# Uncertainty Analysis of Lead Titanate Monodomain Structures

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# Ferroelectrics

- Applications:
  - Energy harvesting
  - Structural health monitoring
  - Flow control
  - Ultrasound
  - Robotics
  - Sonar
  - Nanopositioning


Figure: Piezoelectric ceramics are mechanically deformed when in the presence of an electric field. The reverse mechanism is also true, in that an electrical response is generated if a mechanical load is applied.

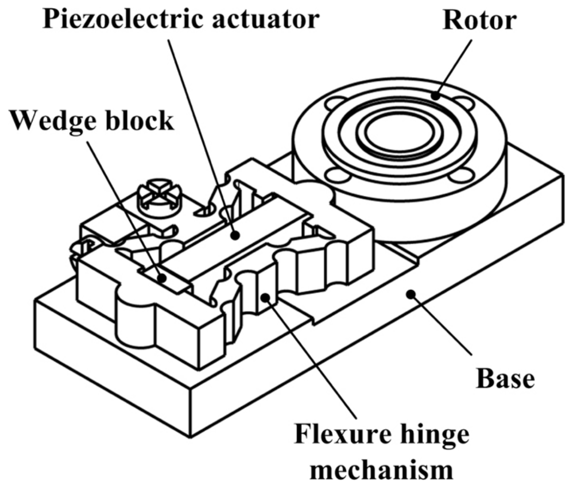



Figure: Schematic of nanoposition stage[1].

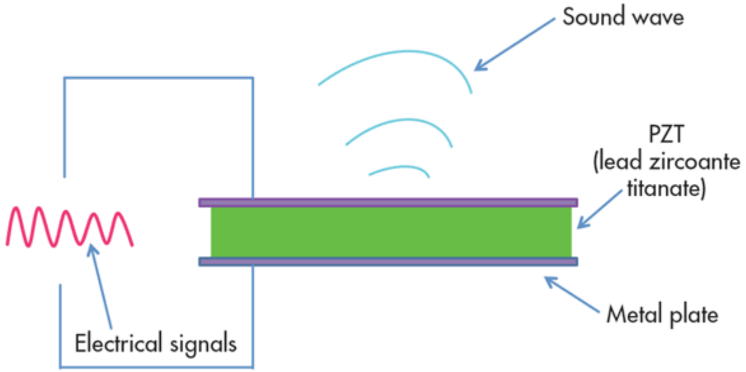



Figure: Schematic of piezoelectric in sonar transducer[2].

1. Li, Jianping, et al. "Design and experimental tests of a dual-servo piezoelectric nanopositioning stage for rotary motion." *Review of Scientific Instruments* 86.4 (2015): 045002.
2. http://www.electronicdesign.com/power/what-piezoelectric-effect

# Motivation

- Density Functional Theory (DFT)
  - Computational limitations
  - Important quantum information
- Continuum modeling
  - Approximations across spatial scales increase uncertainty
- Goal: Inform continuum model parameters using DFT calculations

# Density Functional Theory (DFT)

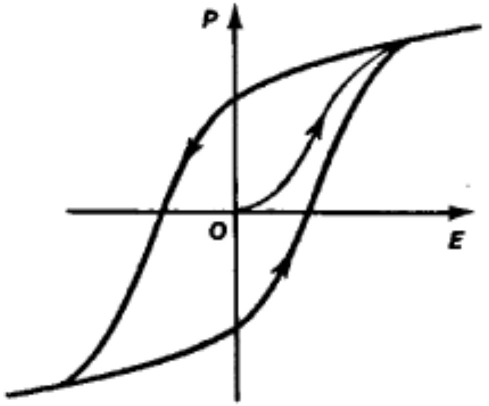



Figure: Polarization versus electric field measurements for ferroelectric material[1].

- Lead Titanate - $PbTiO_3$
- Different atomic positions lead to different polarization states
- Uncertainty:
  - Nuclei positions and electron density (5 atoms, each with 3 degrees of freedom)
  - Approximate as a polarization vector

