MechMet-Based Optimization for Single Crystal Elastic Moduli

MechModuli intent:

- Evaluate the single-crystal elastic constants from HEXD lattice strain measurements

Anisotropic Hooke's law

$$\sigma = \mathbf{C}\epsilon$$
$$\epsilon = \mathbf{S}\sigma$$

where $\mathbf{C}$ is the stiffness tensor and $\mathbf{S}$ is the compliance tensor.

Required input data:

- Neper mesh of diffraction volume; domain must span the entire load-bearing cross-section and have grain-to-grain correspondence with lattice strain data.
- Lattice strain data for a change in applied load taken from lattice strain change at two load levels both in the elastic domain.
- The macroscopic load change corresponding to the lattice strain change: must be specified within 0.1% (to a minimum of 3 significant figures; 4 sig figs would be better).

MechModuli methodology:

- Optimization based on an objective function defined by the difference between measured and simulated lattice strains:

$$R(\mathbf{S}) = \sum_{Grains} (\varepsilon^{\mathbf{m}} - \varepsilon^{\mathbf{s}}(\mathbf{S}))^{\mathbf{T}}(\varepsilon^{\mathbf{m}} - \varepsilon^{\mathbf{s}}(\mathbf{S}))$$

- Univariant descent of compliance components with line search*

$$\frac{\partial R}{\partial S_{kl}} = 2(\boldsymbol{\varepsilon}^m - \boldsymbol{\varepsilon}^s(\mathbf{S}))\frac{\partial \boldsymbol{\varepsilon}^s}{\partial S_{kl}}$$

where

$$\frac{\partial R}{\partial S_{kl}} = 2(\boldsymbol{\varepsilon}^m - \boldsymbol{\varepsilon}^s(\mathbf{S}))\frac{\partial \boldsymbol{\varepsilon}^s}{\partial S_{kl}}$$

and

$$\frac{\partial \boldsymbol{\varepsilon}^s}{\partial S_{kl}} \approx \frac{\Delta \boldsymbol{\varepsilon}^s}{\Delta S_{kl}}$$

- Initial guess computed from a combination of the data and an assumed anisotropic ratio: Young's modulus, bulk modulus and anisotropic ratio are related to compliance components using Voigt average and then re-scaled to match average axial strain.

*Adapted from: C. Efstathiou, D. E. Boyce, J.-S. Park, U. Lienert, P. R. Dawson, and M. P. Miller. A method for measuring single-crystal elastic moduli using high-energy x-ray diffraction and a crystal-based finite element model. Acta Materialia, 58:5806–5816, 2010.

Mechanical Moduli (MechMod)

