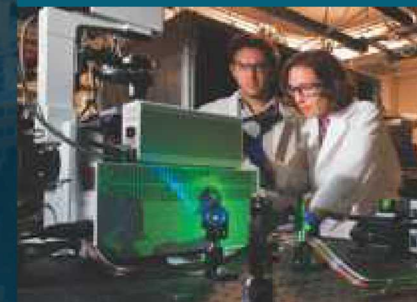
SAND2019-6177C

ADJOINT-ENABLED MULTIDIMENSIONAL OPTIMIZATION OF SATELLITE RADIATION SHIELDS



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ANS Annual Meeting

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PRESENTED BY

Shawn Pautz

SAND2019-??? C

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OUTLINE

Context

Optimization approaches

Derivation of 2D transport sensitivities

Results

Conclusions

CONTEXT

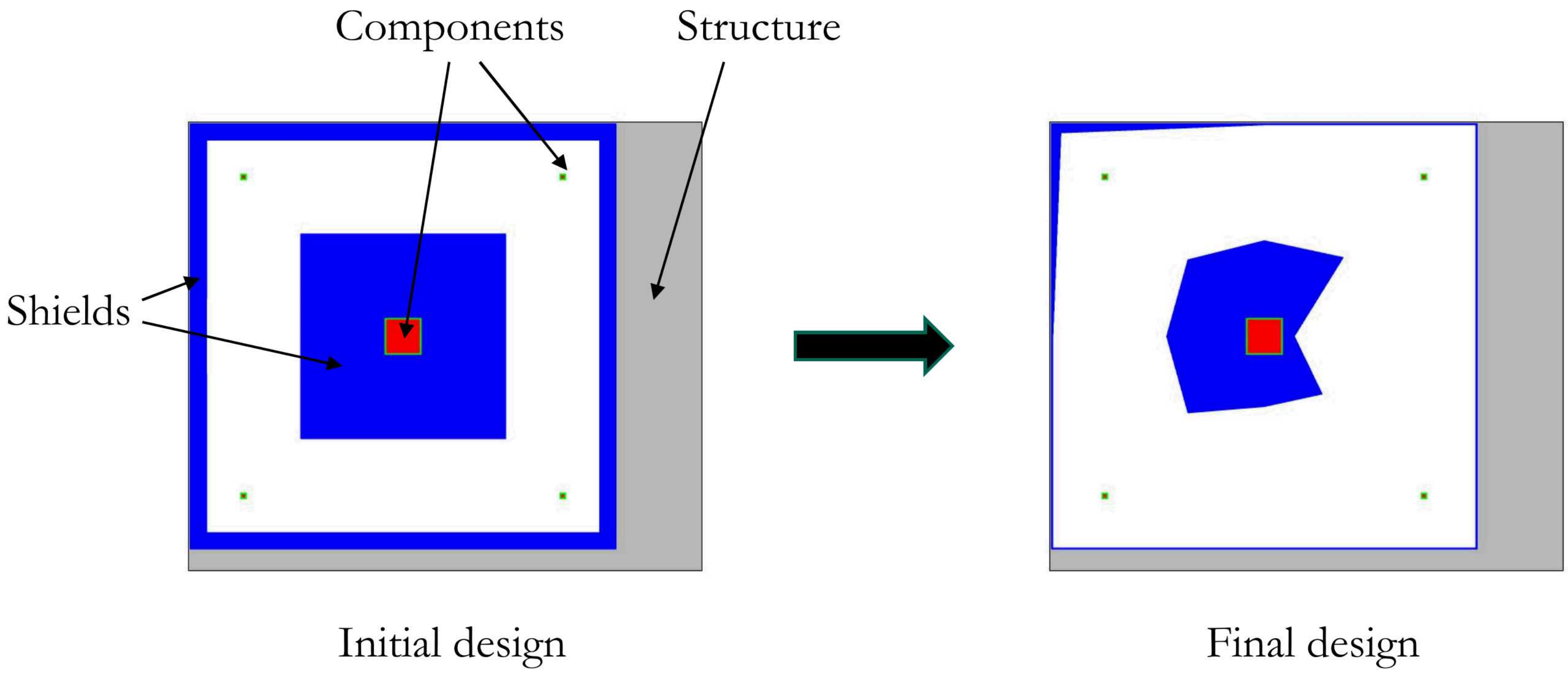
- Increased demand for optimization and UQ
- Increasing interest in advanced materials/manufacturing
- Recent advances in transport community with adjoint-based sensitivities

Opportunity: use adjoint-based transport methods to efficiently determine parameter sensitivities, which will be used to drive design optimization and/or UQ calculations in high-dimensional spaces.

- Enable consideration of larger design/trade space
- Provide greater insight to designers

