SAND2015-10604C

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Sandia National Laboratories

Virtual Science-based Technical Strategy

Goodyear/Sandia Leadership Meeting

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3 Dec 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Motivation: Discussion Question

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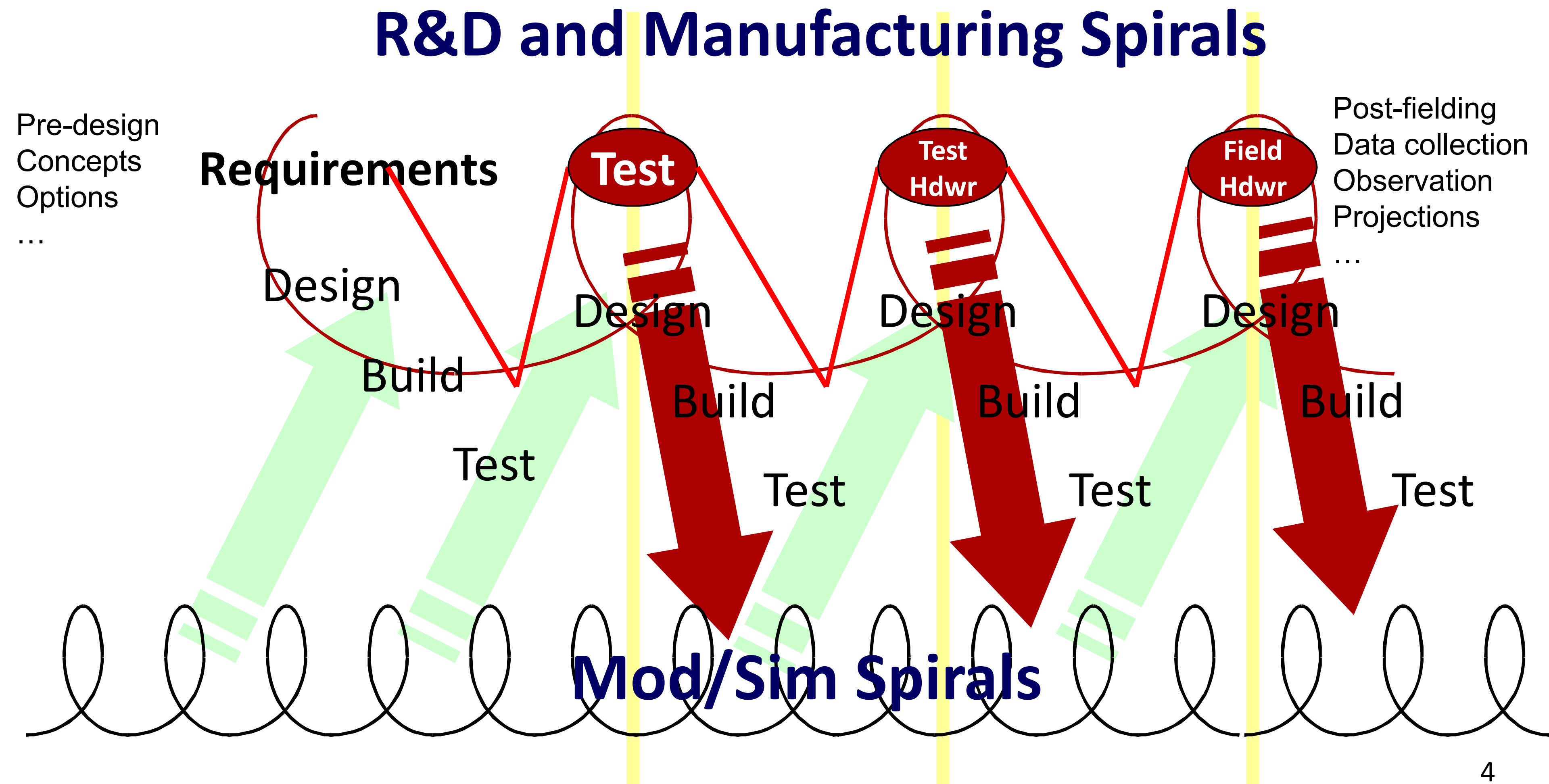
"How do we merge testing and simulation for best decision making, considering both effectives and efficiency?"

Motivation: Discussion Question

- Merge testing and simulation – Some thoughts
  - We desire effectiveness and efficiency from this objective (by definition for this meeting)
  - Clearly testing can be improved by simulation and simulation can be improved by testing
    - How? Where? When?
    - How does synergy of "merge" exceed independent test and simulation?
  - Potential to rejuvenate and revitalize existing test infrastructure and fixtures

Motivation: Discussion Question

- How do we improve existing concepts of test & simulation?

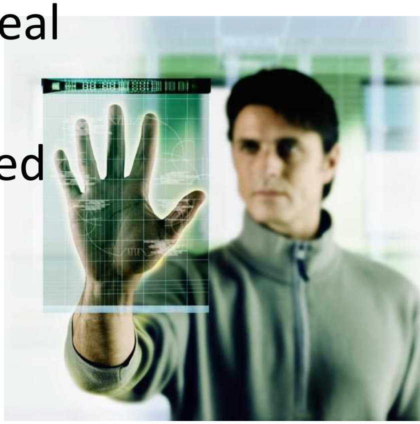


Motivation: Discussion Question

- Merge testing and simulation – Some thoughts (continued)
  - Strong potential for new IP in this pursuit
  - Uniqueness claims should exist in technology and process
  - Validation of simulation for intended use can be critical
  - How do we move data between test and simulation environment?