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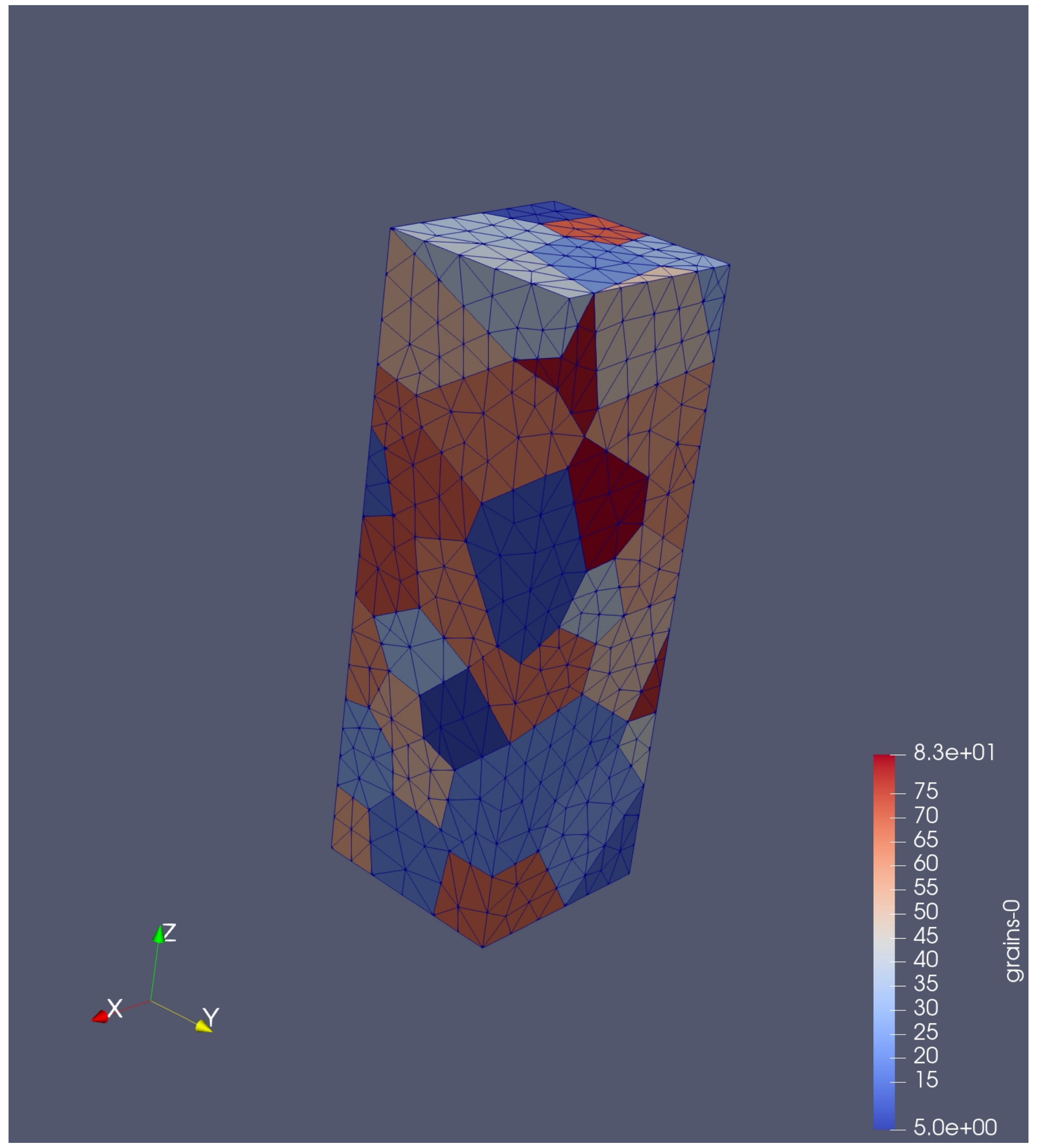
