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Title: AN INVERSE METHOD FOR RADIATION TRANSPORT

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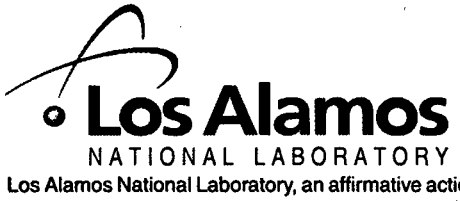

AN INVERSE METHOD FOR RADIATION TRANSPORT

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Abstract – Adjoint functions have been used with forward functions to compute gradients in implicit (iterative) solution methods for inverse problems in optical tomography, geoscience, thermal science, and other fields, but only once has this approach been used for inverse solutions to the Boltzmann transport equation. In this paper, this approach is used to develop an inverse method that requires only angle-independent flux measurements, rather than angle-dependent measurements as was done previously. The method is applied to a simplified form of the transport equation that does not include scattering. The resulting procedure uses measured values of gamma-ray fluxes of discrete, characteristic energies to determine interface locations in a multilayer shield. The method was implemented with a Newton-Raphson optimization algorithm, and it worked very well in numerical one-dimensional spherical test cases. A more sophisticated optimization method would better exploit the potential of the inverse method.

INTRODUCTION

The most widely used approach to solving inverse problems of all kinds, in many different fields, is the *implicit* or *iterative* one, in which the direct problem is solved repeatedly, with different values of the unknown model parameters. One common method of updating the unknown model parameters in each iteration is based on computing the gradient of some error functional with respect to the unknown parameters. The gradient information is then used in one of a multitude of methods (conjugate gradient, steepest descent, etc.) to minimize the error functional.

For many problems, calculating these gradients directly with a finite-difference scheme is extremely expensive, requiring many function evaluations with very small changes of system parameters. The question of how small of a change to make in each parameter for an accurate gradient calculation must also be answered. At the very least, one extra forward calculation is required for each unknown parameter.

In many different fields, this difficulty has been avoided by employing adjoint functions. In optical tomography [e.g., Ref. (1)], *adjoint* or *automatic differentiation* has been used to compute gradients of cost or error functionals with respect to system parameters directly from the computer code used in the forward modeling. In thermal science [e.g., Ref. (2)] and geoscience [e.g., Ref. (3)] applications, explicit equations have been derived and solved for the adjoint functions, which have then been used to compute the required gradients. [Reference (1) discusses the relationship between the two approaches.]

Azmy[4] applied automatic differentiation to the neutral-particle transport problem. Only slightly later, Norton[5] used the adjoint angular flux for calculating the gradient of an error functional in general inverse neutral-particle transport problems (as opposed to the specialized problems of optical tomography). Norton's method requires some measurement of the angular flux distribution exiting the unknown sample and is therefore of limited use when only angle-integrated measurements are available.

In this paper, another method for radiation transport inverse problems is derived. The method is similar to that of Norton[5], but its derivation assumes that detectors provide only the angle-independent flux (i.e., the scalar flux or total leakage).

Given a set of observed gamma-ray fluxes of specific, discrete energies characteristic of the source isotopes, the inverse problem considered is the determination of interface locations in a multilayer source/shield system. The method has been implemented with a Newton-Raphson iteration scheme in one-dimensional spherical geometry, and numerical results are presented.

THE METHOD

Consider a system that includes some source of gamma rays surrounded by some shield. Both the source and the shield may be multilayered but, for simplicity, only homogeneous layers are considered. The source emits gamma rays at discrete energies, which can be resolved quite well using a high-purity germanium detector. Thus we

consider only the transport of photons of discrete energies and assume that any scattered photons lose energy and are removed. The source is also assumed to be isotropic. Under these conditions, the angular flux of photons of the discrete energy (or *line*) denoted by index g is given by

$$\hat{\Omega}\cdot\vec{\nabla}\psi^g(r,\hat{\Omega})+\Sigma_t^g(r)\psi^g(r,\hat{\Omega})=q^g(r),\ g=1,\ldots,G, \tag{1}$$

