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Source Sampling in the Flash Monte Carlo Computer Code

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

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SOURCE SAMPLING IN THE FLASH MONTE CARLO COMPUTER CODE

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ABSTRACT

An estimator algorithm for obtaining the volume source score in the backward Monte Carlo method is presented. The algorithm given uses vector geometry to obtain greater efficiency than the one utilized by Collins and Wells¹ in the original FLASH code. The vector method is easily extended to estimate the score from other source geometries.

I. INTRODUCTION

The volume source FLASH Monte Carlo code developed by Radiation Research Associates¹ (RRA), Fort Worth, Texas, performs a numerical integration along a line through a volume source with cells defined by intersections of cones and spheres. This integration is performed at each statistical particle collision and an efficient integration algorithm is therefore a fundamental requirement to minimize computing time. We present a FORTRAN language vector algorithm for calculating the source score in an atmosphere of uniform refractive index.

II. SOURCE AND ATMOSPHERE GEOMETRIES

The atmosphere is represented by a mesh of concentric spherical shells of radii r_j , $j = 1, 2, 3, \dots, J_H$. The source cell volumes are defined by the mesh intersections of axially concentric cones and concentric spheres. The cones are specified by the cosines of their half-angles, μ_i , $i = 1, 2, \dots, N_{SPA}$, and the spheres by the radii $r'_{k,k} = 1, 2, \dots, N_{SR}$. We assume

that the cone angle cosines are monotonically decreasing with increasing index (increasing cone angle), and that the atmospheric and source radii are monotonic increasing with increasing indices. The source and atmospheric geometry is thus as shown in Fig. 1. The statistical particle collision occurs at $\vec{r}_C$ and is written in the inertial basis in the $\hat{i} - \hat{k}$ plane since the source is azimuthally symmetric:

$$\vec{r}_C = r_C (\sin \beta \hat{i} + 0 \hat{j} + \cos \beta \hat{k}) \quad (1)$$

The integration direction through the source is given by values of the random variables (α_s, γ_s) which define the unit particle propagation vector

$$\vec{v}_k = \sin \gamma_s \cos \alpha_s \vec{\theta} - \sin \gamma_s \sin \alpha_s \vec{\phi} + \cos \gamma_s \vec{R}_C \quad (2)$$

where the unit basis vectors are

Fig. 1. FLASH code source geometry. The source axis and detector directions define the $(\hat{i}, \hat{j}, \hat{k})$ coordinate system. The atmosphere boundaries are labelled r_1, r_2 , etc., and the source layers are r'_1, r'_2 , etc. The source cone angle cosines are μ_1, μ_2, μ_3 .

$$\vec{R}_C = \frac{\vec{r}_C}{r_C},$$

$$\vec{\Theta} = \cos \beta \hat{i} + 0 \hat{j} - \sin \beta \hat{k}, \quad (3)$$

and

$$\vec{\Phi} = \vec{R}_C \times \vec{\Theta}.$$

The propagation direction, in general, intersects the source volume in two places, (at V_1 and V_2), given by $\vec{x}_{V1}$ and $\vec{x}_{V2}$. The source region is defined as the volume enclosed by (r'_1, r'_{NSR}) and the cone angle cosine μ_{NSPA} (Fig. 1). A portion of this

volume may have null emissivity and will not contribute to the source integral. If the collision, $\vec{r}_C$, occurs inside the source volume, there is only one intersection with the source at V_1 with position $\vec{x}_{V1}$. The integration is performed along the line between $\vec{r}_{T1}$ and $\vec{r}_{T2}$, where we have:

i) $\vec{r}_C$ outside source:

$$\vec{r}_{T1} = \vec{x}_{V1}; \vec{r}_{T2} = \vec{x}_{V2}$$

ii) r_C inside source:

$$\vec{r}_{T1} = \vec{r}_C; \vec{r}_{T2} = \vec{x}_{V1}.$$

An integration through the volume source computes the direct intensity component to the source score:¹

$$DI(t) = \int_{\vec{r}_{T1}}^{\vec{r}_{T2}} N(\vec{R}_T, t_e) e^{-\rho(\vec{R}_T - \vec{r}_C)}$$

$$T_W(\vec{R}_T - \vec{r}_C) T_{CO_2}(\vec{R}_T - \vec{r}_C) d\vec{R}_T, \quad (4)$$

