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Adjoint-enabled Optimization and UQ for Radiation Shield Design

Brian M. Adams

Optimization and Uncertainty Quantification Dept.

Shawn Pautz, Laura Swiler, Brian Franke,
Ethan Blansett, Don Bruss

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Simulation-based Radiation Shield Design

- 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: Robust design to 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

Radiation Transport Solver with Adjoint-based Sensitivities

- Boltzmann transport for fluxes ψ, with derived response g

$$\Omega \cdot \nabla\psi + \sigma_t(r,E)\psi = \int_{E'} dE' \int_{4\pi} d\Omega' \sigma_s(r,\Omega' \to \Omega, E' \to E)\psi(r,\Omega',E') + q$$

streaming L collision C scattering S source

$$\psi = \psi_b(r,\Omega,E), \{r \in \partial D | \Omega \cdot \vec{n} < 0\}$$

boundary condition

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

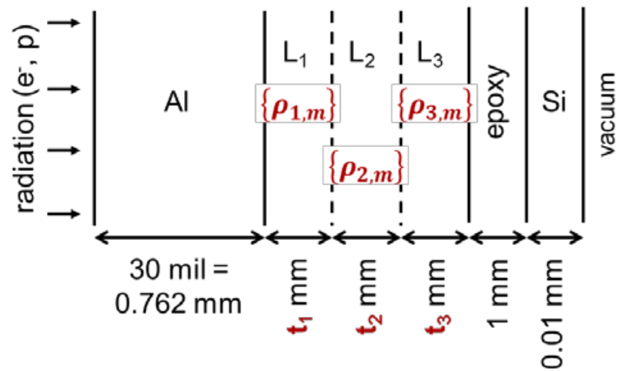
- SCEPTRE simulation of forward/adjoint radiation transport

$$L\psi + C\psi = S\psi + q \qquad (L^\dagger + C^\dagger - S^\dagger)\psi^\dagger = q^\dagger$$

- Post-process fluxes, adjoint fluxes to calculate, e.g.,
  - Dose $g(p)$ in silicon-based microelectronics, $q^\dagger = \sigma_d(r,E)/V$
  - Sensitivities: form a Lagrangian, enforce forward and adjoint solution to get sensitivity $\partial g(p)/\partial p$ of dose to design and uncertain parameters p.

Optimization Formulation

- Goal: What component materials, composite material fractions, and shield layer geometries yield the lightest, sufficiently protective shield?
- Example: 1-D electron/proton shield design
  - Structural aluminum facing space radiation
  - 3-layer designable shield protecting silicon;
    - Thickness $\boldsymbol{t_j}$ of layer j
    - Fraction $\boldsymbol{\rho_j}$ of material m in layer j



- Transport-constrained nonlinear program

$$\min_{t,\rho}\ mass(t,\rho)$$
$$s.t.\ \ g(p) = dose(t,\rho) \leq 10\ krad$$

$$\sum \rho_{j,m} = 1, \forall j$$
$$0 \leq \rho_{j,m} \leq 1$$
$$0 \leq t \leq t_{max}$$

- Adjoint-based sensitivities $\partial g(p)/\partial p$ for gradient-based optimization; nearly constant cost per evaluation for any number parameters
- Solved with Dakota (NPSOL's sequential quadratic programming)

Single Layer Shield Optimization

- Demonstration: single layer shield for 3000km orbit; design
  - Design fraction of UHMWPE (polyethylene), Al, Cu, Mo, Ta; thickness
- Solution cost (6 design parameters)

	Iterations	Forward Solves	Adjoint Solves
Adjoint	17	17	17
Finite difference	19	133	-

Adjoint costs roughly 1.75x forward, for total 2.75x per eval

- Shift from UHMWPE to Ta yields a 4.4% lighter, thinner shield, meeting same dose constraint. Al, Cu, Mo are not selected.
  - Modest gain demonstrated, but significant vs. aluminum shielding

	thickness (cm)	UHMWPE fraction	Ta fraction	mass (g/cm^2)	dose (krad)
initial	13.50	1.0000	0	12.55	10.01
final	12.81	0.9994	0.0006	12.02	10.00

Proton/Electron Environment Varies By Altitude

- Differing requirements, e.g., for weather vs. GPS satellites
- Optimizer determines optimal shield for each altitude

