ADJOINT-BASED UQ AND OPTIMIZATION UNDER UNCERTAINTY FOR SATELLITE SHIELD DESIGNS

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PRESENTED BY
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Objectives

- Motivation: Robust design of satellite radiation shields
- Enabling technology: derivative-enhanced uncertainty quantification (UQ), optimization, and optimization under uncertainty (OUU) methods
- Enabling technology: adjoint-based radiation transport sensitivities
- Demonstration: example UQ and OUU results

Simulation-based robust design

<table>
<thead>
<tr>
<th>Derivative-enhanced UQ</th>
<th>Gradient-based optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radiation transport with adjoint-based sensitivities</td>
<td>dakota.sandia.gov</td>
</tr>
</tbody>
</table>
Satellite shielding problem

- Shields enable use of commodity microelectronics in space systems, but consume precious weight budget
- Combined electron/proton shielding is non-intuitive; graded-Z (atomic number) shields can help
- **Goal: Simulation-based robust design**
  For example: minimize shield mass, ensuring sufficiently low radiation dose to satellite microelectronics
  - Explore advanced/composite materials, manufacturing processes
  - Design optimal shield layer geometries
  - Seek robustness to environment, manufacturing uncertainties
  - Avoid overly conservative safety factors
Satellite shielding problem (1D)

- 1-D electron/proton shield for satellite in 3000 km orbit
- Radiation environment specified with Spenvis AE8/AP8
- Structural aluminum facing space radiation, 3-layer shield protecting silicon
- Need to limit dose to Si to 10 krad/year.

Design and uncertain variables:
- Thickness $t_j$ of layer $j$
- Fraction $\rho_j$ of material $m$ in layer $j$
Satellite shielding problem (2D)

Satellite components (red, green) are protected by shields (blue) contained within aluminum spacecraft structure (gray). Isotropic protons and/or electrons drive the problem. Control points ($r^*::p^*$) define the shield surfaces, and thus the design (for fixed materials).
Basic Classes of Optimization Approaches

**Derivative-Free Local**
- Sampling with bias/rules toward improvement
- Requires only function values
- Good for noisy, unreliable or expensive derivatives
- Converges to local extreme

**Derivative-Free Global**
- Broad exploration with selective exploitation
- Requires only function values
- Typically computationally intensive
- Converges to global extreme

**Gradient Descent**
- Looks for improvement based on derivative
- Requires analytic or numerical derivatives (*more soon*)
- Efficient/scalable for smooth problems
- Converges to local extreme
**Goal:** determine uncertainty in model output, given uncertainty in input parameters

- Assign probability distributions on input parameters $u$, e.g., normal, uniform, histogram

**Monte Carlo / Latin Hypercube Sampling (LHS)**

- Randomly sample *function values only* globally over the uncertain parameter space
- Calculate sample statistics, e.g., mean, percentiles
- Robust, but slow to converge

**Mean Value (MV) Local Reliability**

- Single evaluation of *function value and derivatives* at uncertain variable means
- First-order propagation of moments via “sandwich formula” (higher-order possible as well)
- Exact for multivariate normal uncertain inputs $u$ with a linear map $g(u)$; may be poor for nonlinear problems

\[
\mu_g = \frac{1}{N} \sum_{i} g(u_i)
\]

\[
\sigma_g = \sqrt{\frac{1}{N} \sum_{i} (g(u_i) - \mu_g)^2}
\]

\[
\mu_g = g(\mu_u)
\]

\[
Cov(g) = \nabla_u g(\mu_u)^T Cov(u) \nabla_u g(\mu_u)
\]
Advanced UQ Methods

- **Most-probable point (MPP) Local Reliability:**
  - Reformulate UQ as optimization
  - Numerous variants, including successive approximations
  - More accurate for specific probability levels than MV
  - Uses *function values and derivatives*

- **Polynomial chaos expansions (PCE)**
  - Expand QOI in an uncertainty-optimal orthogonal polynomial basis $\varphi_i$. Statistics can then be calculated exactly from the expansion.
  - Well-suited for smooth responses $g(u)$.
  - Can use function $g(u^i)$ *value only* (PCEf) or *value plus gradient* $\nabla g(u^i)$ data (PCEg) at points $i$ in a regression approach to determine $c_i$
UQ methodology

The UQ information we desire. UQ is applied to a fixed design, perhaps generated with ideal data.

