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Optimal Shielding Design For Minimum Materials Cost or Mass

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INTRODUCTION

Material costs dominate some shielding design problems. This is certainly the case for manned nuclear power space applications for which shielding is essential and the cost of launching by rocket from Earth is high. In such situations or in those where shielding volume or mass is constrained, it is important to optimize the design. Although trial and error synthesis methods may succeed, a more systematic approach is warranted. Design automation may also potentially reduce engineering costs.

The objective is to automate the design of optimal radiation shielding to meet specified attenuation requirements given a menu of allowed shielding materials, their properties and their delivered costs per unit volume. The cost-optimal design is one which, at each location in the shield, chooses the menu material minimizing a particular functional of forward and adjoint angular fluxes plus material cost. Thus a Boltzmann forward and adjoint angular flux solver with additional calculations can evaluate whether a shield design is optimal or whether improvements are possible.

An iterative algorithm based on approximated optimality is proposed to solve for the optimal shield design and numerical experiments with it are discussed.

FORMULATION

Shielding design problem specifications include a radiation source description, a definition of the "detector" regions in which radiation dose rates must be limited along with their limiting dose rate values, and a definition of which shielding materials are allowed and where. If any shield design exists satisfying the requirements, then other admissible designs may also exist. It is useful to choose an optimal design minimizing total mass or cost.

Methodologies: Definitions and Notation

The convex spatial domain $\mathsf{D} \subset \Re^3$ surrounded by vacuum contains a radiation source and subregions $\mathsf{D}_\alpha \subset \mathsf{D}$ indexed by $\alpha \in \mathsf{A}$ in which the dose rate must be limited. The scalar function $q(\vec{r},\hat{\Omega},E)$ specifies the radiation source distribution per unit solid angle per unit energy at location $\vec{r}$ and particle energy E. With the menu represented as a sequenced list of m allowable shielding materials, the volume fraction of material number i, $i \in I$ where I is the material index set, is the scalar function of position, $u_i(\vec{r})$. A complete design of a shield is given by specifying all m of these volume fraction scalar functions of position, or equivalently, by the single m-vector function of position, $\underline{u}(\vec{r}) \equiv (u_1(\vec{r}) \quad u_2(\vec{r}) \quad \ldots \quad u_m(\vec{r}))^T$.

Volume fractions are by definition constrained as $0 \le u_i(\vec{r}) \le 1,, \quad i \in I$ and $\sum_{i \in I} u_i(\vec{r}) \le 1$. This is stated succinctly as $\underline{u}(\vec{r}) \in U$, where $U \subset \Re^m$ is the set equivalent to those definitional constraints. In practical shielding design situations there may be other position-dependent constraints further restricting the materials choices in portions of the spatial domain, stated as $\underline{u}(\vec{r}) \in U_c(\vec{r}) \subset U$. Here, $U_c(\vec{r})$ is the position-dependent set of material choice options under the control of the shielding designer. Total materials cost, C, is modeled in terms of volumetric cost rates c_i assigned for each material $i \in I$. Defining the materials cost vector as $\underline{c} = (c_1 \quad c_2 \quad \ldots \quad c_m)^T$, the total materials cost is

$$C = \underline{c}^T \iiint_{\mathsf{D}} \underline{u}(\vec{r}) dV \tag{1}$$

Scattering and total cross sections are also vectorized as $\underline{\sigma}_t(E) \equiv \left(\sigma_t^{(1)}(E) \quad \sigma_t^{(2)}(E) \quad \ldots \quad \sigma_t^{(m)}(E)\right)^T$ and

$$\underline{\sigma}_s(\hat{\Omega}' \to \hat{\Omega}, E' \to E) \equiv \begin{pmatrix} \sigma_s^{(1)}(\hat{\Omega}' \to \hat{\Omega}, E' \to E) \\ \sigma_s^{(2)}(\hat{\Omega}' \to \hat{\Omega}, E' \to E) \\ \vdots \\ \sigma_s^{(m)}(\hat{\Omega}' \to \hat{\Omega}, E' \to E) \end{pmatrix}$$

