Solution of Stochastic Media Transport Problems by Means of Deterministic Generation of Realizations

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Outline

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- Stochastic problem decompositions
- Quadrature generation of realizations
- Results
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- Conclusions

Background/motivation

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We have been attempting to develop methods and benchmarks for multi-dimensional transport in stochastic media.

The generation of realizations in 2D for Monte Carlo sampling with Markovian media requires a process different than the "obvious" one for 1D; we have applied it in 1D as well.

We serendipitously realized that the alternative process has useful properties for decomposing stochastic media problems into stratified problems.

For some problems a deterministic "sampling" technique on these strata is quite efficient.

Stochastic problem descriptions

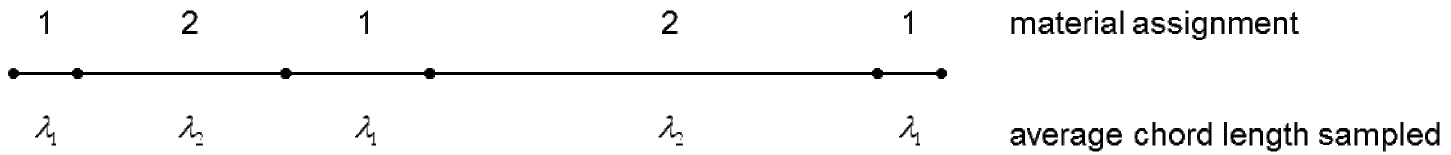
The realizations of a given stochastic media problem obey some statistical distribution. Descriptions of these distributions may not be unique. Some descriptions may have more useful properties than others. Such properties may include:

- Easily stratified
- Easily computed probabilities of strata
- Easy generation of realizations

Interface description and generation of realizations

One method for generation of realizations in 1D Markovian media directly determines interface locations:

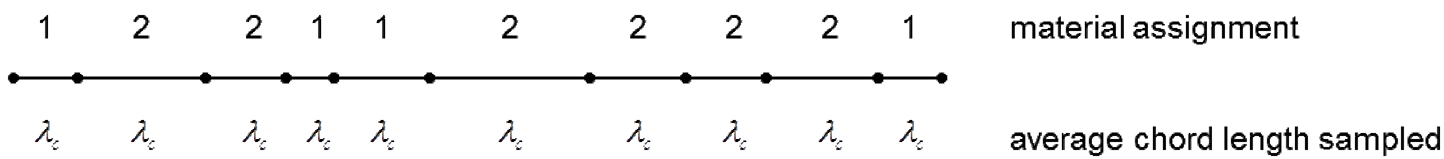
- Sample material at left boundary (e.g. material 1)
- Determine distance to first interface by sampling from $\lambda_1^{-1} e^{-\xi/\lambda_1}$, where λ_1 is the average chord length
- Determine distance to second interface by sampling from $\lambda_2^{-1} e^{-\xi/\lambda_2}$



Pseudo-interface description and generation of realizations

A different method for generation of realizations in 1D Markovian media directly determines "pseudo-interface" locations:

- Determine distance to each pseudo-interface by sampling from $\lambda_c^{-1} e^{-\xi/\lambda_c}$, where $\lambda_c = \lambda_1 \lambda_2 / (\lambda_1 + \lambda_2)$ is the combined (effective) chord length between pseudo-interfaces
- Randomly assign materials afterwards (pseudo-interfaces between identical materials disappear)



Pseudo-interface description and generation of realizations

The two descriptions/processes (interface vs. pseudo-interface) are statistically equivalent. But the pseudo-interface description has two useful properties:

- The frequency with which *I* pseudo-interfaces occur is governed by the Poisson distribution $f(I;\lambda_c) = e^{-\lambda_c}{\lambda_c}^I/I!$
- The location of pseudo-interfaces is uniformly distributed, and thus independent of the location of other pseudo-interfaces.

