Model Development, Uncertainty Quantification, and Control Design for Nonlinear Smart Material Systems

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Applications

**Ferroelectric (e.g., PZT)**
- High Speed Nano-positioning
- Membrane mirrors/antennas

**Ferromagnetic (e.g., Terfenol-D)**
- High Speed Milling
- Catheters for Laser Ablation
- SMA Hinges for Solar Arrays
- Chevrons for Noise Reduction

**Ferroelastic (e.g., Shape Memory Alloy)**
Ferroelectric Model Development -- Mesoscopic Level

Helmholtz Energy Density: \( \alpha = \pm 180, 90 \)

\[ \psi_{\alpha}(P, \varepsilon) = \frac{1}{2} \eta_{\alpha}(P - P_{R}^{\alpha})^2 + \frac{1}{2} c_{\alpha}^P (\varepsilon - \varepsilon_{R}^{\alpha})^2 + h_{\alpha}(P - P_{R}^{\alpha})(\varepsilon - \varepsilon_{R}^{\alpha}) \]

Gibbs Energy Density:

\[ G_{\alpha}(E, \sigma; P, \varepsilon) = \psi_{\alpha}(P, \varepsilon) - EP - \sigma \varepsilon \]

Thermodynamic Equilibria: \( \frac{\partial G}{\partial P} = 0, \frac{\partial G}{\partial \varepsilon} = 0 \)

\[ P^{\alpha} = P_{R}^{\alpha} + \chi_{\alpha}^E E + d_{\alpha} \sigma \]

\[ \varepsilon^{\alpha} = \varepsilon_{R}^{\alpha} + d_{\alpha} E + s_{\alpha}^E \sigma \]

Note:
- Linear in each well
- Hysteresis, nonlinearities due to switching between wells
Model Development -- Mesoscopic Level

Thermodynamic Behavior:

\[ P^\alpha = P^\alpha_R + \chi^\sigma_\alpha E + d_\alpha \sigma \]

\[ \varepsilon^\alpha = \varepsilon^\alpha_R + d_\alpha E + s^E_\alpha \sigma \]
**Model Development -- Mesoscopic Level**

**Problem:** Kinetics produce creep

**Solution:** Theory of thermally activated processes. E.g., minimize

$$G = \phi(p) - K(T) - TS - Ep$$

$$= \phi(p) - K(T) - Tk \ln \frac{N_-}{\prod_{p \in S_-} N_p} - Ep$$

**Dipole Fractions:**

$$\dot{x}_- = -p_{-90}x_- + p_{90-}x_{90}$$

$$\dot{x}_{90} = p_{-90}x_- - (p_{90-} + p_{90+})x_{90} + p_{+90}x_+$$

$$\dot{x}_+ = p_{90+}x_{90} - p_{+90}x_+$$

**Transition Likelihoods:**

$$p_{\alpha\beta} = \frac{1}{\tau} e^{-\Delta G_{\alpha\beta} V/kT}$$

**Polarization and Strain Kernels:**

$$\overline{P} = \sum_{\alpha = \pm, 90} x_\alpha P^\alpha \quad \overline{\varepsilon} = \sum_{\alpha = \pm, 90} x_\alpha \varepsilon^\alpha$$
Model Development -- Macroscopic Level

Ferroelectric Materials:
• Incorporate grains, polycrystallinity, variable interaction fields

Homogenized Energy Model (HEM):
\[ \varepsilon(E(t), \sigma(t); x_+) = \int_0^\infty \int_{-\infty}^\infty \bar{\varepsilon}(E(t) + E_I; F_c) \nu_I(E_I) \nu_c(F_c) dE_I dF_c \]

Note:
\[ \bar{\varepsilon} = \sum_{\alpha = \pm, 90} x_{\alpha}(E, \sigma) \left[ E + d_{\alpha} E + s^E \sigma \right] \]
\[ = S^E \sigma + \bar{d}(E, \sigma) E + \bar{\varepsilon}_{irr}(E, \sigma) \]

Constitutive Relation:
\[ \varepsilon(E, \sigma) = S^E \sigma + \bar{d}(E, \sigma_0) E + \varepsilon_{irr}(E, \sigma_0) \]
\[ \Rightarrow \sigma(E, \varepsilon) = c^E \varepsilon - e(E, \sigma_0) E - c^E \varepsilon_{irr}(E, \sigma_0) \]

Examples:
• Beams, shells, structural-acoustic systems
Model Development -- Macroscopic Level

Ferroelectric Materials:
• Incorporate grains, polycrystallinity, variable interaction fields

Homogenized Energy Model (HEM):
\[ \varepsilon(E(t), \sigma(t); x_+) = \int_0^{\infty} \int_{-\infty}^{\infty} \varepsilon(E(t) + E_I; F_c) \nu_I(E_I)\nu_c(F_c) dE_I dF_c \]

Interaction, coercive field densities

Density Representations:
\[ \nu_I(E_I) = c_2 \sum_{j=1}^{N_\beta} \beta_j \phi_j(E_I), \quad \nu_c(E_c) = c_1 \sum_{i=1}^{N_\alpha} \alpha_i \varphi_i(E_c) \]

