

SAND2012-2491C
**Solving Large-Scale Inverse Problems in Elasticity
Using Sequential Quadratic Programming (SQP)**

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March 28, 2012

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National Nuclear Security Administration under contract DE-AC04-94AL85000.
Research sponsored by the NNSA Advanced Scientific Computing Program under the Computer Science Research Foundation



Outline

Introduction

- Motivation
- Full-Space SQP Review

Linear Elastodynamics

- Problem Overview
- Nonlinear Programming Problem
- Results

Nonlinear Elastostatics

- Problem Overview
- Nonlinear Programming Problem
- Results

Summary

- Further Advances
- Conclusions

Introduction

Motivation

- Direct characterization of material properties is not always possible or desirable
- Nondestructive/noninvasive material characterization is important in many engineering applications, e.g. bio, aero
- Variations in structural response can be induced by
 - Disease; or
 - Damage



Wellington Hospital Cardiac Service

Challenges

- Solution of large-scale inverse problems with models given by partial differential equations (PDEs)
- Characterization of the uncertainties in the model inputs for high-dimensional parameter spaces



Aloha Airlines Flight 243, 1988

SQP Summary

- Matrix-free full-space SQP algorithm with trust regions.
- Handles inequality constraints – control *and* state constraints.
- Linear solver accuracy adjusted dynamically, based on SQP progress.
- Approximate Schur preconditioning reuses forward PDE solvers.
- Fully scalable – assuming scalable forward PDE solvers.



Inverse Estimation of Parameters in Linear Elastodynamics

Problem Overview

NLP Problem

Results

Problem Overview

Find the shear modulus μ and bulk modulus κ from measurements $\{\hat{u}_i\}_{i=1,\dots,d}$ related to the solution $\{u_i\}_{i=1,\dots,d}$ of the boundary value problem

$$\begin{aligned} -\sigma_{ij,j} &= \omega^2 \rho u_i & \text{in } \Omega, \\ u_i &= 0 & \text{on } \Gamma_u, \\ \sigma_{ij} n_j &= \tau_i & \text{on } \Gamma_\tau. \end{aligned}$$

The stress tensor σ_{ij} is defined as

$$\sigma_{ij} = \mu C_{ijkl}^\mu \epsilon_{kl}(u) + \kappa C_{ijkl}^\kappa \epsilon_{kl}(u)$$

$$C_{ijkl}^\mu = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \quad C_{ijkl}^\kappa = \delta_{ij}\delta_{kl}$$

and the strain tensor is defined to be the symmetric part of the displacement gradient, as follows,

$$\epsilon_{ij}(u) = \frac{1}{2}(u_{i,j} + u_{j,i}).$$

Here, $\Omega \subseteq \mathbb{R}^d$, $d = \{1, 2, 3\}$ is the computational domain with boundary $\partial\Omega$ and indices i, j, k , and l take on values $1, \dots, d$.

Full-Space L^2 Formulation

Problem

We consider the following nonlinear programming problem (NLP):

$$\begin{aligned} & \underset{(u, \mu, \kappa) \in \mathcal{U} \times \mathcal{G} \times \mathcal{B}}{\text{minimize}} && \left\{ \frac{1}{2} \|u_i - \hat{u}_i\|^2 + R(\mu) + R(\kappa) \right\} \\ & \text{subject to} && -\sigma_{ij,j} = \omega^2 \rho u_i \quad \text{in } \Omega \\ & && \sigma_{ij} n_j = \tau_i \quad \text{on } \Gamma_\tau \end{aligned}$$

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

Lagrangian

$$\mathcal{L}(u_i, \mu, \kappa, \lambda_i) = \frac{1}{2} \|u_i - \hat{u}_i\|^2 + R(\mu) + R(\kappa) + \langle \lambda_i, -\sigma_{ij,j} - \omega^2 \rho u_i \rangle + \langle \lambda_i, \tau_i - \sigma_{ij} n_j \rangle_{\Gamma_\tau}$$