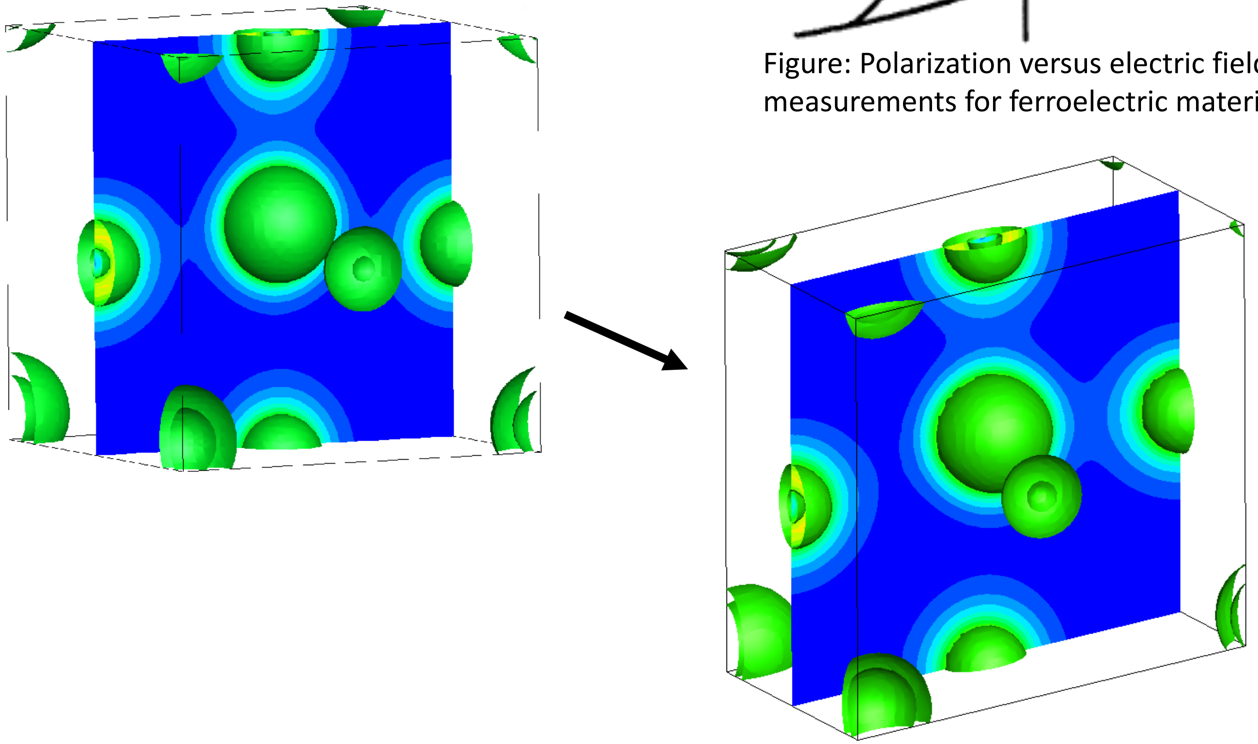


Figure: Example of the electron density solutions: (Left) Reference undeformed cubic structure and (Right) shear deformed state where the unit cell has been sheared such that the deformation gradient component $F_{23}$ is non-zero.

1. http://encyclopedia2.thefreedictionary.com/Hysteresis+(electric)

# Density Functional Theory (DFT)

- Polarization states:
  - Atoms moved based on estimates from shear deformation
  - Positive $P_2$ generated, $P_3$ reduced
  - Polarization uniform in entire domain
- Calculate energy and stress at each polarization state

