Uncertainty Quantification in MEMS

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Introduction

Various sources of uncertainties in MEMS:
- Material properties such as Young’s modulus, Poisson’s ratio etc.
- Geometrical features such as dimensions, gap between electrodes etc.
- Operating environment and Boundary conditions

Objectives: In order to design reliable and efficient MEMS devices
- Quantify the effect of uncertainties on various performance parameters
- Use UQ information to identify critical design parameters

Treatment of uncertainties in MEMS:
- Safety factors: over conservative designs
- Monte Carlo (MC) simulations: computationally expensive
Coupled Electro-Mechanical Problem

Electromechanical coupling

Mechanical Analysis
\[ \nabla \cdot (FS) = 0 \text{ in } \Omega \]
\[ u = G \text{ on } \Gamma_g \]
\[ P \cdot N = H \text{ on } \Gamma_h \]
\[ H = \frac{\sigma^2}{2\epsilon} JF^{-T}N \]

Electrostatic Analysis
\[ \phi(p) = \int_{d\omega} G(p, q)\sigma(q)d\gamma_q + C \]
\[ C_T = \int_{d\omega} \sigma(q)d\gamma_q \]
\[ G(p, q) = -\frac{1}{2\pi\epsilon} \ln |p - q| \text{ in 2D} \]
Mathematical Representation of Uncertainty

- **Probability space** \((\mathcal{F}, \mathbb{P})\)  
  Elementary event \(\theta \in \Theta\)

- **Random variable** \(\xi : \Theta \rightarrow \mathbb{R}\)
  uncertain parameters can be modeled as random variables

- **Random field or process** \(w : (x, t, \Theta) \rightarrow \mathbb{R}\)
  uncertain spatial or temporal functions can be represented as random fields

**Generalized Polynomial Chaos**

\[
w(x, \theta) = \sum_{i=0}^{\infty} w_i(x) \Psi_i(\xi(\theta))
\]

Stochastic input  
Stochastic process  
Deterministic functions  
Orthogonal polynomials  
From Askey scheme

Total number of terms
\[
N + 1 = \frac{(n + p)!}{n! p!}
\]

\(n: \) dimension; \(p: \) order

[N. Wiener, 1938], [Ghanem and Spanos, 1991], [Xiu and Karniadakis, SIAM, 2002]
In order to model stochastic electro-mechanical interaction, we need two components

- **Stochastic Electrostatic Analysis**
  - Input: uncertain geometry or deformation
  - Output: uncertain electrostatic pressure

- **Stochastic Mechanical Analysis**
  - Input: uncertain material properties, geometry and/or loading
  - Output: uncertain deformation

**Challenges**

- Geometrical uncertainty: random computational domain
- Multiphysics: uncertainty propagation across various physical fields
Objective: To quantify the uncertainty in surface charge density and output parameters such as capacitance and electrostatic pressure.

Uncertain geometry

Conductor 1  Conductor 2

Lagrangian Electrostatics

Uncertain geometry

Conductor 1  Conductor 2

Lagrangian BIE

\[ \phi(p) = \int_{d\omega} G(p, q)\sigma(q)d\gamma_q + C \]

\[ C_T = \int_{d\omega} \sigma(q)d\gamma_q \]

\[ \phi(P) = \int_{\sigma_{\Omega}} G(P, Q)\sigma(Q)d\gamma_Q + C \]

\[ C_T = \int_{\sigma_{\Omega}} \mathcal{H}(Q)\sigma(Q)d\gamma_Q \]

[Li and Aluru, 2002]
Stochastic Lagrangian Electrostatics

Expand uncertain displacement in terms of GPC basis functions:

\[ u(X, \theta) = \sum_{m=0}^{M} u_m(X) \Psi_m(\theta) \]

Position of a point on the uncertain boundary:

\[ x(\theta) = X + u(X, \theta) \]

Stochastic Green’s function

\[ G(p, q, \theta) = -\frac{1}{2\pi\epsilon} \ln |P - Q + u_P(\theta) - u_Q(\theta)| \]