The basic UQ process. Samples (whether randomly drawn or generated through more sophisticated algorithms) are used for transport calculations. Transport quantities, perhaps augmented with gradients, are supplied to the UQ algorithm.
The OUU information we desire.
Instead of applying an arbitrary safety factor and determining a probability of failure, we want to choose a failure rate and design to that rate.

The basic OUU process. An outer optimization loop determines nominal designs. Each is subjected to a UQ study to determine its characteristics (e.g. failure probabilities). Transport quantities, perhaps augmented with gradients, are supplied to both the UQ and optimization algorithms to create an OUU process.
Transport Theory: Problem

Problem:
\[ \Omega \cdot \nabla \psi + \sigma_t \psi = \int dE \int_{\Omega'} d\Omega \sigma_s (r, \Omega' \rightarrow \Omega, E' \rightarrow E) \psi (r, \Omega', E') + q, r \in D \]
\[ \psi = \psi_b (r, \Omega, E), \{ r \in \partial D | \Omega \cdot \vec{n} < 0 \} \]

\[ R = \int_D dr \int_E dE \int_{4\pi} d\Omega \psi (r, \Omega, E) q^\dagger (r, E) \]

Simplifications/definitions:

\[ L\psi + C\psi = S\psi + q \]
\[ \int_D dr \int_E dE \int_{4\pi} d\Omega ab \equiv \langle a, b \rangle \]
Transport Theory: Sensitivities

Lagrangian:

\[ \mathcal{L} = \langle \psi, q^\dagger \rangle - \langle \psi^\dagger, L\psi + C\psi - S\psi - q \rangle \]

Derivatives (sensitivities):

\[ \frac{d\mathcal{L}}{dp} = \frac{\partial \mathcal{L}}{\partial p} + \frac{\partial \mathcal{L}}{\partial \psi} \frac{\partial \psi}{\partial p} \]

\( p \) is any uncertain and/or design parameter. In general it is a vector.
Theory: Sensitivities

We then find that if the following equations are satisfied:

\[(L + C - S)\psi = q\] (forward problem)

\[(L^\dagger + C^\dagger - S^\dagger)\psi^\dagger = q^\dagger\] (adjoint problem)

then \(\frac{dL}{dp}\) reduces to:

\[
\frac{dL}{dp} = \left[ \left\langle \psi, \frac{\partial q^\dagger}{\partial p} \right\rangle + \left\langle \psi^\dagger, \frac{\partial q}{\partial p} \right\rangle - \left\langle \psi^\dagger, \left( \frac{\partial}{\partial p} (L + C - S) \right) \psi \right\rangle \right] = \frac{dR}{dp}
\]

The sensitivities of any \(R\) to any \(p\) are obtained by various inner products involving the forward solution \(\psi\), the adjoint solution \(\psi^\dagger\), and derivatives of input (i.e. known) quantities.
We have derived sensitivity expressions for several relevant parameters:

- Material fractions
  - We can examine the entire periodic table concurrently if we desire
- Geometric terms
  - 1D thicknesses
  - 2D parametrized surface
Goal: with what probability will a proposed design meet dose requirements? Ultimately, account for variability in:
- manufacturing (mixtures, layer geometry)
- state of knowledge (transport cross sections)
- operating environment (source spectrum)

Demonstration: UQ for optimally-designed 3-layer shield
- Assuming imperfect material mixtures
- 5% manufacturing variability = 1σ

Use adjoint-based derivatives with gradient-enhanced UQ methods

<table>
<thead>
<tr>
<th>Layer: Mixture</th>
<th>mean $\mu$ (g/cm$^2$)</th>
<th>standard deviation $\sigma$ (g/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1: UHMWPE</td>
<td>3.4424e+00</td>
<td>1.7212e-01</td>
</tr>
<tr>
<td>L1: Ta</td>
<td>1.3198e-02</td>
<td>6.5992e-04</td>
</tr>
<tr>
<td>L2: UHMWPE</td>
<td>3.6750e+00</td>
<td>1.8375e-01</td>
</tr>
<tr>
<td>L2: Ta</td>
<td>6.1353e-03</td>
<td>3.0677e-04</td>
</tr>
<tr>
<td>L3: UHMWPE</td>
<td>4.8077e+00</td>
<td>2.4039e-01</td>
</tr>
<tr>
<td>L3: Ta</td>
<td>9.7317e-02</td>
<td>4.8658e-03</td>
</tr>
</tbody>
</table>
Application of UQ for 1D Shield

- While most methods agree well near the median, under-resolved LHS demonstrates challenges predicting tail probabilities.