Basis Choices:
\[ \phi_j(E_I) = \frac{1}{\sigma_I^j \sqrt{2\pi}} e^{-E_I^2/2(\sigma_I^j)^2} \]
\[ \varphi_i(E_c) = \frac{1}{\sigma_c^i E_c \sqrt{2\pi}} e^{-[\ln(E_c) - \mu_c^i]^2/2(\sigma_c^i)^2} \]
Homogenized Energy Model: Experimental Validation

PZT Data: York 2008

[Graphs showing polarization vs. time, strain vs. time, and electric field vs. polarization and strain.]
Structural Model: Macro-Fiber Composites (MFC)

Experimental Structure:

Beam Model:

\[ \rho \frac{\partial^2 w}{\partial t^2} - \frac{\partial^2 M}{\partial x^2} = f \]

Constitutive Relation: (Kelvin-Voigt damping)

\[ \sigma(E, \varepsilon) = c^E \varepsilon + c_D \dot{\varepsilon} - \epsilon(E, \sigma_0) E - c^E \varepsilon_{irr}(E, \sigma_0) \]

Here

\[ \varepsilon = \kappa z = -\frac{\partial^2 w}{\partial x^2} z \]

Moment:

\[ M = \int_{\text{thickness}} \sigma z dz \]

\[ \Rightarrow M = -c^E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} - [k_1 \epsilon(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)] \chi_{MFC}(x) \]
Uncertainty Quantification and Parameter Estimation

Sources of Uncertainty:
- Model
- Sensor measurements
- Initial/boundary conditions

Initial Strategy:
- Quantify uncertainty in parameters
- Propagate uncertainty through model

Parameters: $q = (q_{\text{beam}}, q_{\text{hys}})$
  - Beam: $q_{\text{beam}} = (\rho, c^E I, C_D I, k_1, k_2)$
  - HEM: $q_{\text{hys}} = (\varepsilon_R, \eta, \tau, \gamma, \sigma_c, \mu_c, \sigma_I, \alpha_i, \beta_j)$

Data-Driven Techniques:
- Used to obtain initial parameter estimates

Observation Process: Consider

$$w_j = w(t_j, \bar{x}; q) + \varepsilon_j$$

 IID Random Variable
$$E(\varepsilon_j) = 0$$
$$\text{var}(\varepsilon_j) = \sigma_0^2$$

Strategy: Treat $q$ as random variable and determine covariance matrix or densities
Nonlinear Ordinary Least Squares

Parameter Values:

\[ \hat{q} = \arg \min_{q \in Q} \sum_{j=1}^{N} [w_j - w(t_j, \bar{x}; q)]^2 \]

Covariance Estimate:

\[ \text{cov}(\hat{q}) = \hat{s}^2 \left[ \chi^T(\hat{q})\chi(\hat{q}) \right]^{-1} \]

Variance
Fisher Information
Matrix

\[ \chi_{jk}(\hat{q}) = \frac{\partial w(t_j, \bar{x}; \hat{q})}{\partial q_k} \]

Sensitivity
Matrix

Problem:

- Fisher information matrix ill-conditioned
- Redundant information

One Solution:

- Bootstrapping (resampling) techniques

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Residual Bootstrapping to Construct Parameter Densities

Algorithm:

1. Compute
   \[ \hat{q} = \arg \min_{q \in Q} \sum_{j=1}^{N} [w_j - w(t_j, \bar{x}; q)]^2 \]

2. Compute residuals
   \[ r_j = w_j - w(t_j, \bar{x}; \hat{q}), \quad j = 1 \cdots N \]

3. Compute bootstrapped data values
   \[ \hat{w}_j^k = w(t_j, \bar{x}; \hat{q}) + r_j v_j \]
   where \( v_j \) satisfies \( E(v_j) = 0, E(v_j^2) = E(v_j^3) = 1 \)

4. Compute
   \[ \hat{q} = \arg \min_{q \in Q} \sum_{j=1}^{N} [\hat{w}_j^k - w(t_j, \bar{x}; q)]^2 \]

5. This yields \( K \) estimates of \( q \)
Simplistic Strategy:

Employ gains from linearized system

\[
\frac{dy}{dt} = Ay(t) + Bu(t) + G(t)
\]

in nonlinear system

\[
\frac{dy}{dt} = Ay(t) + [B(u, y)](t) + G(t)
\]
Simplistic Strategy:

Employ gains from linearized system

\[ \frac{dy}{dt} = Ay(t) + Bu(t) + G(t) \]

in nonlinear system

\[ \frac{dy}{dt} = Ay(t) + [B(u, y)](t) + G(t) \]

Deployment, Control and Vibration Attenuation for Radar Masts Using Shape Memory Polymers
Nonlinear Model-Based Control Designs

Nonlinear Inverse Filter/Linear Control:

- Employed by a number of researchers

Nonlinear Control:

