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An Atomic Mix Closure for Stochastic Media Transport Problems

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Outline

- Background
- Development of atomic mix closure
- Results
- Conclusions

Background: Statistical transport equation

The statistical transport equation exactly describes averaged fluxes in a (binary) stochastic medium:

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

$\langle \psi_i(\vec{r}, \vec{\Omega}) \rangle$: the ensemble-averaged angular flux conditioned on the existence of material *i* at location $\vec{r}$

$\langle \psi_{s,i}(\vec{r}, \vec{\Omega}) \rangle$: the ensemble-averaged angular flux conditioned on the existence of material *i* at location $\vec{r}$ and the existence of an interface/surface between material *i* and material *j*

Background: Generalized closure

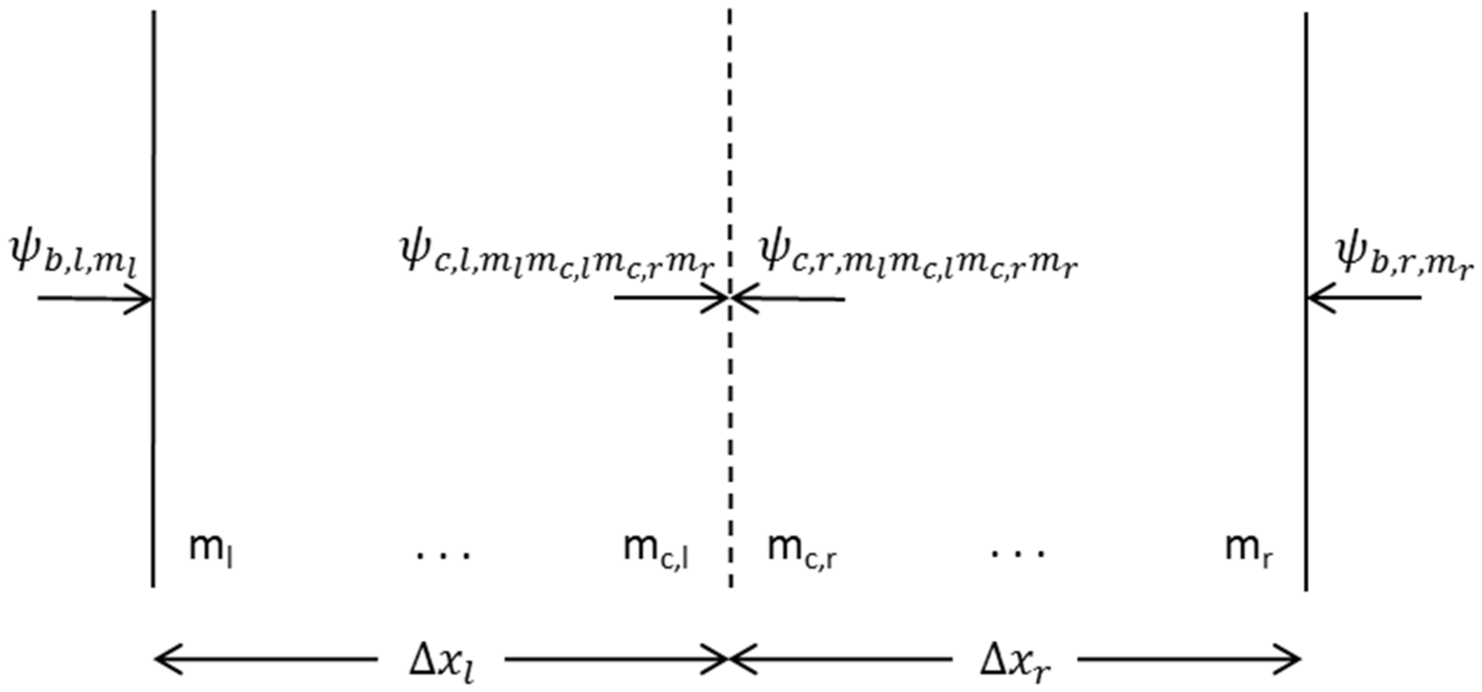
We previously proposed a generalized family of closures for the statistical transport equation:

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

where [] indicates a vector/operator in both angular and material space and *R* is a response matrix, which may in general be dense.

