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Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products in Arbitrary Three-Dimensional Geometries Using MCNP

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INTRODUCTION

Ray analysis techniques are standard for computing the uncollided component of a detector response to radiation [1]. Monte Carlo next-event or point detector tallies [2], when scoring uncollided fluxes, are stochastic ray-tracing methods. Uncollided adjoint flux integrals are sometimes easier to obtain more accurately than the equivalent uncollided point-detector tallies. In addition, uncollided adjoint flux integrals and forward-adjoint inner product integrals in volumes and on surfaces are associated with the derivatives of uncollided detector fluxes and are useful for sensitivity studies and optimization problems.

The forms that these integrals take in general three-dimensional geometries were recently presented [3]. These forms have been specialized to one-dimensional spherical and two-dimensional cylindrical (*r*-*z*) geometries and evaluated deterministically. For arbitrary three-dimensional geometries, however, it makes sense to evaluate them stochastically.

This paper describes the evaluation of these useful integrals using a patch for MCNP5 [2]. The terminology in this paper is necessarily specific to MCNP, but the integrals derived in [3] can be implemented in any neutral-particle Monte Carlo code that can use continuous- or discrete-energy cross sections.

UNCOLLIDED FLUX INTEGRALS

The angular flux $\psi(r,\hat{\mathbf{\Omega}})$ of uncollided neutrons or gamma rays is the solution to the monoenergetic, continuous-angle transport equation

$$\hat{\mathbf{\Omega}}\cdot\nabla\psi(r,\hat{\mathbf{\Omega}})+\Sigma_t(r)\psi(r,\hat{\mathbf{\Omega}})=q(r), \qquad (1)$$

and the uncollided adjoint flux $\psi^*(r,\hat{\mathbf{\Omega}})$ is given by

$$-\hat{\mathbf{\Omega}}\cdot\nabla\psi^*(r,\hat{\mathbf{\Omega}})+\Sigma_t(r)\psi^*(r,\hat{\mathbf{\Omega}})=\Sigma_d(r,\hat{\mathbf{\Omega}}). \qquad (2)$$

The notation is standard and vacuum boundary conditions are assumed. If the quantity of interest is the scalar flux at a point r_d, the adjoint source (detector response function) is $\Sigma_d(r,\hat{\mathbf{\Omega}})=\delta(r-r_d)$.

It can easily be shown that the quantity of interest $M=\langle\Sigma_d,\psi\rangle$ (the inner product notation indicates an integral over all phase space; i.e., angle and volume) is equal to the adjoint integral $\langle\psi^*,q\rangle$. For many physically realizable situations, the source density is isotropic and uniformly distributed by material, and $\langle\psi^*,q\rangle$ can be calculated as the sum of products of cell-integrated scalar adjoint fluxes and cell-dependent source densities. In many cases, $\langle\psi^*,q\rangle$ may be easier to obtain more accurately than $\langle\Sigma_d,\psi\rangle$.

Uncollided forward-adjoint integrals are useful in sensitivity analysis. For example, the derivative of *M* with respect to the mass density of cell *k*, ρ_k, is [4]

$$\frac{\partial M}{\partial\rho_k}=\frac{1}{\rho_k}\left(\langle\psi^*,q_k\rangle_{V_k}-\langle\psi^*,\Sigma_{t,k}\psi\rangle_{V_k}\right), \qquad (3)$$

where subscript V_k indicates a volume integral in cell *k*. The derivative of *M* with respect to the location of interface *k* is [5]

$$\frac{\partial M}{\partial r_k}=\langle\psi^*,\Delta q_k\rangle_{S_k}-\langle\psi^*,\Delta\Sigma_{t,k}\psi\rangle_{S_k} \qquad (4)$$

(if the shape of the interface does not change), where subscript S_k indicates an integral on surface *k* and ΔX is the difference in quantity *X* across the surface.

The derivations of the uncollided adjoint integrals and forward-adjoint inner products have been given [3].