The Boltzman equation for angular flux, $\psi(\vec{r},\hat{\Omega},E)$, is:

$$\hat{\Omega} \bullet \nabla \psi(\vec{r},\hat{\Omega},E) + \underline{\sigma}_t^{\,T}(E)\underline{u}(\vec{r})\psi(\vec{r},\hat{\Omega},E) - q(\vec{r},\hat{\Omega},E) =$$

$$\oint\!\!\!\!\!\!\int d\Omega' \int_0^\infty dE' \underline{\sigma}_s^{\,T}(\hat{\Omega}' \to \hat{\Omega}, E' \to E)\underline{u}(\vec{r})\psi(\vec{r},\hat{\Omega}',E')$$

for $\vec{r} \in \mathsf{D}, \underline{u} \in U$; (2)

boundary condition $\psi(\vec{r},\hat{\Omega},E)\big|_{\vec{r} \in \partial\mathsf{D},\ \hat{n}\bullet\hat{\Omega}<0} = 0$ (3)

where $\hat{n}$ is the outer-directed unit normal on the domain boundary $\partial\mathsf{D}$. Eqs (1)-(3) describe neutron or gamma ray transport which may be combined by redefining E. The dose rate D_α, within region D_α, is the response of an omnidirectional detector separable in energy and position. Its energy weighting function $w(E)$ takes into account

tissue absorption and quality factors. Its position weighting function, $W_\alpha(\vec{r})$, is normalized as $\iiint_{D_\alpha} W_\alpha(\vec{r})dV = 1$. Then

$$D_\alpha = \iiint_{D_\alpha} dV \oiint d\Omega \int_0^\infty dE\, W_\alpha(\vec{r}) w(E) \psi(\vec{r},\hat{\Omega},E) \quad (4)$$

Radiation dose rate constraints required of the shielding design are:

$$D_\alpha \le D_\alpha^{MAX} \quad \forall\, \alpha \in A \quad (5)$$

Optimal Design Problem

The shield cost optimization design problem is to choose $\underline{u}(\vec{r}) \in U_c(\vec{r})$ so that the functional C in Eq. (1) is minimized while Eqs (2), (3), (4) and (5) are satisfied.

Derivation of Optimality Conditions

Eq. (1) is augmented with two zero value terms:

$$C = \underline{c}^T \iiint_D dV\, \underline{u}(\vec{r}) + \sum_{\alpha\in A} \tau_\alpha \left(D_\alpha - D_\alpha^{MAX}\right) + \iiint_D dV \oiint d\Omega \int_0^\infty dE \lambda(\vec{r},\hat{\Omega},E) \times \left[\left(-\underline{\sigma}_t^{\,T}(E)\psi(\vec{r},\hat{\Omega},E) + \oiint d\Omega' \int_0^\infty dE' \underline{\sigma}_s^{\,T}(\hat{\Omega}'\to\hat{\Omega}, E'\to E)\psi(\vec{r},\hat{\Omega}',E') \right) \underline{u}(\vec{r}) + q(\vec{r},\hat{\Omega},E) - \hat{\Omega}\bullet\nabla\psi(\vec{r},\hat{\Omega},E) \right] \quad (6)$$

The first added term includes Kuhn-Tucker multipliers τ_α

$$\tau_\alpha \begin{cases} = 0 \text{ if } D_\alpha - D_\alpha^{MAX} < 0 \\ \ge 0 \text{ if } D_\alpha - D_\alpha^{MAX} = 0 \end{cases} \quad (7)$$

Inequalities (5) and (7) together guarantee that the first added term in Eq. (6) is identically zero. The second added term, including the Lagrange multiplier function $\lambda \equiv \lambda(\vec{r},\hat{\Omega},E)$, is identically zero because of Eq.(2). It is useful to define a Hamiltonian function:

$$H = \underline{c}^T \underline{u}(\vec{r}) + \oiint d\Omega \int_0^\infty dE \left(\begin{array}{l} \lambda(\vec{r},\hat{\Omega},E) \times \\ \left[\left(-\underline{\sigma}_t^{\,T}(E)\psi(\vec{r},\hat{\Omega},E) + \oiint d\Omega' \int_0^\infty dE' \underline{\sigma}_s^{\,T}(\hat{\Omega}'\to\hat{\Omega}, E'\to E)\psi(\vec{r},\hat{\Omega}',E') \right) \underline{u}(\vec{r}) + q(\vec{r},\hat{\Omega},E) \right] \\ + \sum_{\alpha\in A} \tau_\alpha W_\alpha(\vec{r}) w(E) \psi(\vec{r},\hat{\Omega},E) \end{array} \right) \quad (8)$$

