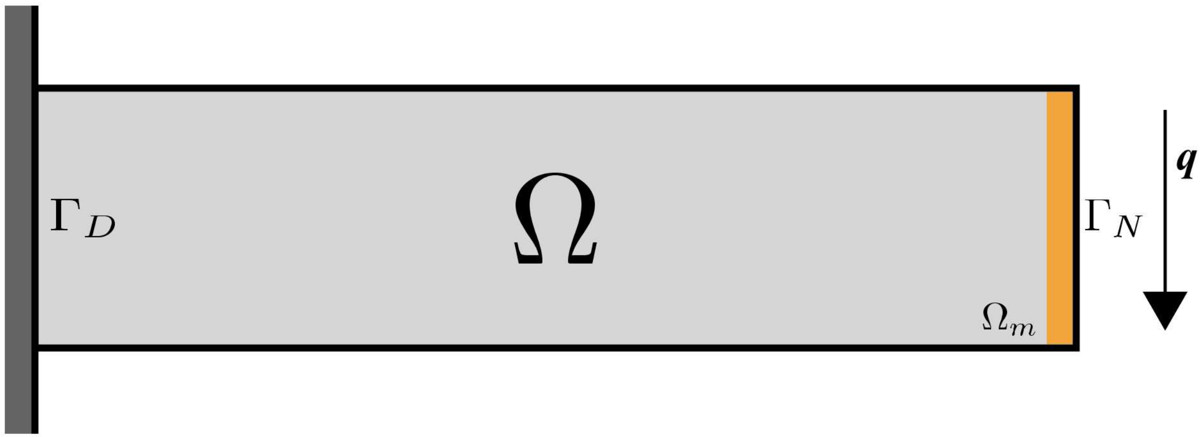
1. **Optimal Penalty Parameter**: Select an optimal \kappa parameter to design, entailing possible violation of constitutive laws
2. **Continuation Approach**: Solve a sequence of optimization problems, with decreasing kappa, to converge to original least-squares problem solution

We'll focus on the second approach.

Design Example: Cantilever Beam Design

Objective:

Minimize vibrational response at end of cantilever beam experiencing forced vibration at multiple frequencies.



Parameters:

Material 0: $\{G_0, b_0, \rho_0\} = \{1, 2, 1e-4\}$

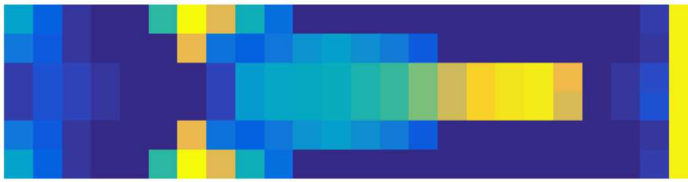
Material 1: $\{G_1, b_1, \rho_0\} = \{1e-2, 2e-2, 1e-6\}$

Initial Guess: $\boldsymbol{\beta} = \mathbf{1}$

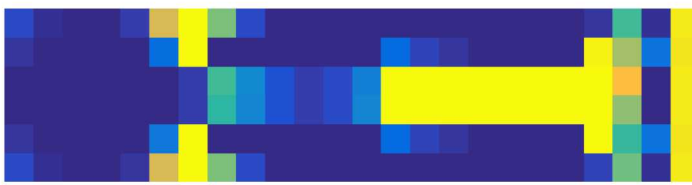
Loading Frequencies:

- Case 1: Single Frequency, $5\ \mathrm{Hz}$
- Case 2: Multiple Frequencies, $\{2, 4, 6\}\ \mathrm{Hz}$

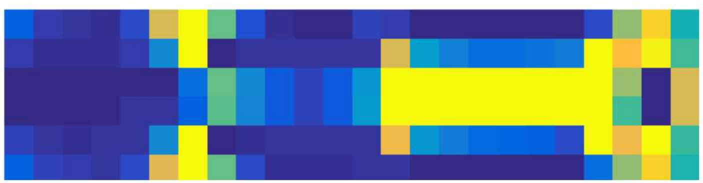
Single-Frequency Optimization: Design Iterations