The LP closure may be expressed as $R \approx I$.

Background: Generalized rod problem



Our approach is to relate the interior fluxes (with or without interfaces) to the boundary fluxes. From this we relate $[\langle\psi_s(\vec{r},\vec{\Omega})\rangle]$ and $[\langle\psi(\vec{r},\vec{\Omega})\rangle]$.

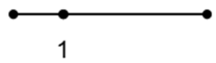
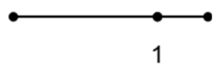
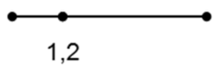
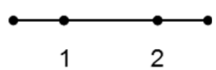
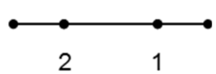
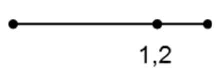
Background: Deterministic generation of realizations and construction of *R*

- Use a numerical quadrature to determine the location of each pseudo-interface for a given *P*. There will be as many quadratures as pseudo-interfaces (*P*-dimensional product quadrature). This yields an ensemble of realizations.
- Solve the transport problems for each generated realization, and combine results according to quadrature integration rules. Repeat for all *P* to obtain $[\langle\psi_s(\vec{r},\vec{\Omega})\rangle]$ and $[\langle\psi(\vec{r},\vec{\Omega})\rangle]$.
- Construct *R*:

$$[\langle\psi\rangle] = R_u[\langle\psi_b\rangle]$$

$$[\langle\psi_s\rangle] = R_s[\langle\psi_b\rangle] = R_s {R_u}^{-1}[\langle\psi\rangle] \equiv R[\langle\psi\rangle]$$