First-Order Necessary Optimality Conditions

$$F(u_i, \mu, \kappa, \lambda_i) = \left\{ \begin{array}{l} (u_i - \hat{u}_i) - (C_{ijkl} \epsilon_{kl}(\lambda)),_j - \omega^2 \rho u_i \quad \text{in } \Omega \\ \nabla_\mu R(\mu) + \epsilon_{ij}(\lambda) C_{ijkl}^\mu \epsilon_{kl}(u) \\ \nabla_\kappa R(\kappa) + \epsilon_{ij}(\lambda) C_{ijkl}^\kappa \epsilon_{kl}(u) \\ -(C_{ijkl} \epsilon_{kl}(u)),_j - \omega^2 \rho u_i \quad \text{in } \Omega; \tau_i - \sigma_{ij} n_j \quad \text{on } \Gamma_\tau \end{array} \right\} = 0$$

Full-Space L^2 Formulation

Hessian of the Lagrangian

$$F'(u_i, \mu, \kappa, \lambda_i)(\delta u_i, \delta \mu, \delta \kappa, \delta \lambda_i) = \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} & \mathbf{D} \\ \mathbf{E} & \mathbf{F} & 0 & \mathbf{G} \\ \mathbf{H} & 0 & \mathbf{I} & \mathbf{J} \\ \mathbf{K} & \mathbf{L} & \mathbf{M} & 0 \end{bmatrix}$$

Jacobian

$$\begin{aligned} \mathbf{D} &= -(C_{ijkl}\epsilon_{kl}(\widehat{\delta\lambda}))_{,j} - \omega^2 \rho \widehat{\delta\lambda}_i & \mathbf{G} &= \epsilon_{ij}(\widehat{\delta\lambda}) C_{ijkl}^\mu \epsilon_{kl}(u) & \mathbf{J} &= \epsilon_{ij}(\widehat{\delta\lambda}) C_{ijkl}^\kappa \epsilon_{kl}(u) \\ \mathbf{K} &= -(C_{ijkl}\epsilon_{kl}(\widehat{\delta u}))_{,j} - \omega^2 \rho \widehat{\delta u}_i & \mathbf{L} &= -(\widehat{\delta\mu} C_{ijkl}^\mu \epsilon_{kl}(u))_{,j} & \mathbf{M} &= -(\widehat{\delta\kappa} C_{ijkl}^\kappa \epsilon_{kl}(u))_{,j} \end{aligned}$$

Full-Space L^2 Formulation

Hessian of the Lagrangian

$$F'(u_i, \mu, \kappa, \lambda_i)(\delta u_i, \delta \mu, \delta \kappa, \delta \lambda_i) = \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} & \mathbf{D} \\ \mathbf{E} & \mathbf{F} & \mathbf{0} & \mathbf{G} \\ \mathbf{H} & \mathbf{0} & \mathbf{I} & \mathbf{J} \\ \mathbf{K} & \mathbf{L} & \mathbf{M} & \mathbf{0} \end{bmatrix}$$

Hessian Operator

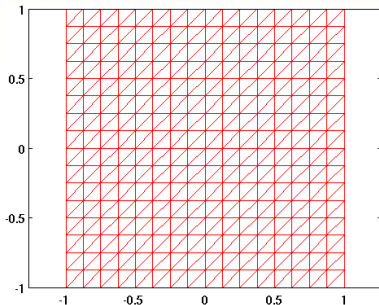
$$\mathbf{A} = \beta \widehat{\delta u}_i \quad \mathbf{B} = -(\widehat{\delta \mu} C_{ijkl}^{\mu} \epsilon_{kl}(\lambda)),_j \quad \mathbf{C} = -(\widehat{\delta \kappa} C_{ijkl}^{\kappa} \epsilon_{kl}(\lambda)),_j$$

$$\mathbf{E} = \epsilon_{ij}(\lambda) C_{ijkl}^{\mu} \epsilon_{kl}(\widehat{\delta u}) \quad \mathbf{F} = \nabla_{\mu}^2 R(\mu) \widehat{\delta \mu}$$