USING MCNP TO COMPUTE INNER PRODUCTS OF UNCOLLIDED FLUXES

The basic idea of using MCNP to compute the inner products of uncollided fluxes is to set up the problem as an adjoint one in the sense that the source is a point source located at the detector point r_d. However, the MGOPT card is not used as it would be in a real adjoint calculation. Flux tallies are made in volumes (F4) and on surfaces (F2) as usual.

NOTRN Switch

In the normal version of MCNP5, the NOTRN card causes the code to do only uncollided point detector tallies and no normal transport (i.e., no scattering). In the patch, a blank NOTRN card or "NOTRN 1" has the same effect. Using "NOTRN 2" causes the patched MCNP to

do only uncollided flux integrals as described in this paper.

LINES Card

The source densities are input on a new data card, LINES. The LINES card has $G \times N$ entries (where G is the number of discrete energy lines and N the number of cells in the problem) consisting of the volumetric line source densities q_n^g (in particles/cm^3·s) for cell n and line index g. The format of the LINES card is

$$\text{LINES} \quad q_1^1 \cdots q_N^1 \; q_1^2 \cdots q_N^2 \cdots q_1^G \cdots q_N^G$$

The code calculates G using the number of entries.

Source

The source is a point source at the detector location r_d; its angular distribution is $\Sigma_d(\hat{\mathbf{\Omega}})$. In MCNP the starting direction is chosen by sampling the polar angle cosine cos θ rather than the polar angle θ and by sampling the azimuthal angle φ uniformly in 2π; thus the weight of each history must be

$$\text{wgt} = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\theta_{max}} d\theta \sin\theta \, \Sigma_d(\hat{\mathbf{\Omega}}) = \frac{1-\cos\theta_{max}}{2} \qquad (5)$$

if the quantity of interest is the scalar flux at point r_d. θ_{max} is an angle chosen, along with a line r_0 from r_d to an arbitrary fixed point in the geometry, to completely cover the geometry with rays [6]. The line r_0 is input as the SDEF parameter VEC. The value of cos θ_{max} is input as the lower limit on the SP distribution for the SDEF parameter DIR [assuming that r_0 (i.e., VEC) actually points into the system].

The line energies E^g, $g = 1,\ldots,G$, are input as a discrete SDEF distribution as usual. The order of the lines on the SDEF distribution must match their order on the LINES card, and the code has no way of checking for consistency. If the number of lines in the SDEF source does not match the number from the LINES card, the number from SDEF is used.

If there are G lines uniformly sampled, then the weight sourced into each line per source particle would be wgt from Eq. (5) divided by G. Thus the weight needs to be multiplied by G. This is done automatically when the particle is started, so the balance tables reflect the modified weight.

Tallies

Tallies are done in a TALLYX subroutine. The quantities to compute are controlled by entries on the FU card as shown in Table I. The NT entry should be used on the FU cards since the sum of these integrals is not meaningful [the difference is normally required, as in Eqs. (3) and (4)]. Tally divisor SD entries of 1 should normally be used for all cells and surfaces; otherwise, volume and surface averages will be computed, which are not normally useful. [On the other hand, some applications may call for a different tally divisor, such as the density in Eq. (3).]

TABLE I. FU Entries for Uncollided Adjoint and Forward-Adjoint Flux Integrals.

Type of Tally	FU Entry	Integral
Volume (F4)	1	$\left\langle \psi^*, q_k \right\rangle_{V_k}$
	2	$\left\langle \psi^*, \Sigma_{t,k}\psi \right\rangle_{V_k}$
	3	$\left\langle \psi^* \right\rangle_{V_k}$
	4	$\left\langle \psi^*, \psi \right\rangle_{V_k}$
	5	$\left\langle \psi^*, q_k \right\rangle_{V_k} - \left\langle \psi^*, \Sigma_{t,k}\psi \right\rangle_{V_k}$
Surface (F2)	1	$\left\langle \psi^*, \Delta q_k \right\rangle_{S_k}$
	2	$\left\langle \psi^*, \Delta\Sigma_{t,k}\psi \right\rangle_{S_k}$
	3	$\left\langle \psi^* \right\rangle_{S_k}$
	4	$\left\langle \psi^*, \psi \right\rangle_{S_k}$
	5	$\left\langle \psi^*, \Delta q_k \right\rangle_{S_k} - \left\langle \psi^*, \Delta\Sigma_{t,k}\psi \right\rangle_{S_k}$