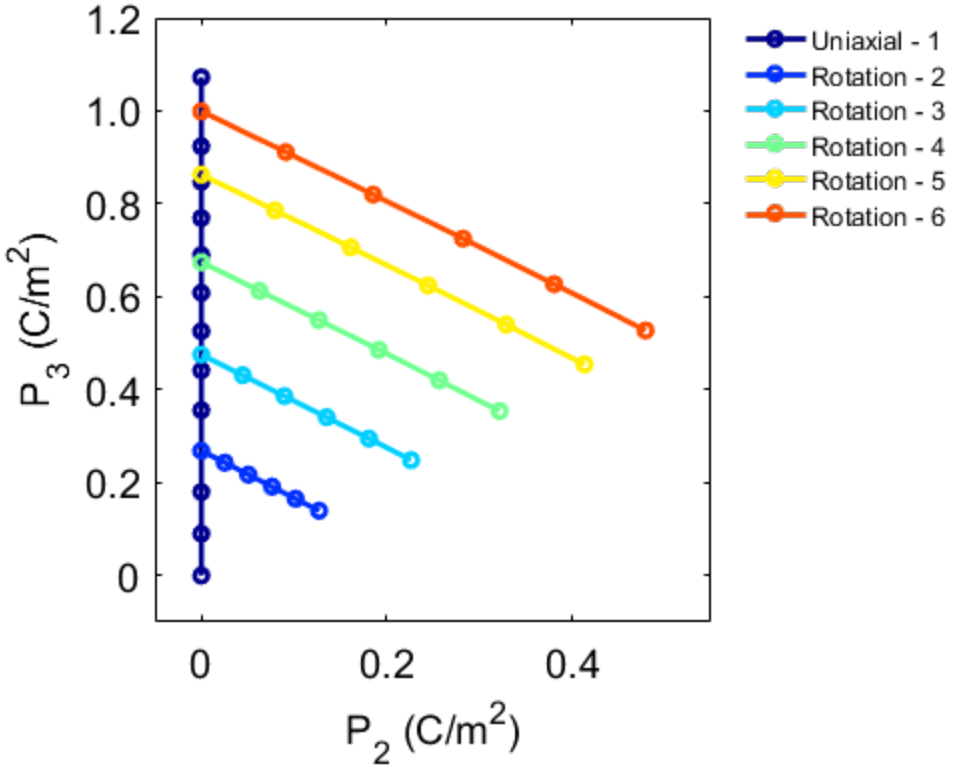
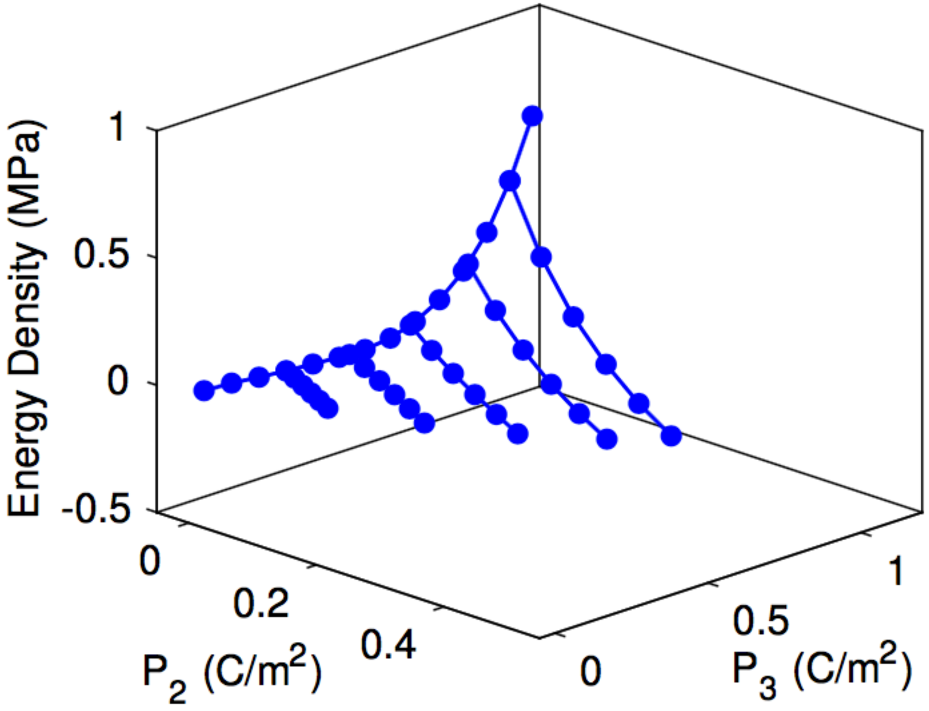