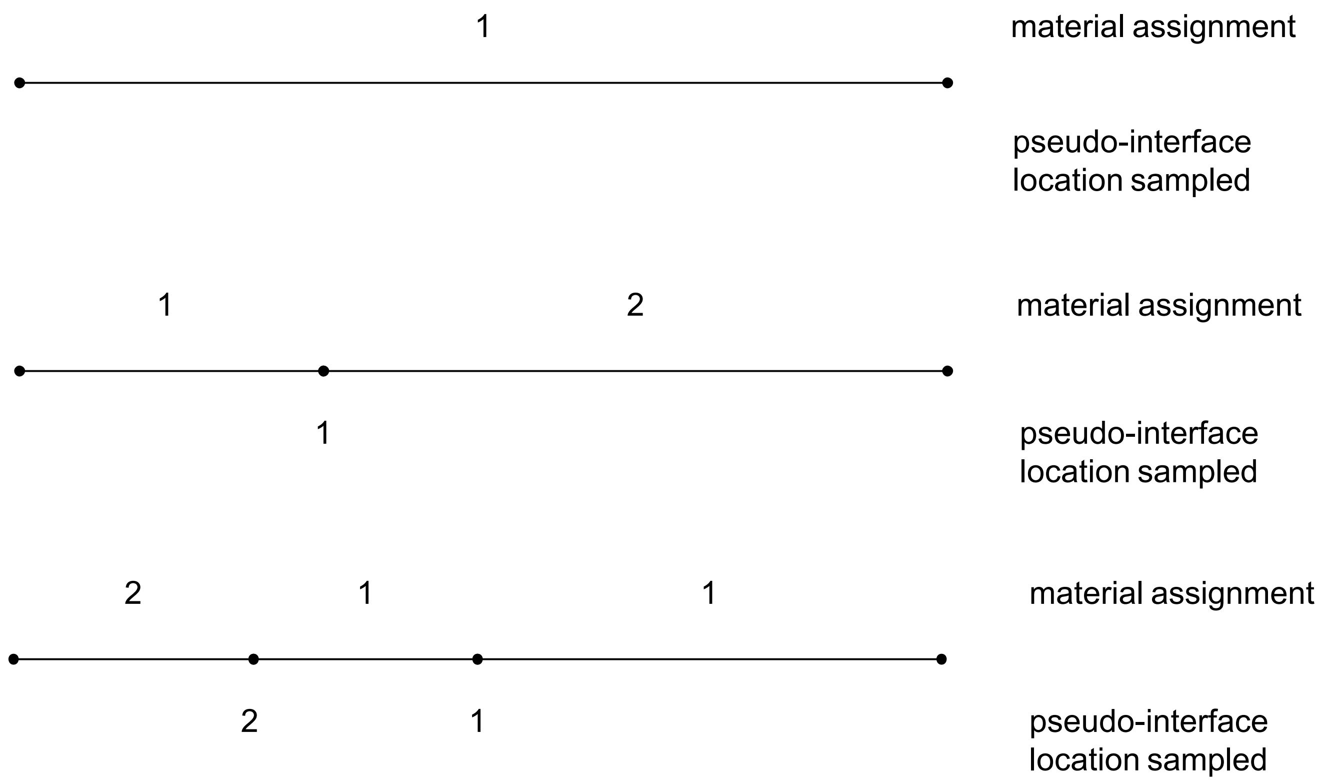
This allows us to divide the problem into strata characterized by the number of pseudo-interfaces (with known probabilities), and also to generate realizations based on pseudo-interface location rather than region width.

Pseudo-interface description and generation of realizations

stratum I, $f(I;\lambda_c)$

Example realizations

- $0,\ e^{-\lambda_c}$
- $1,\ e^{-\lambda_c}\lambda_c$
- $2,\ e^{-\lambda_c}\lambda_c{}^2/2$



Pseudo-interface approaches to the generation of realizations

- Monte Carlo sampling of the number of pseudo-interfaces, followed by Monte Carlo sampling of a realization, is equivalent to the original process.
- Alternative: Stratified sampling of the number of pseudo-interfaces, followed by Monte Carlo sampling of a realization, may offer some variance reduction.
- Alternative: Instead of stratified *sampling*, use a stratified *decomposition* – solve each stratified subproblem independently using the best solution technique.
  - ➢ Our approach: Within a stratum, use deterministic techniques to generate realizations instead of Monte Carlo sampling.