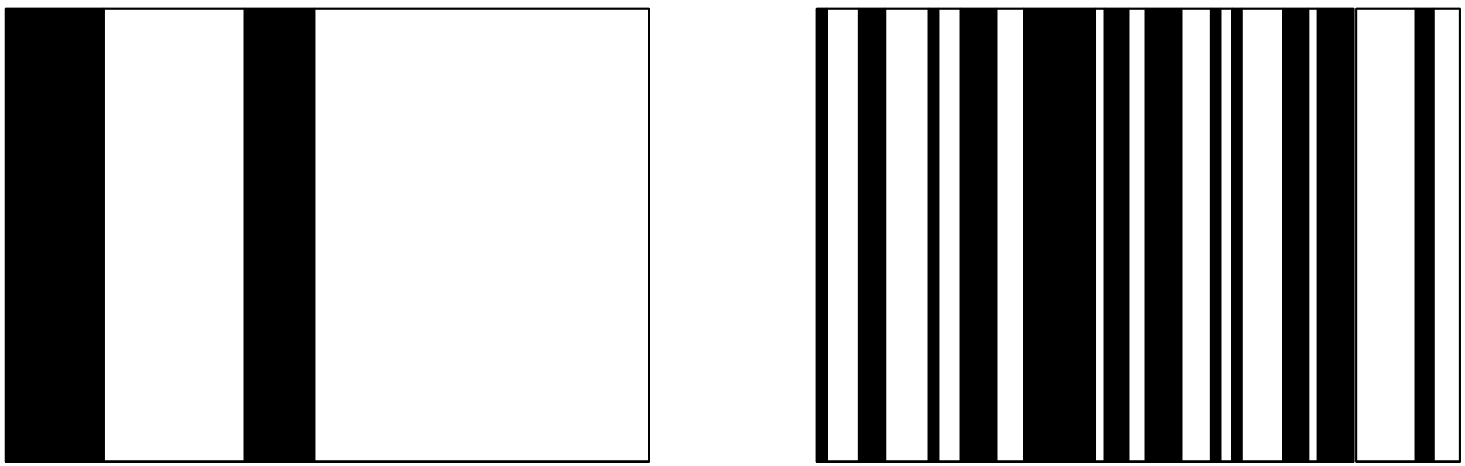
Background: Example problem

Pseudointerfaces		Pseudointerface distribution		Material distribution		Problem
Number	Probability	Configuration	Probability	Configuration	Probability	
0	0.903924		1	1	0.9	1
				2	0.1	2
1	0.091305		0.5	1,1	0.81	1
				1,2	0.09	3
				2,1	0.09	4
				2,2	0.01	2
			0.5	1,1	0.81	1
				1,2	0.09	5
				2,1	0.09	6
				2,2	0.01	2
2	0.004611		0.25	1,1	0.81	1
				1,2	0.09	3
				2,1	0.09	4
				2,2	0.01	2
			0.25	1,1,1	0.729	1
				1,1,2	0.081	5
				1,2,1	0.081	7
				1,2,2	0.009	3
				2,1,1	0.081	4
				2,1,2	0.009	8
				2,2,1	0.009	6
				2,2,2	0.001	2
			0.25	1,1,1	0.0729	1
				1,1,2	0.081	5
				1,2,1	0.081	7
				1,2,2	0.009	3
				2,1,1	0.081	4
				2,1,2	0.009	8
				2,2,1	0.009	6
				2,2,2	0.001	2
			0.25	1,1	0.81	1
				1,2	0.09	5
				2,1	0.09	6
				2,2	0.01	2

Motivation for less expensive closure

Algorithmic complexity of generalized closure : $\leq O(2^{N+1})$

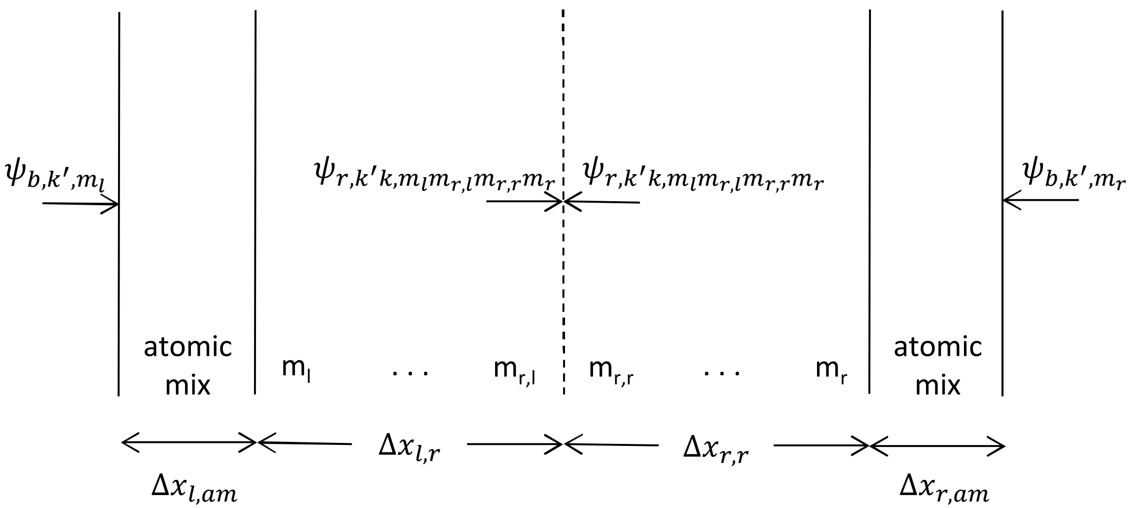
Tractable Intractable



We desire an approach with lower algorithmic complexity.