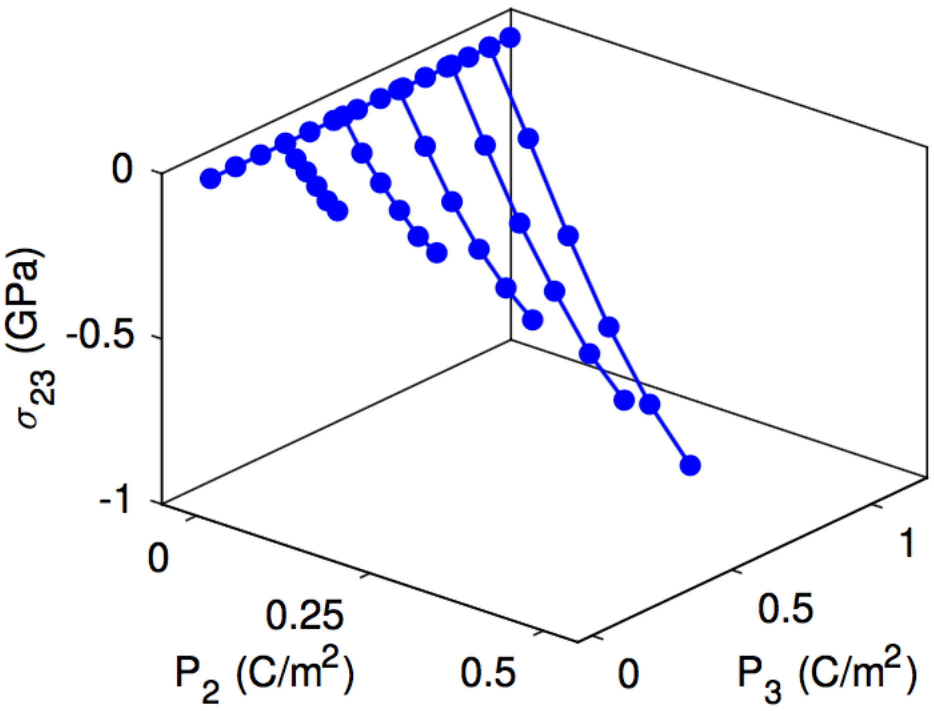

Figure: Polarization rotation – starting from five different locations of nonzero $P_3$ and $P_2 = 0$. Atoms moved along directions estimated from shear deformation states to generate positive $P_2$ values while reducing $P_3$. DFT computations performed by Justin Collins.

# Quantities of Interest

## Energy Density




## Stress



# Continuum Model

- Free energy density

$$u(P_i, \varepsilon_{ij}) = u_L(P_i) + u_M(\varepsilon_{ij}) + u_C(P_i, \varepsilon_{ij}) + u_R(\varepsilon_{ij})$$

- $u_L$ – polarization energy
- $u_M$ - elastic energy
- $u_C$ - electrostrictive energy
- $u_{\mathrm{R}}$ - residual energy

- $P_i$ - polarization in $i^{th}$ direction
- $\varepsilon_{ij}$ - strain

Stress: $\sigma_{ij} = \left(\frac{\partial u}{\partial \varepsilon_{ij}}\right)$

# Continuum Model

- Landau energy density

$$u_L(P_i) = \alpha_1(P_1^2 + P_2^2 + P_3^2) + \alpha_{11}(P_1^2 + P_2^2 + P_3^2)^2$$
$$+ \alpha_{12}(P_1^2 P_2^2 + P_2^2 P_3^2 + P_1^2 P_3^2) + \alpha_{111}(P_1^6 + P_2^6 + P_3^6)$$
$$+ \alpha_{112}[P_1^4(P_2^2 + P_3^2) + P_2^4(P_1^2 + P_3^2) + P_3^4(P_1^2 + P_2^2)]$$
$$+ \alpha_{123} P_1^2 P_2^2 P_3^2$$

- Unknown phenomenological parameters: $\alpha_1, \alpha_{11}, \dots, \alpha_{123}$

# Continuum Model

$$u_M = \frac{c_{11}}{2}(\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2) + c_{12}(\varepsilon_{11}\varepsilon_{22} + \varepsilon_{22}\varepsilon_{33} + \varepsilon_{11}\varepsilon_{33})$$
$$+ 2c_{44}(\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2)$$

$$u_C = -q_{11}(\varepsilon_{11}P_1^2 + \varepsilon_{22}P_2^2 + \varepsilon_{33}P_3^2)$$
$$-q_{12}[\varepsilon_{11}(P_2^2 + P_3^2) + \varepsilon_{22}(P_1^2 + P_3^2) + \varepsilon_{33}(P_1^2 + P_2^2)]$$
$$-q_{44}(\varepsilon_{12}P_1P_2 + \varepsilon_{13}P_1P_3 + \varepsilon_{23}P_2P_3)$$

$$u_R = \sigma_{11}^R\varepsilon_{11} + \sigma_{22}^R\varepsilon_{22} + \sigma_{33}^R\varepsilon_{33} + 2(\sigma_{23}^R\varepsilon_{23} + \sigma_{13}^R\varepsilon_{13} + \sigma_{12}^R\varepsilon_{12})$$

