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- What is ROL?
- Motivation
- Problem formulations
- Application programming interface
- Methods
- Research focus

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.

Motivation

- Optimization of differentiable simulated processes:
  - partial differential equations (PDEs)
  - differential algebraic equations (DAEs)
  - network equations (gas pipelines, electrical networks)
- Inverse problems, model calibration.
- Optimal design, including topology and shape optimization.
- Optimal control, optimal design of experiments, etc.
- Parameter/design/control spaces can be very large, often related to the size of the computational mesh (PDEs) or the size of the device network or graph (DAEs).
- Simulated processes may be subject to uncertainty.

Motivation

- Example cost of deterministic optimization, in terms of "simulation units", such as nonlinear PDE/DAE solves:

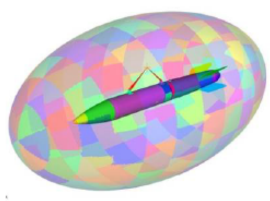
Information	Size of parameter space				Methods
	1	10	10^3	10^6	
Function samples (incl. finite diff's)	100	10,000	∞	∞	Global search or steepest descent
Analytic gradients (hand-coded or AD)	50	100	200	1,000	Quasi-Newton
Analytic Hessians (hand-coded or AD)	50	50	50	50	Newton-Krylov

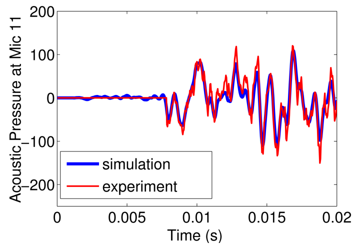
- *We want derivative-based methods.*
- *We want **embedded and matrix-free** methods:*
  - Direct access to application data structures: vectors, etc.
  - Direct use of application methods: (non)linear solvers, etc.

A few current use cases

Inverse problems in acoustics / elasticity.

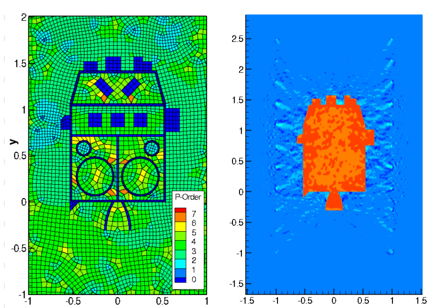
- Interface to the Sierra-SD structural dynamics code (Sandia, Org. 1500).





1M optimization variables, 1M state variables

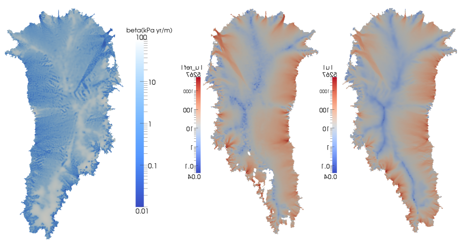
- Interface to DGM, a high-order DG code (Sandia, Org. 1400).



- **175K distributed optimization variables**
- 525K x 10K state variables

Estimating basal friction of ice sheets.

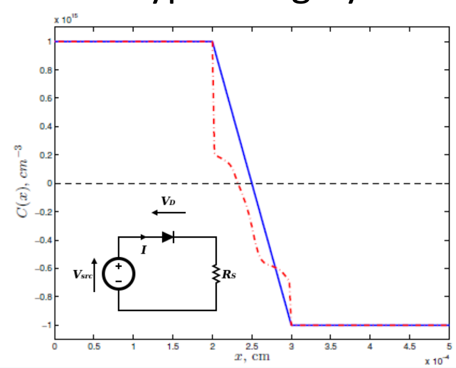
- Interface to LifeV Project (www.lifev.org).



- **65K distributed optimization variables**
- 700,000 state variables

Calibration of electrical device models.

- Prototype using Xyce circuit simulator.



- **50 optimization variables (in-memory or disk storage)**

Mathematical abstraction

- Straight from ROL's documentation:

ROL is used for the numerical solution of smooth optimization problems

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) = 0\,, \\ & a \le x \le b\,, \end{aligned}$$

where:

- $f : \mathcal{X} \to \mathbb{R}$ is a Fréchet differentiable functional,
- $c : \mathcal{X} \to \mathcal{C}$ is a Fréchet differentiable operator,
- $\mathcal{X}$ and $\mathcal{C}$ are Banach spaces of functions, and
- $a \le x \le b$ defines pointwise (componentwise) bounds on x.

- This abstraction is a valuable guiding principle.

