Monte Carlo Simulation of X-ray Transport

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Abstract. An article usually includes an abstract, a concise summary of the work covered at length in the main body of the article. It is used for secondary publications and for information retrieval purposes.

INTRODUCTION

TRANSPORT THEORY

In order to represent the computational domain discretely, space is broken up into a grid of voxels (a pixel with volume), with each voxel being assigned a particular material ID depending on the geometries and compounds/elements in the domain. With our discrete space, given a photon position $\vec{r}$, the corresponding voxel in which the photon resides can be calculated. Therefore, a particular material can be associated with all possible $\vec{r}$'s in the domain.

A photon's position in space after taking the n-th step in the domain $\vec{r}_n$ is represented by the following parametric ray equation:

$$\vec{r}_n = \vec{r}_{n-1} + \hat{d}t_n, \tag{1}$$

where $\vec{r}_{n-1}$ is the initial position before the n-th step, $\hat{d}$ is a unit vector in the direction of the step, and t_n is the distance of the n-th step.

In order to sample t_n, we utilize the following probability distribution function (PDF) $p(t)$ of the distance traveled t by a photon of energy E through material M before interacting:

$$p(t) = n\sigma \exp\left[-t(n\sigma)\right], \tag{2}$$

where n is the number density of M and $\sigma = \sigma(E,M)$ is the microscopic cross-section of M at E.

Using the inversion method for sampling a PDF, it follows that random values of the free path t can be generated with the following equation:

$$t = -\frac{1}{n\sigma}\ln\gamma, \tag{3}$$

where γ is a uniformly distributed random number in the interval $(0,1)$.

SURFACE AND DELTA-TRACKING

If, after taking a step, the photon lands in a voxel with a different material, then the corresponding free path for the new material to be accounted for. This method, called surface-tracking, requires photons to be stopped at voxel boundaries and intersections with surrounding voxels to be calculated, which can be computationally intensive for materials that have a large average free path.

Alternatively, the delta-tracking algorithm offers a solution by sampling the maximum cross-section $\sigma_{\max}$ in the computational domain. This, in turn, brings down the average free path to the minimum in the domain. To account for this decrease in free path, the algorithm introduces delta interactions as an alternative to real interactions, resulting in no change to the energy or direction. The probability of delta interaction P_δ is given by the following equation:

$$P_\delta = \frac{\sigma_{\max}(E) - \sigma(E,M)}{\sigma_{\max}(E)}, \tag{4}$$

where E is the energy of the photon undergoing the step, and M is the material corresponding to the position of the photon at the end of the step. Note that when the photon lands in the material corresponding to the maximum cross-section, $\sigma(E,M) = \sigma_{\max}$ and $P_\delta = 0$. On the contrary, if the photon landed in air and the domain's maximum cross-section corresponded to lead, then $\sigma(E,M) << \sigma_{\max}$, making $P_\sigma \approx 1$.

Overall, delta-tracking is significantly more computationally efficient for domains with similar cross-sections and can be shown to yield equivalent results to surface-tracking.

PHOTON INTERACTIONS

If a delta interaction does not occur, then a real interaction is sampled. Therefore, the probability of a real interaction P_r is directly related to P_δ by

$$P_r = 1 - P_\delta, \tag{5}$$

where P_δ is given by Eq. 4.

If a real interaction occurs in material M, then probability of interaction i occurring is

$$P_i = \frac{\sigma_i(E,M)}{\sigma(E,M)}, \tag{6}$$

where σ_i is the cross-section of interaction i.

If there are N possible interactions for a particular E and M, then $\sigma(E,M)$ is calculated as so

$$\sigma(E,M) = \sum_{i=1}^{N} \sigma_i(E,M). \tag{7}$$

For x-rays, there are three possible photon interactions:

1. Photoelectric Effect

In the photoelectric effect model used in MIDSX, a rather simple approach is taken. When a photon interacts with an atom's electron, the photon is terminated and all energy is deposited at the location of interaction. In general purpose particle transport code systems, when a photoelectric interaction occurs, a photon of energy E is absorbed by an electron in subshell i, causing the electron to leave the atom with energy $E_e = E - U_i$, where U_i is the binding energy of the ith subshell. In addition, photons are emitted due to atomic relaxations. For photon energies in the medical imaging range (30 - 120 keV), the energy of the released electrons does not allow for significant traversal through typically used materials, such as tissue, bone, and fat. This limited traversal results in a localized dose distribution, in turn, validating the model used by MIDSX.

2. Coherent Scattering

Thomson scattering is defined as an incoming photon of energy E elastically scattering with a free electron at rest, resulting in a scattered photon of energy E. The atomic DCS per unit solid angle Ω for the interaction can be derived with classical electrodynamics, and is given by

$$\frac{d\sigma_T}{d\Omega} = r_e^2 \frac{1+\cos^2(\theta)}{2}, \tag{8}$$

where r_e^2 is the classical electron radius.

In an atom, photons scatter off bound electrons rather than the free electrons described by Thomson scattering, resulting in what is known as coherent (Rayleigh) scattering. The DCS per unit solid angle Ω of the interaction, ignoring absorption edge effects, is given by

$$\frac{d\sigma_{Co}}{d\Omega} = \frac{d\sigma_T}{d\Omega} F(x,Z), \tag{9}$$

where x is the momentum transfer between the photon and atom, Z is the atomic number of the atom, and $F(x,Z)$ is the atomic form factor.

$$x = \tag{10}$$

METHODS

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REFERENCES