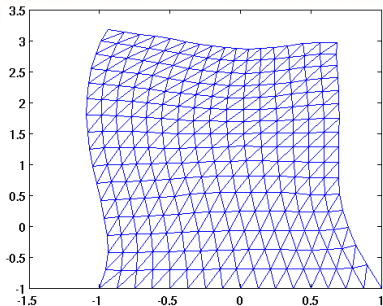
$$\mathbf{H} = \epsilon_{ij}(\lambda) C_{ijkl}^{\kappa} \epsilon_{kl}(\widehat{\delta u}) \quad \mathbf{I} = \nabla_{\kappa}^2 R(\kappa) \widehat{\delta \kappa}$$

Results

Undeformed Grid

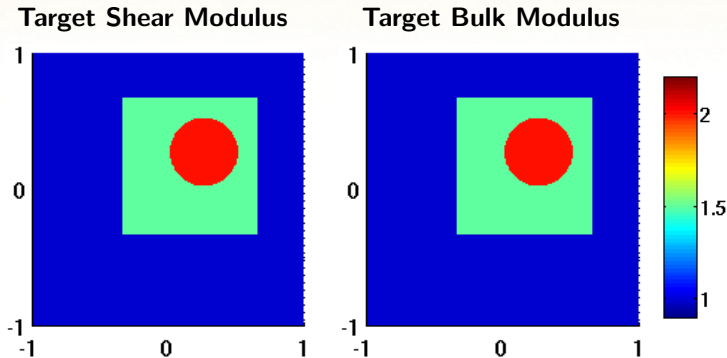


Deformed Grid



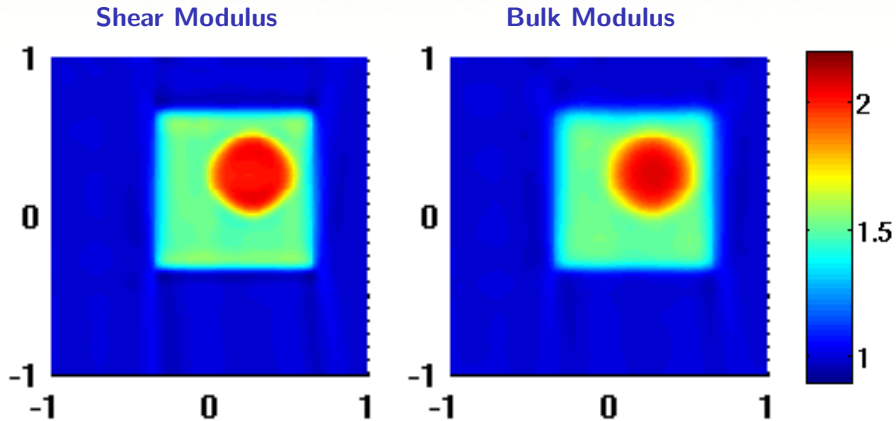
- Our domain D is $[-1, 1]^2$, the grid is uniform triangular, 128×128
- Data is sampled on a finer grid 256×256
- We solve the PDE using Galerkin FEM with a piecewise linear basis
- As the initial guess, we use constant $\mu = 1 \text{ Pa}$ and $\kappa = 1 \text{ Pa}$
- Total number of unknowns is equivalent 99,330

Results

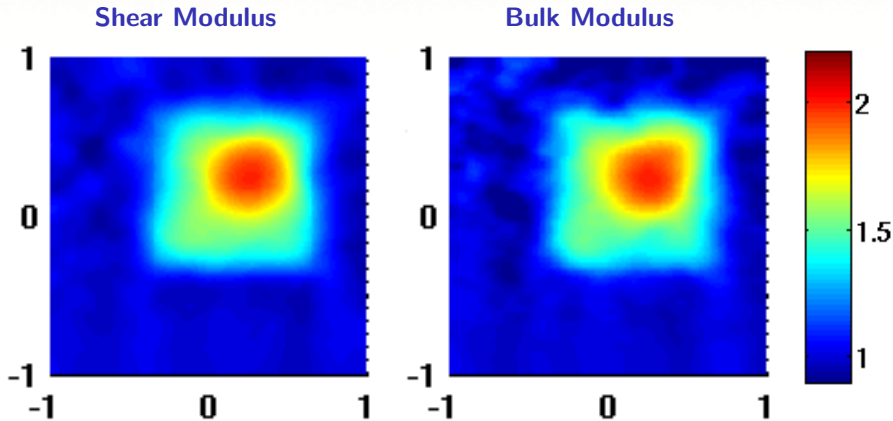


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- Total number of unknowns is equivalent 99,330