- Synthesis between theory and experiments required for real-time implementation
Nonlinear Optimal Control

Function to be Minimized:

\[ J(u) = \frac{1}{2} y^T(t_f) \Pi_f y(t_f) + \frac{1}{2} \int_0^{t_f} [y^T Qy + u^T Ru] \, dt \]

Strategy: Form the Hamiltonian

\[ H(y, \lambda, u) = \frac{1}{2} [y^T Qy + u^T Ru] + \lambda^T [Ay + B(u) + G] \]

Unconstrained optimization yields the necessary conditions

\[ \dot{\lambda} = -\nabla_y H \quad \Rightarrow \quad \dot{\lambda}(t) = -A^T \lambda(t) - Qy(t) \]

\[ 0 = \nabla_u H \quad \Rightarrow \quad Ru^*(t) + [B_u^T(u^*)](t) \lambda(t) = 0 \]

Optimality System:

\[
\begin{bmatrix}
y(t) \\
\lambda(t)
\end{bmatrix} =
\begin{bmatrix}
Ay(t) + [B(u)](t) + G(t) \\
-A^T \lambda(t) - Qy(t)
\end{bmatrix}, \quad y(0) = y_0
\]

\[
\begin{bmatrix}
\lambda(t_f) = \Pi_f y(t_f)
\end{bmatrix}
\]

with \[ u^*(t) = -R^{-1}[B_u^T(u^*)](t) \lambda(t) \]
Numerical Method for Two-Point BVP

**Optimality System:** For \( z = [y, \lambda]^T \), pose as

\[
\dot{z}(t) = F(t, z) \\
E_0 z(0) = [y_0, 0]^T, \quad E_T z(t_f) = [0, \Pi_f y(t_f)]^T
\]

**Solution Technique:**

Discretize with forward difference and solve

\[
\mathcal{F}(z_h) = 0
\]

using the quasi-Newton iteration

\[
z_h^{m+1} = z_h^m + \xi_h^m \quad \text{where} \quad \mathcal{F}'(z_h^m) \xi_h^m = -\mathcal{F}(z_h^m)
\]

**Note:**

- Employ analytic LU decomposition
- 2-D examples: have run over 500,000 unknowns
- Open loop computation for later experimental example: \(~7\) seconds
Nonlinear Control -- Open Loop
**Problem:** Open loop control not robust; e.g., 0.03 second delay
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**Strategy:** Feedback around optimal trajectory \((u^*(t), y^*(t))\)

\[
y^*(0) + \delta y(0) \\
y^*(0) \\
y^*(t) \\
y^*(t) + \delta y(t)
\]

**PI Perturbation Control:** 
\[
\delta u(t) = -k_I e(t) - k_I \int_0^t e(s) ds
\]

**Narrowband Optimal Control:**
**Experimental Implementation --- Tracking at 300 Hz**

**Observation:** PI starts to break down at 300 Hz
Experimental Implementation --- Tracking at 1000 Hz

PI Control

- Commanded Displacement
- Reference Signal

Hysteretic Behavior

Observation:
- Model fit at 300 Hz and 500 Hz
  --- it is predicting at 1000 Hz

Perturbation Control

- Commanded Displacement
- Reference Signal
Narrowband Perturbation Feedback

**Recall:** Hysteresis nonlinearity can produce higher harmonics

**Filter Equations:**

\[
\frac{dx_f}{dt} = A_f x_f(t) + BC x(t)
\]

\[
A_{fi} = \begin{bmatrix}
-2\xi_i \omega_i & -\omega_i^2 \\
1 & 0
\end{bmatrix}
\]

Note: \(\omega_i\) is a frequency being targeted
\(\xi_i\) is an associated damping coefficient

**Control Law:**

\[
u(t) = u^*(t) + u_{NB}(t) + u_I(t)
\]

Optimal Control

Narrowband Feedback

\[
u_{NB} = -[K_f \ K][x_f ; e]
\]
Narrowband Perturbation Feedback --- Experimental Results

**Recall:** Hysteresis nonlinearity can produce higher harmonics

**Filter Equations:**

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\frac{dx_f}{dt} = A_f x_f(t) + BCx(t)
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**Control Law:**

\[
u(t) = u^*(t) + u_{NB}(t) + u_I(t)
\]

Optimal Control

Narrowband Feedback

**Integral Feedback**

\[
u_{NB} = -[K_f \ K][x_f \ ; \ e]
\]

**Note:** 450 \(\mu\)m Max Displacements
Concluding Remarks

Material Properties:
- Hysteresis and constitutive nonlinear inherent to high performance smart materials.
- Hysteresis and nonlinearities can be advantageous

Nonlinear Model Development:
- Physics-based models suitably accurate and efficient for design and control applications.

Uncertainty Quantification:
- Bootstrapping permits characterization of non-Gaussian parameter densities.
- Monte Carlo/bootstrapping methods used to construct confidence bounds for model since not limited by number of parameters.

Control Design:
- Perturbation designs permit real-time implementation.