After swapping scattering integration variables, choosing

$$\lambda(\vec{r},\hat{\Omega},E) \equiv \sum_{\alpha\in A} \tau_\alpha \psi_\alpha^*(\vec{r},\hat{\Omega},E) \quad (9)$$

where the ψ_α^* satisfy adjoint flux equations

$$-\hat{\Omega}\bullet\nabla\psi_\alpha^*(\vec{r},\hat{\Omega},E) + \underline{\sigma}_t^{\,T}\underline{u}(\vec{r})\psi_\alpha^*(\vec{r},\hat{\Omega},E) = \oiint d\Omega' \int_0^\infty dE' \underline{\sigma}_s^{\,T}(\hat{\Omega}\to\hat{\Omega}', E\to E')\psi_\alpha^*(\vec{r},\hat{\Omega}',E')\underline{u}(\vec{r}) + W_\alpha(\vec{r})w(E) \quad (10)$$

with appropriate boundary conditions

$$\psi_\alpha^*(\vec{r},\hat{\Omega},E) = 0, \quad \vec{r}\in\partial D, \hat{n}\bullet\hat{\Omega} > 0 \quad (11)$$

then integrating by parts, Eq. (8) becomes:

$$H = \underline{c}^T \underline{u}(\vec{r}) + \sum_{\alpha\in A} \tau_\alpha \oiint d\Omega \int_0^\infty dE \left(\begin{array}{l} \psi_\alpha^*(\vec{r},\hat{\Omega},E)q(\vec{r},\hat{\Omega},E) + \psi(\vec{r},\hat{\Omega},E) \times \\ \left[\left(\begin{array}{l} -\underline{\sigma}_t^{\,T}(E)\psi_\alpha^*(\vec{r},\hat{\Omega},E) + \\ \oiint d\Omega' \int_0^\infty dE' \underline{\sigma}_s^{\,T}(\hat{\Omega}\to\hat{\Omega}', E\to E')\psi_\alpha^*(\vec{r},\hat{\Omega}',E') \end{array} \right) \underline{u}(\vec{r}) + W_\alpha(\vec{r})w(E) \right] \end{array} \right) \quad (12)$$

A mathematical theorem from the calculus of variations developed as part of optimal control theory, i.e., Pontryagin's Maximum Principle [Pontryagin et al 1962, 17-22] is then invoked as a minimum principle. It states that the necessary *and sufficient* condition for optimality of a particular design, $\underline{u}(\vec{r})$ is that its choice of $\underline{u}$ at each point $\vec{r}\in D$ optimizes the Hamiltonian, *H*, at that point with respect to all other admissible choices of $\underline{u}\in U_c(\vec{r})$ at that point, using the optimal design's own angular flux and adjoint angular flux functions to evaluate *H*. Thus, the optimality condition is as follows:

$\forall \vec{r}\in D, \quad \underline{u}_{opt}(\vec{r}) = \underline{\upsilon}$ where $\underline{\upsilon}$ obeys

$$: \left(\left(\underline{c}^T + \sum_{\alpha\in A} \tau_\alpha \underline{d}_\alpha^{\,T}(\vec{r};\psi_\alpha^*,\psi)\Big|_{opt} \right) \underline{\upsilon} \right) = \min_{\underline{\upsilon}\in U_c(\vec{r})} \left(\left(\underline{c}^T + \sum_{\alpha\in A} \tau_\alpha \underline{d}_\alpha^{\,T}(\vec{r};\psi_\alpha^*,\psi)\Big|_{opt} \right) \underline{\upsilon} \right) \quad (13)$$

where the discriminant vector is

$$\underline{d}_\alpha(\vec{r};\psi_\alpha^*,\psi) \equiv \oiint d\Omega \int_0^\infty dE \psi(\vec{r},\hat{\Omega},E) \times \left(\begin{array}{l} -\underline{\sigma}_t(E)\psi_\alpha^*(\vec{r},\hat{\Omega},E) + \\ \oiint d\Omega' \int_0^\infty dE' \underline{\sigma}_s(\hat{\Omega}\to\hat{\Omega}', E\to E')\psi_\alpha^*(\vec{r},\hat{\Omega},E) \end{array} \right) \quad (14)$$