Altitude (km)	UHMWPE-Al-Cu-Mo-Ta mass (g/cm^2)	Periodic table mass (g/cm^2)
2000	UHMWPE 7.81, Ta 0.126	H 3.95, Ta 0.098
3000	UHMWPE 11.89, Ta 0.138	H 6.03, Ta 0.125
4000	UHMWPE 6.43, Ta 0.166	H 3.19, other 0.290
…	…	…
9000	UHMWPE 0.244, Ta 0.083	H 0.149, At 0.047, Pa trace

- Considered designs with any of 92 materials (H through U)
  - Explore potential options, *without regard to manufacturability*
  - Required ~15 iterations using adjoints (FD impractical): scales well with number of parameters
- *Running many trade studies (see Pautz, et al., ANS M&C 2017)*

Uncertainty Quantification (UQ)

- Goal: with what probability will a proposed design meet dose requirements? Account for variability in
  - manufacturing (mixtures, layer geometry)
  - state of knowledge (transport cross sections)
  - operating environment (source spectrum)

- Use adjoint-based derivatives with advanced UQ methods

- Demonstration: UQ for optimally-designed 3-layer shield, assuming imperfect mixtures

Layer: Mixture	mean μ (g/cm^2)	standard deviation σ (g/cm^2)
L1: UHMWPE	3.4424e+00	1.7212e-01
L1: Ta	1.3198e-02	6.5992e-04
L2: UHMWPE	3.6750e+00	1.8375e-01
L2: Ta	6.1353e-03	3.0677e-04
L3: UHMWPE	4.8077e+00	2.4039e-01
L3: Ta	9.7317e-02	4.8658e-03

Use of Derivatives in UQ

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- Monte Carlo Sampling / LHS to propagate uncertainty in u is robust, but slow to converge; *can't take advantage of adjoint information*

$$\mu_g = \frac{1}{N}\sum_i g(u^i)$$

$$\sigma_g = \sqrt{\frac{1}{N}\sum_i \left(g(u^i) - \mu_g\right)^2}$$

- (Local) Reliability methods use derivatives:
  - Mean value (MV): first- or second-order approximation at uncertain variable means
  - Most-probable point (MPP): reformulate UQ as optimization; apply usual derivative-based methods

$$\mu_g = g(\mu_u)$$

$$Cov(g) = \nabla_u g(\mu_u)^T \mathrm{Cov}(u) \nabla_u g(\mu_u)$$

$$\min_u \; u^T u$$

$$s.t. \; g(u) = g_{target}$$

- Polynomial chaos expansions (PCE)
  - Expand QOI in an uncertainty-optimal orthogonal polynomial basis φ_i; calculate statistics analytically
  - Can use function $g(u^i)$ and gradient $\nabla g(u^i)$ data at points i in a regression approach to determine c_i

$$g(u) \approx \sum_j c_j \varphi_j(u)$$

$$\frac{\partial g}{\partial u}(u) \approx \sum_j c_j \frac{\partial \phi_j}{\partial u}(u)$$

