Improved Monte Carlo modeling of radiation transport through stochastic media

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Radiation propagation through stochastic material is an active topic in transport methods research. By definition, stochastic materials can be characterized only probabilistically, and range from uniform random mixtures (such as concrete) to mixtures with complicated clustering behavior (such as clouds) [1]. Modeling these mixtures accurately and efficiently presents a unique challenge for radiation transport codes.

To address this challenge, we are developing a path-length-sampling (PLS) method specifically designed for transport through stochastic mixtures. The PLS method uses an initial infinite-medium calculation to capture stochastic material effects in the form of tabular PDFs, which are then directly sampled during an Implicit Monte Carlo (IMC) simulation. To date, we have implemented a preliminary version of the PLS method in the Branson IMC mini-app [2]. Initial results demonstrate that the PLS method can accurately capture the effect of material interface refraction in a uniform random medium.

Background and Motivation

The vast majority of existing research on transport through stochastic material considers only two-material mixtures, with code implementations generally limited to a single geometry [3]. While these specialized applications are very valuable from a research perspective, it is not feasible to implement each of these geometries in a general-purpose radiation transport code.

Consequently, there is a need for methods that accurately simulate particle transport through stochastic media, while requiring minimal modifications to existing transport codes. We believe that the PLS method is well-suited to meet these requirements.

Description

To generate path-length distributions for use in IMC simulations, we run a steady-state infinite-medium calculation for the stochastic material of interest. Depending on the properties of the material mixture, this calculation can be done using chord-length sampling, ensemble-averaging of multiple realizations, or other microphysics models.

The output of this material characterization step consists of tabular PDFs for particle path-length and scattering angle. If the material is non-uniform in space, these PDFs can be calculated on a specified sub-cell grid in space and angle.

Figure 1 shows an example cell filled with a non-uniform mixture of two materials (highly-absorbing “clusters” of purple spheres in an optically-thin white background). In Figure 2, we map sub-cell mean free path estimates for this material mix (listed in centimeters, and generated using our material characterization code). The “mean free path” represents the average distance a particle travels between collisions with the material. The colored values in Figure 2 highlight significant variations in the mean free path, which result from the underlying stochasticity of the material.

If we were to treat this cell using the common atomic mix model (i.e. volume-averaging the material opacities), the mean free path would be (i) constant throughout the cell, and (ii) less than a centimeter. Both of these statements are clearly at odds with the data presented in Figure 2; thus, the atomic mix approximation is highly inaccurate for this material cell.

Anticipated Impact

Radiation transport through stochastic material occurs in a number of scenarios of interest to the lab, including climate modeling of atmospheric clouds, ICF capsule experiments, and certain turbulent flows. However, current radiation trans-

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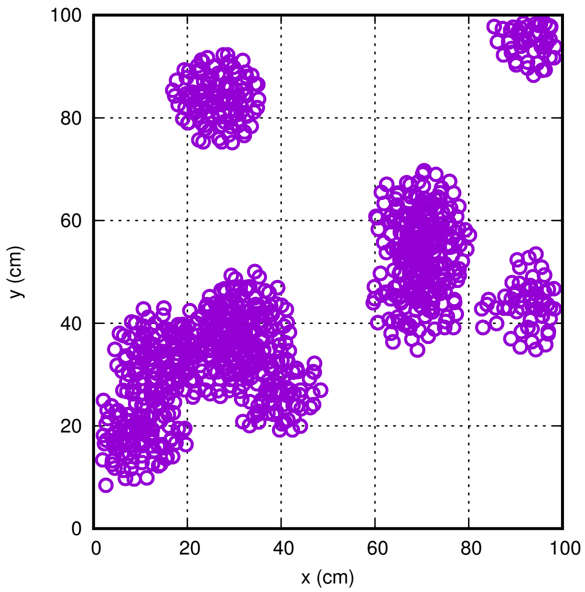

Figure 1: Top view of “clustered” material mix

port capabilities are incapable of capturing subcell variations in material opacity, which can produce unphysical solutions in portions of the problem domain. Implementing an improved stochastic material treatment will lead to more accurate radiation transport solutions in problems with significant sub-cell material heterogeneity.

Path Forward

Once we have completed research work in the Branson mini-app, the PLS method should be straightforward to implement in CCS-2’s Jayenne project software. Porting the PLS implementation to Jayenne will allow us to examine the performance of the method for coupled radiation-hydrodynamics simulations.

Acknowledgements

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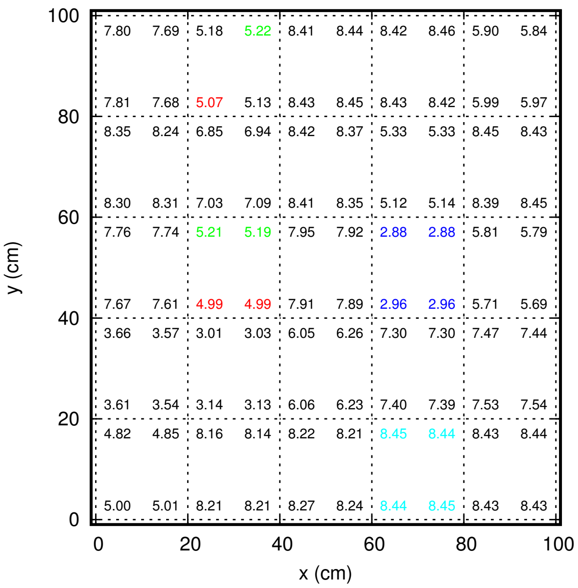

7.80	7.69	5.18	5.22	8.41	8.44	8.42	8.46	5.90	5.84
7.81	7.68	5.07	5.13	8.43	8.45	8.43	8.42	5.99	5.97
8.35	8.24	6.85	6.94	8.42	8.37	5.33	5.33	8.45	8.43
8.30	8.31	7.03	7.09	8.41	8.35	5.12	5.14	8.39	8.45
7.76	7.74	5.21	5.19	7.95	7.92	2.88	2.88	5.81	5.79
7.67	7.61	4.99	4.99	7.91	7.89	2.96	2.96	5.71	5.69
3.66	3.57	3.01	3.03	6.05	6.26	7.30	7.30	7.47	7.44
3.61	3.54	3.14	3.13	6.06	6.23	7.40	7.39	7.53	7.54
4.82	4.85	8.16	8.14	8.22	8.21	8.45	8.44	8.43	8.44
5.00	5.01	8.21	8.21	8.27	8.24	8.44	8.45	8.43	8.43

Figure 2: Sub-cell mean free path estimates

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