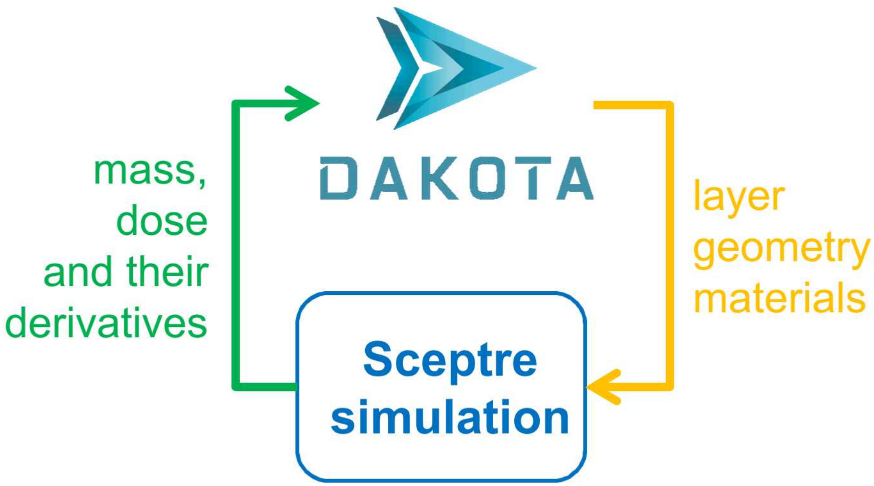
END OBJECTIVE

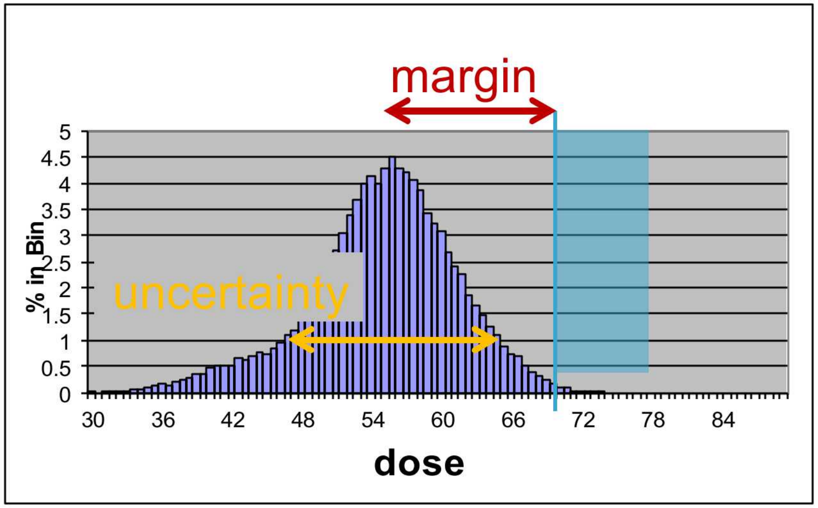
We are interested in satellite electron/proton shielding applications. Mass is at a premium for space missions due to launch costs and/or mass limits. We want to perform design optimization to achieve the required level of protection with the minimum amount of mass. For example, we want to be able to transform the initial design below to a mass-saving one while still meeting the same requirements. This may entail material and/or geometric changes.



SIMULATION-BASED DESIGN EXPLORATION AND ANALYSIS

- Use Dakota with Sceptre (deterministic transport solver) to systematically ask what-if questions: sensitivity, design, uncertainty analyses
- Optimization: What component materials, composite material fractions, and shield layer geometries yield the lightest shield meeting strength and dose requirements?
- Uncertainty Quantification (UQ): Given variability in manufacturing (mixtures, layer geometry) and state of knowledge (transport cross sections), with what probability will a proposed design meet dose requirements?





BASIC CLASSES OF OPTIMIZATION APPROACHES

Gradient Descent

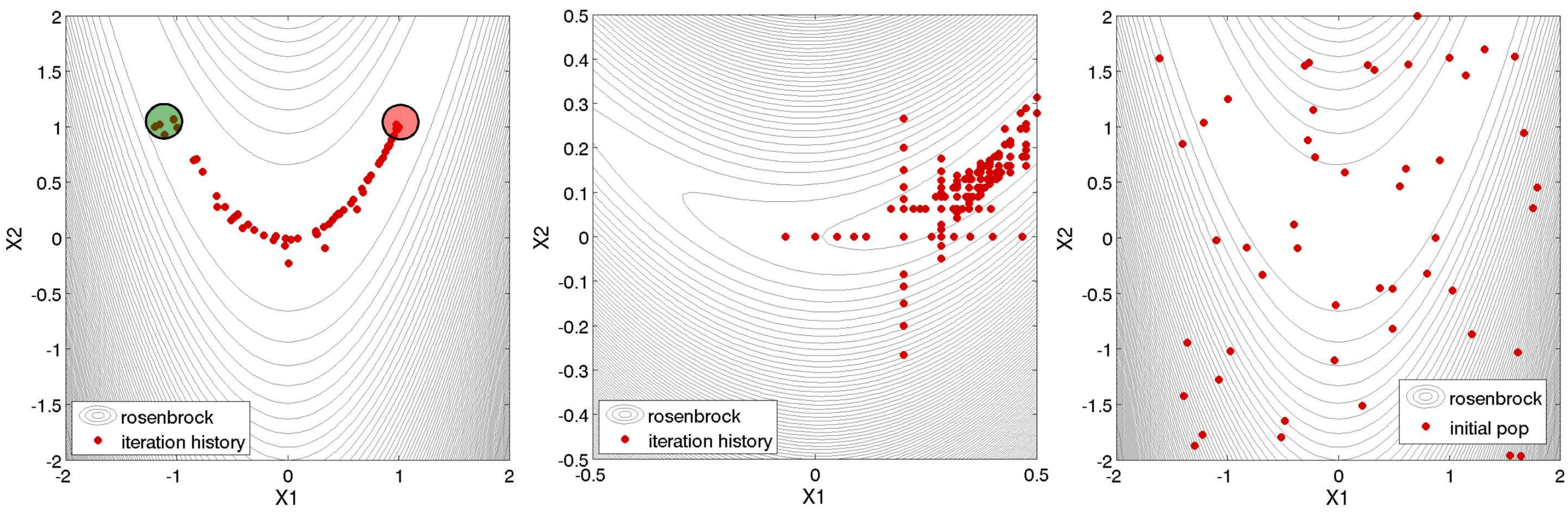
- Looks for improvement based on derivative
- Requires analytic or numerical derivatives *(more soon)*
- Efficient/scalable for smooth problems
- Converges to local extreme