Stochastic deformation gradient

\[ F_{ij} = \delta_{ij} + \sum_{m=0}^{M} \frac{\partial u_{m,i}}{\partial X_j} \Psi_m(\theta) \]

\( i, j = 1, 2 \) in 2D

\[ d\gamma_q = d\gamma_Q \left[ T(Q) \cdot C(Q, \theta) T(Q) \right]^{\frac{1}{2}} \]

\[ C(X, \theta) = F^T F \]

Stochastic Lagrangian BIE

\[ \phi(P) = \int_{d\Omega} G(P, Q, \theta) \sigma(Q, \theta) d\gamma_Q + C(\theta) \]

\[ C_T = \int_{d\Omega} H(Q, \theta) \sigma(Q, \theta) d\gamma_Q \]

[N. Agarwal and Aluru, JCP, 2007]
**Electrostatics: Stochastic Discretization**

**Step 1:** Unknown variables

\[
\sigma(x, \theta) = \sum_{n=0}^{N} \sigma_n(x) \Psi_n(\xi) \quad C(\theta) = \sum_{n=0}^{N} C_n \Psi_n(\xi)
\]

**Step 2:** Expanding the nonlinear functions in terms of GPC basis functions

\[
G(P, Q, \theta) = \sum_{l=0}^{N} G_l(P, Q) \Psi_l(\theta) \quad \mathcal{H}(P, Q, \theta) = \sum_{l=0}^{N} \mathcal{H}_l(P, Q) \Psi_l(\theta)
\]  

[Debusschere et al., *SIAM*, 2004]

**Step 3:** Using Galerkin projection in the space of PC basic functions

\[
\phi(P) \langle \Psi_m \rangle = \int_{d\Omega} \sum_{n=0}^{N} \sum_{l=0}^{N} G_l(P, Q) \sigma_n(Q) e_{lmn} d\gamma_Q + C_m d_{mm}
\]

\[
C_T \langle \Psi_m \rangle = \int_{d\Omega} \sum_{n=0}^{N} \sum_{l=0}^{N} \mathcal{H}_l(Q) \sigma_n(Q) e_{lmn} d\gamma_Q
\]

\[
m \in [0, N] \quad 2(N + 1)
\]

Coupled Integral Eqs.

**Step 4:** Spatial discretization using Boundary Element Method (BEM)

\[
e_{ijk} = \langle \Psi_i \Psi_j \Psi_k \rangle \quad d_{kk} = \langle \Psi_k^2 \rangle
\]

[N. Agarwal and Aluru, *JCP*, 2007]
Numerical Examples: Interconnect Circuits

Effect of uncertain gap on capacitance

\[ H = \bar{H}(1 + \nu_H \xi) \]

Random translational displacement

\[ \mathbf{u} = [0, \nu_H \bar{H} \xi]^T \]

\[ W = 1 \mu m, T = 0.2 \mu m \]

\[ \bar{H} = 0.2 \mu m \]

Mean and SD
For bottom surface
Empirical formula for capacitance:

\[
\frac{C}{\varepsilon} = 1.15 \left(\frac{W}{H}\right) + 2.80 \left(\frac{T}{H}\right)^{0.222}
\]

Mean and standard deviation for capacitance:

<table>
<thead>
<tr>
<th></th>
<th>MC</th>
<th>PC2</th>
<th>PC3</th>
<th>Emp</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>76.8919</td>
<td>76.8918</td>
<td>76.8920</td>
<td>76.2580</td>
</tr>
<tr>
<td>Std</td>
<td>5.7482</td>
<td>5.7423</td>
<td>5.7481</td>
<td>5.8329</td>
</tr>
</tbody>
</table>
Stochastic Mechanics

Deterministic Case:

\[ [K(u)] \Delta u = -R(u) \]

Stiffness matrix

\[ \Delta u \]

Incremental nodal displacement vector

Residual vector

After linearization and spatial discretization

Stochastic Case:

\[ [K(u(\theta))] \Delta u(\theta) = -R(u(\theta)) \]

Stochastic stiffness matrix

\[ \Delta u(\theta) \]