# Bayesian Statistical Analysis

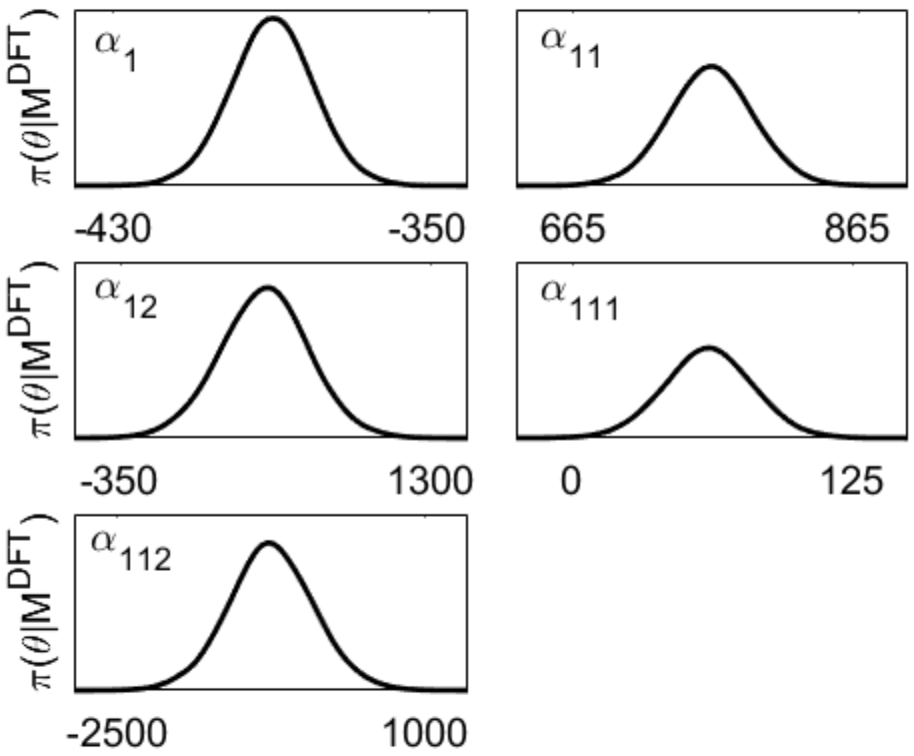
- $\theta_u = [\alpha_1, \alpha_{11}, \dots, \alpha_{123}], \theta_\sigma = [q_{11}, q_{12}, q_{44}, \sigma_{11}^R, \sigma_{22}^R, \sigma_{33}^R, \sigma_{23}^R]$
- Statistical Model: $M^{data}(i) = M(i;\theta) + \varepsilon_i, \quad i = 1, \dots, N$
- Bayes' Relation

$$\pi(\theta | M^{data}) = \frac{p(M|\theta)\pi_0(\theta)}{\int_{\mathbb{R}_p} p(M|\theta)\,\pi_0(\theta) d\theta}$$

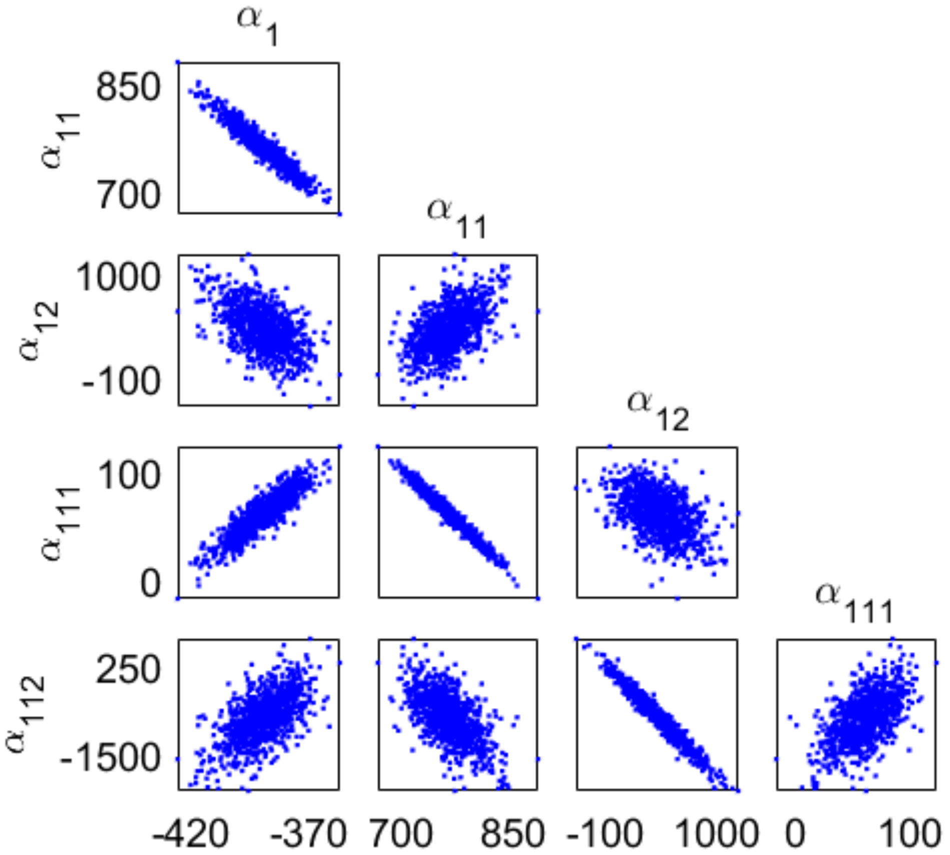
- Posterior Density: $\pi(\theta | M^{data})$
- Prior Density: $\pi_0(\theta)$
- Likelihood Function: $p(M|\theta) = e^{-\sum_{i=1}^{n}[M^{data}(i) - M(i;\theta)]^2/(2\sigma^2)}$
  - Assume observation errors are independent and identically distributed (iid): $\varepsilon_i \sim N(0, \sigma^2)$.