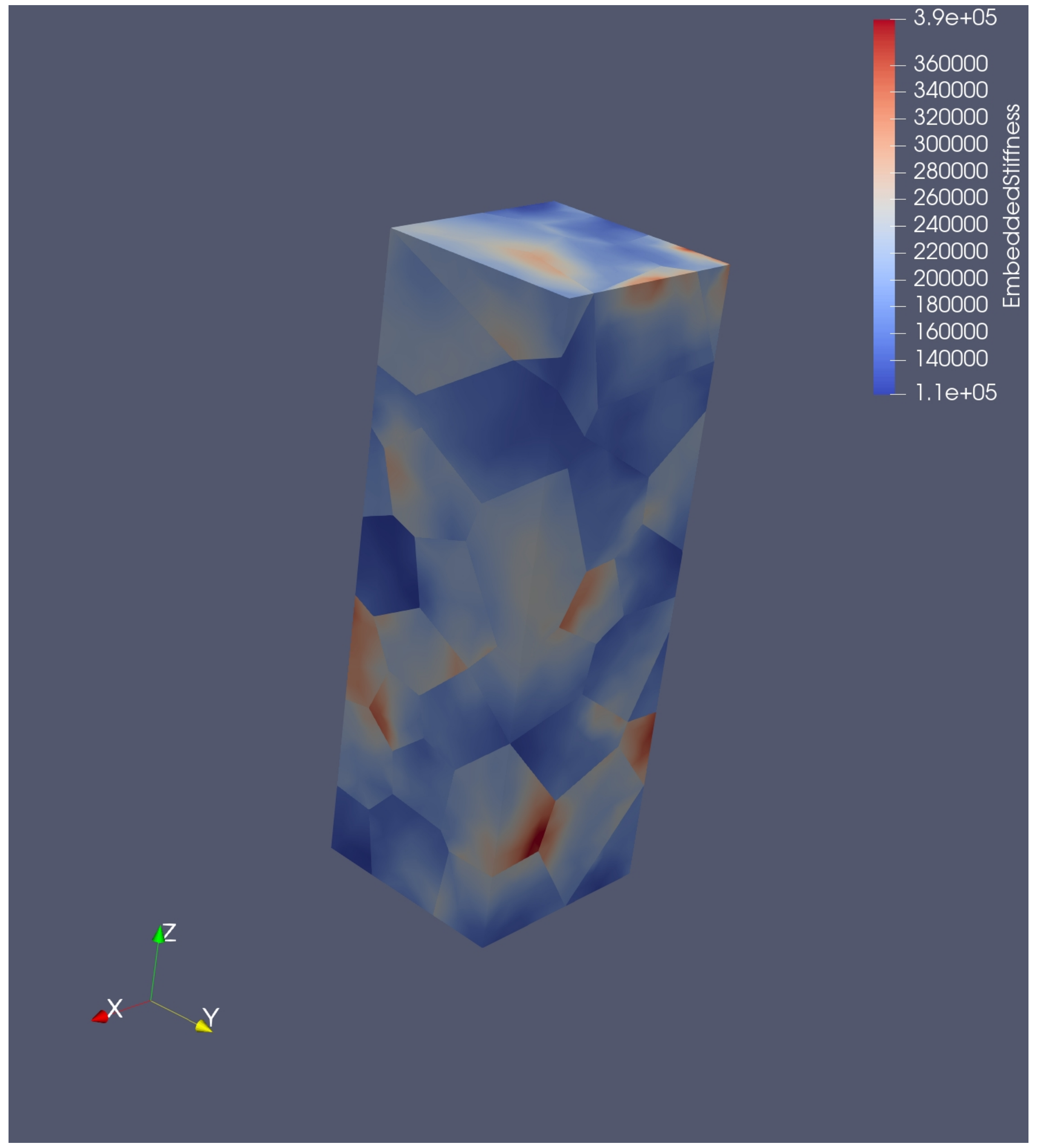
Test Case:

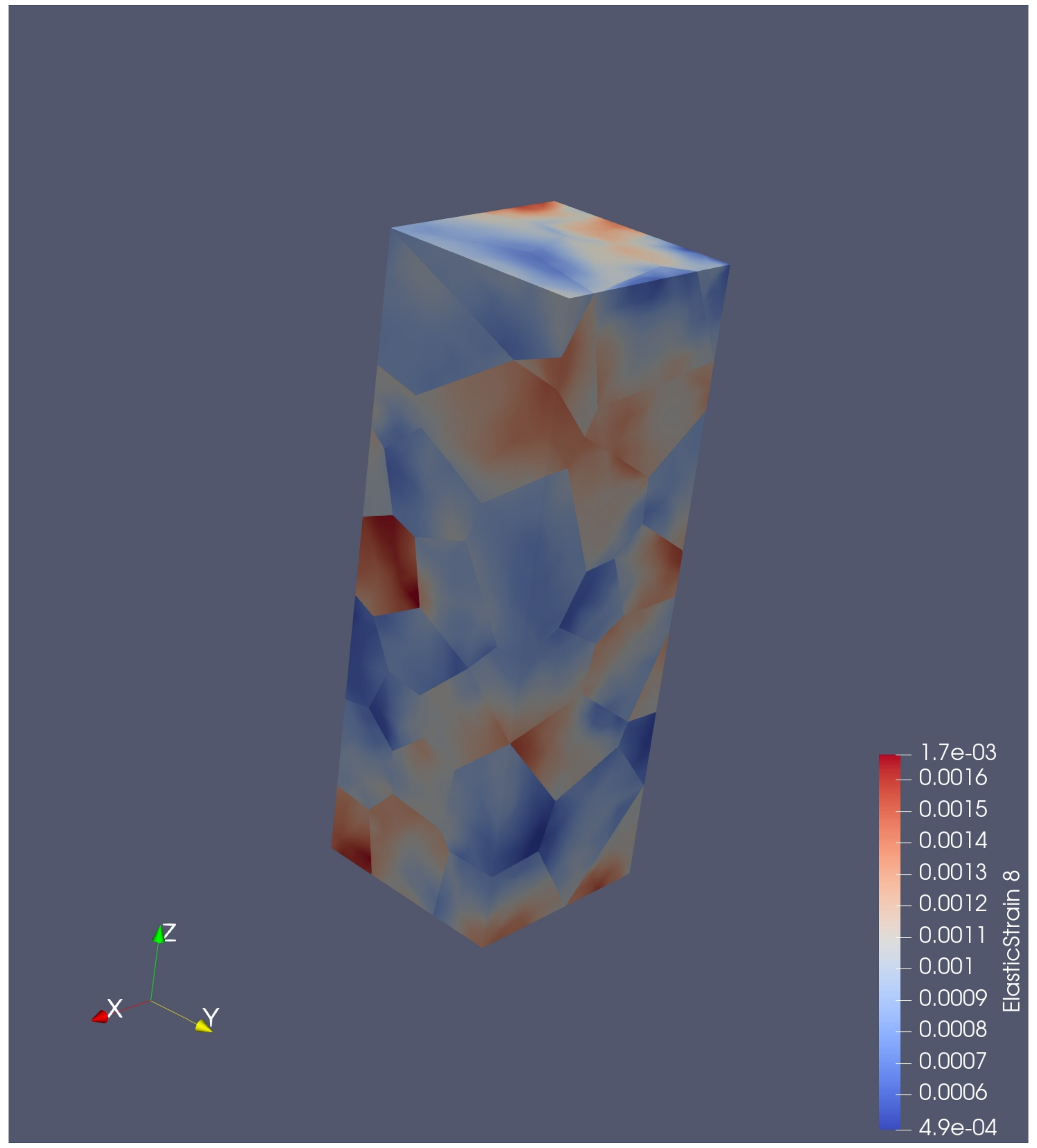
- Synthetic data generated by MechMet
- 83 Grains with 5451 elements and 8337 nodes
- Tensile loading using traction BC
- FCC properties similar to stainless steel
- Lattice strains computed for applied 200N load
- Strains volume-weighted to obtain grain averages
- Strain file exported from MechMet and used as data file
- All grains used in optimization