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

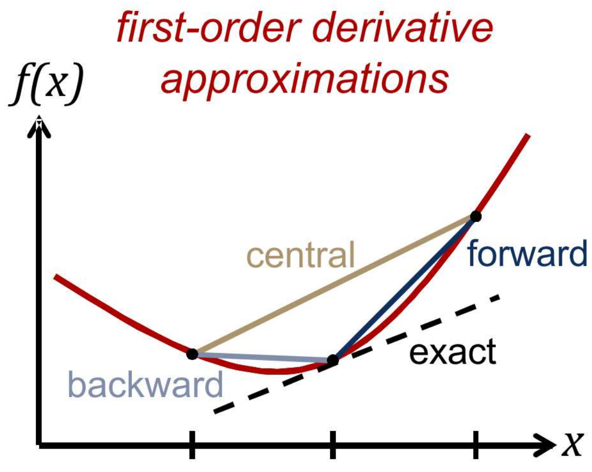


GRADIENTS FOR DERIVATIVE-BASED METHODS

- Akin to Newton's method for root-finding, minimize the objective by going "downhill" based on the gradient of the objective function:

$$\nabla f_x(x) = \left[\frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_N} \right]$$

- Most simulations don't calculate derivatives
- Dakota approximates gradients (and Hessians if needed) by running the simulation at $x \pm \Delta x$ as needed



First-order Forward Difference	Second-order Central Difference
$\frac{\partial f}{\partial x} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$	$\frac{\partial f}{\partial x} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$

`responses`
`  numerical_gradients`
`    forward`
`    fd_step_size 1.0e-3`
	`responses`
	`  numerical_gradients`
	`    central`
	`    fd_step_size 1.0e-3`

ADJOINT-ENABLED OPTIMIZATION

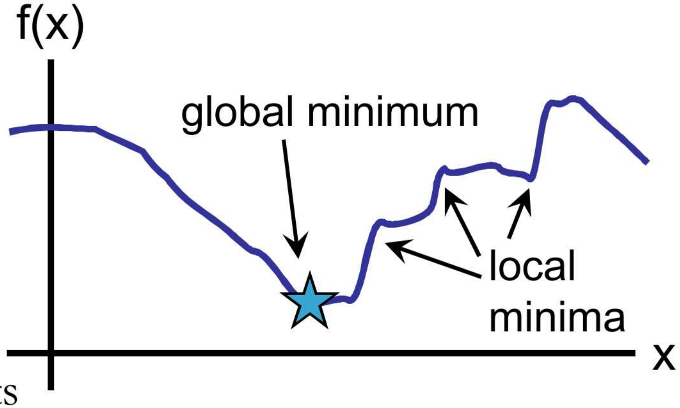
- Goal: minimize mass subject to dose constraint, given design variables x:
  - location t_j of surface point j
  - fraction $p_{j,m}$ of material m in layer j

$$\min\ f(x) = mass(p,t)$$
$$\text{s.t. } g(x) = dose(p,t) \le d_{max}$$

- We find local minima with Newton-like gradient-based methods; loosely

$$x_{k+1} = x_k - [Hf(x)]^{-1}\nabla_x f(x)$$

where explicit adjoints alleviate finite differencing for $\nabla_x f(x)$



- Solve the constrained problem with sequential quadratic programming (NPSOL) and $f(x)$, $g(x)$ adjoints
- Address non-smoothness or multiple minima with multi-start local optimization, trust region surrogate-based optimization instead of pattern search or genetic algorithms…

THEORY: PROBLEM

Problem:

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

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

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

Simplifications/definitions:

$$L\psi + C\psi = S\psi + q$$

$$\int_D dr \int_E dE \int_{4\pi} d\Omega ab \equiv \langle a, b\rangle$$

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

Substituting in the expression for the Lagrangian and carrying out several steps yields:

$$
\begin{aligned}
\frac{d\mathcal{L}}{dp}
&= \left[\left\langle \psi, \frac{\partial q^\dagger}{\partial p} \right\rangle + \left\langle \psi^\dagger, \frac{\partial q}{\partial p} \right\rangle - \left\langle \psi^\dagger, \left(\frac{\partial}{\partial p} (L + C - S) \right) \psi \right\rangle \right. \\
&\quad \left. + \left\langle \frac{\partial \psi}{\partial p}, q^\dagger - (L^\dagger + C^\dagger - S^\dagger)\psi^\dagger \right\rangle + \left\langle \frac{\partial \psi^\dagger}{\partial p}, q - (L + C - S)\psi \right\rangle \right] \\
&\quad + \left[\langle I, q^\dagger - (L^\dagger + C^\dagger - S^\dagger)\psi^\dagger \rangle + \left\langle \frac{\partial \psi^\dagger}{\partial \psi}, q - (L + C - S)\psi \right\rangle \right] \frac{\partial \psi}{\partial p}
\end{aligned}
$$

The derivatives of output quantities (e.g. $\frac{\partial \psi}{\partial p}$) are unknown.

THEORY: SENSITIVITIES

If the following equations are satisfied:

$$(L + C - S)\psi = q \qquad \text{(forward Boltzmann problem)}$$

$$\left(L^{\dagger} + C^{\dagger} - S^{\dagger}\right)\psi^{\dagger} = q^{\dagger} \qquad \text{(adjoint Boltzmannproblem)}$$

then $\frac{d\mathcal{L}}{dp}$ reduces to :

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

The sensitivities of *any* R to *any p* are obtained by various inner products involving the forward solution ψ, the adjoint solution $\psi^{\dagger}$, and derivatives of *input* (i.e. known) quantities.