# Energy Calibration:

- Posterior densities: $\pi(\theta_u|M^{data})$

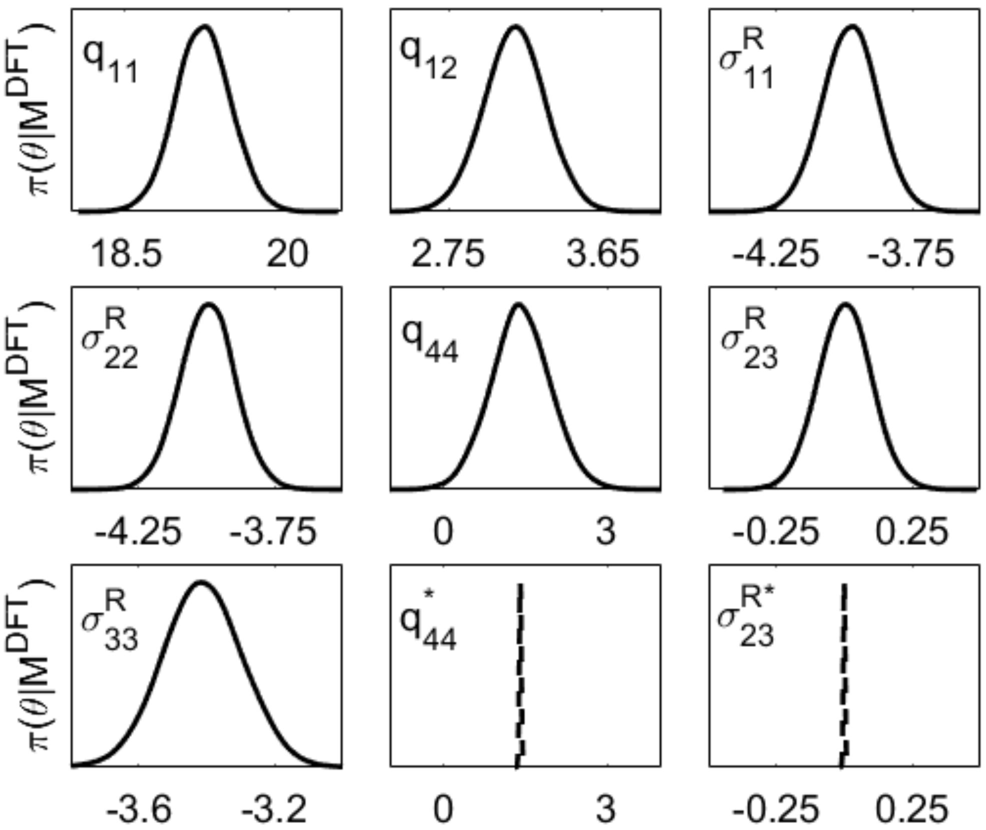



- Pairwise correlation:

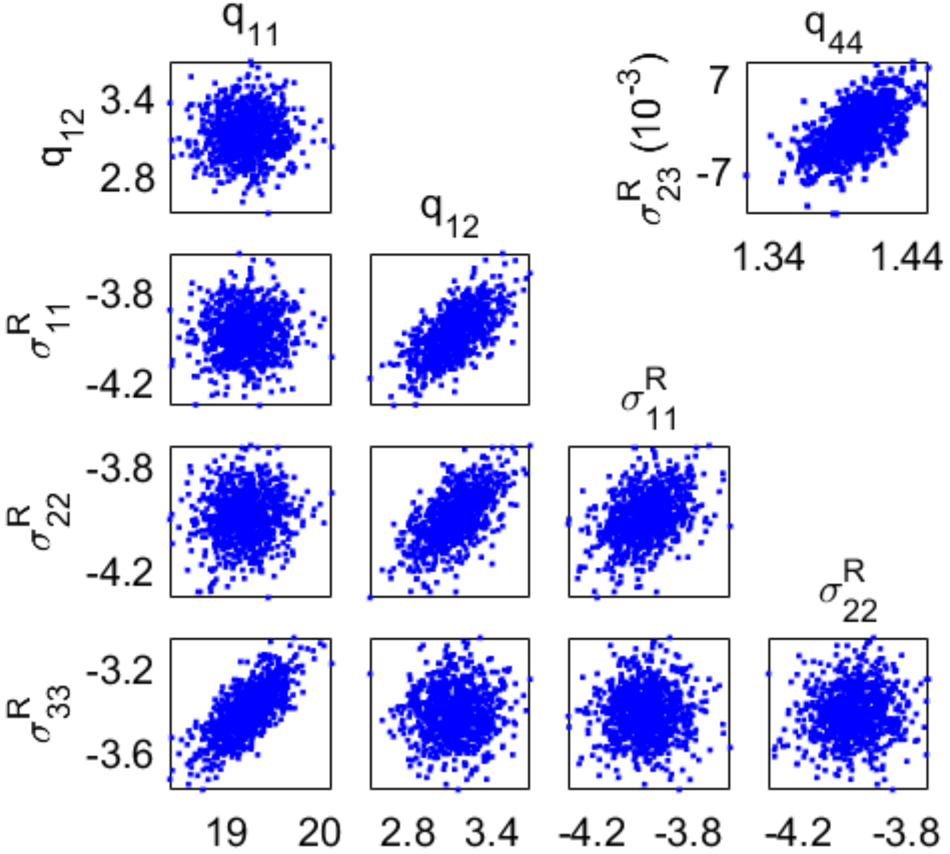


# Stress Calibration

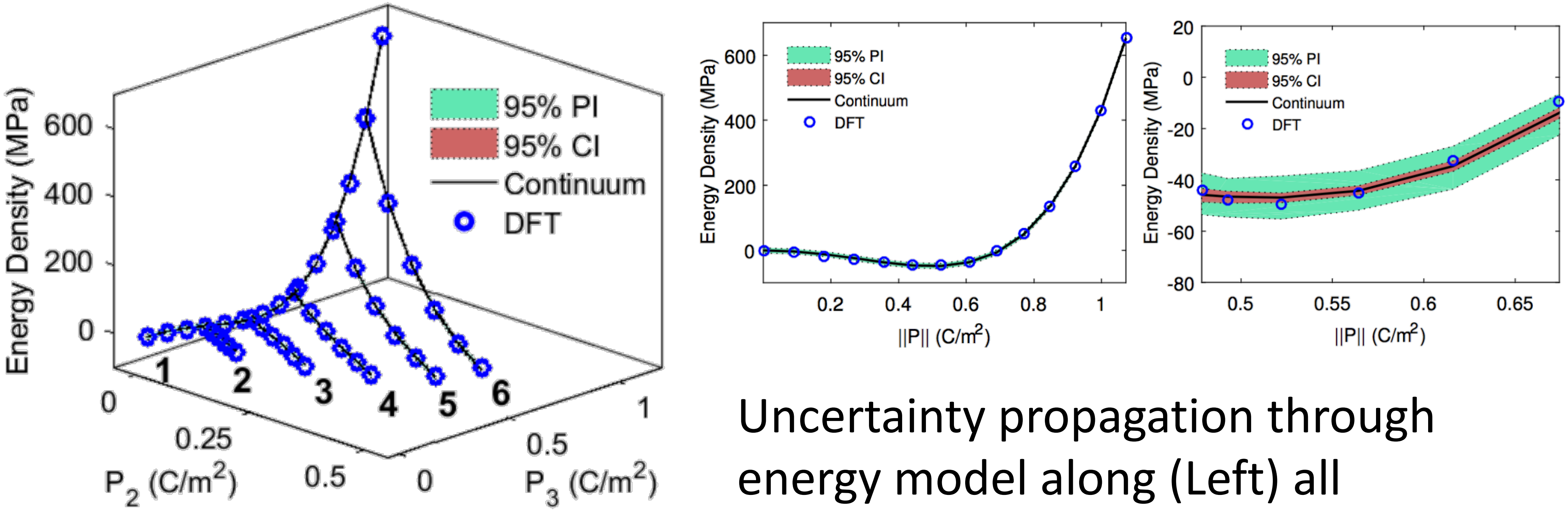
- Posterior densities: $\pi(\theta_\sigma | M^{data})$