Problem formulations

- ROL supports four basic NLP problem types:

Type-U: Unconstrained.

$$\min_{x} \quad f(x)$$

Type-B: Bound constrained.

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & a \le x \le b \end{aligned}$$

Type-E: Equality constrained.

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) = 0 \end{aligned}$$

Type-EB: Equalities + bounds.

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) = 0 \\ & a \le x \le b \end{aligned}$$

Note:

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) \le 0 \end{aligned} \qquad \longleftrightarrow \qquad \begin{aligned} \min_{x,s} \quad & f(x) \\ \text{subject to} \quad & c(x) + s = 0\,, \\ & s \ge 0\,. \end{aligned}$$

Design of ROL

Application programming interface

Linear algebra interface	Functional interface		Algorithmic interface
Vector	Objective BoundConstraint EqualityConstraint	SimOpt Middleware	StatusTest **Step** DefaultAlgorithm

Methods – Implementations of Step instances

Linear algebra interface

- ROL::Vector is designed to enable direct use of application data structures (serial, parallel, in-memory, disk-based, etc.).
- Methods:
  plus, scale, dot, norm, clone (pure virtual)
  axpy, zero, set (virtual)
  basis, dimension (optional)
- Nothing new. History: HCL/RVL, TSFCore, Thyra.
- Recent applications of ROL require dual-space operations:
  dual **(virtual)**
- Note: Other Trilinos packages have similar linear algebra interfaces, but may not be able to take advantage of dual-space operations, such as Riesz maps.

Functional interface

$$\begin{aligned} \min_{x} \quad & \boxed{f(x)} \\ \text{subject to} \quad & c(x) = 0 \\ & a \le x \le b \end{aligned}$$

- ROL::Objective provides the objective function interface.
- Methods:
  value (pure virtual)
  gradient, hessVec (virtual)
  update, invHessVec, precond, dirDeriv (optional)
- We can use finite differences to approximate missing derivative information (default implementation).
- For best performance, implement analytic derivatives.
- Tools: checkGradient, checkHessVec, checkHessSym.
- ROL::BoundConstraint enables pointwise bounds on optimization variables, in support of projected gradient, projected Newton, and primal-dual active set methods.

Functional interface

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & \boxed{c(x) = 0} \\ & a \le x \le b \end{aligned}$$

- ROL::EqualityConstraint enables equality constraints.
- Methods:

  value (pure virtual)

  applyJacobian, applyAdjointJacobian, applyAdjointHessian (virtual)

  update, applyPreconditioner, solveAugmentedSystem (optional)
- We can use finite differences to approximate missing derivative information (default implementation).
- For best performance, implement analytic derivatives.
- Tools: checkApplyJacobian, etc.

Functional interface

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & \boxed{c(x) = 0} \\ & a \le x \le b \end{aligned}$$

- Documentation excerpt:

template<class Real >

```
void ROL::EqualityConstraint< Real >::applyAdjointHessian ( Vector< Real > &        ahuv,
                                                             const Vector< Real > &  u,
                                                             const Vector< Real > &  v,
                                                             const Vector< Real > &  x,
                                                             Real &                  tol
                                                           )
```

virtual

Apply the derivative of the adjoint of the constraint Jacobian at x to vector u in direction v, according to $\boxed{v \mapsto c''(x)(v,\cdot)^* u.}$

Parameters

[out]	**ahuv**	is the result of applying the derivative of the adjoint of the constraint Jacobian at **x** to vector **u** in direction **v**; a dual optimization-space vector
[in]	**u**	is the direction vector; a dual constraint-space vector
[in]	**v**	is an optimization-space vector
[in]	**x**	is the constraint argument; an optimization-space vector
[in,out]	**tol**	is a tolerance for inexact evaluations; currently unused

On return, ahuv $= c''(x)(v,\cdot)^* u$, where $u \in C^*$, $v \in \mathcal{X}$, and ahuv $\in \mathcal{X}^*$.

The default implementation is a finite-difference approximation based on the adjoint Jacobian.

SimOpt: The middleware for engineering optimization

- Many simulation-based Type-E problems have the form:

$$\min_{u,z} \; f(u,z) \quad \text{subject to} \quad c(u,z) = 0$$

  - u denote simulation variables (state variables, **basic, Sim**)
  - z denote optimization variables (controls, parameters, **nonbasic, Opt**)

- A common Type-U reformulation, by nonlinear elimination, is:

$$\min_{z} \; f(u(z),z) \quad \text{where } u(z) \text{ solves } c(u,z) = 0$$

- For these cases, the SimOpt interface enables direct use of methods for **both** unconstrained and constrained problems.