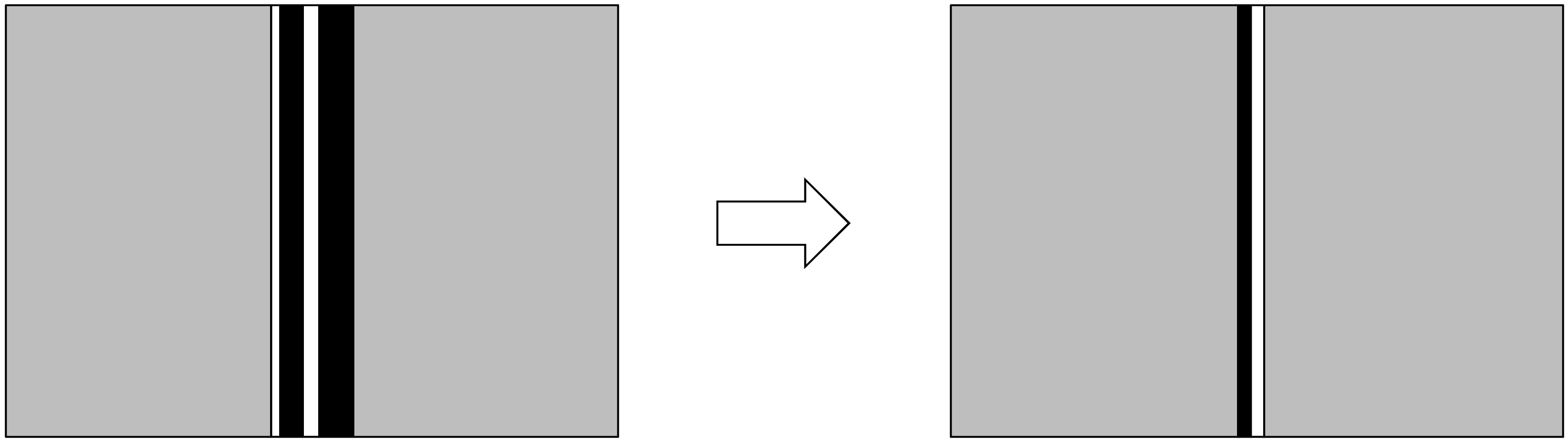
Proposed solution: atomic mix buffer layers

We explicitly model the interfaces in a region of interest and atomically mix elsewhere. This greatly reduces the algorithmic complexity, hopefully without sacrificing too much accuracy.



We discovered an interesting limit…

Let the width of the "sensitive" region shrink to zero:



Near this "atomic mix" limit:

- There is a single unmixed material in that region (without interfaces), or two unmixed materials (with one interface).
- Transport results are governed completely by a single atomically mixed realization