WHY WE CARE ABOUT ADJOINT SENSITIVITIES

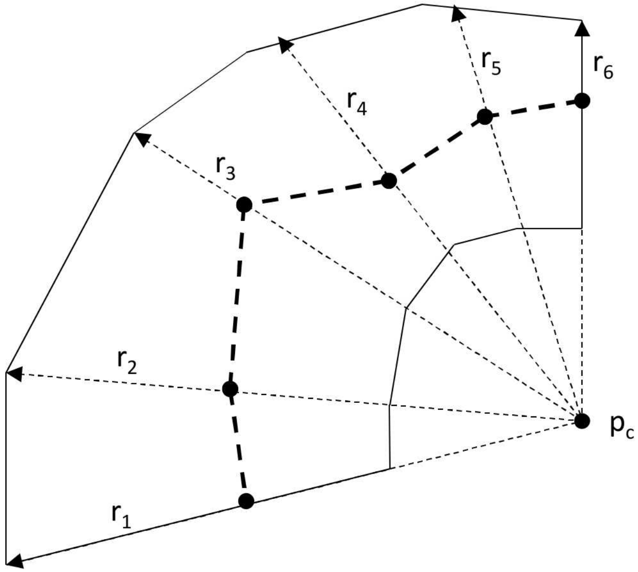
Solver behavior for some 1D optimization runs

Problem	Design Parameters	Transport solves for finite differences	Transport solves for adjoint approach
1	1	8	8
2	1	4	4
3	2	33	22
4	3	20	10
5	5	84	44
6	6	133	34
7	12	377	60
8	92	-	26
9	184	-	30

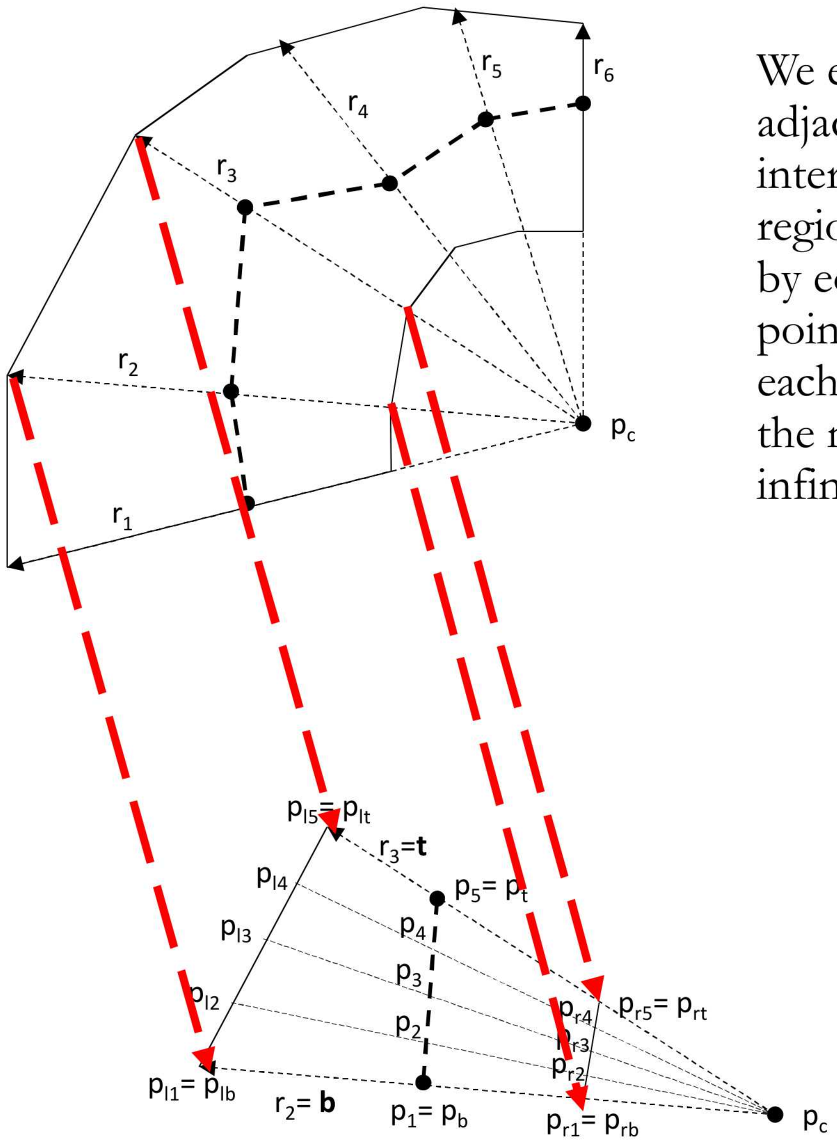
Adjoint-based approach scales much better than finite-difference approach for large number of parameters (2 < p+1)

APPLICATION OF SENSITIVITIES: 2D "RADIAL" GEOMETRIES

We want to know the effect of geometric changes in satellite electron/proton shields. We postulate a variable-thickness shield surrounding an electronic component or package (a portion of the geometry is depicted below). The shield surface is parametrized by some number of "control" points, each lying some distance along unique rays emanating from a "central" point (perhaps within the package to be protected). The points are connected by line segments to define the surface. We need to drive the sensitivity of the dose to the component to changes in the location of each point.