**Reasonable agreement near median**

**Poorer agreement in tails**
Application of UQ for 1D Shield

- LHS converges fairly quickly to mean, less so for other statistics
- Gradient-based MPP and PCE methods resolve statistics with lower compute cost, see, e.g., 99\textsuperscript{th} percentile f vs. g.
- Offer accuracy advantages over MC/LHS for tail probabilities
Optimized 2D Designs

Proton-only environment (for simplicity) at 2000 km circular equatorial orbit
Environment generated by Spenvis
Transport calculations performed by Sceptre code, optimization algorithms in Dakota

Optimal design (no geometric uncertainties) for polyethylene (UHMWPE) shields.
Inner dose requirement: 40 krad/year
Outer dose requirement: 100 krad/year

Optimal design (no geometric uncertainties) for copper shields.
Inner dose requirement: 20 krad/year
Outer dose requirement: 100 krad/year
Geometric Uncertainties

We used nominal designs for 2D UQ studies. We arbitrarily assumed 2 mm uncertainties on the locations of the control points of the inner shield. We also imposed upper and lower limits on the radii of the control points.

<table>
<thead>
<tr>
<th>Control Point</th>
<th>UHMWPE Radius Mean</th>
<th>Copper Radius Mean</th>
<th>Radius Std. Dev.</th>
<th>Lower Bound</th>
<th>Upper Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>r1::p2</td>
<td>6.416</td>
<td>3.372</td>
<td>0.2</td>
<td>1.697</td>
<td>13.011</td>
</tr>
<tr>
<td>r2::p2</td>
<td>4.242</td>
<td>2.957</td>
<td>0.2</td>
<td>1.2</td>
<td>9.2</td>
</tr>
<tr>
<td>r3::p2</td>
<td>4.81</td>
<td>2.988</td>
<td>0.2</td>
<td>1.697</td>
<td>13.011</td>
</tr>
<tr>
<td>r4::p2</td>
<td>1.757</td>
<td>1.930</td>
<td>0.2</td>
<td>1.2</td>
<td>9.2</td>
</tr>
<tr>
<td>r5::p2</td>
<td>6.726</td>
<td>3.367</td>
<td>0.2</td>
<td>1.697</td>
<td>13.011</td>
</tr>
<tr>
<td>r6::p2</td>
<td>5.695</td>
<td>3.316</td>
<td>0.2</td>
<td>1.2</td>
<td>9.2</td>
</tr>
<tr>
<td>r7::p2</td>
<td>6.351</td>
<td>3.441</td>
<td>0.2</td>
<td>1.697</td>
<td>13.011</td>
</tr>
<tr>
<td>r8::p2</td>
<td>5.854</td>
<td>3.316</td>
<td>0.2</td>
<td>1.2</td>
<td>9.2</td>
</tr>
</tbody>
</table>
Several UQ methods (some that use gradients, other that don’t) used to study previous designs. Note that MPP, though more expensive than other methods, gives more detailed information about the tail of the distribution than the nominal case.

<table>
<thead>
<tr>
<th>Material</th>
<th>UQ Method</th>
<th>Transport calculations</th>
<th>Sensor 1</th>
<th>Sensor 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Dose Mean / p50</td>
<td>Dose Std. Dev.</td>
</tr>
<tr>
<td>UHMWPE</td>
<td>LHS10</td>
<td>10</td>
<td>40.06</td>
<td>0.399</td>
</tr>
<tr>
<td></td>
<td>LHS80</td>
<td>80</td>
<td>40.07</td>
<td>0.366</td>
</tr>
<tr>
<td></td>
<td>MV</td>
<td>6</td>
<td>40.03</td>
<td>0.358</td>
</tr>
<tr>
<td></td>
<td>MPP</td>
<td>varies (≈300)</td>
<td>40.04</td>
<td>-</td>
</tr>
<tr>
<td>Cu</td>
<td>LHS10</td>
<td>10</td>
<td>20.13</td>
<td>0.762</td>
</tr>
<tr>
<td></td>
<td>LHS80</td>
<td>80</td>
<td>20.14</td>
<td>0.690</td>
</tr>
<tr>
<td></td>
<td>MV</td>
<td>6</td>
<td>20.02</td>
<td>0.670</td>
</tr>
<tr>
<td></td>
<td>MPP</td>
<td>varies (≈300)</td>
<td>20.02</td>
<td>-</td>
</tr>
</tbody>
</table>