Quadrature generation of realizations

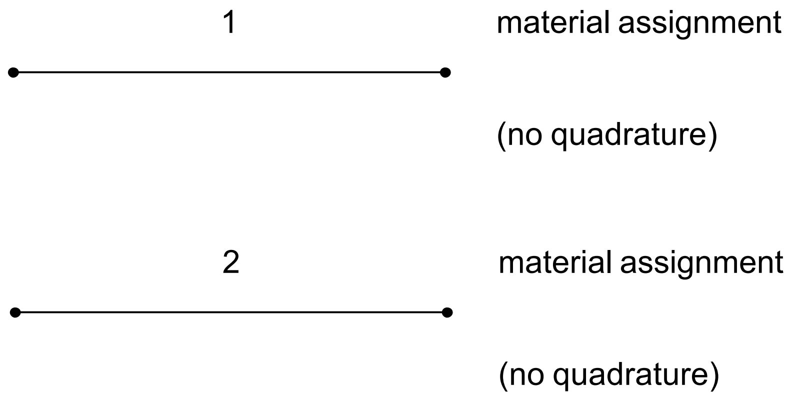
Technique:

- Use a numerical quadrature (e.g. Gauss-Legendre) to determine the location of each pseudo-interface for a given *I*. There will be as many quadratures as pseudo-interfaces (*I*-dimensional product quadrature). The accuracy will be governed by the quadrature order(s).
- Solve the transport problem for each generated realization, and combine results according to quadrature integration rules to solve the *I*th subproblem.