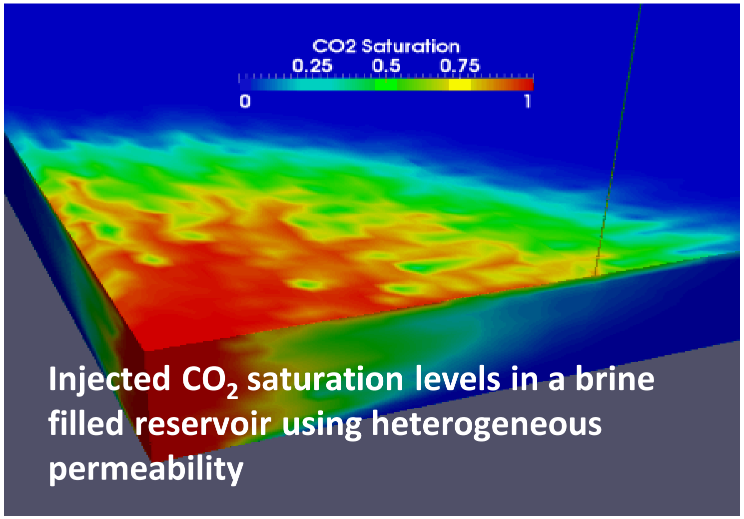
Motivation: Discussion Question

- Borrowing from "Live Virtual Constructive" (LVC), often used by DoD as taxonomy for classifying models & simulations.
  - **Live** – (analogy to "Test?") A "simulation" involving live people and things – still a simulation because it is not a real environment. A live wargame.
  - **Virtual** – Real people and things interacting with simulated systems. e.g., simulation with "human in the loop," or physical asset interacting with a simulation. Data moves back and forth between simulation and the real world.
  - **Constructive** – Simulated people operating simulated systems. Pure simulation.
- A fully merged Test-Simulation environment would allow one to flow back and forth across these domains as needed to achieve testing objectives.



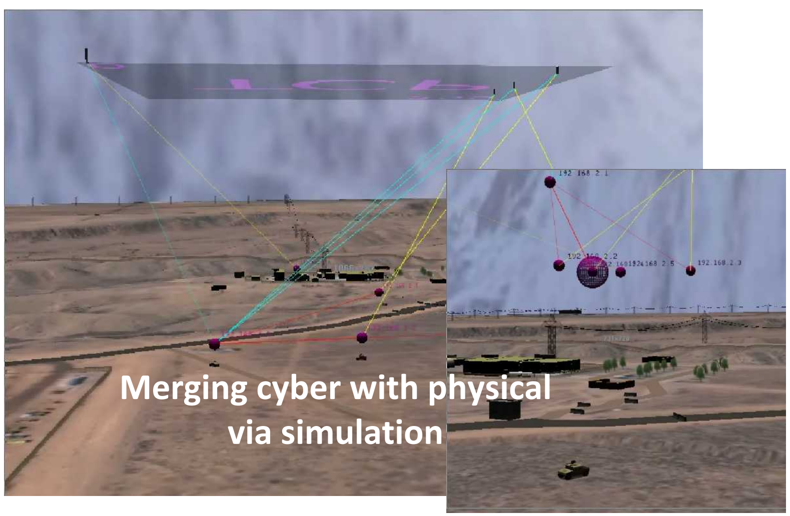
Motivation: Discussion Question

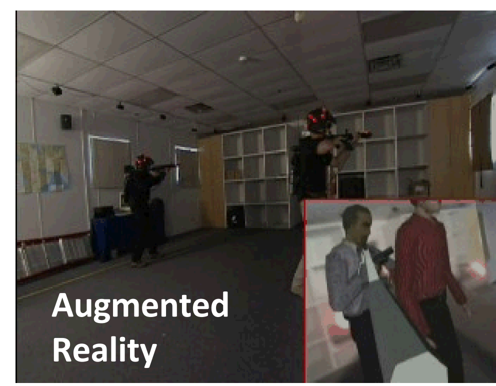
- A few examples at Sandia



Injected CO_2 saturation levels in a brine filled reservoir using heterogeneous permeability


LNG Test 2 - De-coupled LNG pool spreading and fire spreading


Merging cyber with physical via simulation


Augmented Reality

Brainstorming a Test-Sim Merge Spectrum

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MORE LIKE TEST | **TEST-SIMULATION MERGE** | **MORE LIKE SIMULATION**

DIFFICULT (future)

EASIER (now)

As one way to map ideas related to a merge of Test and Simulation, consider a space with these dimensions…

Brainstorming a Test-Sim Merge Spectrum

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MORE LIKE TEST

TEST-SIMULATION MERGE

MORE LIKE SIMULATION

MORE DIFFICULT

EASIER

Live-Virtual-Constructive Test Systems "Holodeck"