where $\psi^g(r,\hat{\Omega})$ is the angular flux of gamma rays of energy g, position r, and angle $\hat{\Omega}$; $\Sigma_t^g(r)$ is the total cross section at energy g and position r; $q^g(r)$ is the source ($\gamma/cm^3\cdot s$), at position r, of gamma rays of energy g; and G is the number of discrete energies considered. It should be stressed that there is no coupling among the energy "groups" in Eq. (1). Also useful is the equation for the adjoint flux, $\psi^{*g}(r,\hat{\Omega})$,

$$-\hat{\Omega}\cdot\vec{\nabla}\psi^{*g}(r,\hat{\Omega})+\Sigma_t^g(r)\psi^{*g}(r,\hat{\Omega})=q^{*g}(r,\hat{\Omega}), \tag{2}$$

where the adjoint source is to be defined. For the present purpose, vacuum boundary conditions are imposed. [It is understood that Eq. (2) and each subsequent equation represents G equations.]

Suppose the flux for each energy line g is measured at a detector external to the source/shield system. The quantity of interest is

$$M^g=\int dV\int d\hat{\Omega}\Sigma_d^g(r,\hat{\Omega})\psi^g(r,\hat{\Omega}), \tag{3}$$

where the detector response function $\Sigma_d^g(r,\hat{\Omega})$ is zero outside the detector volume. We define the detector response function as

$$\Sigma_d^g(r,\hat{\Omega})\equiv\hat{\Omega}\cdot\hat{\mathbf{n}}_d\delta(r-r_d), \tag{4}$$

where $\hat{\mathbf{n}}_d$ is the outward unit normal vector at point r on the surface $r=r_d$, so that the detector measurement M^g becomes the system leakage.

Now let the symbol $\psi_o^g(r,\hat{\Omega})$ represent the actual, as opposed to the calculated, angular flux. The measured leakage, M_o^g, is

$$M_o^g=\int dV\int d\hat{\Omega}\Sigma_d^g(r,\hat{\Omega})\psi_o^g(r,\hat{\Omega}). \tag{5}$$

We define the following functional to represent the difference between the actual system and the calculated model:

$$\varepsilon^g=\frac{1}{2}(M^g-M_o^g)^2. \tag{6}$$

A variation in the parameters of the model (Σ_t^g and q^g are perturbed to $\Sigma_t^g+\delta\Sigma_t^g$ and $q^g+\delta q^g$) results in a variation in the calculated model angular flux (ψ^g is perturbed to $\psi^g+\delta\psi^g$) that results in a variation in the calculated leakage (M^g is perturbed to $M^g+\delta M^g$) that results in a variation in the error functional [from Eq. (6), ignoring second-order terms]

$$\delta\varepsilon^g=(M^g-M_o^g)\delta M^g. \tag{7}$$

The variation in the leakage is

$$\delta M^g = \int dV \int d\hat{\Omega} \Sigma_d^g \delta\psi^g. \tag{8}$$

Ignoring second-order terms, the variation in Eq. (1) is

$$\hat{\Omega} \cdot \vec{\nabla} \delta\psi^g(r,\hat{\Omega}) + \Sigma_t^g(r)\delta\psi^g(r,\hat{\Omega}) = \delta q^g(r) - \delta\Sigma_t^g(r)\psi^g(r,\hat{\Omega}). \tag{9}$$

Following Norton[5], the goal is to remove the variation in the flux, $\delta\psi^g$, from Eq. (8). To accomplish this, let the adjoint source be the detector response function, so that Eq. (2) reads

$$-\hat{\Omega} \cdot \vec{\nabla} \psi^{*g}(r,\hat{\Omega}) + \Sigma_t^g(r)\psi^{*g}(r,\hat{\Omega}) = \Sigma_d^g(r,\hat{\Omega}). \tag{10}$$

Using Eq. (10) in Eq. (8) and then using Eq. (9) yields

$$\delta M^g = \int dV \int d\hat{\Omega} \psi^{*g} (\delta q^g - \delta\Sigma_t^g \psi^g). \tag{11}$$