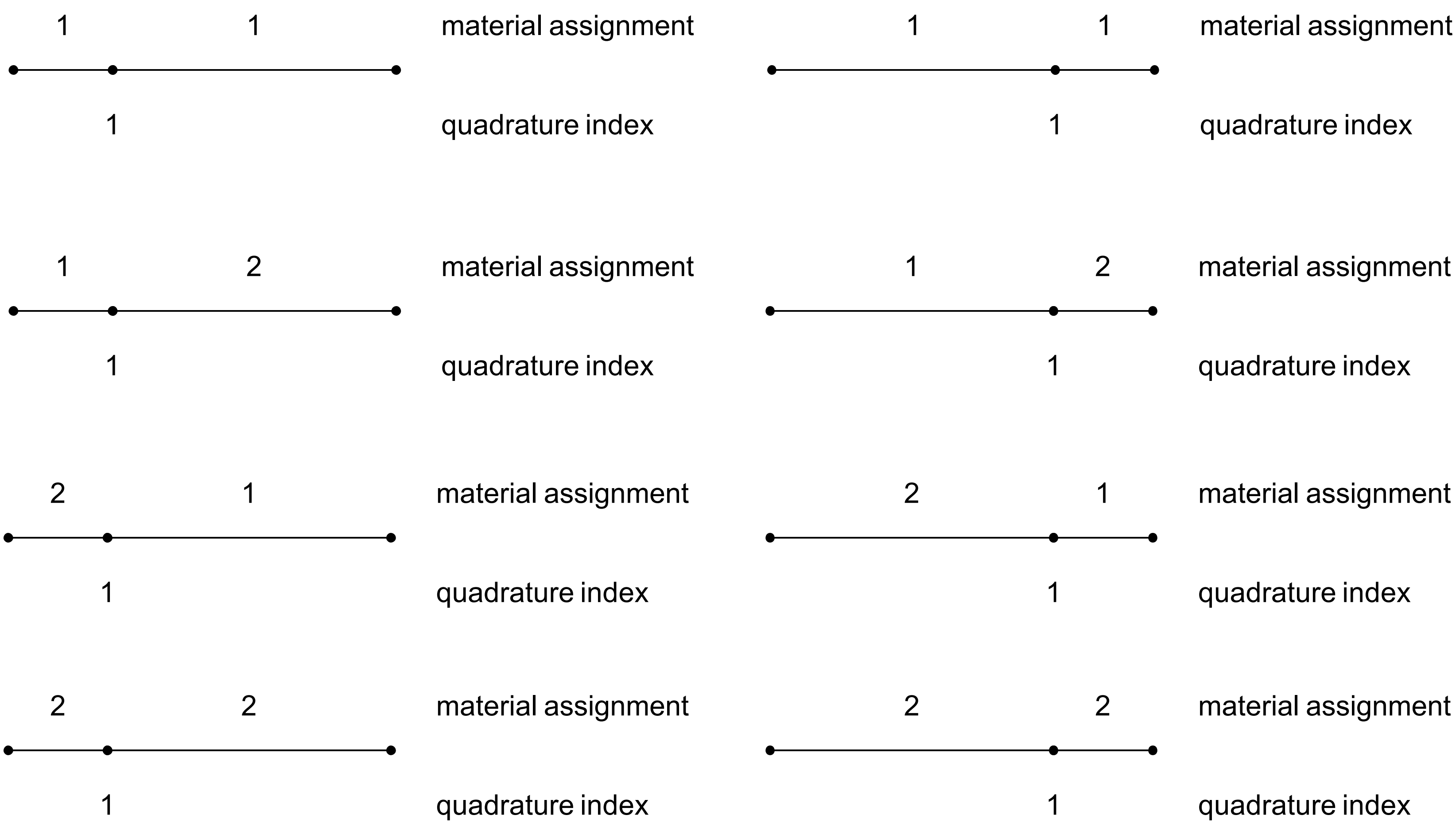
$$R_I = \sum_{n_1=1}^{N} w_{n_1} \sum_{n_2=1}^{N} w_{n_2} \cdots \sum_{n_I=1}^{N} w_{n_I} \sum_{m_0=0}^{1} p(m_0) \cdots \sum_{m_I=0}^{1} p(m_I) R_{n_1 n_2 \cdots n_I m_0 \cdots m_I}$$

- Combine the results over all subproblems according to Poisson weighting: $R = \sum_{I=0}^{I_{max}} R_I f(I; \lambda_c)$

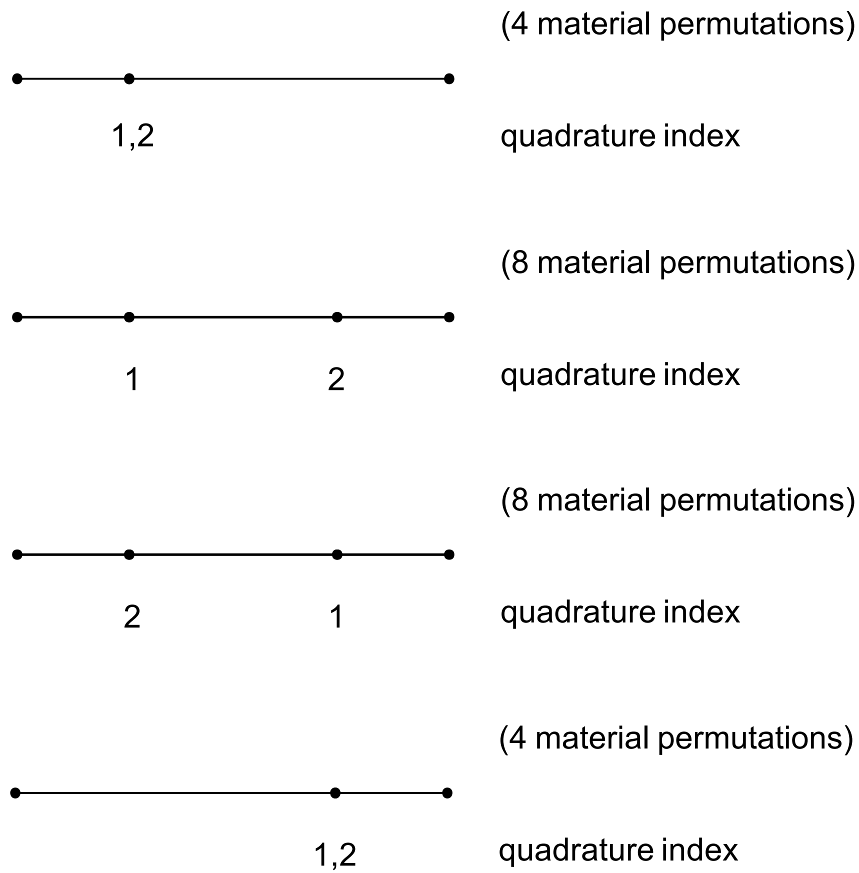
Quadrature generation of realizations with zero pseudo-interfaces (stratum 0)