OUTLINE OF SENSITIVITY DERIVATION



We examine the region between two adjacent control points on both sides of the interface (bottom figure). We subdivide the region into several other subregions defined by equidistant points between the control points. After writing various equations for each subregion, we will examine the limit as the number of subregions increases to infinity.

EXAMPLE: COLLISION TERM

The collision term for one region is given by:

$$C\psi = \sum_n \left[H(x' - x'_{p_{ln}}) - H(x' - x'_{p_n})\right]\left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right]\sum_m p_{ml}(\sigma_{t,g,m,l} - \sigma_{\delta,gg,m,l})\psi_g$$
$$+ \sum_n \left[H(x' - x'_{p_n}) - H(x' - x'_{p_{rn}})\right]\left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right]\sum_m p_{mr}(\sigma_{t,g,m,r} - \sigma_{\delta,gg,m,r})\psi_g$$

The derivative of the collision term with respect to movement of the bottom control point is:

$$\frac{\partial C}{\partial h_b} = \sum_n \delta(x' - x'_{p_n})\nabla_{nc,b}\vec{p}_n\left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right]\sum_m p_{ml}(\sigma_{t,g,m,l} - \sigma_{\delta,gg,m,l})$$
$$- \sum_n \delta(x' - x'_{p_n})\nabla_{nc,b}\vec{p}_n\left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right]\sum_m p_{mr}(\sigma_{t,g,m,r} - \sigma_{\delta,gg,m,r})$$

EXAMPLE: COLLISION TERM (CONTINUED)

The portion of the response sensitivity related to the collision term is given by:

$$\frac{\partial R}{\partial h_b} = -\langle \psi_g^{\dagger}, \left(\frac{\partial C}{\partial h_b}\right) \psi_{g'} \rangle$$

$$= -\int_V dV \sum_g \int_{4\pi} d\Omega\, \psi_g^{\dagger}(r,\Omega) \sum_n \delta(x' - x'_{p_n}) \nabla_{nc,b}\vec{p}_n \left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right] \sum_m p_{ml}(\sigma_{t,g,m,l} - \sigma_{\delta,gg,m,l})\psi_g(r,\Omega)$$

$$+ \int_V dV \sum_g \int_{4\pi} d\Omega\, \psi_g^{\dagger}(r,\Omega) \sum_n \delta(x' - x'_{p_n}) \nabla_{nc,b}\vec{p}_n \left[H\left(y' - y'_{p_n}\right) - H\left(y' - y'_{p_{n+1}}\right)\right] \sum_m p_{mr}(\sigma_{t,g,m,r} - \sigma_{\delta,gg,m,r})\psi_g(r,\Omega)$$

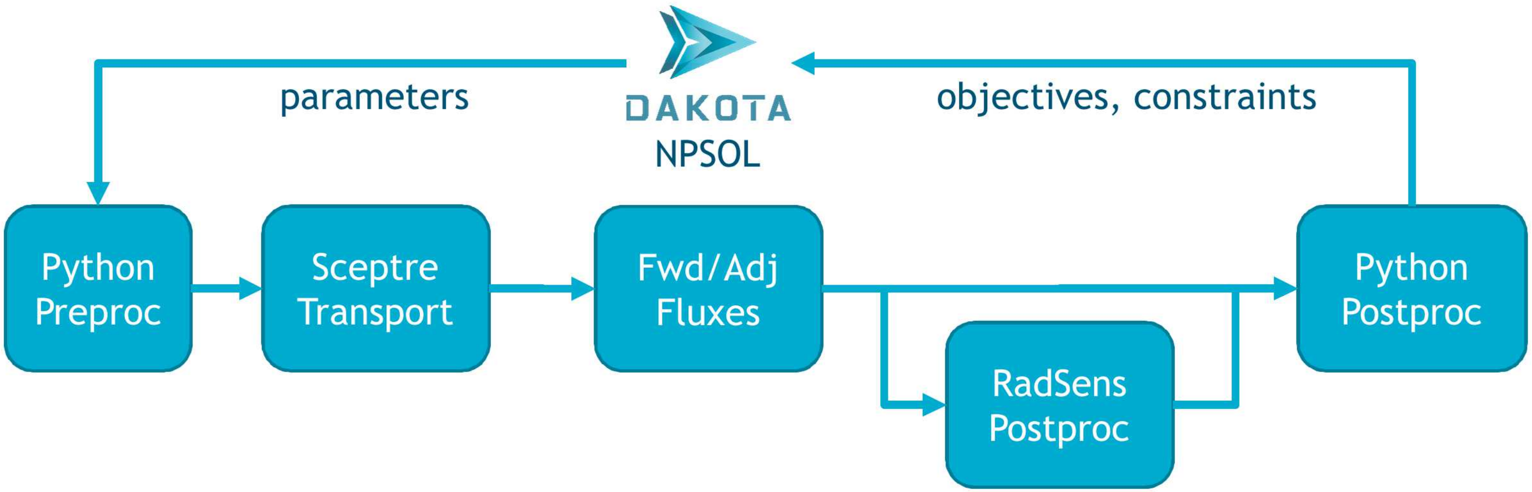
EXAMPLE: COLLISION TERM (CONTINUED)

We take the limit as the number of subregions goes to infinity to obtain the portion of the response sensitivity related to the collision term:

$$\lim_{N\to\infty} \frac{\partial R}{\partial h_b}$$
$$= -\sum_g \sum_m p_{ml}\left(\sigma_{t,g,m,l} - \sigma_{\delta,gg,m,l}\right) \int_{4\pi} d\Omega \int_{\partial D_l} ds \overrightarrow{i'} \cdot \vec{n} \nabla_{nc,b} \vec{p}_n \psi_g^{\dagger}(s,\Omega) \psi_g(s,\Omega)$$
$$+ \sum_g \sum_m p_{mr}\left(\sigma_{t,g,m,r} - \sigma_{\delta,gg,m,r}\right) \int_{4\pi} d\Omega \int_{\partial D_r} ds \overrightarrow{i'} \cdot \vec{n} \nabla_{nc,b} \vec{p}_n \psi_g^{\dagger}(s,\Omega) \psi_g(s,\Omega)$$

Analogous expressions are derived for the scattering and adjoint source terms to obtain the full sensitivity of the response to movement of the control point for one region. Movement of a point may involve more than one region.