Using Eq. (11), Eq. (7) becomes

$$\delta\varepsilon^g = \int dV \nabla_t \varepsilon^g(r)\delta\Sigma_t^g - \int dV \nabla_q \varepsilon^g(r)\delta q^g, \tag{12}$$

where, following Norton, we define

$$\nabla_t \varepsilon^g(r) \equiv -(M^g - M_o^g) \int d\hat{\Omega} \psi^{*g} \psi^g \tag{13}$$

and

$$\nabla_q \varepsilon^g(r) \equiv -(M^g - M_o^g) \int d\hat{\Omega} \psi^{*g}. \tag{14}$$

The quantities $\nabla_t \varepsilon^g$ and $\nabla_q \varepsilon^g$ are the functional gradients (Fréchet derivatives) of the error, ε^g, computed with respect to the total cross section and gamma-ray source, respectively, for each line.

APPLICATION OF THE METHOD TO FIND UNKNOWN INTERFACE LOCATIONS

Suppose that the material composition and order of all the layers in the system are known but the interface locations between layers are unknown[6]. This situation is depicted in Figure 1 for r_3, the interface between layers 3 and 4. The material cross section in the neighborhood of an interface r_n is

$$\Sigma_t^g(r) = \Sigma_{t,n}^g + H(r - r_n)(\Sigma_{t,n+1}^g - \Sigma_{t,n}^g), \tag{15}$$

where $H(r - r_n)$ is the Heaviside step function. The derivative of $\Sigma_t^g(r)$ with respect to the interface location is

$$\frac{\partial\Sigma_t^g(r)}{\partial r_n} = \delta(r - r_n)\Delta\Sigma_{t,n}^g, \tag{16}$$

where $\delta(r - r_n)$ is the Dirac delta function and $\Delta\Sigma_{t,n}^g$ is defined as

$$\Delta\Sigma_{t,n}^g \equiv \Sigma_{t,n}^g - \Sigma_{t,n+1}^g. \tag{17}$$

The total cross section variation (for line g) due to variations in the interface locations is

$$\delta\Sigma_t^g = \sum_{n=1}^{N} \frac{\partial\Sigma_t^g(r)}{\partial r_n} \delta r_n = \sum_{n=1}^{N} \delta(r - r_n)\Delta\Sigma_{t,n}^g \delta r_n, \tag{18}$$

where N is the number of unknown interface locations.

Similarly, the total gamma-ray source variation (for line g) due to variations in the interface locations is

$$\delta q^g = \sum_{n=1}^{N} \frac{\partial q^g(r)}{\partial r_n} \delta r_n = \sum_{n=1}^{N} \delta(r - r_n) \Delta q_n^g \delta r_n, \tag{19}$$

where Δq_n^g is defined as

$$\Delta q_n^g \equiv q_n^g - q_{n+1}^g. \tag{20}$$

Using Eqs. (18) and (19) in Eq. (12), the total variation in the error ε^g due to interface location variations is

$$\delta \varepsilon^g = \sum_{n=1}^{N} \left[\nabla_t \varepsilon^g(r_n) \Delta \Sigma_{t,n}^g - \nabla_q \varepsilon^g(r_n) \Delta q_n^g \right] \delta r_n. \tag{21}$$

Since $\delta \varepsilon^g = \sum_{n=1}^{N} \left(\partial \varepsilon^g / \partial r_n \right) \delta r_n$, it is evident that[5]

$$\frac{\partial \varepsilon^g}{\partial r_n} = \nabla_t \varepsilon^g(r_n) \Delta \Sigma_{t,n}^g - \nabla_q \varepsilon^g(r_n) \Delta q_n^g. \tag{22}$$

A $G \times N$ matrix of the $\partial \varepsilon^g / \partial r_n$ values (i.e., the Jacobian matrix; call it $\underline{\underline{\varepsilon'_r}}$) can be constructed and used to reconstruct the vector of unknown interface locations, $\underline{r} \equiv \{r_1, \ldots, r_N\}$.