- Pairwise correlation:

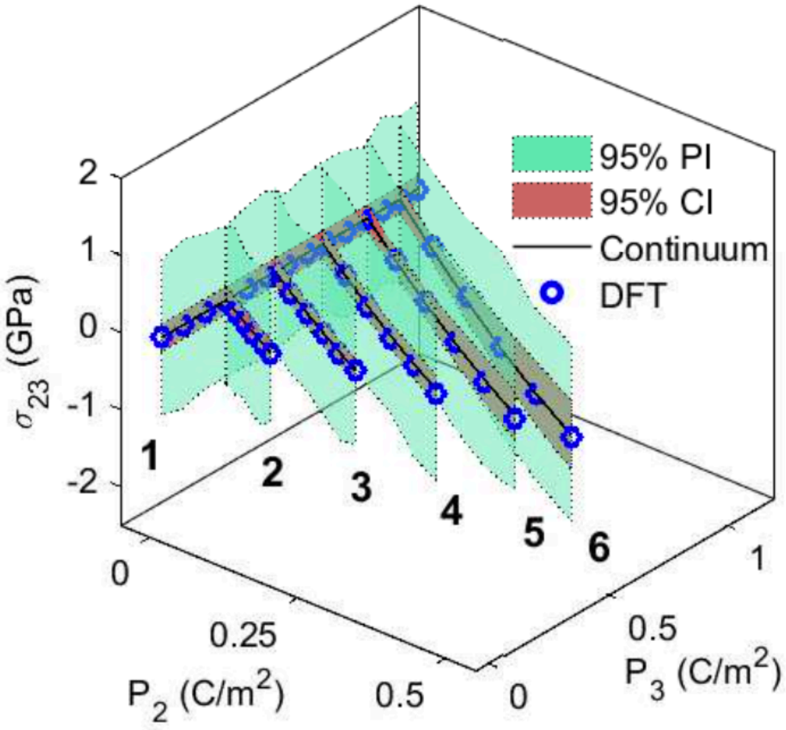


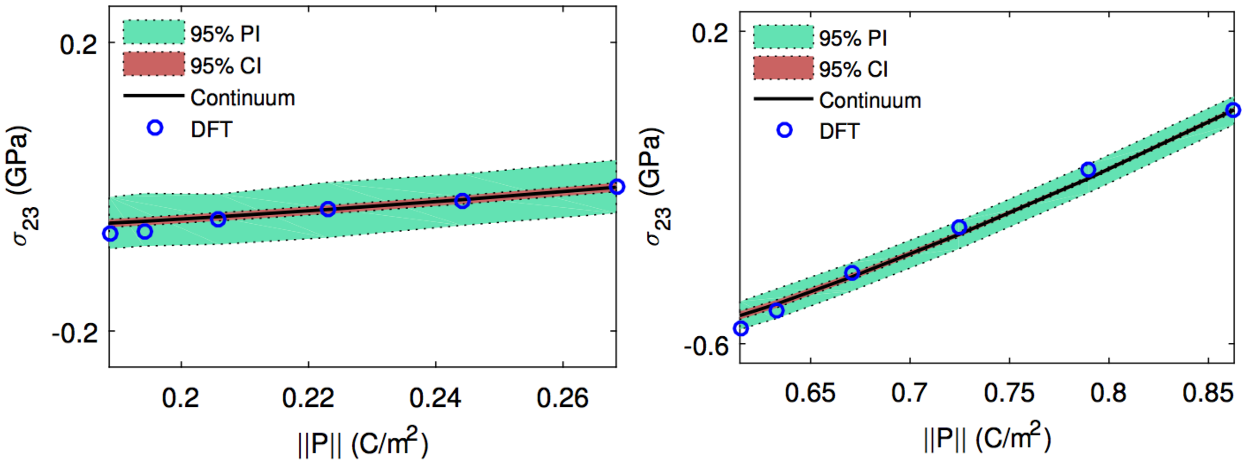
# Uncertainty Propagation: Energy




Uncertainty propagation through energy model along (Left) all thermodynamic paths, (Center) Line 1, and (Right) Line 4.

# Uncertainty Propagation: Stress




Uncertainty propagation through shear stress model along (Left) all thermodynamic paths, (Center) Line 2, and (Right) Line 5.

# Conclusions

- Parameter estimation
- Uncertainty propagation
- Future research:
  - Domain wall structures

# Acknowledgements

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