Computed Parameters, No Noise



Computed Parameters, 3% Noise



SQP Performance

k	f(x_k)	c(x_k)	L_x(x_k, lam_k)	Delta_k	n_k	t_k	itcg
0	6.93090e-01	3.062110e-13	1.781733e-02	1.00e+02			
1	8.10553e-03	7.771920e-03	5.954813e-04	5.33e+02	2.88e-10	7.61e+01	72
2	4.42933e-03	3.788758e-03	1.870175e-04	1.21e+02	4.45e+00	1.66e+01	3
3	3.33968e-03	1.020809e-02	3.779170e-05	1.06e+02	7.87e-01	1.51e+01	6
4	3.18639e-03	1.049432e-02	1.377018e-05	1.32e+01	5.20e-01	1.32e+01	8
5	3.13484e-03	1.069195e-02	5.134040e-06	1.32e+01	2.57e-01	1.32e+01	11
6	3.12505e-03	4.355073e-03	2.525812e-06	1.29e+01	2.16e-01	6.43e+00	12
7	3.12184e-03	3.640399e-03	1.741322e-06	4.56e+00	5.90e-02	4.56e+00	14
8	3.12074e-03	1.006678e-03	1.064661e-06	1.60e+01	2.54e-02	2.28e+00	14
9	3.12026e-03	8.401915e-04	8.417355e-07	2.35e+00	6.01e-03	2.35e+00	16
10	3.12010e-03	3.957708e-04	5.254084e-07	2.35e+00	3.75e-03	1.18e+00	16
11	3.12004e-03	1.138563e-04	2.018372e-07	3.83e+00	9.26e-04	5.47e-01	16
12	3.12002e-03	9.428050e-05	1.820050e-07	4.35e-01	3.12e-04	4.35e-01	16
13	3.12001e-03	1.194862e-04	1.865811e-07	4.35e-01	2.27e-04	4.35e-01	16
14	3.12000e-03	3.342200e-05	7.061537e-08	1.52e+00	2.84e-04	2.17e-01	16
15	3.11999e-03	3.390794e-05	8.867013e-08	2.13e-01	8.19e-05	2.13e-01	16
16	3.11999e-03	4.356250e-05	7.217764e-08	2.13e-01	8.81e-05	2.13e-01	17
17	3.11999e-03	4.831992e-05	7.877364e-08	2.13e-01	1.03e-04	2.13e-01	17
18	3.11999e-03	5.779310e-05	1.907613e-08	2.13e-01	1.29e-04	2.13e-01	21
19	3.11999e-03	5.475901e-06	1.825626e-10	4.24e-01	1.45e-04	6.06e-02	37
20	3.11999e-03	4.199292e-10	6.559367e-12	4.24e-01	1.33e-05	8.24e-04	42

- We observed **quadratic convergence** in all numerical studies



Inverse Estimation of Parameters in Nonlinear Elastostatics

Problem Overview

NLP Problem

Results

Problem Overview

Find the shear modulus μ and bulk modulus κ from measurements $\{\hat{u}_i\}_{i=1,\dots,d}$ related to the solution $\{u_i\}_{i=1,\dots,d}$ of the boundary value problem

$$\begin{aligned} -(F_{iK}S_{KL})_{,L} &= 0 & \text{in } \Omega_0, \\ u_j &= 0 & \text{on } \Gamma_{u_j}^0, \\ (F_{iK}S_{KL})n_L^0 &= \tau_i^0 & \text{on } \Gamma_{\tau}^0. \end{aligned}$$

For a Saint Venant-Kirchhoff Material, the second Piola-Kirchhoff stress tensor S_{KL} is defined as

$$\begin{aligned} S_{KL} &= \mu C_{IJKL}^{\mu} E_{IJ} + \kappa C_{IJKL}^{\kappa} E_{IJ} \\ C_{IJKL}^{\mu} &= \delta_{IK}\delta_{JL} + \delta_{IL}\delta_{JK} - (2/3)\delta_{IJ}\delta_{KL} & C_{IJKL}^{\kappa} &= \delta_{IJ}\delta_{KL} \end{aligned}$$