UQ for an Optimally Designed 3-layer Shield

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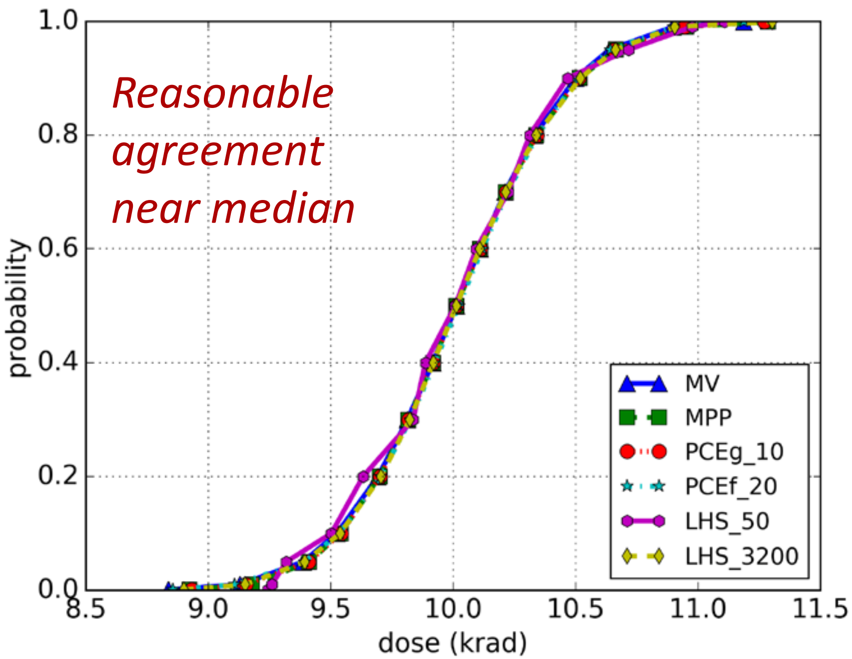
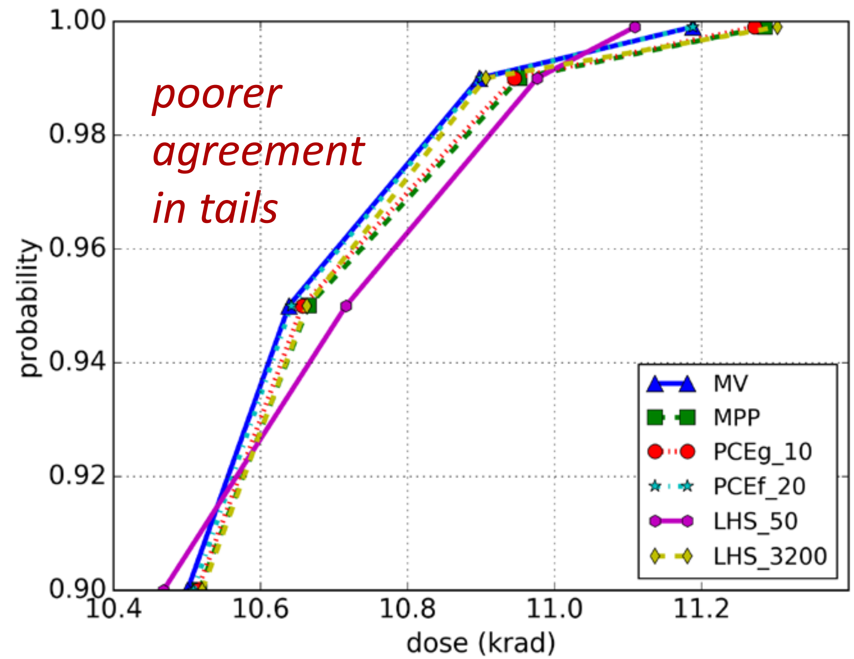
- Advanced, gradient-informed UQ methods offer computational efficiency and accuracy advantages

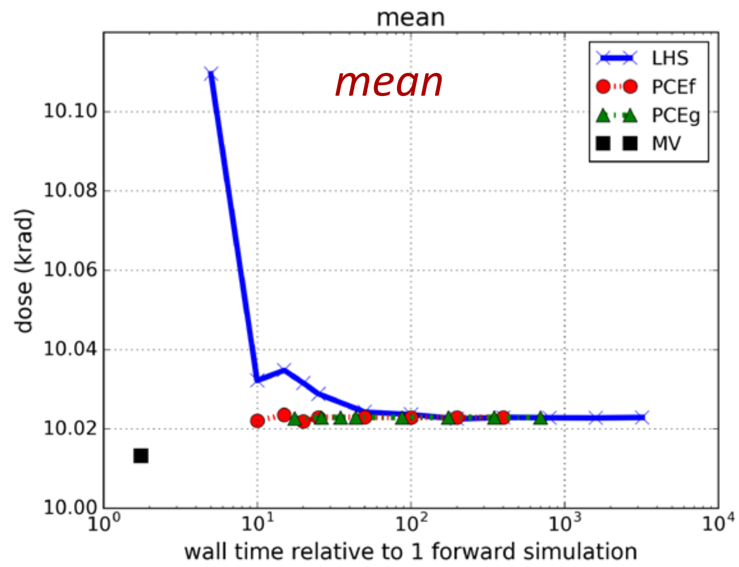
Method	Rel. Wall	Notes
MV	1.75	1 forward + 1 adjoint solve
MPP	4 * 1.75	4 * (fwd. + adj.), 1 prob. level
	54 * 1.75	54 * (fwd. + adj.), 30 levels
LHS_N; PCEf_N	N	N * fwd.
PCEg_N	N * 1.75	N * (fwd. + adj.)