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)

SimOpt: Benefits

- Streamlined modular implementation for a very large class of engineering optimization problems.

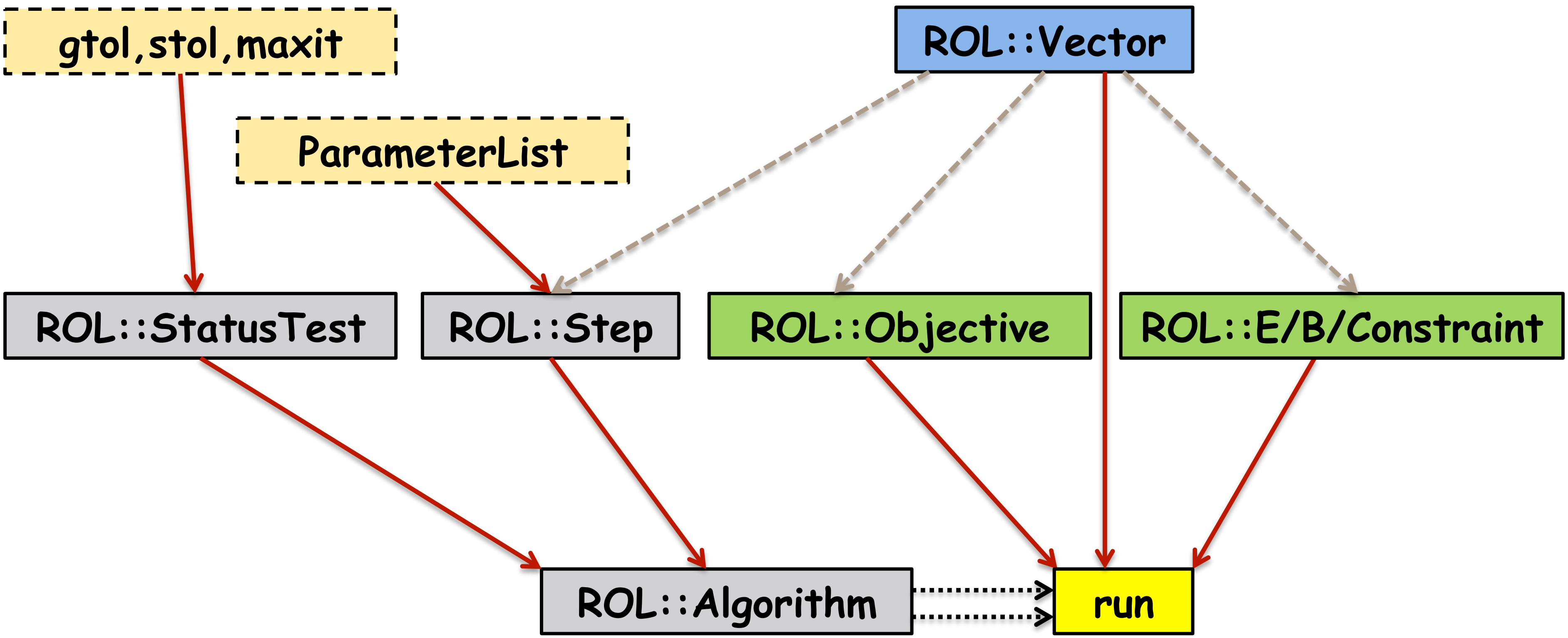
- Implementation verification through a variety of ROL tests:
  - Finite difference checks with high granularity.
  - Consistency checks for operator inverses and adjoints.

- Access to all optimization methods through a **single interface**.

- Enables future ROL interfaces for advanced solution checkpointing and restarting, closer integration with application-specific time integrators, etc.

Algorithmic interface

- Modular design:



Algorithmic interface

- An illustration, sans details, using a sequential quadratic programming (SQP) step for Type-E formulations:

```
RCP<Objective<RealT> > obj;
RCP<EqualityConstraint<RealT> > constr;

RCP<CompositeStepSQP<RealT> > step(parlist);
RCP<StatusTestSQP<RealT> > status(gtol, ctol, stol, maxit);

DefaultAlgorithm<RealT> algo(step, status);

x.zero(); vl.zero();

algo.run(x, vl, *obj, *constr);
```

Methods – Part 1

- **Type-U (unconstrained):**
  - Globalization: LineSearchStep and TrustRegionStep.
  - Gradient descent, quasi-Newton (limited-memory BFGS, DFP, Barzilai-Borwein), nonlinear CG (6 variants), inexact Newton (including finite difference hessVecs), Newton, with line searches and trust regions.
  - Trust-region methods supporting inexact objective functions and inexact gradient evaluations. Enables *adaptive and reduced models*.