The deformation gradient F_{iK} and Green-Lagrangian strain tensor E_{KL} are respectively defined as

$$F_{iK} = \frac{1}{2} \left(\frac{\partial u_i}{\partial X_K^0} + \delta_{iK} \right) \quad E_{IJ} = \frac{1}{2} (F_{iK}F_{iL} + \delta_{KL}).$$

Here, $\Omega_0 \subseteq \mathbb{R}^d$, $d = \{1, 2, 3\}$ is the computational domain on the reference configuration with boundary $\partial\Omega_0$ and indices i, I, J, K and L take on values $1, \dots, d$.

Full-Space L^2 Formulation

Problem

We consider the following NLP:

$$\begin{aligned} & \underset{(u, \mu, \kappa) \in \mathcal{U} \times \mathcal{G} \times \mathcal{B}}{\text{minimize}} && \left\{ \frac{1}{2} \|u_i - \hat{u}_i\|^2 + R(\mu) + R(\kappa) \right\} \\ & \text{subject to} && -(F_{iK} S_{KL})_{,L} = 0 \quad \text{in } \Omega_0 \\ & && (F_{iK} S_{KL}) n_L^0 = \tau_i^0 \quad \text{on } \Gamma_\tau^0 \end{aligned}$$

Lagrangian

$$\mathcal{L}(u_i, \mu, \kappa, \lambda_i) = \frac{1}{2} \|u_i - \hat{u}_i\|^2 + R(\mu) + R(\kappa) + \langle \lambda_i, -(F_{iK} S_{KL})_{,L} \rangle + \langle \lambda_i, \tau_i^0 - (F_{iK} S_{KL}) n_L^0 \rangle_{\Gamma_\tau^0}$$

First-Order Necessary Optimality Conditions

$$F(u_i, \mu, \kappa, \lambda_i) = \left\{ \begin{array}{l} \beta(u_i - \hat{u}_i) - (\lambda_{i,K} S_{KL})_{,L} - (F_{iK} (\mathbf{C}_{IJKL} (F_{jK} \lambda_{j,L} + \lambda_{j,K} F_{jL})))_{,L} \quad \text{in } \Omega_0 \\ \nabla_\mu R(\mu) + \lambda_{i,L} F_{i,K} C_{IJKL}^\mu E_{IJ} \\ \nabla_\kappa R(\kappa) + \lambda_{i,L} F_{i,K} C_{IJKL}^\kappa E_{IJ} \\ -(F_{iK} S_{KL})_{,L} \quad \text{in } \Omega_0 ; \quad \tau_i^0 - (F_{iK} S_{KL}) n_L^0 \quad \text{on } \Gamma_\tau^0 \end{array} \right\} = 0$$

Full-Space L^2 Formulation

Hessian of the Lagrangian

$$F'(u_i, \mu, \kappa, \lambda_i)(\delta u_i, \delta \mu, \delta \kappa, \delta \lambda_i) = \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} & \mathbf{D} \\ \mathbf{E} & \mathbf{F} & 0 & \mathbf{G} \\ \mathbf{H} & 0 & \mathbf{I} & \mathbf{J} \\ \mathbf{K} & \mathbf{L} & \mathbf{M} & 0 \end{bmatrix}$$

Jacobian

$$\mathbf{D} = -(F_{iK} C_{IJKL} (F_{jK} \widehat{\delta \lambda_{j,L}} + \widehat{\delta \lambda_{j,K}} F_{jL})),L \quad \mathbf{G} = \widehat{\delta \lambda_{iL}} F_{iK} C_{IJKL}^\mu E_{IJ} \quad \mathbf{J} = \widehat{\delta \lambda_{iL}} F_{iK} C_{IJKL}^\kappa E_{IJ} \\ -(\widehat{\delta \lambda_{i,K}} S_{KL}),L$$

$$\mathbf{K} = -(F_{iK} C_{IJKL} (F_{jK} \widehat{\delta u_{j,L}} + \widehat{\delta u_{j,K}} F_{jL})),L \quad \mathbf{L} = -(\widehat{\delta \mu} F_{iK} C_{IJKL}^\mu E_{IJ}),L \quad \mathbf{M} = -(\widehat{\delta \kappa} F_{iK} C_{IJKL}^\kappa E_{IJ}),L \\ -(\widehat{\delta u_{i,K}} S_{KL}),L$$