Test Validated by Sim

Sim Validated by Test

Brainstorming a Test-Sim Merge Spectrum

MORE LIKE TEST

TEST-SIMULATION MERGE

MORE LIKE SIMULATION

MORE DIFFICULT

EASIER

Live-Virtual-Constructive Test Systems "Holodeck"

Simulated Test Environments

Design of Experiments (Test)

Extend Test Results to Sensor-denied Areas

Collect field performance data, project future performance

Inverse Problems

Sim Creating System or Test Requirements

Optimize Test Through Sim

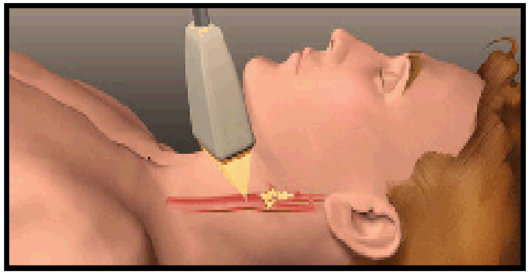
Test Informed by Sim

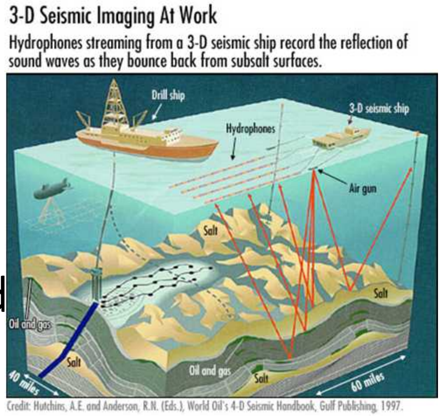
Test Validated by Sim

Sim Validated by Test

Categories of Inverse Problems

- Imaging + shape reconstruction
  - Can be used as a testing tool
  - Ultrasound: medical, seismic
- Calibration of material models
  - Merges test and sim
- Optimal Experimental Design
  - Best placement of sensors, test fixture setups
- Information mining
  - Using physics-based models to interrogate sensor d
- Design of materials
  - E.g. Cloaking, camouflage, noise suppression, etc





Inverse Problems – Effectiveness and Efficiency

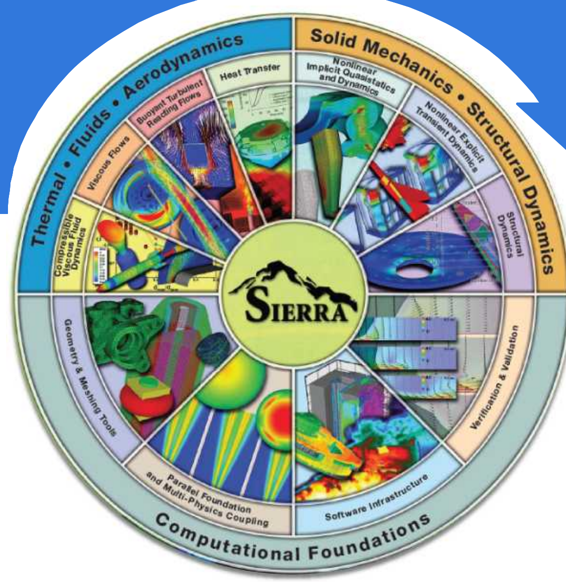
- Cost savings by minimizing testing on actual systems
- Improved understanding of *as-built* systems
  - Material property distribution, metrology, crack detection, etc.
- Decreased uncertainty stemming from robust model calibration.
- Inverse problems provide a natural path to V&V by marrying experiments and simulation.

Experiment + Simulation

- Inverse problems merge experiments and simulation
- Experiment drives the inverse problem, and inverse problem drives the experiments

Experiment

Optimization loop



Series of Forward Problems

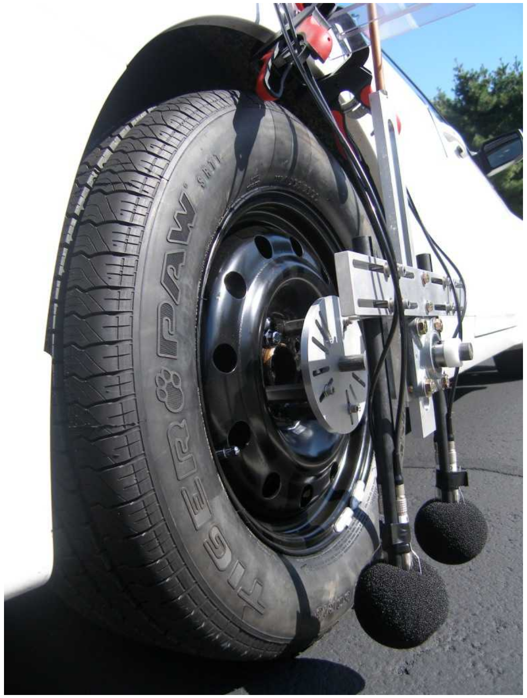
Quantity of Interest

- Material parameters
- Boundary conditions
- Loads
- Etc, etc

Inverse Problems: Potential Collaboration

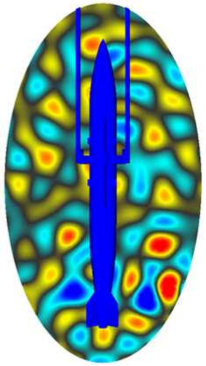
Minimizing noise radiation

- Adjust material properties to minimize vibration-induced noise
- Adjust tire layout parameters (belts, rubber, etc) to minimize structural-borne noise and vibration