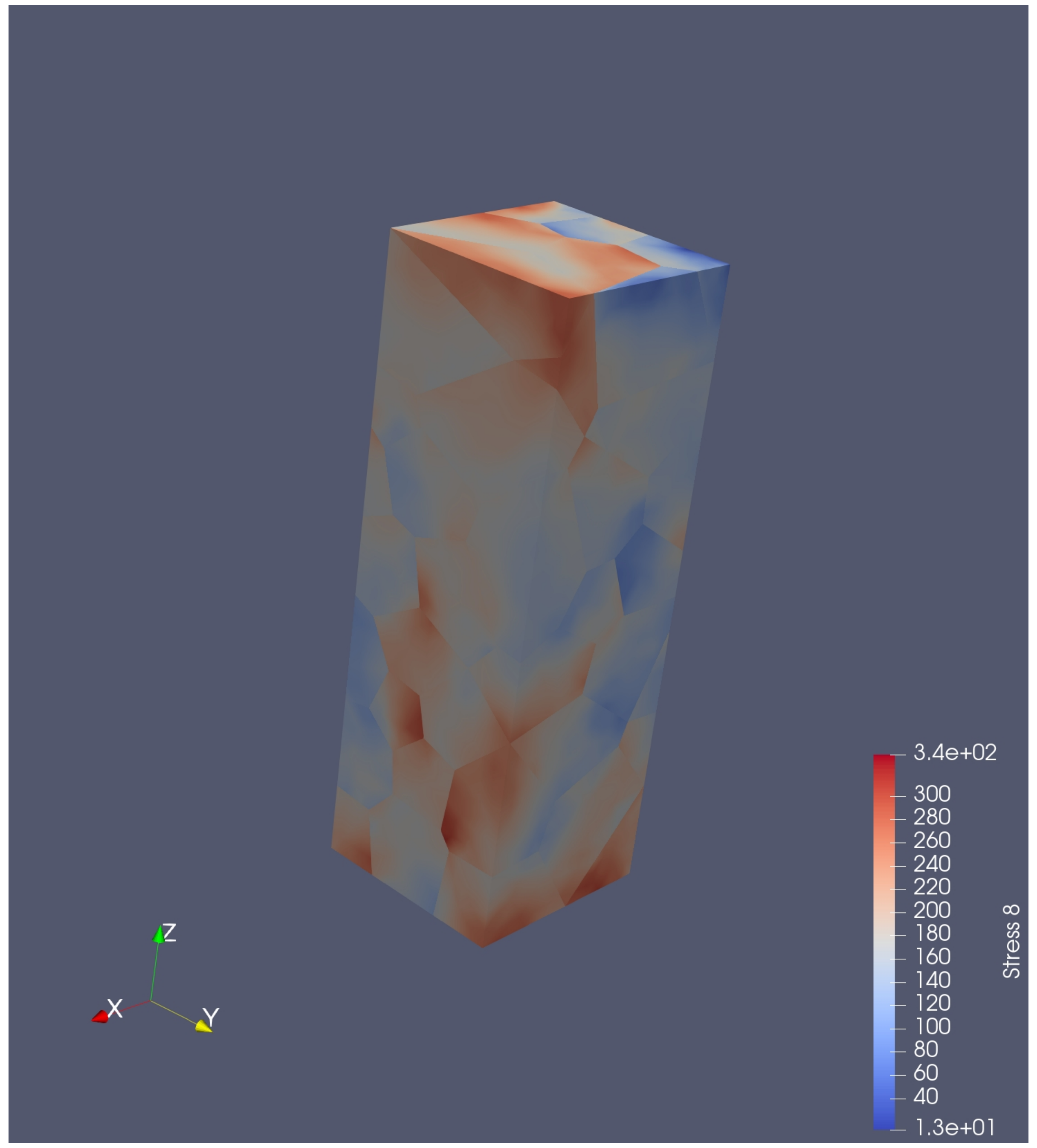
Grains



Embedded (apparent) directional elastic modulus



Axial strain at 0.1% extension in z-direction



Axial stress at 0.1% extension in z-direction

Cornell University
College of Engineering

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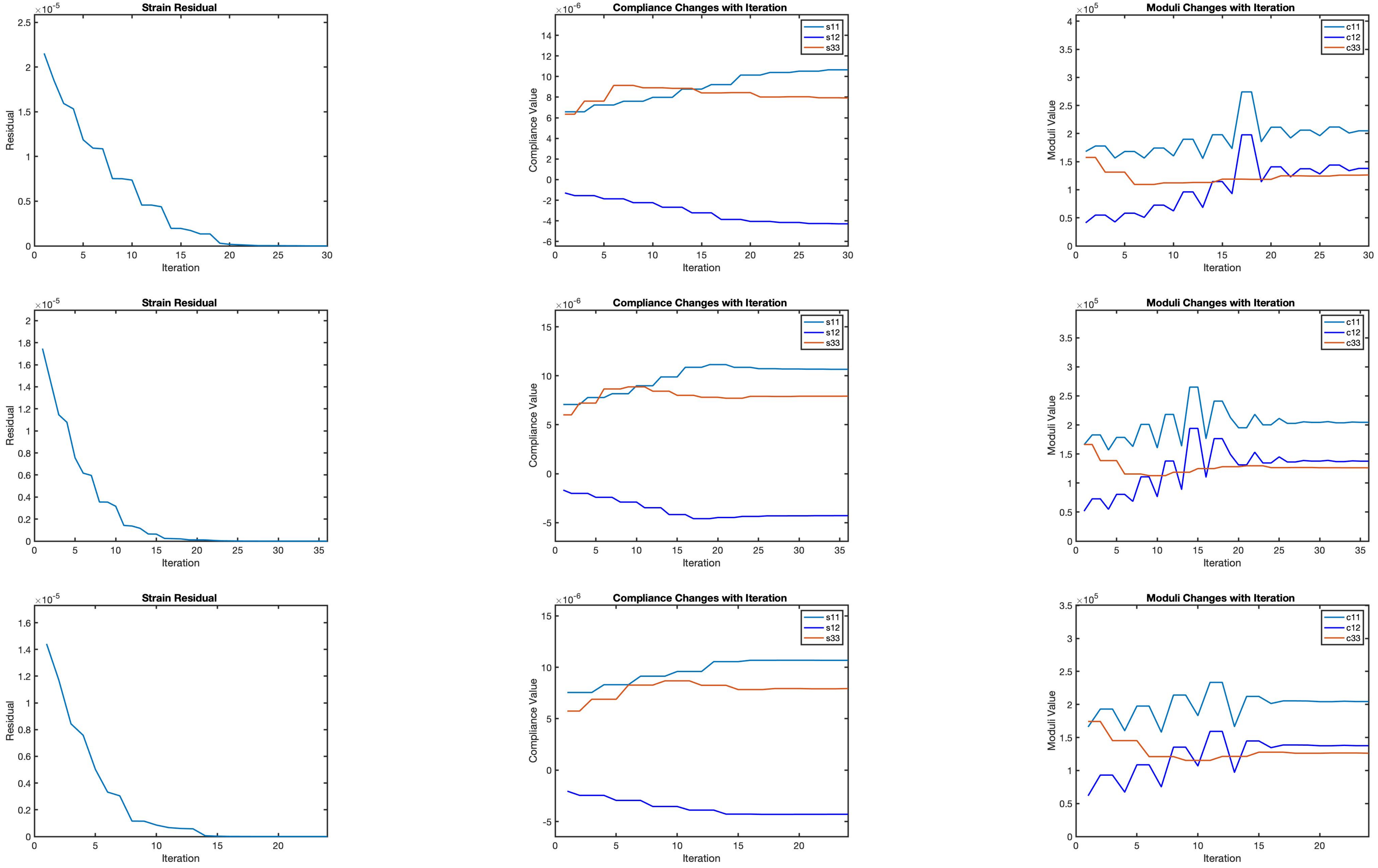
Assumed anisotropy (A):

A=3.0

A=3.5

A=4.0



Strain Residual | Iteration History - Compliances | Iteration History - Stiffnesses

Notes:

- Convergence set to 10^{-5} of lattice strain norm.
- Descent method based on compliance components; stiffness components are derived from compliances.
- An iteration consists of change one compliance component. Descent method cycles through compliance components, sequentially changing S_{11}, S_{12} and S_{44}.

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Converged Moduli

Moduli	C_11	C_12	C_33
A=3.0	204.9	138.0	126.3
A=3.5	204.5	137.6	126.2
A=4.0	204.4	137.8	126.1
MechMet	204.6	137.7	126.2

← A=3.77

Comment:
This is as good as it gets in terms of 'clean' data: a correct set of moduli exists; there is no noise; sample size is small. But it is re-assuring to know that when an 'exact' answer exists, the method does find it.