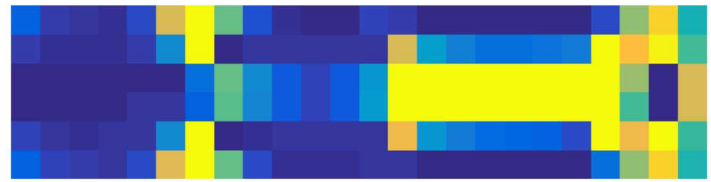
Iteration 1: $\boldsymbol{\kappa}$ = 1.00e+03



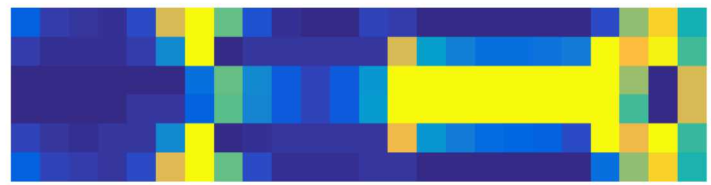
Iteration 2: $\boldsymbol{\kappa}$ = 1.00e+01



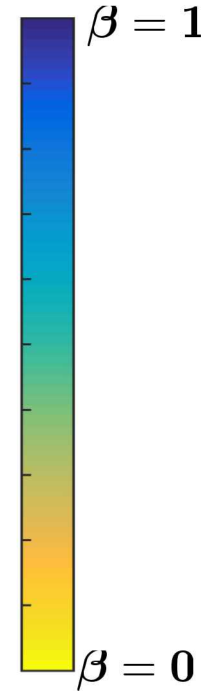
Iteration 3: $\boldsymbol{\kappa}$ = 1.00e-01



Iteration 4: $\boldsymbol{\kappa}$ = 1.00e-03



Iteration 5: $\boldsymbol{\kappa}$ = 1.00e-05



L2 Solution

Single Frequency Design: Displacement Patterns

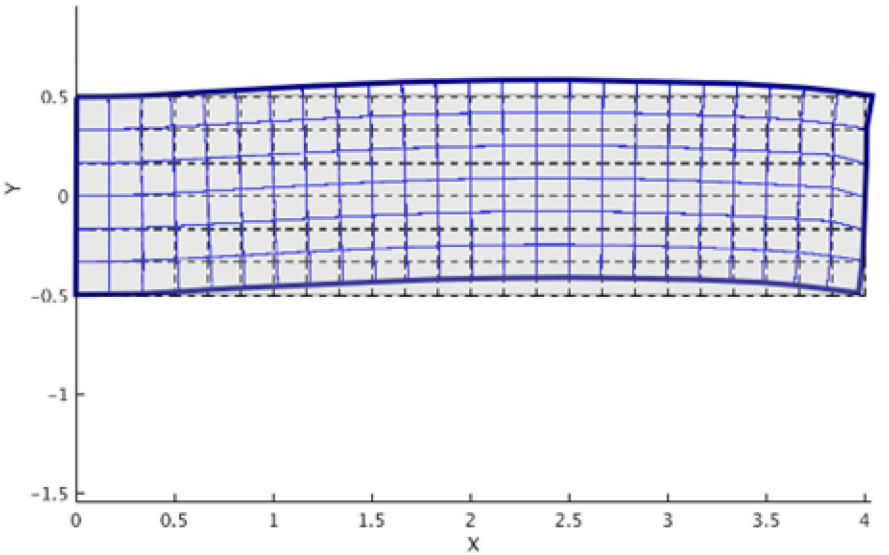


FIGURE: Displacement pattern for L2-problem design
Relative displacement magnitude reduction:

$$\frac{\boldsymbol{u}_{L2}^T[Q]\boldsymbol{u}_{L2}}{\boldsymbol{u}_0^T[Q]\boldsymbol{u}_0} = 0.0906$$