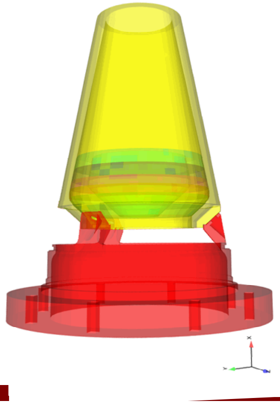


Related inverse problems at Sandia:

Source inversion



Material optimization



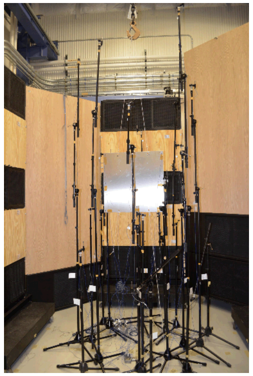
Inverse Problems: Potential Collaboration

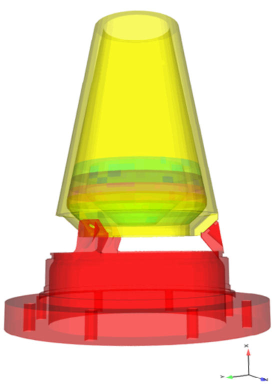
Characterizing boundary conditions

- Determining appropriate friction models for traction (wet, dry, etc)
- Determining traction forces in footprint (validation)

Related inverse problems at Sandia:

Determining impedance boundary conditions





Inverse Problems – Potential CRADA Interactions

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Inverse homogenization

Given a composite of 2 materials, material A (which is known) and material B (which is unknown), find the properties of material B such that the composite has prescribed properties

Material A - rubber
Material B - inclusions

Slide to be provided by M. Sobhanie (GY Akron)

Discussion

"How do we merge testing and simulation for best decision making, considering both effectives and efficiency?"

Technical Concepts (Back-up Slides)

Abstract Optimization Formulation

Abstract optimization formulation

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

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

Objective function

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

Operator-Based Solution Strategy

The Newton Step equations:

$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{up} & g_u^T \\ \mathcal{L}_{pu} & \mathcal{L}_{pp} & g_p^T \\ g_u & g_p & 0 \end{bmatrix} \begin{Bmatrix} \delta u \\ \delta p \\ w^\star \end{Bmatrix} = - \begin{Bmatrix} J_u \\ J_p \\ g \end{Bmatrix} \quad (1)$$

Reduced-space approach:
Static condensation of δu and $w^\star$

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

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

Full-space approach:
Solve equations (1) as is

Key concept: If we can define the action of each of the operators in equation (1) on a vector or vectors, then

1. Software structure can be modularized
2. We can have access to all optimization methods through a single interface[1]

[1]Heinkenschloss and Vicente, "An Interface between Optimization and Application for the Numerical Solution of Optimal Control Problems", ACM Transactions on Mathematical Software, Vol. 25, No. 2, June 1999, Pages 157–190.

Material Inversion Research

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Eigenvalue-based approach

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

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

$$b_i = 0$$

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

$$b_i = b(\boldsymbol{u}_i) = \boldsymbol{u}_i^T \boldsymbol{M}\boldsymbol{u}_i - 1 = 0$$

$$\mathscr{L}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{w},\boldsymbol{\eta}) := J + \boldsymbol{w}^T\boldsymbol{g} + \sum_{i=i}^{n} \eta_i b_i$$

Applicability: stiffness parameters (springs, elastic materials)

Helmholtz-based approach

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

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

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

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

$$\boldsymbol{\sigma}(\omega) = \boldsymbol{D}(\omega)\boldsymbol{\epsilon} = (b(\omega)\boldsymbol{D}_b + G(\omega)\boldsymbol{D}_G)\boldsymbol{\epsilon}(\omega)$$

Applicability: stiffness, mass and damping parameters

Strategy: eigenvalue-based inversion followed by Helmholtz-based inversion

Source Inversion in Sierra-SD

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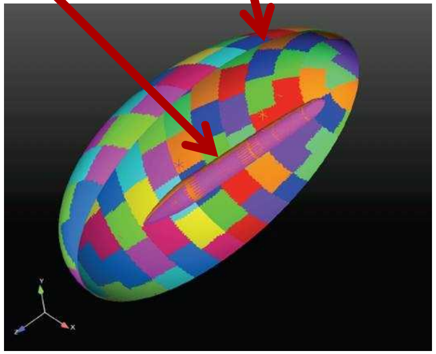
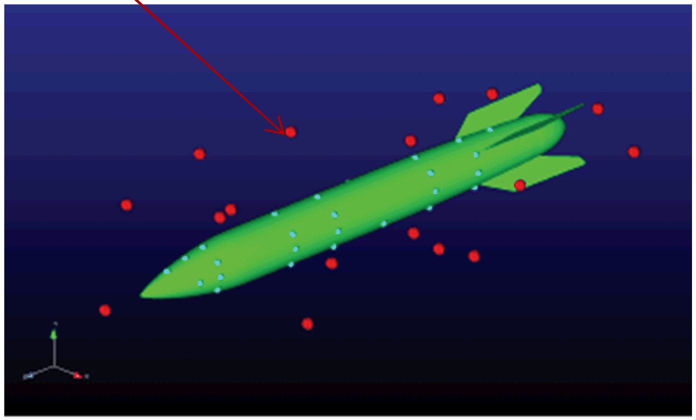
Goal:
Solve inverse problem to obtain acoustic patch inputs that produce the given microphone measurements.