IMPLEMENTATION

The inverse method of this paper has been implemented for symmetric spherical geometries in which the innermost material is the gamma-ray source. Spherical geometries make for good one-dimensional test problems because (for a finite source) it is not only the shell thicknesses that matter, but the shell locations as well.

The forward and adjoint angular fluxes for each line are computed using the discrete-ordinates code PARTISN[7]. Appropriate total cross sections for discrete photon energies are constructed using the continuous-energy photon cross section library MCPLIB02, used by the Monte Carlo code MCNP[8]. A separate FORTRAN code was written to read the PARTISN output files and compute the necessary integrals. A Unix shell script controls the iterations.

A simple Newton-Raphson iteration scheme[9] was implemented to take advantage of the calculated derivatives. The Newton-Raphson formula for finding N unknown radii from G measured lines is, in the notation of this paper,

$$\underline{\underline{\varepsilon'_r}} \underline{\Delta r} = -\underline{\varepsilon}, \tag{23}$$

where $\underline{\underline{\varepsilon'_r}}$ is the $G \times N$ Jacobian matrix, $\underline{\varepsilon}$ is the $G \times 1$ vector of ε^g values, and $\underline{\Delta r}$ is the $N \times 1$ vector of updates to make to the unknown radii at the end of the iteration. This simple scheme was chosen for convenience; finding one that works "the best" is the subject of current research.

The Jacobian $\underline{\underline{\varepsilon'_r}}$ of Eq. (23) is inverted using singular value decomposition (SVD)[9]. The application of SVD to this type of problem is discussed in Ref. (6). Suffice it to say here that SVD handles singular matrices gracefully,

such that it is frequently advantageous to force an ill-conditioned Jacobian to be singular by raising the preset SVD threshold.

TEST CASES

Two test problems for unknown interface locations were run using a spherical Godiva model as a passive (non-fission) gamma ray source. The Godiva model was composed of 94.73% ^{235}U and 5.27% ^{238}U (by weight) and had a mass density of 18.74 g/cm^3 and a radius of 8.741 cm. For these test problems [as in Ref. (6)], Godiva was placed in a spherical lead and aluminum shield. The lead layer had an inner radius of 12.4 cm and a thickness of 0.5 cm; the aluminum layer had an inner radius of 12.9 cm and a thickness of 0.3 cm. The lead and aluminum were modeled as pure elements with densities 11.4 and 2.7 g/cm^3, respectively.

The one-group forward and adjoint calculations used S_{32} gamma-ray transport in one-dimensional spherical geometry. The detector was modeled as a spherical surface with a radius of 100 cm. "Measured" detector responses were calculated for the actual system using the same angle and geometry discretizations. Convergence was declared when the leakage for all lines was within 0.1% of the leakage calculated for the actual model.

Table I gives the results for both test problems.

Case 1: Source radius known

In case 1, the source radius was known but the lead layer was 0.2 cm too thin, the aluminum layer was 2.1 cm too thick, and the shield was 0.1 cm too close to the source (see Table I). The method converged, but only when the Jacobian $\underline{\underline{\varepsilon'_r}}$ of Eq. (23) was allowed to be singular by raising the SVD threshold. Different values of the threshold resulted in different iteration histories. The method converged in 16 iterations to the solution shown in Table I when the threshold was raised to 2×10^{-8}. When the Jacobian was not singular, the method calculated negative radii in the zeroth iteration and could not continue. A different optimization algorithm will allow an automatic solution to this problem.

Case 2: All radii unknown

In case 2, the source radius was 0.341 cm too small, the shield was 0.4 cm too far away from the source, the lead layer was 0.1 cm too thin, and the aluminum layer was 0.7 cm too thick. The method converged to the solution shown in Table I in 20 iterations. This is a very promising result, as this problem is quite difficult solve[6].

This problem also highlights the need for a more efficient optimization algorithm than Newton-Raphson. The models do not improve monotonically. After great improvements through iteration 8, during which the Jacobian matrix is singular (the SVD threshold was 1×10^{-9}), the models diverge when the Jacobian matrix is singular, then improve suddenly after an iteration in which the Jacobian is not singular, and the pattern repeats.