Atomic mix closure

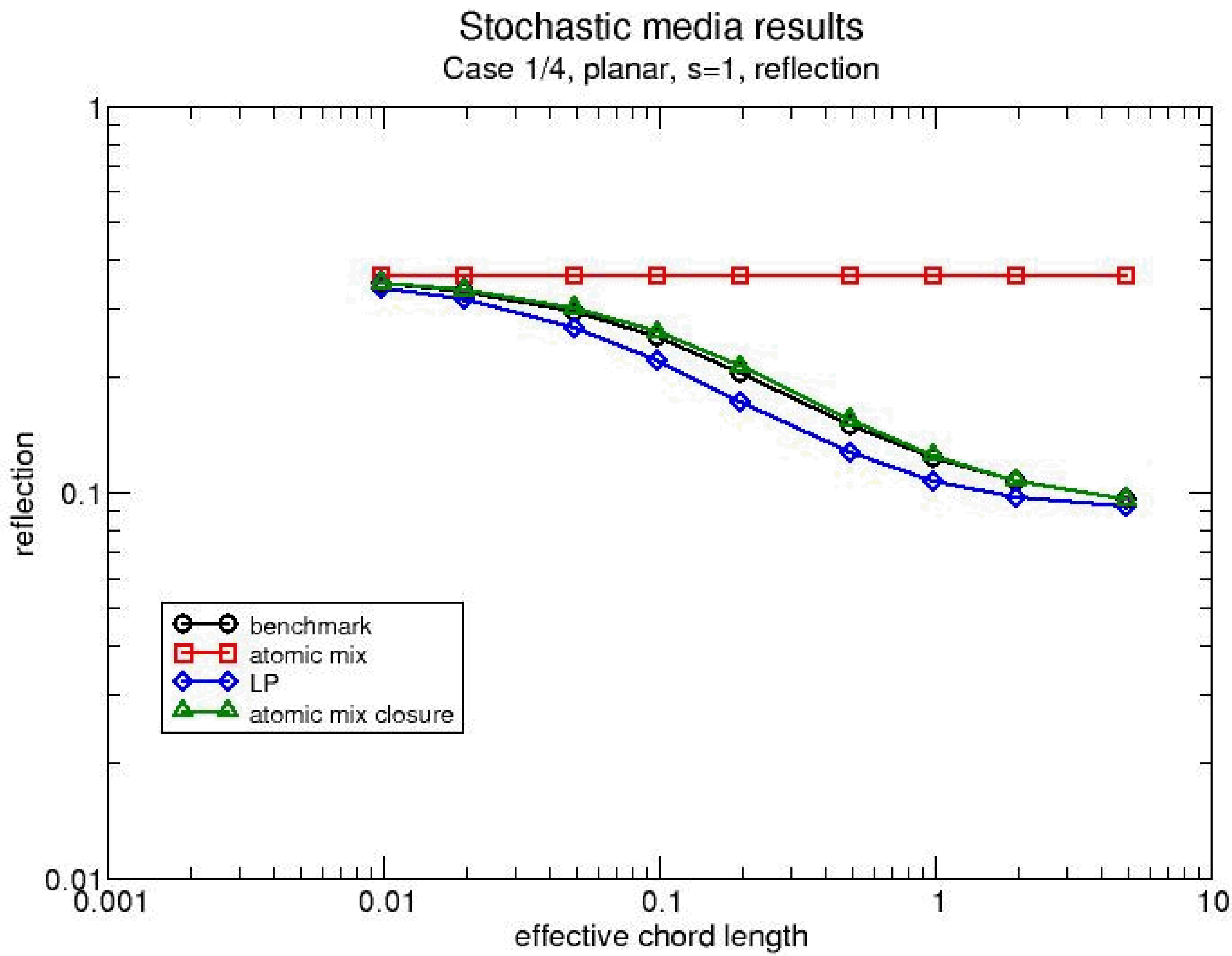
Since we preserved the distinction in material identities as we approach the atomic mix limit, we can relate the average fluxes in a simple manner:

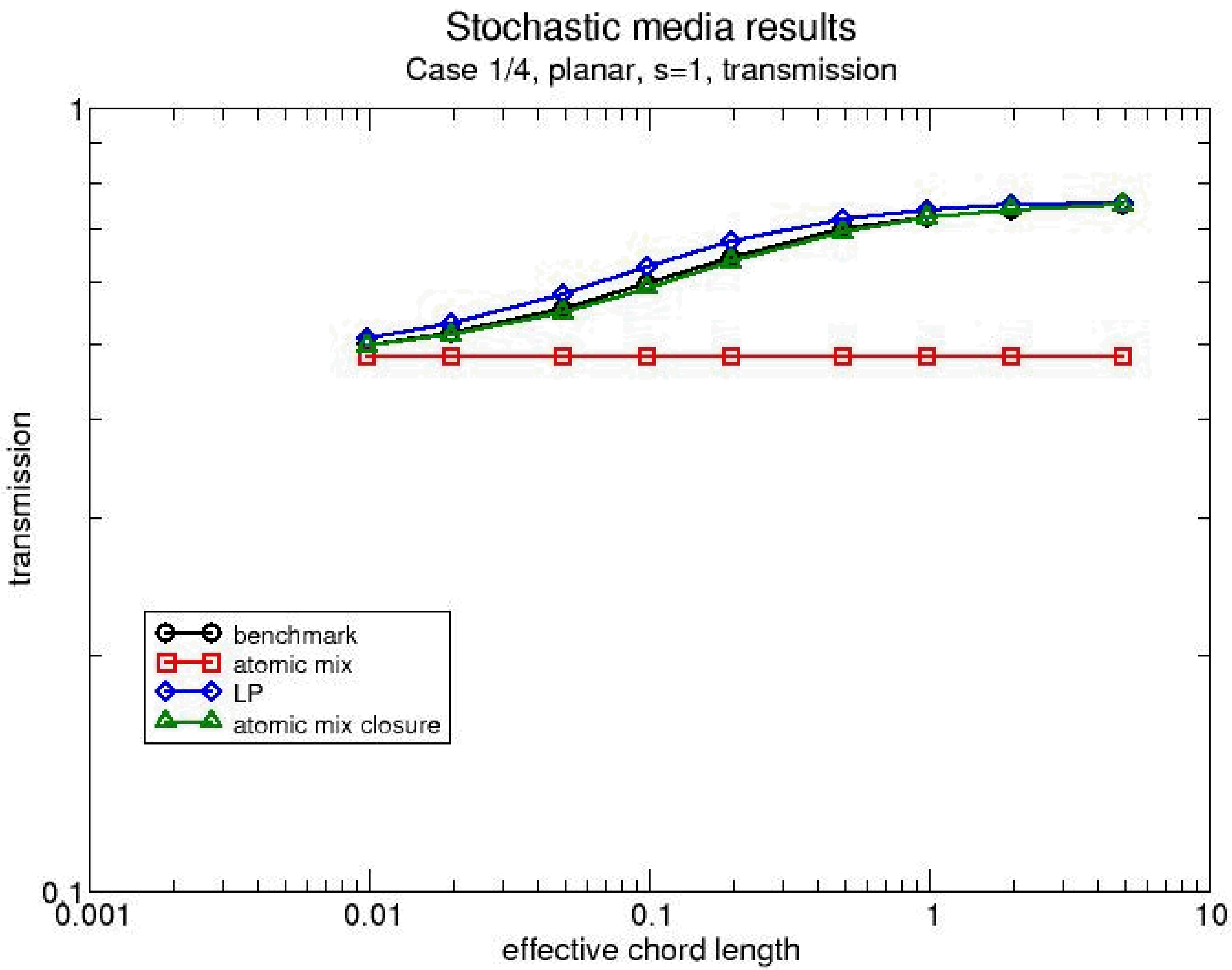
$$\langle \psi_{k,0} \rangle = \sum_{k'} R_{k'k} \psi_{b,k',0}, \quad \langle \psi_{k,1} \rangle = \sum_{k'} R_{k'k} \psi_{b,k',1}, \qquad \Rightarrow \qquad R_u$$