OPTIMIZATION



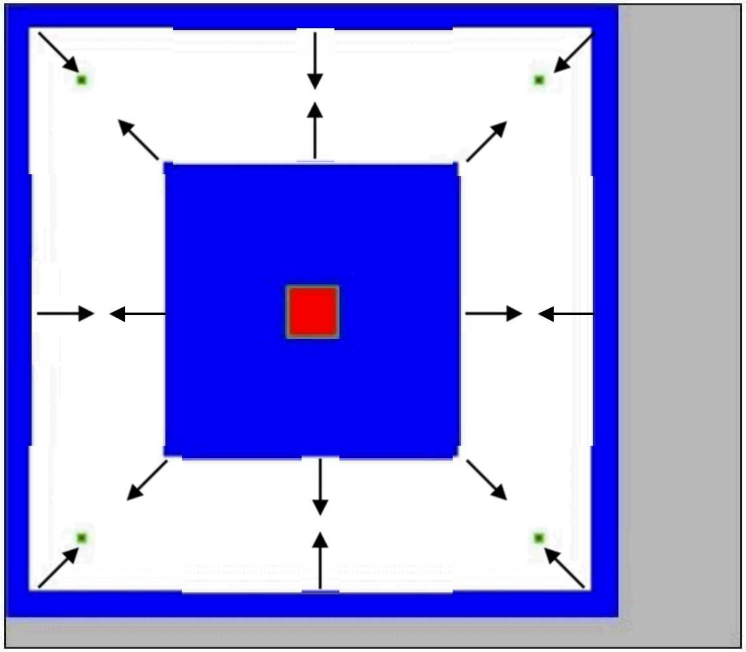
- Dakota NPSOL optimization drives the process
- Python tools translate between Dakota and Sceptre
- Sceptre deterministic transport produces forward and adjoint angular flux fields
- Material and geometric sensitivities are post-processed from these fields

APPLICATION: ELECTRON AND/OR PROTON SATELLITE SHIELDING

We are interested in satellite shielding applications. The problems we will study are:

- 2000 km circular equatorial orbits (arbitrarily chosen to demonstrate optimization)
- Proton and/or electron environments as defined by the AP8 and AE8 models in Spenvis
- Various components to be protected to various levels
- Multiple shielding regions of arbitrary geometry and/or materials

APPLICATION: ELECTRON AND/OR PROTON SATELLITE SHIELDING

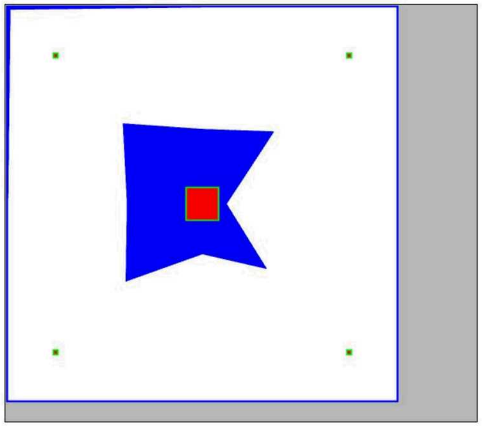


Initial design

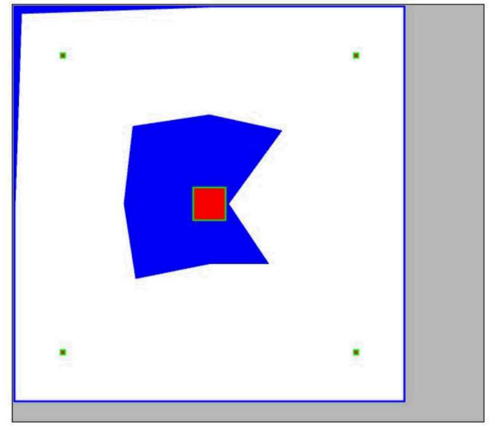
We want to protect components in a satellite. The electron/proton flux is isotropic, but asymmetric aluminum structure produces an asymmetric internal environment. The thick region on the right is an approximation to the satellite structure. The region on the bottom represents other instruments. There are four components in the corners, and a larger fifth component in the middle. Nominal shields are in blue. The location and allowed movement of control points is represented by arrows.