2 approaches:
1. Frequency domain
   - broadband frequency sweep
2. Time domain
   - implicit time integration that covers frequency range of interest

Surface with 172 acoustic patches

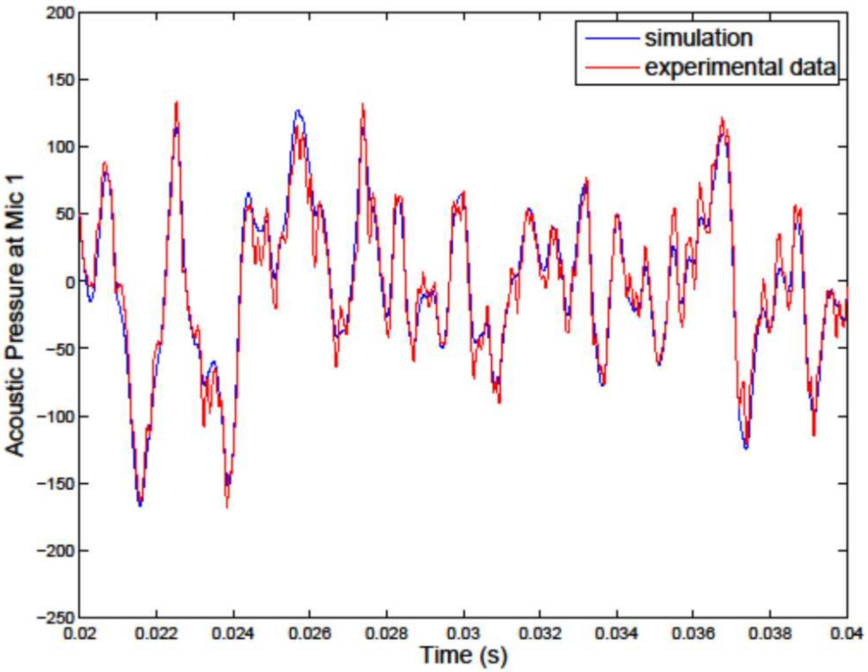


Microphone locations

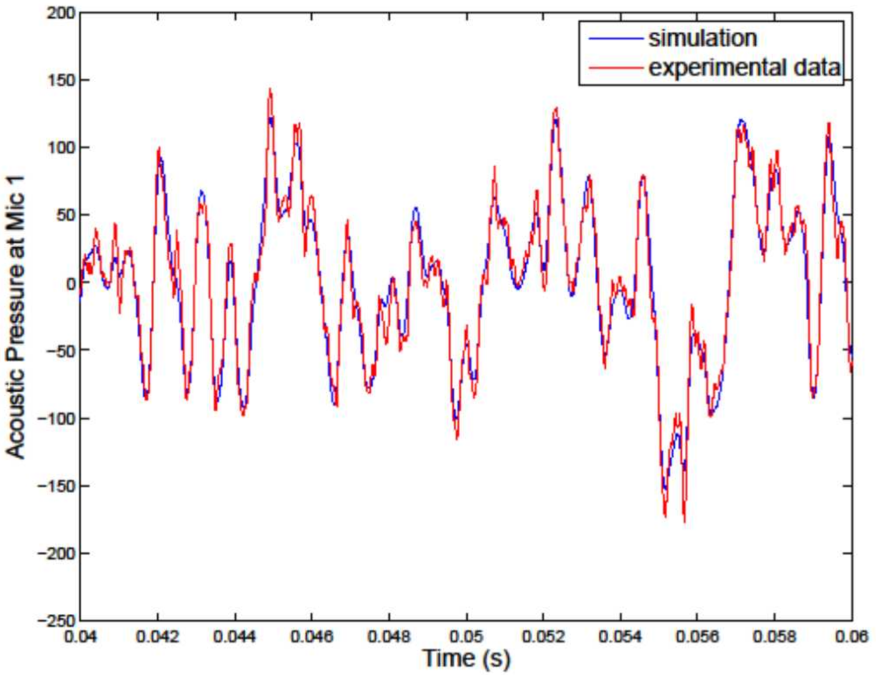


Time Domain Source Inversion Using Sierra-SD/ROL

A Comparison of Experimental Data and Inverse Simulation for Microphone 1



0.02(s) < t < 0.04(s)



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Eigenvalue-Based Material Inversion