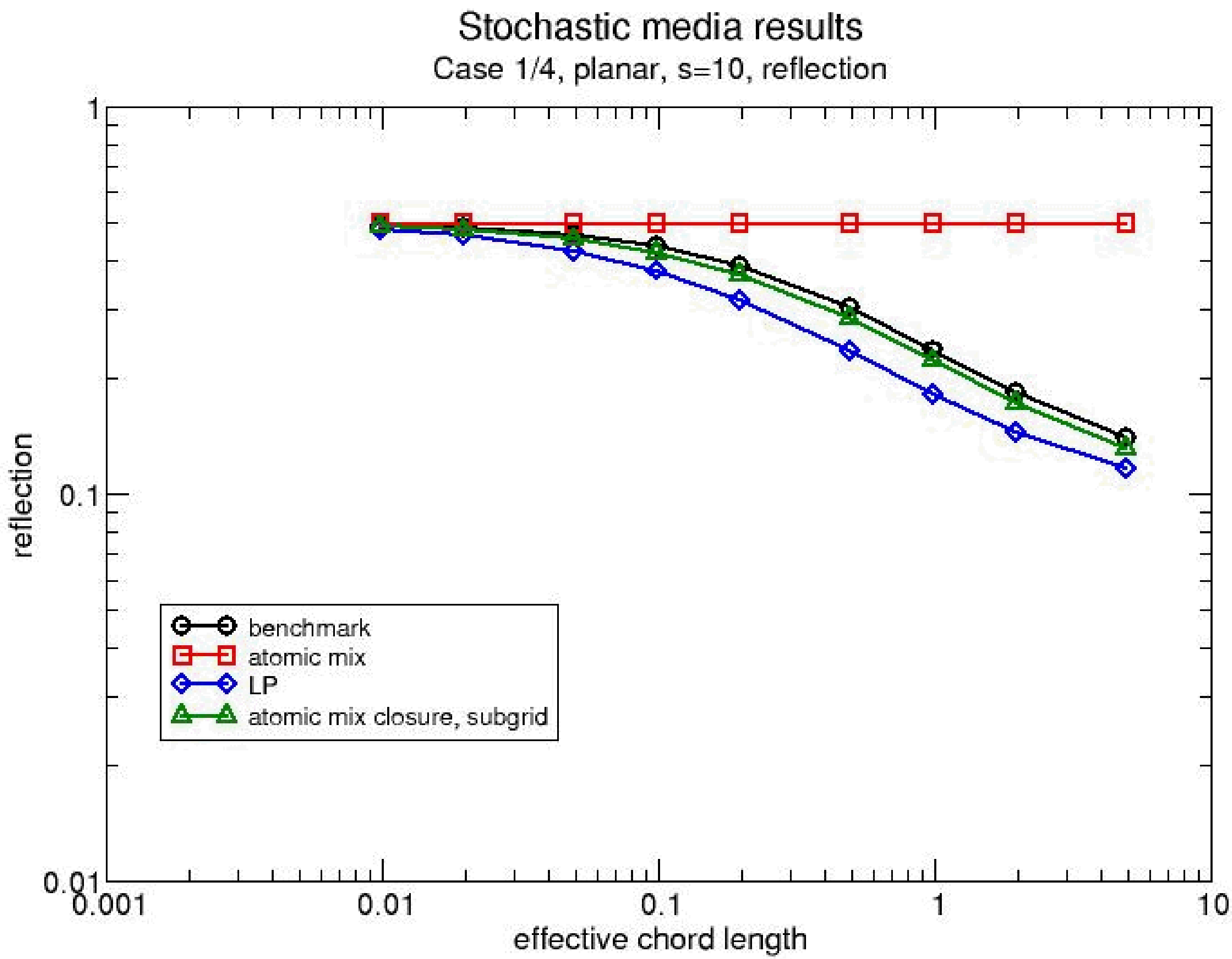
$$\langle \psi_{s,k,0} \rangle = \begin{cases} \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',0} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',1}, & \mu_k > 0 \\ \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',1} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',0}, & \mu_k < 0 \end{cases},$$