Full-Space L^2 Formulation

Hessian of the Lagrangian

$$F'(u_i, \mu, \kappa, \lambda_i)(\delta u_i, \delta \mu, \delta \kappa, \delta \lambda_i) = \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} & \mathbf{D} \\ \mathbf{E} & \mathbf{F} & \mathbf{0} & \mathbf{G} \\ \mathbf{H} & \mathbf{0} & \mathbf{I} & \mathbf{J} \\ \mathbf{K} & \mathbf{L} & \mathbf{M} & \mathbf{0} \end{bmatrix}$$

Hessian Operator

$$\mathbf{A} = \widehat{\delta u_i} - (\lambda_{i,K} C_{IJKL} (F_{jK} \widehat{\delta u_{j,L}} + \widehat{\delta u_{j,K}} F_{jL})),_L - (\widehat{\delta u_{i,K}} C_{IJKL} (F_{jK} \lambda_{j,L} + \lambda_{j,K} F_{jL})),_L \\ - (F_{iK} C_{IJKL} (\widehat{\delta u_{j,K}} \lambda_{j,L} + \lambda_{j,K} \widehat{\delta u_{j,L}})),_L$$

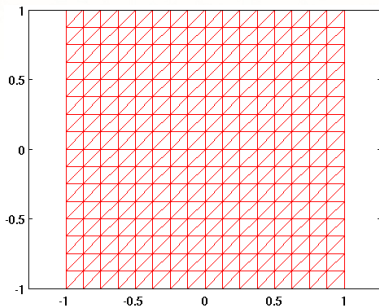
$$\mathbf{B} = -(\widehat{\delta \mu} F_{i,K} C_{IJKL}^\mu (F_{jK} \lambda_{j,L} + \lambda_{j,K} F_{jL})),_L \quad \mathbf{C} = -(\widehat{\delta \kappa} F_{i,K} C_{IJKL}^\kappa (F_{jK} \lambda_{j,L} + \lambda_{j,K} F_{jL})),_L \\ - (\widehat{\delta \mu} \lambda_{i,K} C_{IJKL}^\mu E_{IJ}),_L \quad - (\widehat{\delta \kappa} \lambda_{i,K} C_{IJKL}^\kappa E_{IJ}),_L$$

$$\mathbf{E} = \lambda_{i,L} F_{i,K} C_{IJKL}^\mu (F_{jK} \widehat{\delta u_{j,L}} + \widehat{\delta u_{j,K}} F_{jL}) + \lambda_{i,L} \widehat{\delta u_{i,K}} C_{IJKL}^\mu E_{IJ} \quad \mathbf{F} = \nabla_\mu^2 R(\mu)$$

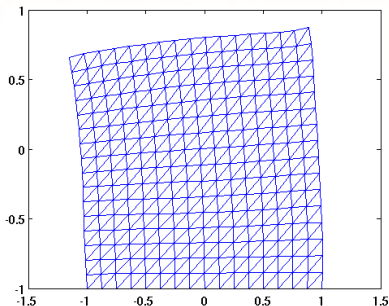
$$\mathbf{H} = \lambda_{i,L} F_{i,K} C_{IJKL}^\kappa (F_{jK} \widehat{\delta u_{j,L}} + \widehat{\delta u_{j,K}} F_{jL}) + \lambda_{i,L} \widehat{\delta u_{i,K}} C_{IJKL}^\kappa E_{IJ} \quad \mathbf{I} = \nabla_\kappa^2 R(\kappa)$$