Discussion of Optimality Conditions

In summary, the optimal shield design is the simultaneous solution to Eqs (2), (3), (4), (5), (7), (13) and (14). Since total cross sections include scattering, the components of $\underline{\mathsf{d}}_\alpha\left(\vec{r};\psi_\alpha^*,\psi\right)$ tend to be negative. Costs listed in the $\underline{c}$ vector are nonnegative as are the Kuhn-Tucker multipliers τ_α. Therefore, components of

$$\underline{b}(\vec{r}) \equiv \underline{c} + \sum_{\alpha\in A} \tau_\alpha \underline{\mathsf{d}}_\alpha\left(\vec{r};\psi_\alpha^*,\psi\right) \qquad (15)$$

may be negative or positive at different locations. Where all m components of $\underline{b}(\vec{r})$ are nonnegative, the optimal shield design minimizes $\underline{b}^T(\vec{r})\underline{u}(\vec{r})$ by setting $\underline{u}_{opt}(\vec{r}) = \underline{0}$, if $\underline{0} \in U_c(\vec{r})$ allows a void to be used there. In other locations where one or more components of $\underline{b}(\vec{r})$ are negative the index of the most negative component specifies the optimal material choice. There can also be equally negative components of $\underline{b}(\vec{r})$. Resulting auction ties between different materials can be awarded arbitrarily if the regions in which this occurs have zero volume as with a material switching boundary.

Increasing the positive value of a Kuhn-Tucker multiplier τ_α decreases the components of $\underline{b}(\vec{r})$ and may result in expanding the region in which some components of $\underline{b}(\vec{r})$ are negative. This has the effect through Eq (13) of adding shielding material at the expense of void regions, thus tending to reduce dose rates D_α. However, Eq. (7) does not allow positive τ_α values unless corresponding dose rates equal their maximum limits. Thus, optimal design solutions include precise τ_α values. Since for each dose rate strictly less than its maximum limit the corresponding τ_α is zero, it follows that Eq.(13) does not allow such inactive constraints to influence the optimal design.

Optimal Design Algorithm

Pontryagin's principle provides a way to determine whether a particular radiation shield design is optimal. Using that design's $\underline{u}(\vec{r})$, solve for the angular flux and adjoint functions, calculate dose rates, then check whether Pontryagin's optimality condition is everywhere met for some set of Kuhn-Tucker multipliers $\{\tau_\alpha, \alpha \in \mathrm{A}\}$ conforming to doserate-dependent positivity limitations. Unfortunately Pontryagin's principle does not provide any algorithm to directly *find* the optimum design. A difficulty is that the logic is circular. To find the optimal shield design, $\underline{u}_{opt}(\vec{r})$ via Eq. (13) one must first compute $\underline{\mathsf{d}}_\alpha\left(\vec{r};\psi_\alpha^*,\psi\right)_{opt}$ via Eq. (14) for which one needs to know optimal angular flux ψ_{opt} and adjoint functions, $\left(\psi_\alpha^*\right)_{opt}$ which in turn, depend on the optimal design, $\underline{u}_{opt}(\vec{r})$.

The iterative algorithm investigated has two nested loops. The inner loop uses old flux functions from the previous iteration's shield design to evaluate Eqs (14)-(15). It should be noted that a better approximation could in principle be obtained by adjusting the old flux functions by perturbations linearly proportional to the design changes. However, that would require making many forward and adjoint runs during each design iteration in order to determine the flux perturbation functions. Using the unmodified old flux functions as a rough approximation to the flux is justified by only allowing a small part of the shield to be redesigned in any iteration. The inner loop then modifies $\underline{u}(\vec{r})$ in this restricted manner to be slightly closer to an optimal design for some set of D_α values. The outer loop adjusts τ_α values to drive D_α towards consistency with D_α^{MAX}.

The inner loop is initialized with values for $\{\tau_\alpha\}_{\alpha\in A}$ and with an initial shield design ${}^{[k]}\underline{u}(\vec{r})$ for iteration count k=0. Eqs (2), (3), (10) and (11) are solved for angular flux ${}^{[k]}\psi\left(\vec{r},\hat{\Omega},E\right)$ and adjoint ${}^{[k]}\psi_\alpha^*\left(\vec{r},\hat{\Omega},E\right)$ functions, then Eqs (14) and (15) are evaluated using these functions to determine ${}^{[k]}\underline{b}(\vec{r})$. Then instead of using Eq. (13) the algorithm evaluates the following:

$$\forall \vec{r} \in \mathsf{D},\quad \underline{v}(\vec{r}) = \underline{\upsilon} \text{ where } \underline{\upsilon} \text{ obeys}$$
$$\left({}^{[k]}\underline{b}^T(\vec{r})\underline{\upsilon}\right) = \min_{\underline{\upsilon}\in U_c(\vec{r})}\left({}^{[k]}\underline{b}^T(\vec{r})\underline{\upsilon}\right) \qquad (16)$$