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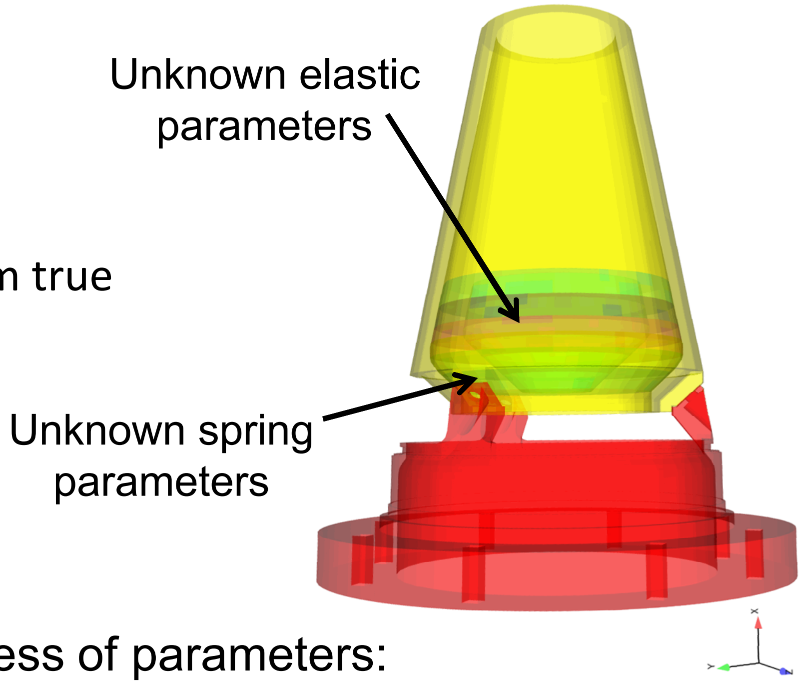
- Spring/foam calibration on mass-mock
- Goal: Match synthetic modes to computed modes
- Synthetic modal data used as input
- Initial guess of parameters a factor of 10 away from true values



Mode number	Initial Guess	Results from inversion	Exact modes
1	2.759e6	1.240e6	1.240e6
2	2.957e6	1.358e6	1.3607e6
3	1.157e7	7.071e6	7.052e6
4	1.186e7	1.041e7	1.043e7
5	1.266e7	1.102e7	1.103e7
6	1.695e7	1.262e7	1.256e7
7	2.041e8	2.025e8	2.025e8

Initial guess of parameters:

Table 1. Joint2G parameters for joint 1 of LFU model.

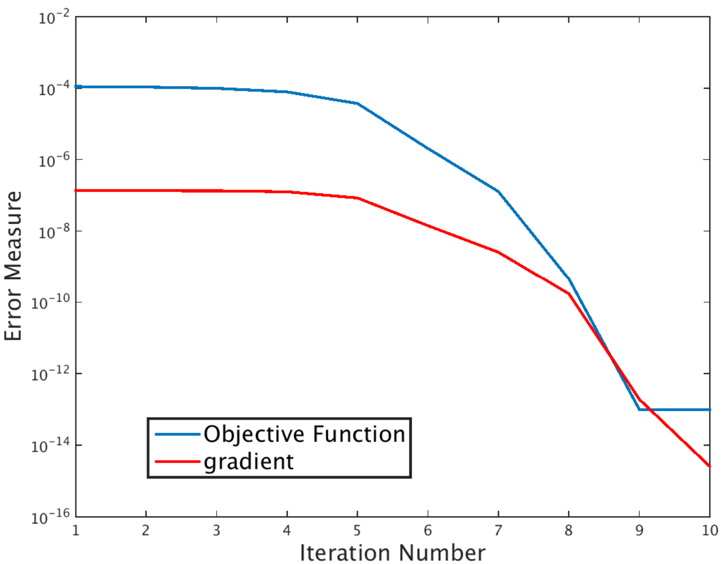
	kx	ky	kz	krz	kry	krz
exact	2.46e6	2.0e8	2.0e8	N/A	N/A	N/A
computed	2.47e6	2.0e8	2.0e8	N/A	N/A	N/A
initial guess	2.46e5	2.0e8	2.0e8	N/A	N/A	N/A

Table 4. Elastic foam parameters for LFU model.

	shear modulus (G)	bulk modulus (K)
exact	1.585e4	4.134e4
computed	1.585e4	4.134e4
initial guess	1.585e3	4.134e3

Frequency-Domain Material Inversion

- Dashpot/foam calibration on mass-mock
- Full Newton with adjoint-based Hessians
- Measured displacements on foam block
- Stiffness parameters from previous slide
- Initial guess: zero damping