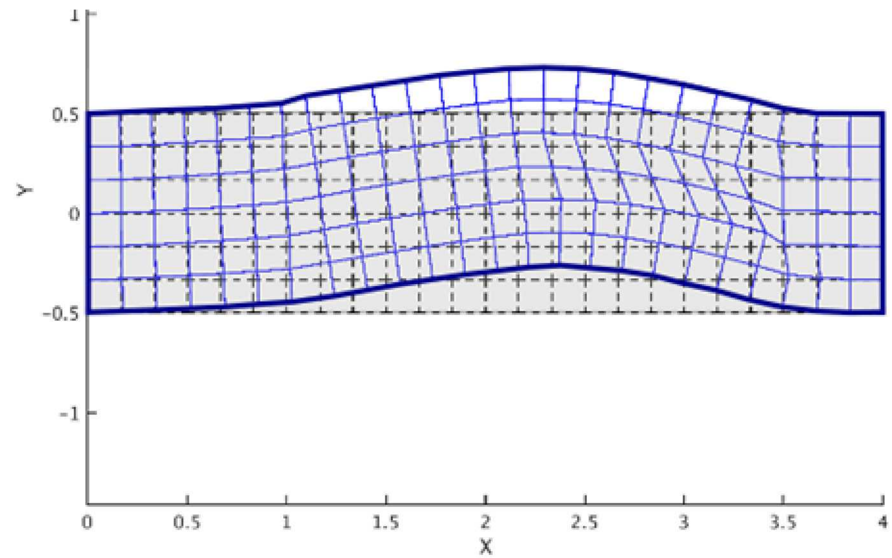


FIGURE: Displacement pattern for C-MECE problem design.
Relative displacement magnitude reduction:

$$\frac{\boldsymbol{u}_{M}^T[Q]\boldsymbol{u}_{M}}{\boldsymbol{u}_0^T[Q]\boldsymbol{u}_0} = 3.2660\text{e-}05$$

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Multi-Frequency Optimization: Design Iterations