- **Type-B (bound constrained):**
  - Projected gradient and projected Newton methods.
  - Primal-dual active set methods.

Methods – Part 2

- **Type-E (equality constrained):**
  - Sequential quadratic programming (SQP) with trust regions, supporting inexact linear system solves.
  - A hierarchy of full-space SQP methods, based on the constraint null-space representation (summer 2015):
    (1) sim/opt splitting with simple linearized forward and adjoint solves,
    (2) simple optimality systems with forward/adjoint preconditioners,
    (3) full KKT (optimality) system solves.

- **Type-EB (equality + bound constrained):**
  - Augmented Lagrangian methods.
  - Semismooth Newton methods (summer 2015).
  - Interior-point methods (summer 2015).

Methods – Part 3

- **Optimization under uncertainty:**

$$\min_{z} \ \sigma(f(z,\vartheta))$$

$$\min_{z} \ \sigma(f(u(z,\vartheta),z,\vartheta)) \quad \text{where } u(z,\vartheta) \text{ solves } c(u,z,\vartheta)=0$$

  - Compute controls/designs that are risk-averse or robust to uncertainty in the parameters ϑ. Here σ is some **risk measure**.
  - Risk measures: Conditional value-at-risk (CVaR), Expectation (mean), Mean plus deviation, Mean plus variance, Exponential disutility.
  - Incorporate sampling and adaptive quadrature approaches from uncertainty quantification. Flexible sampling interface through SampleGenerator and BatchManager.
  - Control inexactness and adaptivity through **trust-region** framework.

Research focus

- Optimization under uncertainty, risk-averse optimization.
- Treatment of general constraints in large-scale optimization.
- Sequential subspace methods, continuation, regularization.
- Inexact and adaptive methods for large-scale optimization.
- Tighter application integration through SimOpt.

Miscellaneous

- Efficient computations, restarts and checkpointing enabled through `AlgorithmState` and `StepState`.
- Flexible output using user-defined streams.
- Soft and hard iteration updates are possible, for efficiency.

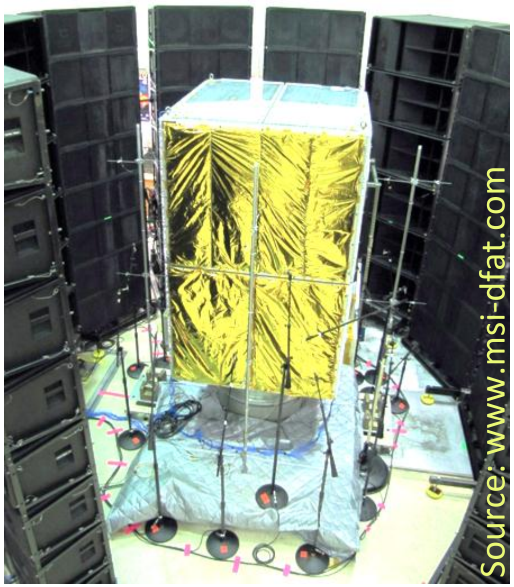
- Coming in 2015:
  - Specialized techniques for topology optimization, such as generalizations of method of moving asymptotes (MMA).
  - Computing conservative estimates of probability of failure, through buffered probabilities.
  - Methods for general constraints.
  - Hierarchy of full-space SQP methods.
  - User’s guide.

ROL

Supplementary material

Another important application: Direct-field acoustic testing (DFAT)

The purpose of DFAT in the weapon program is to simulate in the lab *liftoff/in-flight/reentry environments (W78) and vibrational conditions (B61)* enabling: (1) reduction in cost of testing & (2) predictive component analysis.



Full-system testing facility

Mobile facility

Computational simulation must aid lab experiments:

model calibration, material/source inversion, loudspeaker control

→ OPTIMAL DESIGN AND INVERSE PROBLEMS

Optimal design

Given:
- a set of loudspeakers;
- a waveform generator;
- a mixer board;
can we create a specified acoustic pressure field in a region of interest?