SUMMARY AND CONCLUSIONS

An adjoint-based method of computing the gradient of an error functional has been applied to develop an iterative inverse method for radiation transport. The method is closely related to previous methods in the thermal and geological sciences and to a previous method in radiation transport due to Norton. Unlike Norton's method, however, the present method does not require angle-dependent flux measurements.

The iterative inverse transport method has been applied to develop a solution method for the problem of determining interface locations in a multilayer source/shield system. The method is based on precise measurements of the gamma flux at discrete energies characteristic of the source. Application of the method to solve for other unknowns is conceivable.

The method has been implemented in one-dimensional (spherical) geometry with Newton-Raphson optimization. Very good results have been obtained for test problems with unknown interface locations. In addition, the method is much more efficient than a direct finite-difference approach. Problems with four unknown parameters can be solved with two transport calculations per iteration (one forward and one adjoint), rather than at least five (one extra forward calculation per unknown).

REFERENCES

1. Klose, A. D. and Hielscher, A. H. *Optical tomography using the time-independent equation of radiative transfer – Part 2: inverse model.* J. Quant. Spectrosc. Radiat. Transfer **72**(5), 715–732 (2002).

2. Alifanov, O. M. *Methods of solving ill-posed inverse problems.* J. Eng. Phys. **45**(5), 1237–1245 (1983).

3. Bunge, H.-P., Hagelberg, C. R., and Travis, B. J. *Mantle circulation models with variational data assimilation: inferring past mantle flow and structure from plate motion histories and seismic tomography.* Geophys. J. Int. **152**(2), 280–301 (2003).

4. Y. Azmy, Y. Y. *Post-convergence automatic differentiation of iterative schemes.* Nucl. Sci. Eng. **125**(1), 12–18 (1997).

5. Norton, S. J. *A general nonlinear inverse transport algorithm using forward and adjoint flux computations.* IEEE Trans. Nucl. Sci. **44**(2), 153–162 (1997).

6. Favorite, J. A. *Using the Schwinger variational functional for the solution of inverse transport problems.* Nucl. Sci. Eng. **146**(1), 51–70 (2004).

7. Alcouffe, R. E., Baker, R. S., and Turner, S. A. *PARTISN.* LA–CC–98–62, Los Alamos National Laboratory (1997).

8. X-5 Monte Carlo Team. *MCNP–A general Monte Carlo N–particle transport code, version 5.* Vol. I, LA–UR–03–1987, Los Alamos National Laboratory (2003).

9. Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P. *Numerical recipes in FORTRAN: The art of scientific computing,* 2nd Ed. (reprinted with corrections). (Cambridge: Cambridge University Press) (1994) ISBN 0 521 43064 X.

Table I. Results for Unknown Interface Test Problems

		Outer Radii (cm)[a]			
Descriptor	Model	Godiva	Void	Lead	Aluminum
Actual Model		8.7410	12.400	12.9000	13.2000
Case 1	Initial	*8.7410*	12.3	12.6	15.0
	Converged	*8.7410*	12.4072	12.9073	13.2078
Case 2	Initial	8.4	12.8	13.2	14.2
	Converged	8.7421	12.4299	12.9301	13.2328

[a]Italics represent quantities that are known.

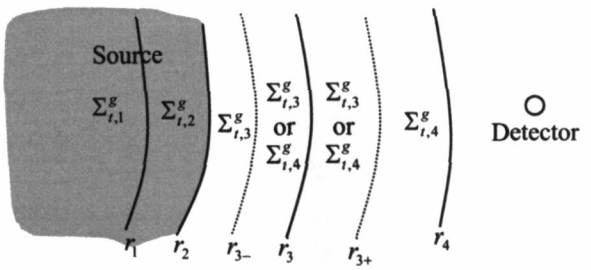

Figure 1. Depiction of source problem when the source and shield compositions are known but one interface location is not.