2-point quadrature generation of realizations with one pseudo-interface (stratum 1)



2-point quadrature generation of realizations with two pseudo-interfaces (stratum 2)



Algorithmic complexity of quadrature approach

Expense of approach for *I* pseudo-interfaces and *N*th-order quadratures:

- Simple implementation: $O(2^{N+1}N^I), I \geq N$
  $O(2^{I+1}N^I), I < N$
- Solve only unique problems: $\leq O(2^{N+1})$
- Ignore low-weight problems: ???

Example: benchmark problem, reflection

Nine 1D, S_{16} benchmarks with isotropic source on left from M.L. Adams, E. W. Larsen and G.C. Pomraning, “Benchmark Results for Particle Transport in a Binary Markov Statistical Medium,” *J. Quant. Spectrosc. Radiat. Transfer*, **42**, pp. 253-266 (1989).

First benchmark: $\sigma_0 = \frac{10}{99}, \sigma_1 = \frac{100}{11}, c_0 = 0, c_1 = 1, \frac{\lambda_0}{\lambda_1} = 9, \Delta x = 0.1$

Results

I	N			
	2	4	8	16
0	0.04270	0.04270	0.04270	0.04270
1	0.05074	0.05056	0.05056	0.05056
2	0.05410	0.05475	0.05511	0.05522
3	0.05578	0.05730	0.05811	0.05836
4	0.05662	0.05896	0.06022	---
5	0.05704	0.06008	---	---

Estimated errors

I	N		
	2	4	8
0	0	0	0
1	0.0036	0.0000	0.0000
2	-0.0203	-0.0085	-0.0020
3	-0.0442	-0.0182	-0.0043
4	*-0.0598*	*-0.0209*	---
5	*-0.0506*	---	---

Benchmark results, reflection (Poisson summation over strata)

(Number of realizations in parentheses)

$\Delta x = 0.1$

problem	method		
	quadrature, order 2	quadrature, order 4	Monte Carlo (1%)
1	0.04887 (210)	0.04906 (4578)	0.0493 (58000)
2	0.008681 (210)	0.008679 (4578)	0.00874 (1100)
3	0.04824 (210)	0.04843 (4578)	0.0484 (37800)
4	0.04349 (34)	0.04348 (130)	0.0442 (83900)
5	0.008898 (34)	0.008900 (130)	0.00895 (1100)
6	0.04290 (34)	0.04289 (130)	0.0431 (53200)
7	0.07600 (10)	0.07600 (18)	0.0771 (9600)
8	0.0009835 (10)	0.0009836 (18)	0.000967 (10300)
9	0.06715 (10)	0.06715 (18)	0.0680 (9200)