Requirements:
- UHMWPE: 40/100 krad
- Copper: 20/100 krad
Fix outer shield at optimal deterministic design

Manufactured radii assumed truncated normal with $1\sigma = 0.2\text{cm}$

Require 95\textsuperscript{th} percentile of dose at center less than requirement

<table>
<thead>
<tr>
<th>Control Point</th>
<th>UHMWPE</th>
<th>Copper</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Nominal Design (deterministic radii)</td>
<td>Reliable Design (mean radii)</td>
</tr>
<tr>
<td>r1::p2 (cm)</td>
<td>6.416</td>
<td>6.496</td>
</tr>
<tr>
<td>r2::p2 (cm)</td>
<td>4.242</td>
<td>4.352</td>
</tr>
<tr>
<td>r3::p2 (cm)</td>
<td>4.81</td>
<td>4.885</td>
</tr>
<tr>
<td>r4::p2 (cm)</td>
<td>1.757</td>
<td>1.741</td>
</tr>
<tr>
<td>r5::p2 (cm)</td>
<td>6.726</td>
<td>6.962</td>
</tr>
<tr>
<td>r6::p2 (cm)</td>
<td>5.695</td>
<td>5.854</td>
</tr>
<tr>
<td>r7::p2 (cm)</td>
<td>6.351</td>
<td>6.620</td>
</tr>
<tr>
<td>r8::p2 (cm)</td>
<td>5.854</td>
<td>5.946</td>
</tr>
<tr>
<td>Mass (g/cm)</td>
<td>81.85 (nom)</td>
<td>85.32 (mean)</td>
</tr>
<tr>
<td>Dose to Sensor 1 (krad)</td>
<td>40.04 (nom)</td>
<td>39.99 (p95)</td>
</tr>
</tbody>
</table>
Below is a UQ study of the robust design. Note the differences between the mean cases and the 95th percentile cases.

<table>
<thead>
<tr>
<th>Material</th>
<th>UQ Method</th>
<th>Transport calculations</th>
<th>Dose Mean / p50</th>
<th>Dose Std. Dev.</th>
<th>Dose p95</th>
<th>Mass Mean / p50</th>
<th>Mass Std. Dev.</th>
<th>Mass p95</th>
</tr>
</thead>
<tbody>
<tr>
<td>UHMWPE</td>
<td>MV</td>
<td>6</td>
<td>39.421</td>
<td>0.3481</td>
<td>39.99</td>
<td>85.317</td>
<td>2.0402</td>
<td>88.67</td>
</tr>
<tr>
<td>Cu</td>
<td>MV</td>
<td>6</td>
<td>18.977</td>
<td>0.6222</td>
<td>20.00</td>
<td>307.04</td>
<td>11.534</td>
<td>326.0</td>
</tr>
</tbody>
</table>

**More Features of Reliable Designs:**

**UHMWPE (40 krad/yr):**
- 18 iterations (feasible after only 4)
- About 2% greater radius, 4% more massive

**Copper (20 krad / yr):**
- 29 iterations (feasible after 28)
- About 4% greater radius (range 2% -- 6%), 6% more massive

Copper more mass efficient, but reliable design requires more material in a relative sense
Conclusions

• Recent advances in transport sensitivity analysis may be combined with advanced derivative-enhanced UQ/OUU algorithms

• We have applied gradient information to UQ studies; compares favorably with more expensive (e.g. LHS) methods

• We also have applied gradients to optimization under uncertainty.

• Future work
  • 3D geometric sensitivities
  • Examine additional UQ algorithms within OUU studies
  • Examine other uncertain variables, e.g. boundary conditions