Then

$${}^{[k+1]}\underline{u}(\vec{r}) = \begin{cases} \underline{v}(\vec{r}) & \forall \vec{r} \in \mathsf{E}_k \subset \mathsf{D} \\ {}^{[k]}\underline{u}(\vec{r}) & \forall \vec{r} \in \mathsf{D} - \mathsf{E}_k \end{cases}$$

It is appropriate to choose E_k based on the projected reduction in the Hamiltonian if change were allowed, equivalent to adding the following definition to Eqs (16):

$$\mathsf{E}_k = \left\{\vec{r} \in \mathsf{D}: \quad {}^{[k]}\underline{b}^T(\vec{r})\left({}^{[k]}\underline{u}(\vec{r}) - \underline{v}(\vec{r})\right) \geq \varepsilon_k\right\} \qquad (17)$$

Here, ε_k is a threshold value for deciding whether departures from optimality are severe enough to merit changing material at a location during the current redesign iteration. An automated method sorts the ${}^{[k]}\underline{b}^T(\vec{r})\left({}^{[k]}\underline{u}(\vec{r}) - \underline{v}(\vec{r})\right)$ values for the domain, then sets ε_k based on highest percentile improvements.

RESULTS

The optimal design algorithms were implemented for the spherically symmetric case in SCALE 5.0 in a custom fortran code module SAS1XOPT, by modifying the SAS1X control sequence. The implementation accommodates the sum of both neutron and gamma dose rates via SCALE's XSDOSE module.

The chosen model problem is the design of shielding for a family of mobile fission reactor engines powering manned Mars surface vehicles. This application is interesting in its own right but illustrates a situation in which a large amount of shielding is essential but its delivery cost is very high. Engines developing rated shaft output powers ranging from 100 to 10,000 horsepower would enable Mars surface missions ranging from excursions in pressurized rover vehicles lasting for long durations to large scale ground excavation, mining, or deep drilling. Fission reactors would use unmoderated HEU in uranium nitride plate fuel elements operating at high temperature, similar to the SP100 design. An Open Brayton Cycle implemented in three radial flow compressors and turbine stages transfers reactor heat in lithium-7 coolant through a heat exchanger into compressed Martian air which then expands through turbines extracting work and exits carrying the waste heat.

Radiation requirements for all engines were chosen to limit the shielded dose rate (neutron + gamma) at R=6 meters from the reactor center to 1.375 mR/hr, i.e., to 12 rem per full power Earth-year. The menu of possible shielding materials was provided, with all costs per unit volume set proportional to material density.

Table 1: Shielding Materials Menu Choices by SAS1XOPT in Minimum-Mass designs

Admissible Shielding Material	Use in min.mass designs
Tungsten	Used
Boron-10	Used
Beryllium	Not used
Iron	Not used
Polyethyleneplastic	Not used
Lead	Not used
6Lithium Hydride	Used
Uranium-238	Used
Graphite carbon	Not used
7Lithium Hydride	Not used
Boron-10 Carbide	Not used
Water	Not used

Summaries of minimum-mass design results are given in Table 2. Because water is expected to be abundantly available on Mars as near-surface buried ice, the 316 hp case was rerun with the cost for water reset to $0.01/g while all other material costs were held at $50/g. The resulting design uses 4.80 tonnes of water plus 17.85 tonnes of other shielding materials, thus increasing mass by 0.862 tonnes while reducing cost.

Table 2: SAS1XOPT Designed Minimum-Mass Spherical Shields Limiting R=6 m Dose Rate (neutron+Gamma) to 1.375 mr/hr (12 R/yr)

#	Shaft Power (hp)	Reactor Thermal Power (MW)	Reactor+ Shield Mass (Tonnes)	Shield Outer Radius (cm)
1	100	0.310	18.949	133.14
2	178	0.4958	20.220	133.51
3	316	0.8217	21.788	134.44
4	562	1.368	23.676	135.09
5	1000	2.291	26.154	135.62
6	1780	3.931	29.320	136.15
7	3160	6.879	34.178	136.77
8	5620	12.136	38.219	137.59
9	10000	21.274	45.671	138.43

CONCLUSIONS

The future use of 3D Boltzmann solvers will allow extending results to shaped shield designs in which material is not wasted to maintain unneeded spherical symmetry. The largest cost savings of automated optimal design of shielding is expected to be for applications involving nuclear powered manned space missions where the required shielding attenuation of radiation and costs are both large. However, less exotic applications such as the shielding of radiation facilities on Earth could also benefit from optimal shielding design, and automation of the design process may reduce engineering costs.

ENDNOTES

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