EXAMPLE: PROTON SHIELDING WITH POLYETHYLENE REQUIREMENTS: 100 KRAD/YR AT CORNERS, 40 KRAD/YR AT CENTER

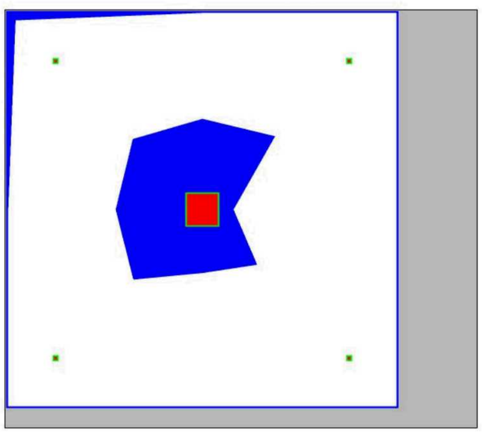
(The initial design is overdesigned and requires 225 g/cm)



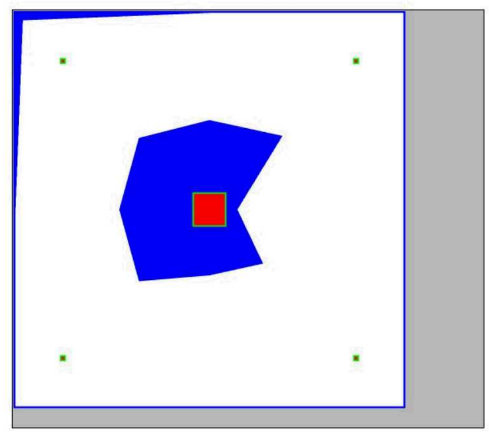
Second design iteration (71 g/cm)



Third design iteration (81 g/cm)

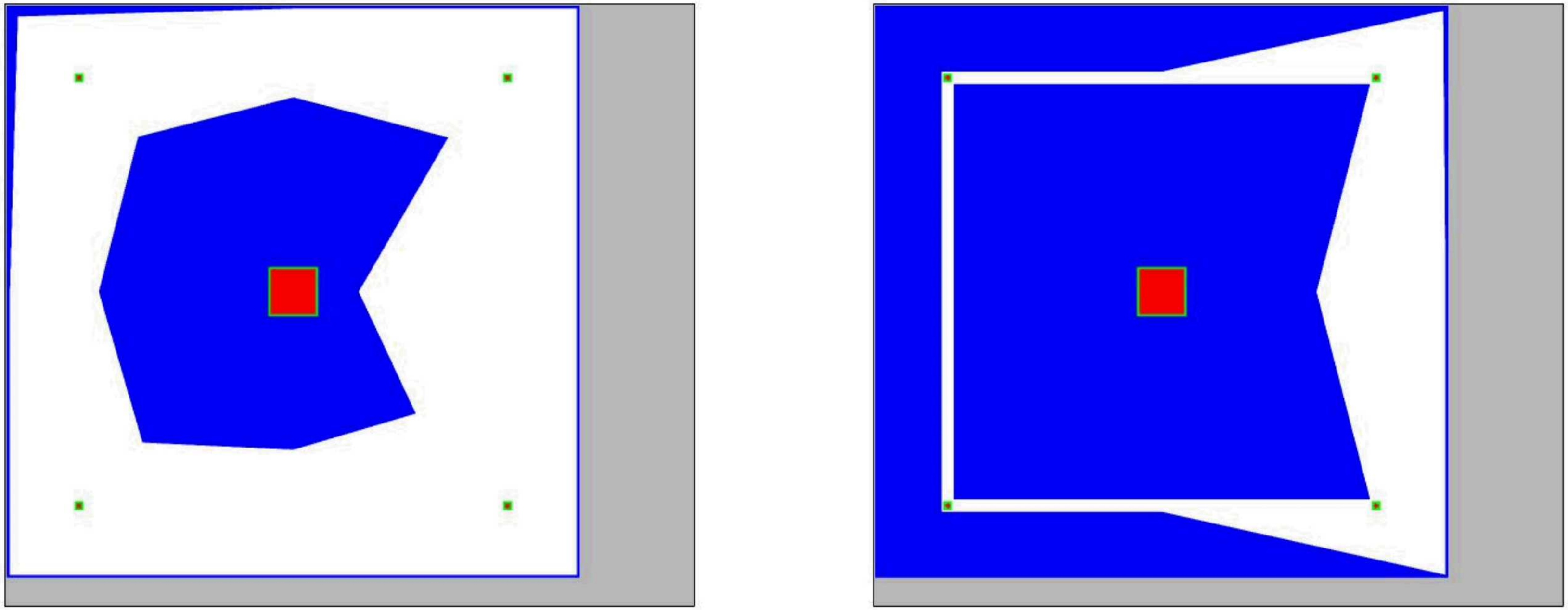


Fourth design iteration (81 g/cm)