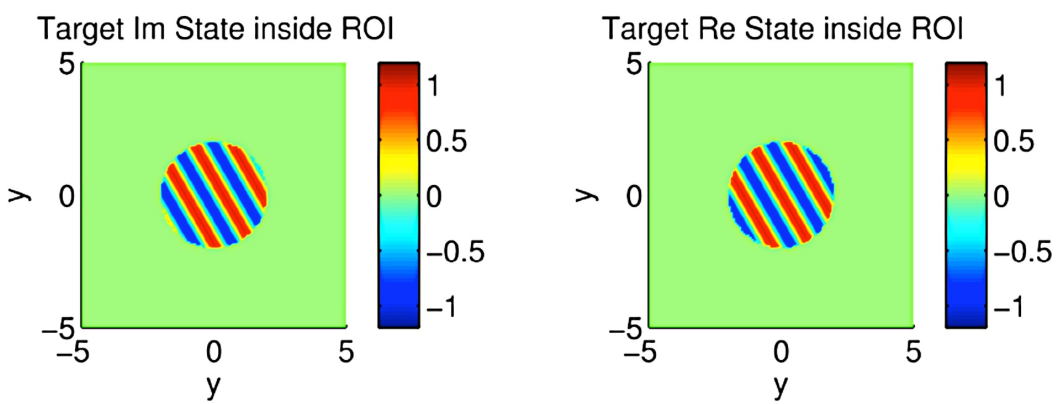
Optimal design

$$\underset{p,g}{\text{Minimize}} \quad \frac{1}{2}\int_{\widehat{\Omega}} (p-\widehat{p})\overline{(p-\widehat{p})}\,dx + \frac{\alpha}{2}\int_{\Omega_c} g\overline{g}\,dx$$

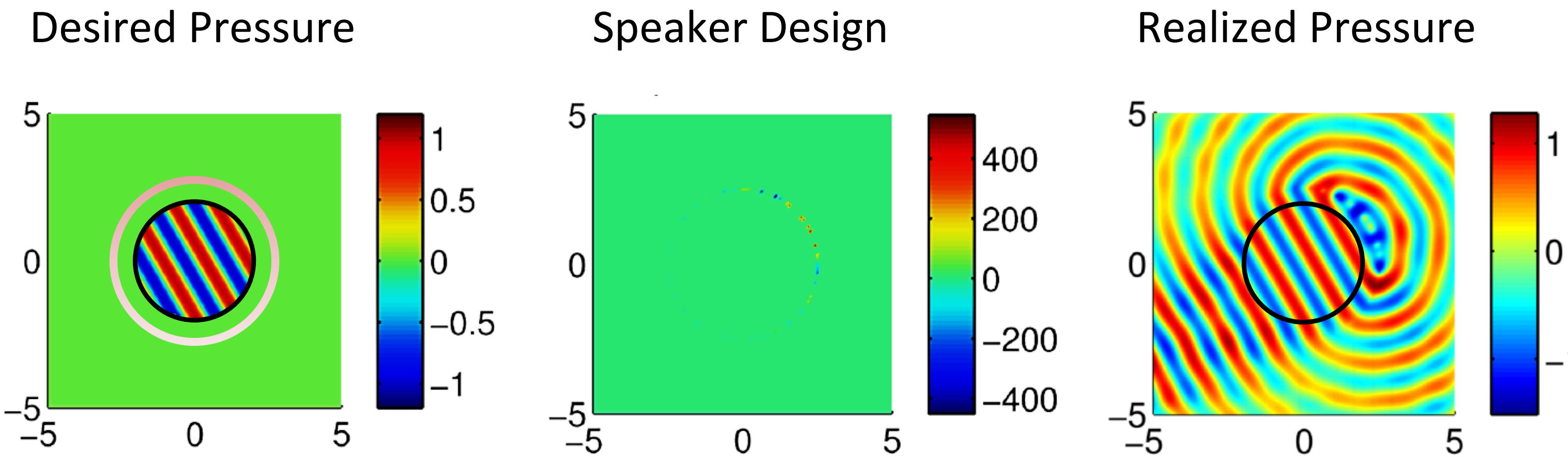
subject to

$$\begin{aligned} -\Delta p - k^2 p &= g && \text{in} \quad \Omega, \\ \frac{\partial p}{\partial n} &= -ikp && \text{on} \quad \partial\Omega, \end{aligned}$$

where p is the simulated acoustic pressure, g is the acoustic control, k is the wave number, $\widehat{p}$ is the desired pressure, $\widehat{\Omega}$ is a disk-shaped region of interest (ROI), Ω_c is an outer control annulus, and $\alpha = 10^{-5}$.