The uncollided flux surface integrals of Eq. (4) and Table I suffer from the same difficulty that plagues normal Monte Carlo surface flux tallies [2, 7]. For rays that graze the surface, the integrand blows up, so a lower limit has to be placed on the cosine of the grazing angle, reducing the accuracy of the numerical integral.

VERIFICATION

The ability to compute uncollided inner product and adjoint-only integrals in volumes and on surfaces was verified [3] by comparing stochastic results with deterministic ones (including one semi-analytic problem) for a one-dimensional spherical and a two-dimensional (r-z) cylindrical problem. Here, derivatives with respect to interface locations [Eq. (4)] are compared with deterministic values for a sphere.

The sphere was made of seven shells. Starting from the inside, the material and outer radius of each shell were: void, 20 cm; high-enriched uranium (HEU), 25 cm; void, 30 cm; HEU, 35 cm; void, 40 cm; HEU, 45 cm; ^{27}Al, 50 cm. The HEU and ^{27}Al mass densities were 4 and 2.7 g/cm^3, respectively.

Results are shown in Table II. The deterministic spherical surface integrals do not require the cosine division that causes integrals to blow up and so are more exact [3], but the difference is calculated relative to the average; i.e.,

$$\text{Diff.} = \frac{R_{sto} - R_{det}}{\frac{1}{2}(R_{sto} + R_{det})}. \quad (6)$$

A lower cosine limit of 0.0001 and a substitute cosine divisor of 0.00005 were used in the MCNP patch, replacing the standard MCNP values of 0.10 and 0.05. The stochastic results are generally well within one standard deviation of the deterministic results. (Interestingly, when the standard MCNP minimum cosine and divisor were used, surfaces 2 and 4 had differences of –14.3% and –45.9%, respectively.)

TABLE II. $\partial M/\partial r_k$ for the Spherical Test Problem.

k	Deterministic	Stochastic[a]	Diff.
1	-1.14606×10^{-2}	$-1.14620 \times 10^{-2} \pm 0.01\%$	0.012%
2	2.16342×10^{-2}	$2.16479 \times 10^{-2} \pm 0.12\%$	0.063%
3	-3.79882×10^{-2}	$-3.79892 \times 10^{-2} \pm 0.01\%$	0.003%
4	8.40208×10^{-1}	$8.37366 \times 10^{-1} \pm 0.21\%$	–0.339%
5	-2.32152×10^{0}	$-2.32148 \times 10^{0} \pm 0.01\%$	–0.002%
6	9.79807×10^{3}	$9.79814 \times 10^{3} \pm 0.00\%$	0.001%
7	-8.25002×10^{3}	$-8.25013 \times 10^{3} \pm 0.00\%$	0.001%

[a] 1σ relative errors are given.

For this spherical problem, the deterministic integrator took less than ½ s on one processor, but the MCNP5 calculation took ~100 minutes on 32 processors to reach the precision shown on Table II. A spherical test problem was chosen because the deterministic values were available. As usual, the Monte Carlo method would be most useful for complicated three-dimensional problems for which deterministic results are not available.

CONCLUSIONS

A patch to MCNP5 has been developed to compute uncollided adjoint flux integrals and forward-adjoint flux product integrals on surfaces and in volumes for arbitrary three-dimensional geometries. The adjoint integral sometimes offers a more accurate estimate of the quantity of interest than a direct calculation. In addition, these quantities are useful for sensitivity and perturbation applications.

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