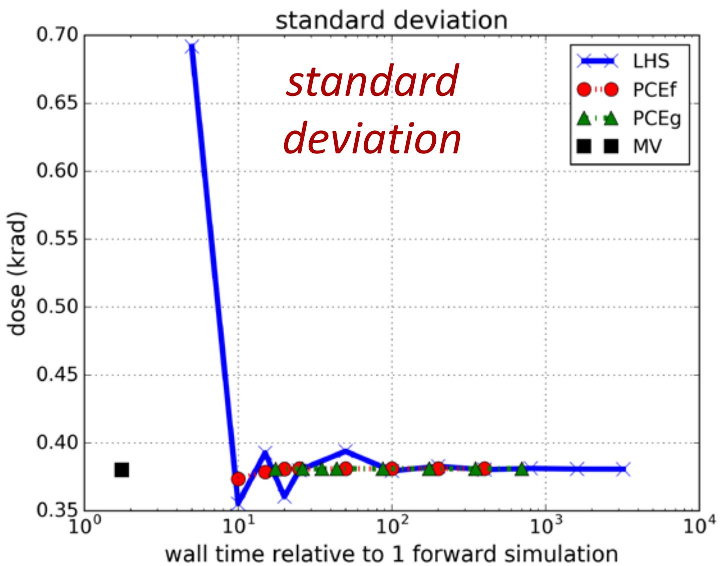


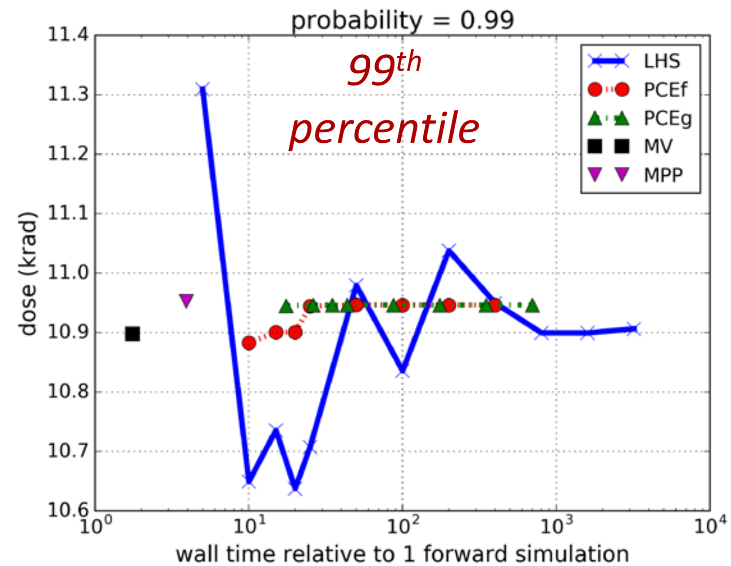


Convergence of UQ Methods

- Gradient-based MPP and PCE methods show promise in resolving statistics with lower cost
- Should offer accuracy advantages over MC/LHS for tail probabilities
- *Details: Adams, et al., ANS M&C 2017*

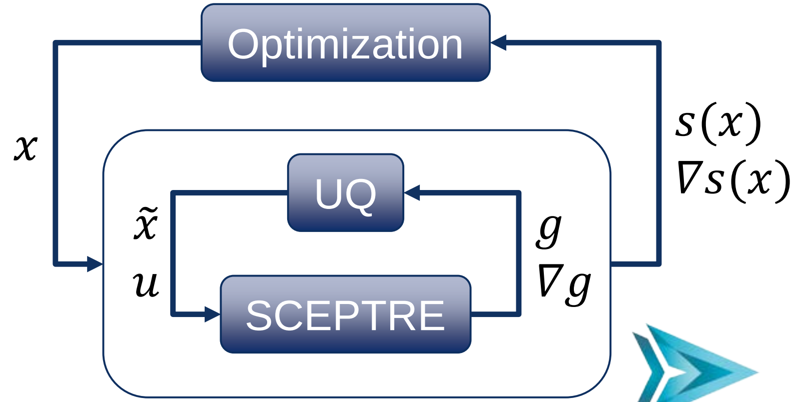






Work in Progress:
Adjoint-enabled Radiation Shield Design

- Design with 2-D and 3-D geometries, allow spot shielding
- Multiple dose constraints for differing component requirements
- Uncertainties in source spectrum (how to parameterize?)
- Nested analysis to directly seek designs x that satisfy statistical robustness or reliability constraints $s(x)$
  - Reliability, polynomial chaos take advantage of algebraic statistics form to propagate simulation adjoints to derivatives of statistics without finite differences
  - Also benefits bounding or interval analysis with aleatory + epistemic



Thanks for your attention!

briadam@sandia.gov