$\Delta x = 1$

problem	method		
	quadrature, order 2	quadrature, order 4	Monte Carlo (1%)
4	0.1196 (210)	0.1201 (4578)	0.123 (49700)
5	0.07503 (210)	0.07481 (4578)	0.0744 (1500)
6	0.1424 (210)	0.1425 (4578)	0.145 (10200)
7	0.3221 (90)	0.3219 (818)	0.319 (8200)
8	0.008829 (90)	0.008864 (818)	0.00888 (10700)
9	0.2444 (90)	0.2442 (818)	0.242 (6900)

Potential application: improved LP closure

The Levermore-Pomraning (LP) equations describing particle transport in stochastic media would be exact except for the "LP closure":

$$\hat{\psi}_{s,m}(r,\Omega_k) \approx \hat{\psi}_m(r,\Omega_k)$$

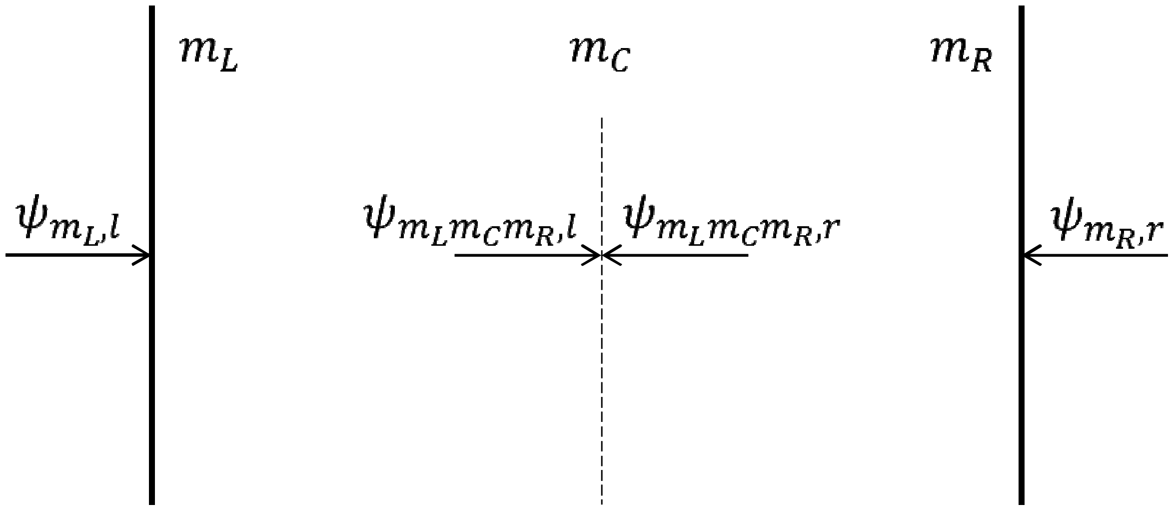
where $\hat{\psi}_m(r,\Omega_k)$ is the ensemble-averaged angular flux, conditioned on material *m* existing at *r*, and $\hat{\psi}_{s,m}(r,\Omega_k)$ is the same average but also conditioned on a surface (material interface) existing at *r* oriented such that the flux is leaving material *m*.

More generally, we may write $\vec{\hat{\psi}}_{s,m}(r,\Omega_k) \approx I\vec{\hat{\psi}}_m(r,\Omega_k)$

Modeling interface effects

- We wish to find a more general relationship between $\vec{\hat{\psi}}_{s,m}(r,\Omega_k)$ and $\vec{\hat{\psi}}_m(r,\Omega_k)$.
- To do this we will relate both to the boundary conditions, then combine the relationships to eliminate the boundary terms (we will ignore internal sources for now).

