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An Atomic Mix Closure for Stochastic Media Transport Problems

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INTRODUCTION

The accurate modeling of stochastic media in radiation transport calculations remains on ongoing research challenge. The Levermore-Pomraning (LP) closure for the statistical transport equation is simple and inexpensive, but it is often inaccurate [1-2]. More accurate closures have been proposed, but they can be prohibitively expensive [3]. In this work we present a relatively inexpensive closure that we have observed to be more accurate than LP in almost all cases studied.

DESCRIPTION OF THE ACTUAL WORK

The statistical transport equation governing transport in binary stochastic media is given by (adapted from [2]):

$$\vec{\Omega}\cdot\nabla\left\langle\psi_i\left(\vec{r},\vec{\Omega}\right)\right\rangle+\sigma_{t,i}\left\langle\psi_i\left(\vec{r},\vec{\Omega}\right)\right\rangle=$$
$$\frac{\sigma_{s,i}}{4\pi}\int d\vec{\Omega}'\left\langle\psi_i\left(\vec{r},\vec{\Omega}'\right)\right\rangle+\lambda_i^{-1}\left(\left\langle\psi_{s,j}\left(\vec{r},\vec{\Omega}'\right)\right\rangle-\left\langle\psi_{s,i}\left(\vec{r},\vec{\Omega}'\right)\right\rangle\right) \quad (1)$$

This equation is formally exact for arbitrary mixing statistics. Unfortunately an additional set of equations is needed to relate the two types of conditional averages.

In [3] we proposed a family of closures of the following form:

$$\left[\left\langle\psi_s\left(\vec{r},\vec{\Omega}\right)\right\rangle\right]=R\left(\vec{r}\right)\left[\left\langle\psi\left(\vec{r},\vec{\Omega}\right)\right\rangle\right] \quad (2)$$

To determine R we proposed a set of subsidiary calculations to relate $\left[\left\langle\psi_s\right\rangle\right]$ and $\left[\left\langle\psi\right\rangle\right]$ to boundary fluxes $\left[\psi_b\right]$:

$$\left[\left\langle\psi\right\rangle\right]=R_u\left[\psi_b\right],$$
$$\left[\left\langle\psi_s\right\rangle\right]=R_s\left[\psi_b\right]=R_sR_u^{-1}\left[\left\langle\psi\right\rangle\right]\equiv R\left[\left\langle\psi\right\rangle\right] \quad (3)$$

These subsidiary calculations involve a deterministically-generated ensemble of geometric realizations; weighted transport calculations on this ensemble yield numerical approximations to R. Depending on the problem this ensemble can be quite large.

We note that the LP closure uses the identity matrix for R in Equation (2).

New Closure

In order to develop our new model for R we depict an arbitrary realization in Figure 1 for a stochastic transport problem in one-dimensional slab geometry. In the regions centered around location r we explicitly note the distinct materials at the extremities and on either side of r; there may be material interfaces within these regions (not depicted). These are surrounded by "buffer" regions extending to the problem boundary in which we replace distinct material regions with atomically mixed material. The motivation for the atomic mix layers is to reduce the number of explicit material regions and interfaces that we will eventually need to computationally model; we assume that material distribution details near r are more important. We depict the (known) boundary fluxes and the (unknown) fluxes at r. This is a generalization of the approach we took in [3], which did not include any atomic mix layers and was specialized for the "rod" (two-point angular quadrature) problem.

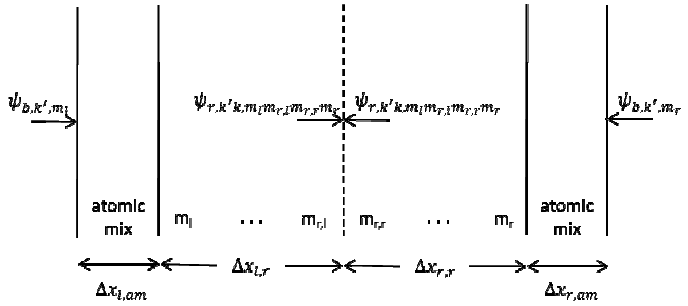

Fig. 1. General slab-geometry stochastic transport model.