Iteration 1: **κ** = 1.00e+04

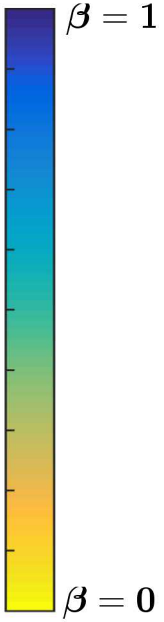
Iteration 2: **κ** = 1.00e+02

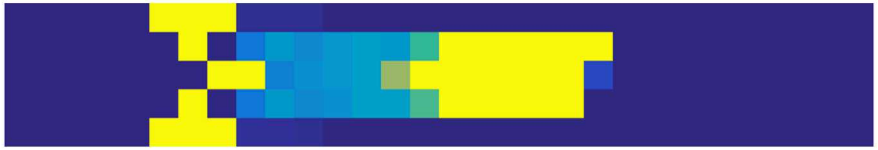
Iteration 3: **κ** = 1.00e+00

Iteration 4: **κ** = 1.00e-02

Iteration 5: **κ** = 1.00e-02

Iteration 6: **κ** = 1.00e-02





L2 Solution

Multi-Frequency Optimization: Displacement Patterns

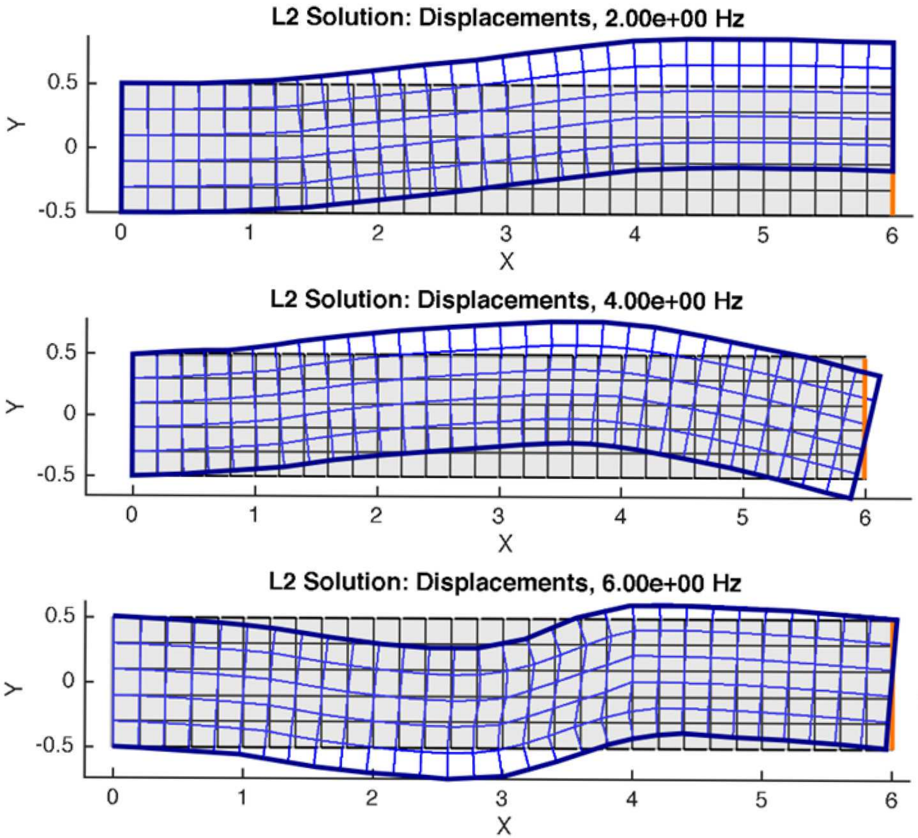


FIGURE: Displacement pattern for L2-problem design
Relative end displacement magnitude:

$$\frac{\boldsymbol{u}_{L2}^T[Q]\boldsymbol{u}_{L2}}{\boldsymbol{u}_0^T[Q]\boldsymbol{u}_0} = 0.1545$$

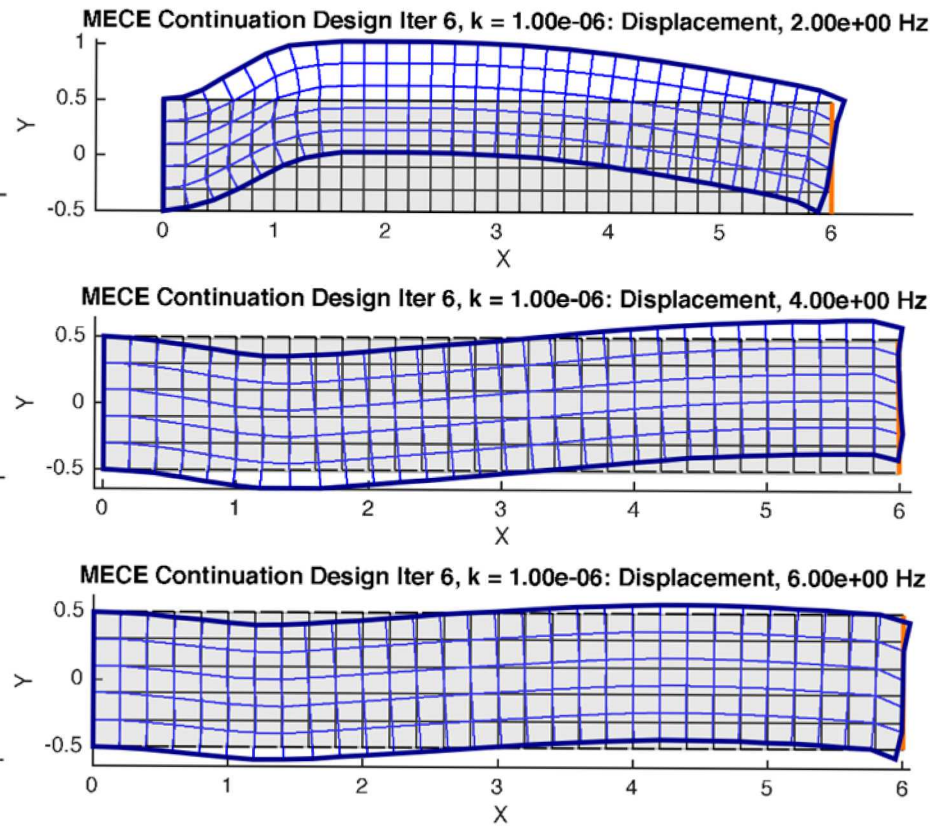


FIGURE: Displacement pattern for C-MECE problem design.
Relative end displacement magnitude: 0.0186

$$\frac{\boldsymbol{u}_{M}^T[Q]\boldsymbol{u}_{M}}{\boldsymbol{u}_0^T[Q]\boldsymbol{u}_0} = 0.0186$$