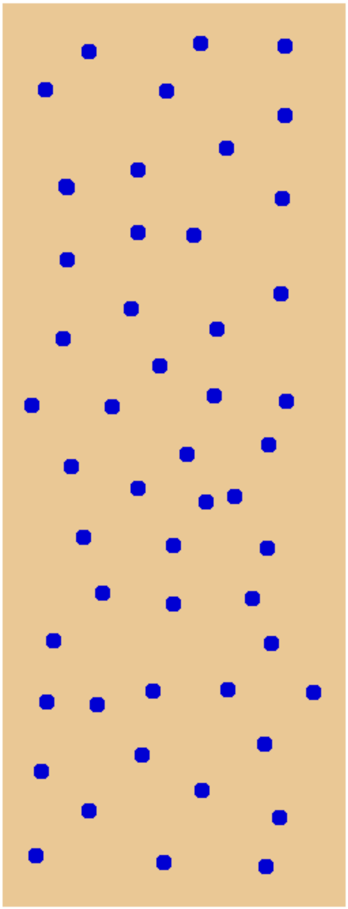


Optimal design

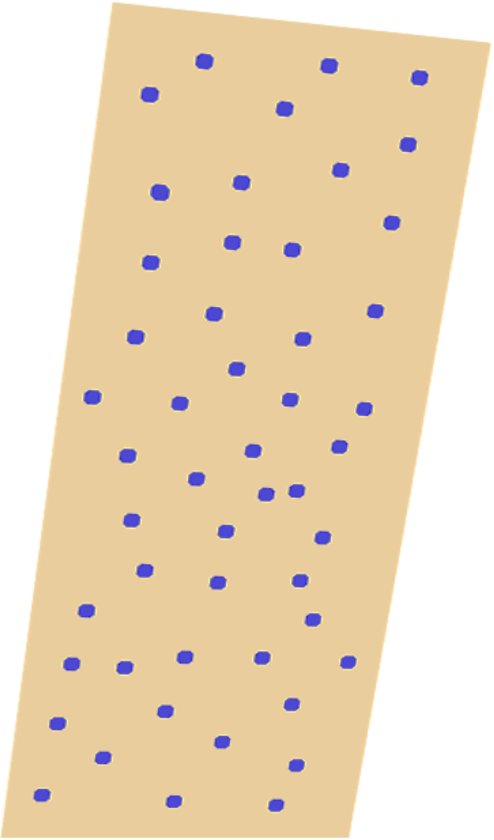


Inversion

Foam block at rest



Deformed foam block



Inversion

$$\underset{\{u,\mu,\kappa\}\in\,\mathcal{U}\times\mathcal{G}\times\mathcal{K}}{\text{Minimize}} \quad \frac{1}{2}\int_{\Omega^0}(u_i-\widehat{u}_i)^2\,dx + R(\mu) + R(\kappa)$$

subject to

$$\begin{aligned} -(F_{ik}S_{kj})_{,j} &= 0 && \text{in} \quad \Omega^0, \\ (F_{ik}S_{kj})\,n_j &= \tau_i && \text{in} \quad \partial\Omega^0_\tau \end{aligned}$$

where $\mathcal{U} = \left\{u_i : u_i \in H^1\left(\Omega^0\right),\ u_i = 0 \text{ on } \partial\Omega^0_u\right\}$, $\mathcal{G} = \{\mu : \mu \in L^2(\Omega^0),\ \mu > 0\}$, and $\mathcal{B} = \{\kappa : \kappa \in L^2(\Omega^0),\ \kappa > 0\}$.

— Here $\{u_i\}_{i=1,\ldots,d}$ is the displacement in the i-th direction and τ_i is the surface traction in the i-th direction.

— The second Piola-Kirchhoff stress tensor for a Saint-Venant Kirchhoff material is given by $S_{ij} = \mathbf{C}_{ijkl}\,E_{kl}$, where the fourth-order tensor of elastic moduli is

$$\mathbf{C}_{ijkl} = (\kappa - \frac{2}{3})\,\delta_{ij}\,\delta_{kl} + \mu\,(\delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk})\,.$$

The Green strain tensor is given by $E_{ij} = \frac{1}{2}\left(F_{ki}F_{kj} - \delta_{ij}\right)$, with the deformation gradient $F_{ij} = \frac{\partial u_i}{\partial x^0_j} + \delta_{ij}$, Kronecker delta δ_{ij}, and a reference material point x^0.