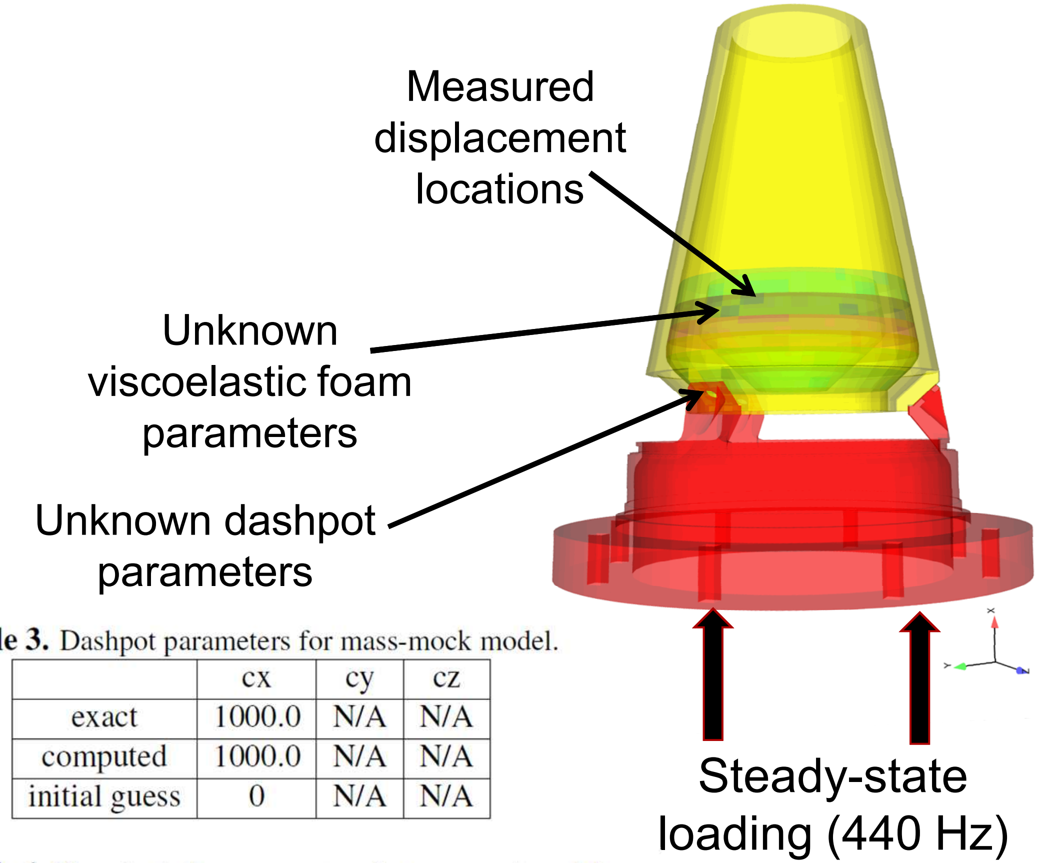


Table 3. Dashpot parameters for mass-mock model.

	cx	cy	cz
exact	1000.0	N/A	N/A
computed	1000.0	N/A	N/A
initial guess	0	N/A	N/A

Table 4. Viscoelastic foam parameters for mass-mock model.

	Imaginary part of G	Imaginary part of K
exact	362.4	785.2
computed	362.3	785.0
initial guess	0	0

SimOpt: The middleware for engineering optimization

Objective_SimOpt

value(u,z)
gradient_1(g,u,z)
gradient_2(g,u,z)
hessVec_11(hv,v,u,z)
hessVec_12(hv,v,u,z)
hessVec_21(hv,v,u,z)
hessVec_22(hv,v,u,z)

Note: 1 = Sim = u
2 = Opt = z

EqualityConstraint_SimOpt

value(c,u,z)
applyJacobian_1(jv,v,u,z)
applyJacobian_2(jv,v,u,z)
applyInverseJacobian_1(ijv,v,u,z)
applyAdjointJacobian_1(ajv,v,u,z)
applyAdjointJacobian_2(ajv,v,u,z)
applyInverseAdjointJacobian_1(iajv,v,u,z)
applyAdjointHessian_11(ahwv,w,v,u,z)
applyAdjointHessian_12(ahwv,w,v,u,z)
applyAdjointHessian_21(ahwv,w,v,u,z)
applyAdjointHessian_22(ahwv,w,v,u,z)
solve(u,z)

Rapid Optimization Library (ROL)

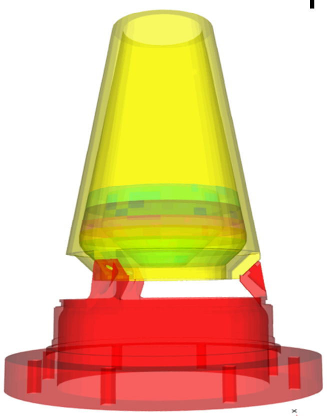
- ROL is a Trilinos package for large-scale continuous optimization, a.k.a. nonlinear programming (NLP).
- Available in Trilinos since 10/21/2014.
- ROL includes:
  - A rewrite and consolidation of existing optimization tools in Trilinos: *Aristos, MOOCHO, Optipack, Globipack.*
  - Hardened, production-ready algorithms for unconstrained and equality-constrained continuous optimization.
  - Methods for efficient handling of inequality constraints.
  - A unified interface for simulation-based optimization.
  - New methods for efficient handling of inexact computations.
  - New methods for optimization under uncertainty.