Evolution of Design Performance in Continuation Method

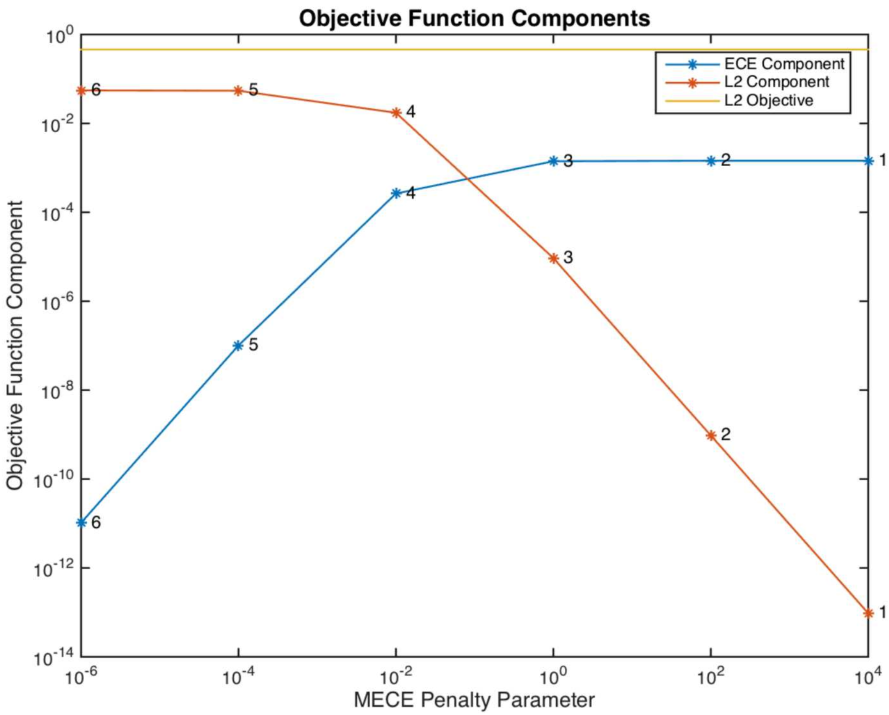


FIGURE: Evolution of objective function components for successive continuation iterations

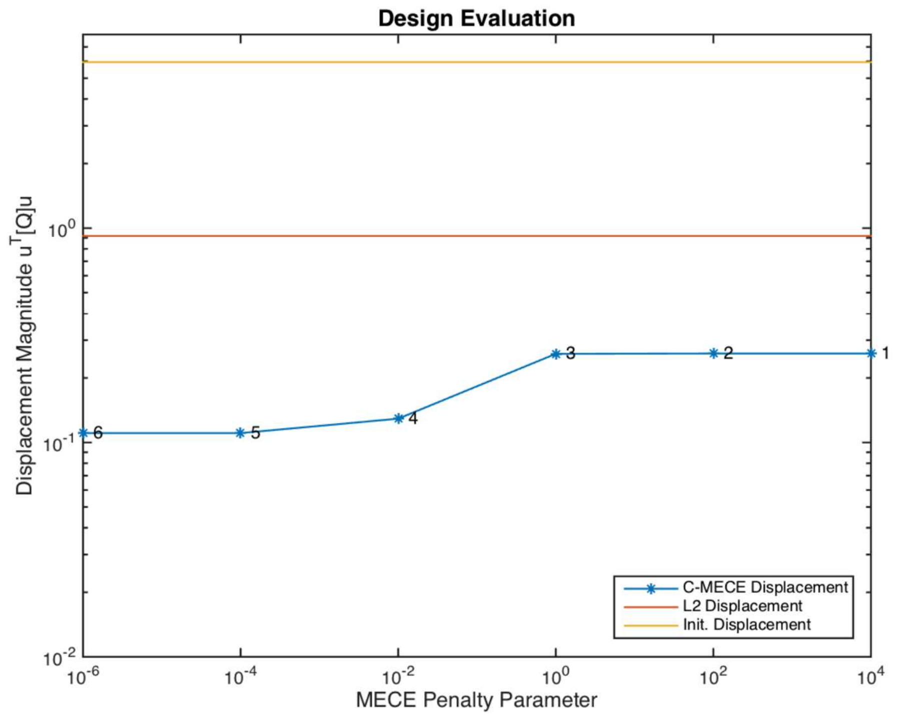


FIGURE: Design performance, measured with displacement magnitude, for successive continuation iterations.

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Conclusions

- Presented a Modified Error in Constitutive Equations approach to material and structural design
- Continuation scheme solves sequence of MECE optimization problems, reducing the penalty parameter and converging to L2 problem
- Continuation scheme approach can converge to a unique local minimum from L2 problem
- Multi-frequency problems especially promising for MECE; superposition of FRF's in L2 problem makes problem less convex
- Future directions:
  - Extension to acoustic-structural interaction for acoustic cloaking applications
  - Transient problem implementation

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