With the above description of the problem we can relate the conditionally-averaged interior fluxes to the boundary fluxes as a function of the material distributions:

$$\left\langle\psi_{k,m_r^-}\right\rangle=p_{m_r^-}^{-1}\sum_{k'}\sum_{m_r^+}\sum_{m^-}\sum_{m^+}p_{r,m_r^-m_r^+m^-m^+}R_{r,k'k,m_r^-m_r^+m^-m^+}\psi_{b,k',m^-},$$
$$\left\langle\psi_{s,k,m_r^-}\right\rangle=p_{m_r^-}^{-1}\sum_{k'}\sum_{m^-}\sum_{m^+}p_{r,m_r^-\overline{m}_r^-m^-m^+}R_{s,r,k'k,m_r^-\overline{m}_r^-m^-m^+}\psi_{b,k',m^-} \quad (4)$$

The various response functions R in Equation (4) are derived from ensemble-averages of the conditional interior fluxes depicted in Figure 1 and are in general unknown.

In [3] Equation (4) was approximately solved by creating a finite ensemble of realizations, performing transport calculations on each realization for each boundary flux, and then using the computed interior fluxes to obtain R. We had intended (and still do intend) to perform a similar process in the present work, which we hope will obtain reasonable accuracy at reduced computational cost. However, we have discovered an interesting limit which has proved quite fruitful and is the main topic of this paper.

If we allow $\Delta x_{l,r} \to \Delta x_{r,r} \to 0$ and the atomic mix buffer regions to grow accordingly, we find that $m_l \to m_{r,l}$ and $m_r \to m_{r,r}$. In this limit we find that Equation (4) simplifies to

$$\left\langle \psi_{k,0} \right\rangle = \sum_{k'} R_{k'k} \psi_{b,k',0}, \quad \left\langle \psi_{k,1} \right\rangle = \sum_{k'} R_{k'k} \psi_{b,k',1},$$

$$\left\langle \psi_{s,k,0} \right\rangle = \begin{cases} \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',0} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',1}, & \mu_k > 0 \\ \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',1} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',0}, & \mu_k < 0 \end{cases},$$

$$\left\langle \psi_{s,k,1} \right\rangle = \begin{cases} \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',1} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',0}, & \mu_k > 0 \\ \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',0} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',1}, & \mu_k < 0 \end{cases} \tag{5}$$

where the first two equations define the elements of R_u and the other two define R_S. We note two important properties of this equation. First, R_u and R_S contain identical matrix elements but with permuted rows and columns. This results directly from the fact that in this thin limit there are either no material interfaces (and thus the driving boundary flux initially transports through the same material as the interior fluxes), or there is a single material interface and the boundary flux will initially transport through one or the other material depending on which half-space it is in. Interestingly, if we do not make this distinction then R_u=R_s and we obtain the LP closure. Second, each $R_{k'k}$ can be obtained by transport calculations on a *single* realization, namely one filled entirely with atomically mixed materials. This can be accomplished with N transport calculations, where N is the number of angular quadrature points, if one is interested only in a single representation for R throughout the domain (R in general is spatially dependent). If the angular quadrature is symmetric one may use only $N/2$ calculations.

RESULTS

In order to test the atomic mix closure we reexamine the benchmark problems first reported in [2]. These problems consist of nine different combinations of binary media and mixing statistics for three different slab widths. The problems are monoenergetic in one-dimensional slab geometry; both the rod and S_{16} variants were studied. The problems are driven by an isotropic flux on the left boundary. All scattering is isotropic. The reflected and transmitted currents are the transport quantities examined. In the present work we do not restrict ourselves to the particular chord lengths reported in [2]; instead we examine a variety of length scales.

We generated the atomic mix response matrices in Equation (5) with the Sceptre deterministic code [4] using its discretization of the first-order form of the linear monoenergetic Boltzmann equation, controlling the iterative errors to be less than 10^{-7} and spatial errors to be less than 10^{-6}. These response matrices were then used in a variant of Sceptre that can solve Equations (1) and (2). We also used Sceptre to generate benchmarks using Monte Carlo sampling to create ensembles of realizations.