Final design: 82 g/cm

DESIGNS WITH OTHER DOSE CONSTRAINTS



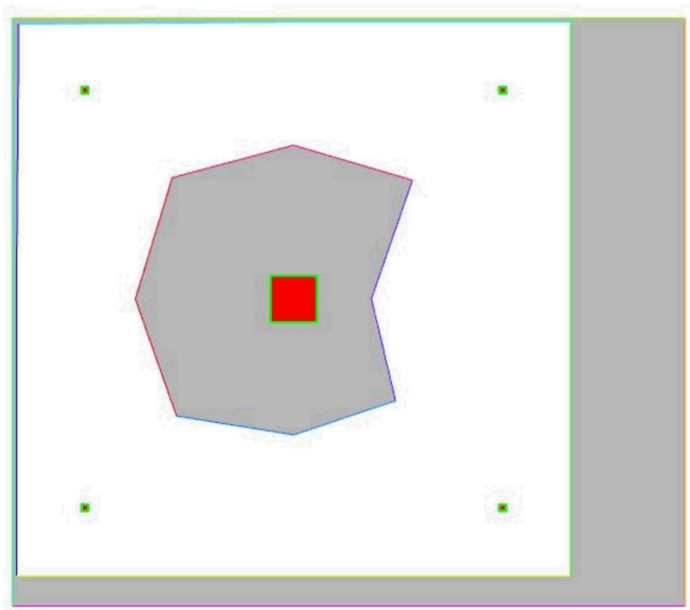
Center dose requirement: 30 krad/yr

Final design: 174 g/cm

Center dose requirement: 20 krad/yr

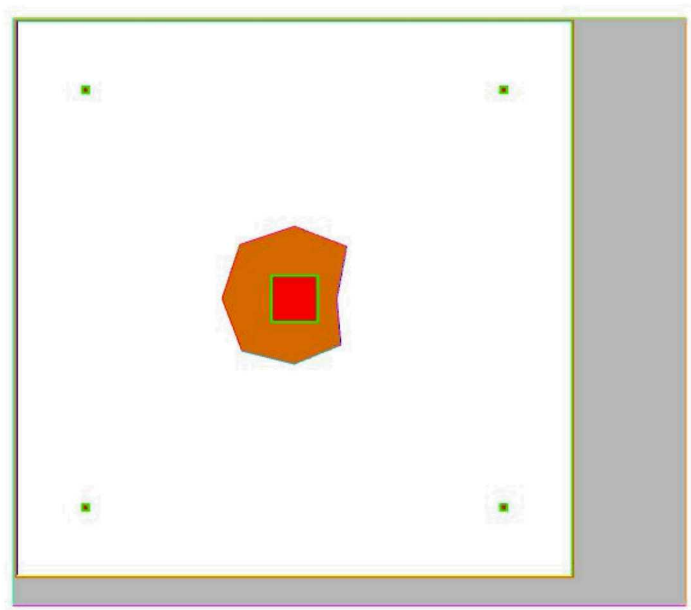
Final design: 450 g/cm

DESIGNS WITH OTHER MATERIALS



Aluminum shields, 20 krad/yr at center

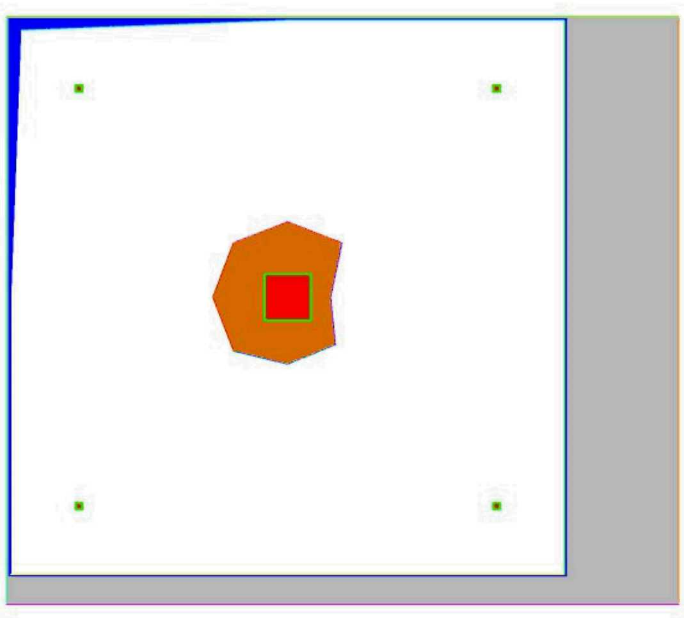
Final design: 357 g/cm



Copper shields, 20 krad/yr at center

Final design: 289 g/cm

COMBINED MATERIAL AND GEOMETRY OPTIMIZATION

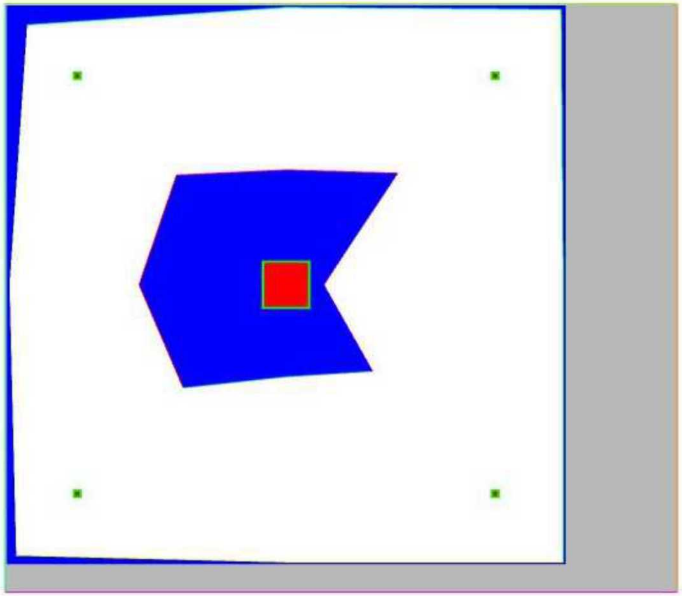


Requirement: 20 krad/yr at center

For this design we arbitrarily allowed for the use of polyethylene, aluminum, copper, molybdenum, and/or tantalum

Final design: Polyethylene outer shield, copper inner shield, 226 g/cm

COMBINED PROTON/ELECTRON ENVIRONMENT



Requirement: 40 krad/yr at center

For this design we only allowed for the use of polyethylene

Final design: 97 g/cm

CONCLUSIONS

- Our previous work demonstrated our ability to compute geometric and material sensitivities in 1D slab geometry and to incorporate them into satellite shield design optimization
- In the current work we derived sensitivities for parametrized 2D geometries and incorporated them into our design optimization tools
- We have demonstrated the use of these tools for a variety of satellite problems:
  - combined environments
  - multiple materials
  - numerous control points
- Future work:
  - More combined environment studies with multiple materials
  - 3D sensitivities/optimization
  - Robust design