Random incremental nodal displacement vector

Random residual vector

[Acharjee and Zabaras, CMAME, 2006]
Mechanics: Stochastic Discretization

- **Step 1**: Expand the unknown using GPC:
  \[ \Delta u(\theta) = \sum_{j=0}^{N} \Delta u_j \Psi_j(\theta) \]

- **Step 2**: Express the random stiffness matrix and residual vector in terms of GPC basis functions:
  \[ K(\theta) = \sum_{i=0}^{N} K_i \Psi_i(\theta) \quad R(\theta) = \sum_{i=0}^{N} R_i \Psi_i(\theta) \]

- **Step 3**: Galerkin projection in the space of GPC basis functions:
  \[ \sum_{i} \sum_{j} K_{ij} \Delta u_j \langle \Psi_i \Psi_j \Psi_k \rangle = -R_k \langle \Psi^2_k \rangle \quad k = 0, \ldots, N \]
Numerical Example: Fixed Beam

Effect of uncertain Young’s modulus

\[ E = E_0 (1 + \nu E \xi) \text{ where, } \xi \in [-1, 1] \nu E = 0.2 \]

Uniformly distributed between limits

\[ [E_0 - \Delta E, E_0 + \Delta E] \]

\[ E_0 = 169 \text{ GPa} \]

\[ \Delta E = 0.2E_0 \]

PDF of midpoint vertical displacement

Mean vertical displacement with error bars
1: Identify uncertain parameters (material properties and geometrical parameters) and represent them in terms of independent random variables $\xi = [\xi_1, \xi_2, \ldots, \xi_n]^T$, such that $n$ represents the dimension of the random domain.
2: Represent undeformed (or mean) initial domains as $\Omega_i$ with boundary $d\Omega_i$ and discretize.
3: Model geometrical uncertainties in initial configuration as random deformation field $\mathbf{u}(\mathbf{X}, \theta)$ applied to conductors defined using mean configuration.
4: **Initialization** Set $i = 0$ and the spectral modes for the uncertain surface charge density $[\sigma_k]^i = 0$.
5: Expand uncertain material tensor $\mathbf{C}(\theta) = \sum_{k=0}^{N} \mathbf{C}_k \Psi_k$ and uncertain deformation field $[\mathbf{u}(\mathbf{X}, \theta)]^i = \sum_{k=0}^{N} [\mathbf{u}_k]^i \Psi_k$ in terms of GPC basis functions, where $N+1$ is the total number of terms considered.
6: **repeat**
7: **Stochastic electrostatic analysis**
   a. Using $[\mathbf{u}_k]^i \Psi_k$, solve for the spectral modes $[\sigma_k]^{i+1}$, such that the uncertain surface charge density is given as $\sigma(\mathbf{x}, \theta)^{i+1} = \sum_{k=0}^{N} [\sigma_k]^{i+1} \Psi_k$.
   b. Using $[\sigma_k]^{i+1} \Psi_k$, expand the electrostatic pressure $\mathbf{H}^{i+1} = \sum_{k=0}^{N} [\mathbf{H}_k]^{i+1} \Psi_k$.
8: **Stochastic mechanical analysis**
   Using $\mathbf{C} = \mathbf{C}_k \Psi_k$, $[\mathbf{u}_k]^i \Psi_k$ and $\mathbf{H}^{i+1} = [\mathbf{H}_k]^{i+1} \Psi_k$, compute the spectral modes $[\mathbf{u}_k]^{i+1}$, such that the uncertain deformation field is represented as $[\mathbf{u}]^{i+1} = \sum_{k=0}^{N} [\mathbf{u}_k]^{i+1} \Psi_k$.
9: Update $i = i + 1$.
10: **until** A self-consistent solution is obtained, such that $|[\mathbf{u}_k]^{i+1} - [\mathbf{u}_k]^i| < tol$ and $|[\sigma_k]^{i+1} - [\sigma_k]^i| < tol$, $\forall k$.
11: **Post-processing** Compute the statistics (such as mean and standard deviation) of the deformation $\mathbf{u}(\mathbf{X}, \theta)$ and surface charge density $\sigma(\mathbf{x}, \theta)$.