where $N(\vec{R}_T, t_e)$ is the number of source photons emitted per steradian at $\vec{R}_T$ in the integration path, at time t_e ; $\rho(\vec{R}_T - \vec{r}_C)$ is the optical distance along the integration path from $\vec{r}_C$; and $T_W T_{CO_2}$ are water vapor and carbon dioxide transmissions from $\vec{r}_C$ to $\vec{R}_T$. The integral is approximated by a sum over individual emission segments within the source and multiplied by the path average attenuation from the collision point to the exterior source volume:

$$DI(t) = \sum_{i=1}^{NS} \left(\int_{\vec{r}_{T1i}}^{\vec{r}_{T2i}} N e^{-\rho} dS_i \right) \langle T_W T_{CO_2} \rangle_{avg}, \quad (5)$$

where the segment dS_i is given by

$$dS_i = |d\vec{R}_{T_i}| = |\vec{R}_{T_{2i}} - \vec{R}_{T_{1i}}|, \quad (6)$$

lies within the spherical shell of the atmospheric mesh bounded by r_i and r_{i+1} (Fig. 2). Since we assume the atmosphere constant over a shell, we obtain:¹

$$\int_{\vec{R}_{T_{1i}}}^{\vec{R}_{T_{2i}}} = \left[\frac{N \vec{R}_{T_{1i}} t_e}{\Sigma_i} \right] \begin{bmatrix} -\rho \vec{R}_{T_{1i}} & -\rho \vec{R}_{T_{2i}} \\ e & -e \end{bmatrix}, \quad (7)$$

where Σ_i is the extinction coefficient in the interval dS_i given by

$$\Sigma_i \approx \frac{\rho \vec{R}_{T_{2i}} - \rho \vec{R}_{T_{1i}}}{dS_i}. \quad (8)$$

Clearly, some changes in the notation are required if the integration path has the opposite direction ($-\vec{v}_k$) of that shown in Fig. 2, but the principle remains the same.

Fig. 2. Integration geometry for the source layer between r_j' and r_{j+1}' . The integration begins at the collision vector, $\vec{r}_c$.

III. SOURCE INTERSECTIONS

We determine the vectors $\vec{x}_{v_1}$ and $\vec{x}_{v_2}$ by first calculating the intersections of the propagation line, $t\vec{v}_k$, with the source volume spherical surfaces of radii r_1' and $r_{N_{SR}}'$; and the intersections with the conical surface having half-angle $\theta_{\max}$ where

$$\mu_{N_{SPA}} = \cos(\theta_{\max}).$$

Consider Fig. 3A which illustrates the geometry of a line intersecting a sphere. The equation of the line is $t\vec{v}_k$ and the intersections occur at

$$\vec{r}_{1,2} = t_{1,2} \vec{v}_k + \vec{r}_c \quad (9)$$

which on squaring yields

$$t_{1,2}^2 = r^2 = t_{1,2}^2 \vec{v}_k^2 + 2t_{1,2} \vec{r}_c \cdot \vec{v}_k + r_c^2, \quad (10)$$

which solves as

$$t_{1,2} = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}, \quad (11)$$

where

$$A = 1; B = 2 r_c \cos \gamma_s; C = r_c^2 - r^2. \quad (12)$$

We clearly reject intersections that give $t_{1,2} < 0$ (or imaginary) because these are either in the $-\vec{v}_k$ direction (or do not exist).

Figure 3B shows the intersection of the line $t'\vec{v}_k$ with a cone. We write the intersections as

$$\vec{r}_{1,2} = \vec{r}_c + t'_{1,2} \vec{v}_k, \quad (13)$$

and have to determine $t'_{1,2}$.

Fig. 3.a. Geometry of a line intersection with a sphere.

b. Geometry of a line intersection with a cone.