Results

Undeformed Grid

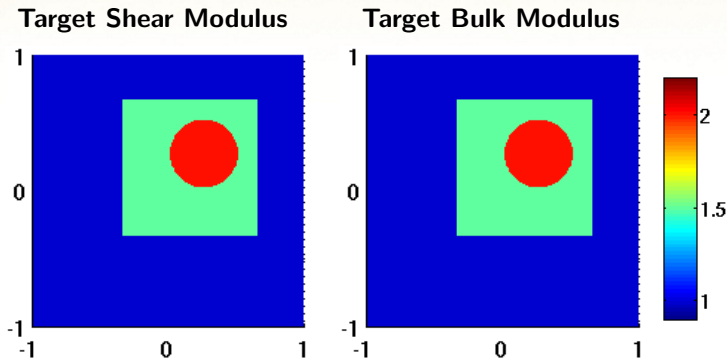


Deformed Grid



- Our domain D is $[-1, 1]^2$, the grid is uniform triangular, 200×200
- Data is sampled on a finer grid 400×400
- We solve the PDE using Galerkin FEM with a piecewise linear basis
- As the initial guess, we use constant $\mu = 1 \text{ Pa}$ and $\kappa = 1 \text{ Pa}$
- Total number of unknowns is equivalent 161,202

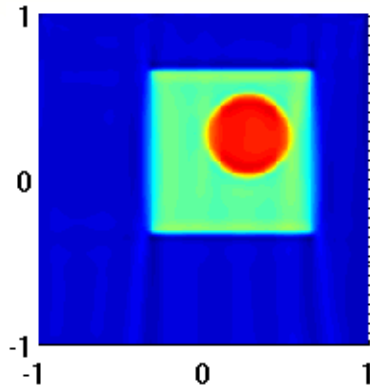
Results



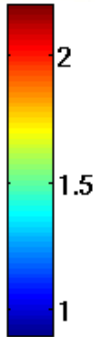
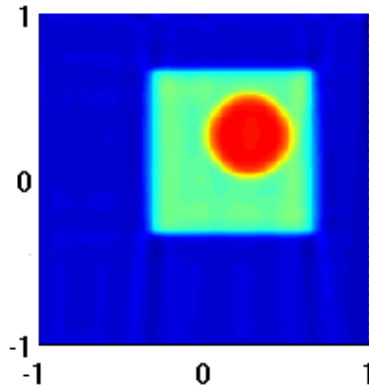
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Computed Parameters, No Noise

Shear Modulus

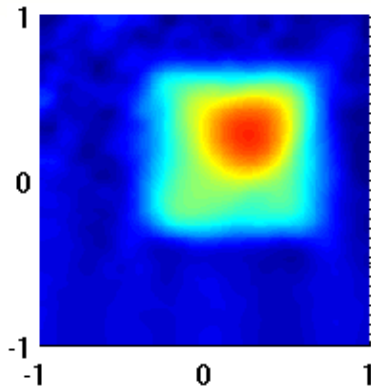


Bulk Modulus

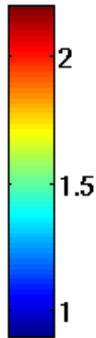
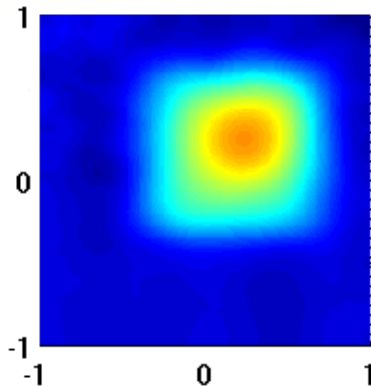