We present a few selected results below. In Figures 2 and 3 we depict the reflected and transmitted fluxes, respectively, for a series of stochastic problems ("cases" 1 and 4) that correspond to Tables 10 and 13 in [2] for a problem thickness of 1 (average optical thickness of 1) and S_{16} Gauss-Legendre quadrature. We plot results for our benchmark calculations, for an atomic mix calculation, for the LP treatment, and for the atomic mix closure (using the response matrix computed in the center of the geometry). Note that the "atomic mix" results are the directly computed reflection and transmission from an atomic mix realization, not the results generated by means of the corresponding closure. We see here that the atomic mix closure is quite accurate; in particular, it is more accurate than LP. Similar results have been observed for all of the other problems with this problem thickness. Only occasionally is LP slightly more accurate in the limit of very large chord lengths.

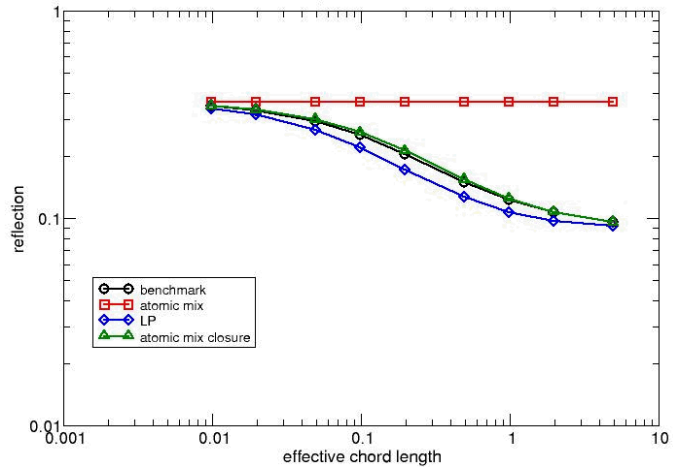

Fig. 2. Reflection results, cases 1/4, S_{16}, thickness=1.

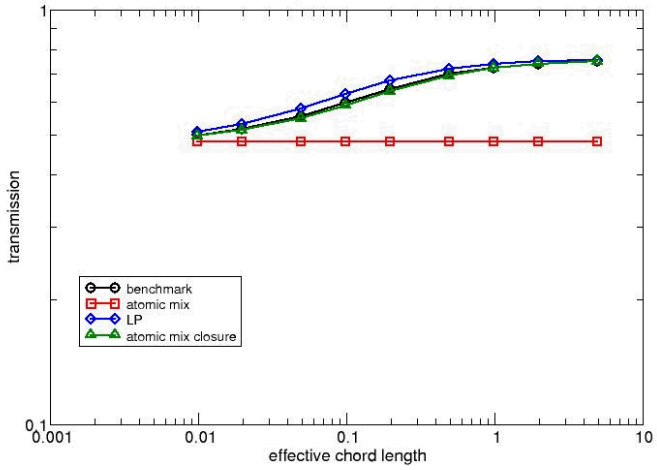

Fig. 3. Transmission results, cases 1/4, S_{16}, thickness=1.

For problem thicknesses of 10 we find comparable results for the rod problems: although the relative errors of both are larger, the atomic mix closure is more accurate than LP. For the S_{16} problems, however, we find that source iteration with the atomic mix closure is unstable. Inspection of the closure matrices shows that they are not diagonally dominant. We instead elect to use the closures generated previously for problem thicknesses of 1 as subgrid models. Results for the same stochastic problems depicted in Figures 2 and 3 but with a thickness of 10 are shown in Figures 4 and 5. We again find that the atomic mix closure is more accurate than LP, even though the closure was generated with a thinner problem. Comparable results are obtained for all of the other stochastic problems studied.