Writing $\vec{r}_{1,2}$ in component form yields

$$\begin{aligned} \vec{r}_{1,2} = r_{1,2} [& \sin\theta \cos\phi_{1,2} \hat{i} \\ & + \sin\theta \sin\phi_{1,2} \hat{j} + \cos\theta \hat{k}] , \end{aligned} \quad (14a)$$

or

$$\begin{aligned} \vec{r}_{1,2} = & (t'_{1,2} v_{k1} + r_{c1}) \hat{i} \\ & + (t'_{1,2} v_{k2} + r_{c2}) \hat{j} \\ & + (t'_{1,2} v_{k3} + r_{c3}) \hat{k} . \end{aligned} \quad (14b)$$

Equate the components of (14a,b) to obtain three equations:

$$t'_{1,2} v_{k1} + r_{c1} = \sin\theta \cos\phi_{1,2} r_{1,2} , \quad (15)$$

$$t'_{1,2} v_{k2} + r_{c2} = \sin\theta \sin\phi_{1,2} r_{1,2} , \quad (16)$$

$$t'_{1,2} v_{k3} + r_{c3} = \cos\theta r_{1,2} . \quad (17)$$

Solving these for $t'_{1,2}$ yields the quadratic

$$\begin{aligned} t_{1,2}^2 [v_{k1}^2 + v_{k2}^2 - v_{k3}^2 \tan^2 \theta] \\ + t'_{1,2} 2[v_{k1}r_{c1} + v_{k2}r_{c2} - v_{k3}r_{c3} \tan^2 \theta] \\ + [r_{c1}^2 + r_{c2}^2 - r_{c3}^2 \tan^2 \theta] = 0 , \end{aligned}$$

which solves as

$$t'_{1,2} = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} \quad (18)$$

with

$$A = [v_{k1}^2 + v_{k2}^2 - v_{k3}^2 \tan^2 \theta] ,$$

$$B = 2[v_{k1}r_{c1} + v_{k2}r_{c2} - v_{k3}r_{c3} \tan^2 \theta] ,$$

$$C = [r_{c1}^2 + r_{c2}^2 - r_{c3}^2 \tan^2 \theta] .$$

As in the case of a spherical intersection, we ignore negative and imaginary solutions.

The first source volume intersection vector, $\vec{x}_{v1}$, is that corresponding to the minimum, positive distance along the line $t\vec{v}_k$ to the two spheres and the cone that define the source. The second intersection, $\vec{x}_{v2}$, is the next largest value.

IV. INTEGRATION SEGMENTS

To determine the path length through each spherical shell, the geometry shown in Fig. 4 must be solved; namely, one must know if the line $t\vec{V}_k$ intersects the $(i+1)^{\text{th}}$ or the i^{th} shell. We determine this by computing the vector tangent to r_i , $\vec{V}_t$, and testing the condition

$$\vec{V}_k \cdot \vec{R}_c > \vec{V}_t \cdot \vec{R}_c .$$

The condition is true if the intersection is with the upper $(i+1)^{\text{th}}$ radius. Note that a line segment can traverse the atmospheric boundaries such that the radial intersection index, i , decreases to a minimum and then increases along the path. This test must therefore be performed at each step in the integration. The tangent vector to a sphere from $\vec{r}_c$ must be known to apply this test; and Fig. 5 shows the requisite geometry for the line $t\vec{V}_t$ tangent at $\vec{r}_t$. One has by inspection of Fig. 5:

$$t\vec{V}_t = \vec{r}_t - \vec{r}_c , \quad (19)$$

Fig. 4. Particle propagation directions from a collision at $\vec{r}_c$.

subject to the condition

$$\vec{r}_t \cdot \vec{V}_t = 0 . \quad (20)$$

Dotting (19) by $\vec{r}_t$ and using (20) we find

$$0 = r_t^2 - r_t r_c \cos \alpha ,$$

or

$$\cos \alpha = \frac{r_t}{r_c} . \quad (21)$$

We clearly have the Pythagorean relation

$$t = + \sqrt{r_c^2 - r_t^2} , \quad (22)$$

which solves the intersection since we express

$$\vec{r}_t = (\cos \alpha \vec{R}_c + \sin \alpha \vec{M}) r_t , \quad (23)$$

where

$$\vec{M} = \frac{\hat{z} \times \vec{R}_c}{|\hat{z} \times \vec{R}_c|} . \quad (24)$$

Fig. 5. Geometry of a line tangent to a sphere at $\vec{r}_t$.

Once one has ascertained which sphere (i or i+1) is intersected by the line, the distance dS_i and intersection vector $R_{T_{2i}}$ can be calculated.

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