[Agarwal and Aluru, *CMAME*, 2008]
Numerical Example: MEMS Switch

Effect of uncertain Young’s modulus and gap, assumed uniformly distributed

\[ [E_0 - \Delta E, E_0 + \Delta E], \quad E_0 = 169 \text{ GPa}, \quad \Delta E = 0.1E_0 \]
\[ [g_0 - \Delta g, g_0 + \Delta g], \quad g_0 = 1 \mu m, \quad \Delta g = 0.1 \mu m \]

\[ u(X, \theta) = u_0 + u_1 \xi_1 + u_2 \xi_2 + u_3 \frac{1}{2} (3\xi_1^2 - 1) + u_4 \xi_1 \xi_2 + u_5 \frac{1}{2} (3\xi_2^2 - 1) + \ldots \]

PDF of tip displacement using GPC and MC, \( V=7.0 \text{ V} \)
Vertical displacement with error bars, \( V=7.0 \text{ V} \)
MEMS Switch: Verification using MC

Mean and std for peak displacement, $V=7.0$ V

<table>
<thead>
<tr>
<th></th>
<th>MC</th>
<th>GPC2</th>
<th>GPC3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean $[\mu m]$</td>
<td>-0.1381</td>
<td>-0.1380</td>
<td>-0.1381</td>
</tr>
<tr>
<td>Std $[\mu m]$</td>
<td>0.0299</td>
<td>0.0292</td>
<td>0.0293</td>
</tr>
</tbody>
</table>

MC simulations using 10,000 realizations

PDF of tip displacement using GPC for different applied voltage

$V=5.0$ V

$V=7.4$ V

$V=7.8$ V
MEMS Switch: Sensitivity Analysis

Sensitivity of tip displacement to variations in Young’s modulus and gap

\[ E = E_0(1 + \nu_E \xi_1) \]
\[ g = g_0(1 + \nu_g \xi_2) \]

\[ v = f(\xi_1, \xi_2) \]

Sensitivity w.r.t. Young’s modulus

\[ \frac{1}{\nu_E} \left[ \frac{\partial v}{\partial \xi_1} \right]_{(\xi_1, \xi_2) = (0, 0)} \]

Sensitivity w.r.t. gap

\[ \frac{1}{\nu_g} \left[ \frac{\partial v}{\partial \xi_2} \right]_{(\xi_1, \xi_2) = (0, 0)} \]

Observations

- Tip displacement is more sensitive to variations in gap than Young’s modulus
- Sensitivity information can be used to identify critical design parameters
Comb Drive

Effect of uncertain Young’s modulus

\[ [E_0 - \Delta E, E_0 + \Delta E], \ E_0 = 200 \ GPa, \ \Delta E = 0.1E_0 \]

PDF of capacitance, \( V=4.6 \ V \)

Mean and standard deviation of capacitance, \( V=4.6 \ V \)

<table>
<thead>
<tr>
<th></th>
<th>MC</th>
<th>GPC3</th>
<th>GPC4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Std(\times 10^{-3} [pF/m])</td>
<td>0.1918</td>
<td>0.1885</td>
<td>0.1894</td>
</tr>
</tbody>
</table>

Mean and standard deviation of displacement, \( V=4.6 \ V \)

<table>
<thead>
<tr>
<th></th>
<th>MC</th>
<th>GPC3</th>
<th>GPC4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean [(\mu m)]</td>
<td>0.1541</td>
<td>0.1542</td>
<td>0.1542</td>
</tr>
<tr>
<td>Std [(\mu m)]</td>
<td>0.0208</td>
<td>0.0206</td>
<td>0.0207</td>
</tr>
</tbody>
</table>
Summary

- *Stochastic Lagrangian framework* based on generalized polynomial chaos (GPC) to handle uncertainties in mechanical properties and geometrical parameters for static analysis of electrostatic MEMS.

- Propagation of uncertainties from one energy domain to other energy domains.

- Effect of uncertainties on various design parameters can be easily computed.

- Verification using Monte Carlo (MC) simulation.