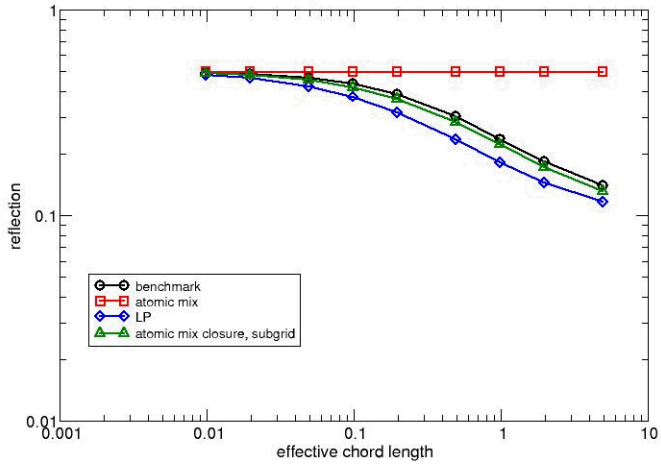

Fig. 4. Reflection results, cases 1/4, S_{16}, thickness=10.

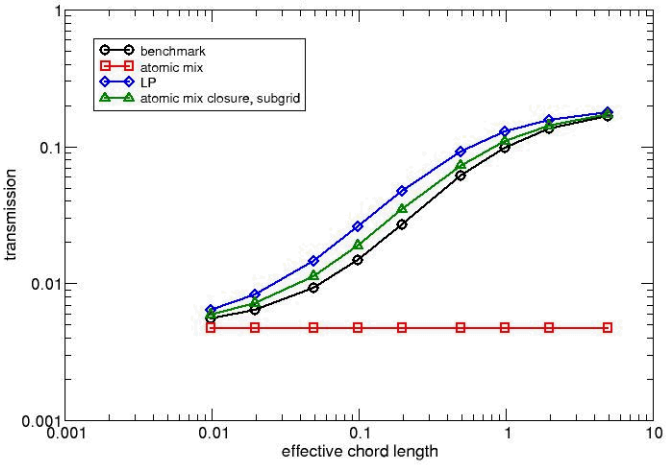

Fig. 5. Transmission results, cases 1/4, S_{16}, thickness=10.

These results show that the atomic mix closure is a promising alternative to LP. It requires a modest number of subsidiary calculations on a single homogenized realization, which if done as a subgrid model will be less expensive than the full-geometry calculations. The same closure may be used for any chord length as long as the relative material proportions remain the same. In almost every case we have studied it is more accurate than LP.

CONCLUSIONS

Obtaining solutions to stochastic transport problems can be quite difficult. Transport calculations on an ensemble of explicit realizations generated by Monte Carlo sampling can be prohibitively expensive. Atomic mix or LP calculations are relatively inexpensive, but they can be inaccurate. The present work illustrates an approach that is less expensive

than Monte Carlo sampling yet more accurate than atomic mix or LP approximations.

We still need to analyze the reasons why the atomic mix closures derived for thicker problems lead to source iteration instabilities. It is not clear if the closure itself induces an ill-posed problem or if it is merely the iterative process that is problematic. We hope to examine alternative source terms to drive the subsidiary calculations. We also want to extend the work to multigroup and multidimensional problems.

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NOMENCLATURE

$\Delta x_{l,am}$ = width of left atomic mix buffer region
$\Delta x_{l,r}$ = width of region(s) to left of *r*
$\Delta x_{r,am}$ = width of right atomic mix buffer region
$\Delta x_{r,r}$ = width of region(s) to right of *r*

λ_i = average chord length in material *i*

m_l = material at left boundary
m_r = material at right boundary
$m_{r,l}$ = material to left of *r*
$m_{r,r}$ = material to right of *r*
m^- = material at upstream boundary
m^+ = material at downstream boundary
m_r^- = material upstream of *r*

$\bar{m}_r^-$ = opposite of material upstream of *r*
m_r^+ = material downstream of *r*

μ_k = direction *k* of angular quadrature
Ω = direction of particle travel
p_m = probability of material *m*

$\psi_{b,k',m}$ = boundary flux in direction k' entering material *m*

$\langle \psi_i \rangle$ = ensemble-averaged angular flux in material *i*

$\langle \psi_{s,i} \rangle$ = ensemble-averaged angular flux at a surface leaving material *i*

r = spatial location
R = response matrix
R_s = surface-averaged response matrix
R_u = unconditionally-averaged response matrix

$\sigma_{s,i}$ = scattering cross section in material *i*

$\sigma_{t,i}$ = total cross section in material *i*

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