Computed Parameters, 3% Noise

Shear Modulus



Bulk Modulus



SQP Performance

k	f(x_k)	c(x_k)	L_x(x_k, lam_k)	Delta_k	n_k	t_k	itcg
0	1.21121e-02	1.418450e-13	1.501655e-03	1.00e+02			
1	9.18257e-05	8.198400e-03	8.177939e-06	1.75e+02	7.65e-11	2.50e+01	3
2	1.00124e-05	1.281381e-03	1.438794e-06	2.45e+02	4.52e+00	3.47e+01	4
3	3.00828e-06	6.600252e-04	3.330121e-07	2.45e+02	8.05e-01	1.85e+01	6
4	1.79307e-06	1.086107e-03	2.098207e-07	1.03e+01	8.05e-02	1.03e+01	6
5	9.72900e-07	1.804024e-04	2.018572e-07	7.20e+01	5.72e-02	1.03e+01	6
6	1.76429e-08	9.444912e-04	6.134319e-09	7.20e+01	2.24e-02	2.91e+01	21
7	2.34142e-08	1.549139e-05	2.226323e-08	7.20e+01	8.81e-02	8.96e-01	5
8	9.14361e-09	8.921297e-05	2.967412e-09	6.59e+00	1.38e-04	6.59e+00	19
9	6.09451e-09	4.709693e-05	1.808598e-09	6.59e+00	6.44e-03	5.02e+00	23
10	5.17726e-09	3.097234e-05	6.411598e-10	6.59e+00	2.41e-03	4.14e+00	31
11	5.11002e-09	4.721732e-07	3.776935e-10	6.59e+00	2.41e-03	4.34e-01	17
12	4.97759e-09	6.359808e-06	6.916146e-11	3.29e+00	2.98e-05	3.29e+00	62
13	4.97340e-09	1.623117e-07	1.259521e-11	3.86e+00	6.39e-05	5.51e-01	76
14	4.97334e-09	3.230133e-09	1.555454e-12	3.86e+00	3.33e-06	5.25e-02	66
15	4.97334e-09	1.433939e-10	6.650761e-13	2.37e-02	7.79e-08	1.18e-02	58

Further Advances

Precise Embedding of Uncertainty into the Inverse Problem Formulation

To directly incorporate the notion of uncertainty into the mathematical formulation of the inverse problem we require

- **Research:** Advances in algorithmic research such as new optimization algorithms, parallel solvers, and numerical methods for stochastic computation
- **Numerical Tools:** Use of the best available numerical tools for a rigorous implementation of the advances in algorithmic research

Conclusions

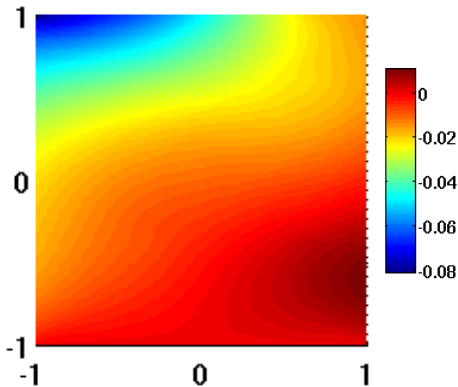
For large-scale PDE-constrained inverse problems:

- We can successfully apply the SQP to relevant **large-scale** inverse problems in solid mechanics
- We can successfully apply the SQP to large-scale inverse problems in nonlinear elasticity **without** using continuation methods
- Second-order optimization algorithms can achieve **quadratic** convergence rates [1]
- **Advances** in algorithmic research are required to accomplish a precise embedding of stochastic discretizations into our mathematical models

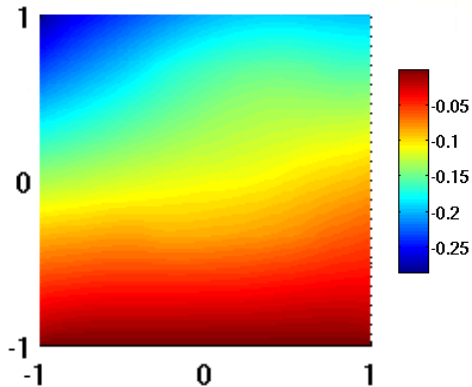
- 1 D. Ridzal, M. Aguiló, and M. Heinkenschloss "Numerical study of a matrix-free trust-region SQP method for equality constrained optimization," Sandia Technical Report SAND2011-9346, December 2011

Computed Displacement Field, No Noise

U_1 Field

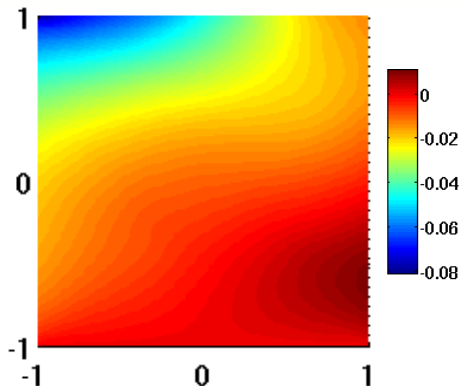


U_2 Field



Computed Displacement Field, 3% Noise

U_1 Field



U_2 Field