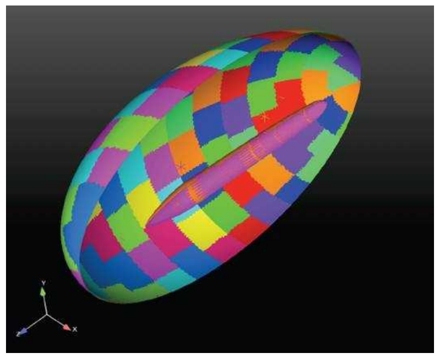
http://trilinos.org/packages/rol/

Contacts: Denis Ridzal, Drew Kouri (Sandia)

Generality of Operator-Based Optimization

Applications





operators

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

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

Elastic parameters

Residual Stress fields

Impedance boundaries

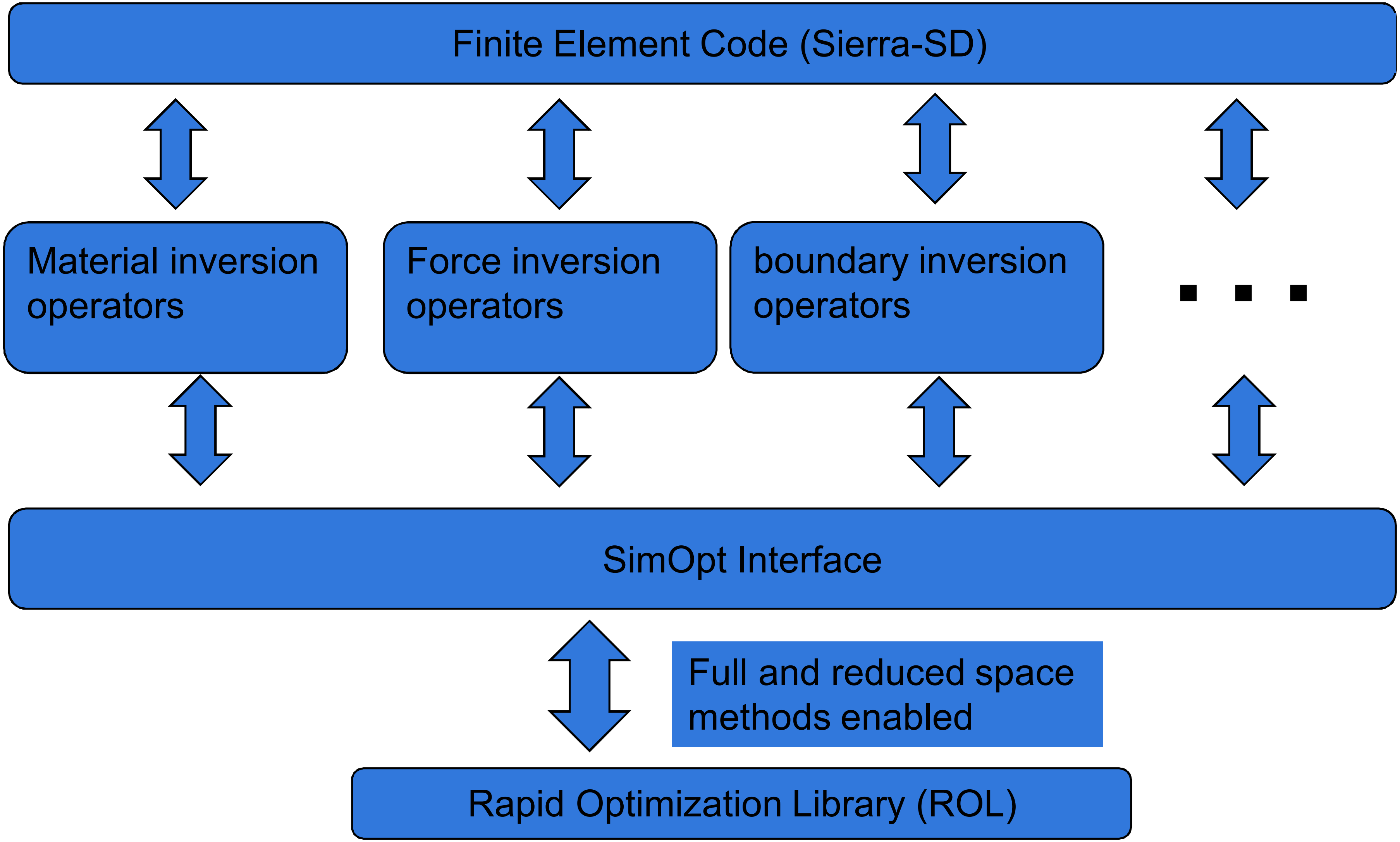
Viscoelastic parameters

density

Loads/ forces

Applications → operators → optimization

Operator-Based Inverse Problems



Inverse Problems in Sierra-SD

Three modalities are available:

Time-domain

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

- Stiffness, damping parameters
- Linear or nonlinear
- Force/Material identification

Frequency-domain

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

- Stiffness, damping, parameters
- Linear only
- Force/material identification

Eigenvalue (modal)

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

- Stiffness parameters
- Linear only
- Material identification

Conclusions

- Wide-range of potential applications for inverse problems at Sandia
- Massively parallel structural dynamics and acoustics (Sierra-SD) and optimization software(ROL) have been loosely coupled through SimOpt interface for the solution of a variety of inverse problems.
- Operator-based approach for both mathematical formulation and software development allows for:
  - Modular software infrastructure
  - Allows various optimization methods to be accessed through a single interface