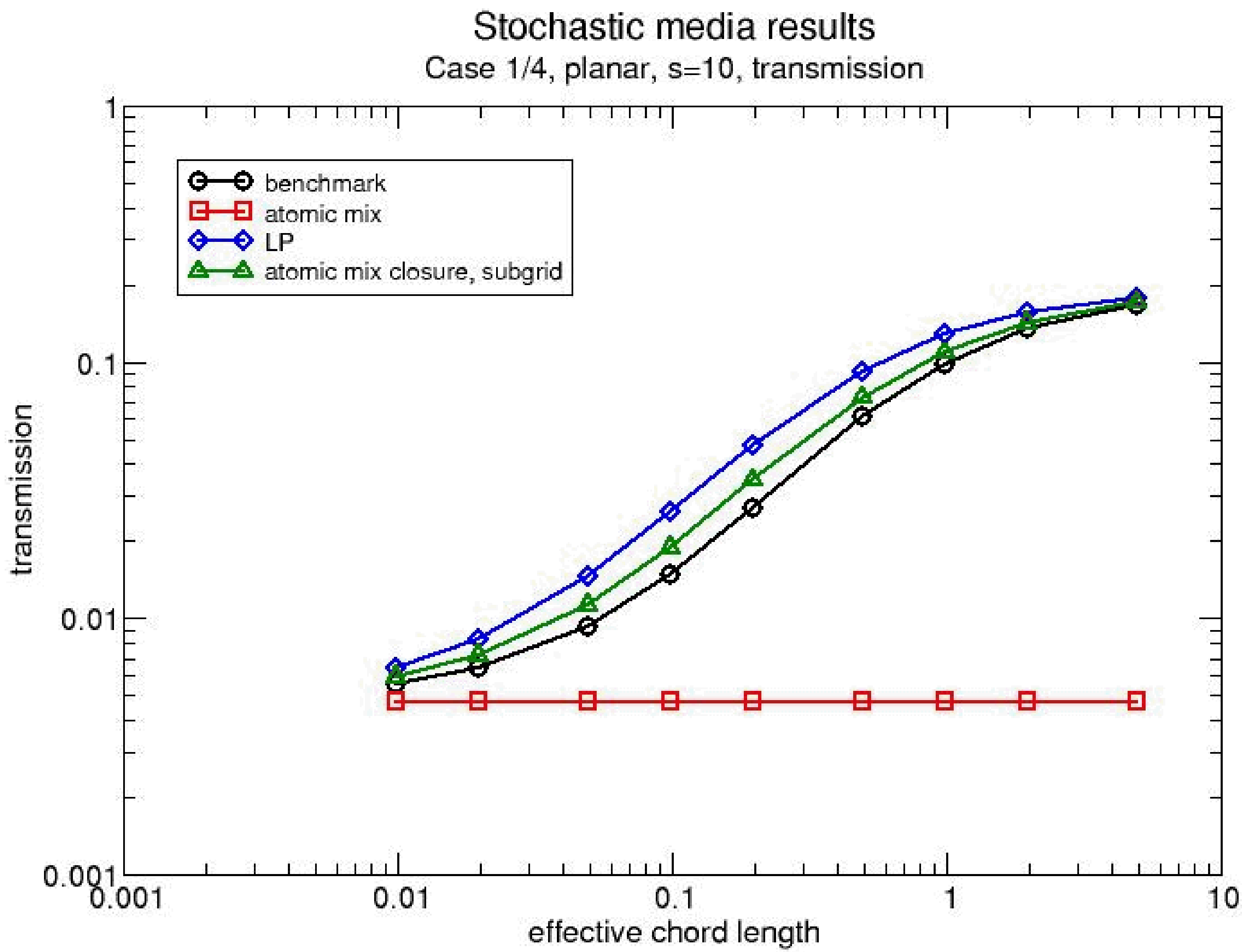
$$\langle \psi_{s,k,1} \rangle = \begin{cases} \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',1} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',0}, & \mu_k > 0 \\ \sum_{\mu_{k'}>0} R_{k'k} \psi_{b,k',0} + \sum_{\mu_{k'}<0} R_{k'k} \psi_{b,k',1}, & \mu_k < 0 \end{cases} \qquad \Rightarrow \qquad R_s$$

A few transport calculations and some matrix math yield the atomic mix closure.


Stochastic media results
Case 1/4, planar, s=1, reflection
reflection
1
0.1
0.01
0.001
0.01
0.1
1
10
effective chord length
benchmark
atomic mix
LP
atomic mix closure


Stochastic media results
Case 1/4, planar, s=1, transmission
transmission
effective chord length
1
0.1
0.001
0.01
0.1
1
10
benchmark
atomic mix
LP
atomic mix closure


Stochastic media results
Case 1/4, planar, s=10, reflection
reflection
effective chord length
1
0.1
0.01
0.001
0.01
0.1
1
10
benchmark
atomic mix
LP
atomic mix closure, subgrid


Stochastic media results
Case 1/4, planar, s=10, transmission
benchmark
atomic mix
LP
atomic mix closure, subgrid
transmission
effective chord length
1
0.1
0.01
0.001
0.001
0.01
0.1
1
10

Conclusions

- In our attempt to find more sophisticated closures to the statistical transport equation, we have discovered a simple closure.
- This closure is generally more accurate than LP and requires only a modest amount of pre-computation.
- The atomic mix *closure* is much more accurate than atomic mix *results*: the functional form retains important properties as chord lengths increase.
- The closure is subject to instabilities in thick problems (diagonal dominance issues) that can be addressed with subgrid approaches.

Future work

- Improve the theory, e.g. formal asymptotic derivation
- Gain better understanding of instabilities
- Correct for boundary effects
- Extend to higher-order angular quadratures and multigroup