Modeling the general case (material interface *may* exist at *r)*



By performing transport calculations we may derive/approximate the following response matrix:

$$\begin{bmatrix} \psi_{m_L m_C m_R,l} \\ \psi_{m_L m_C m_R,r} \end{bmatrix} = R_{m_L m_C m_R} \begin{bmatrix} \psi_{m_L,l} \\ \psi_{m_R,r} \end{bmatrix}$$

Modeling the general case (material interface *may* exist at *r*)

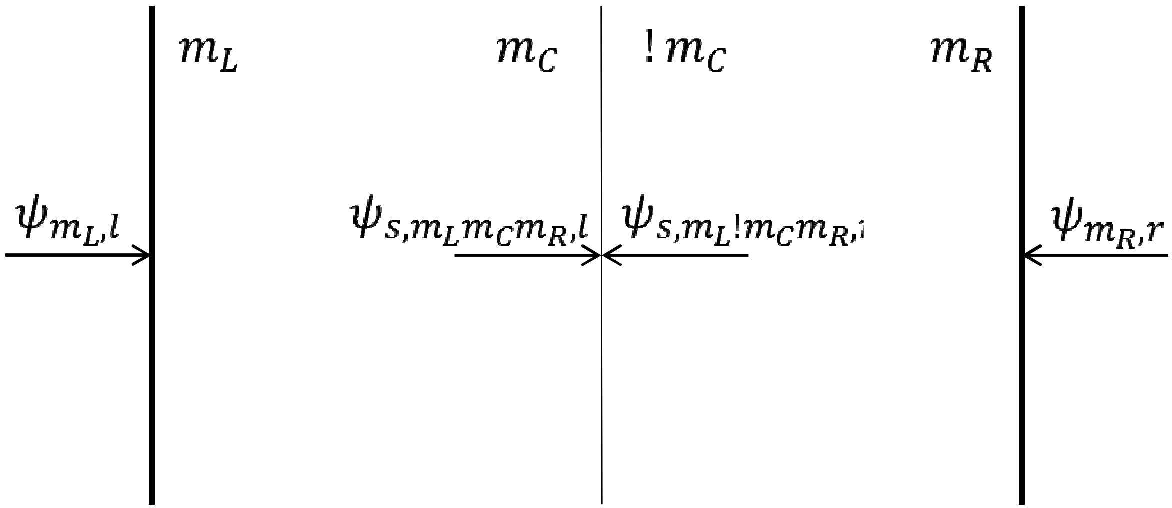
Ensemble-averaged interior flux

$$\hat{\psi}_{i,1,l} = p_{111}\psi_{111,l} + p_{112}\psi_{112,l} + p_{211}\psi_{211,l} + p_{212}\psi_{212,l}$$

By combining the above equation(s) with the various material configuration-dependent response matrices we can determine the overall average interior response of the system:

$$\begin{bmatrix} \hat{\psi}_{i,1,l} \\ \hat{\psi}_{i,1,r} \\ \hat{\psi}_{i,2,l} \\ \hat{\psi}_{i,2,r} \end{bmatrix} = R_i \begin{bmatrix} \psi_{1,l} \\ \psi_{1,r} \\ \psi_{2,l} \\ \psi_{2,r} \end{bmatrix}$$

Modeling the special case (material interface *must* exist at *r*)



By performing transport calculations we may derive/approximate the following response matrix:

$$\begin{bmatrix} \psi_{s,m_L m_C m_R,l} \\ \psi_{s,m_L!m_C m_R,r} \end{bmatrix} = R_{s,m_L m_C m_R} \begin{bmatrix} \psi_{m_L,l} \\ \psi_{m_R,r} \end{bmatrix}$$

Modeling the special case (material interface *must* exist at *r*)

Ensemble-averaged interior surface flux

$$\hat{\psi}_{s,1,l} = p_{s,111}\psi_{s,111,l} + p_{s,112}\psi_{s,112,l} + p_{s,211}\psi_{s,211,l} + p_{s,212}\psi_{s,212,l}$$

By combining the above equation(s) with the various material configuration-dependent response matrices we can determine the overall average interior surface response of the system. Combining the two responses (surface/general) then provides the correct closure for the LP equations:

$$\begin{bmatrix} \hat{\psi}_{s,1,l} \\ \hat{\psi}_{s,1,r} \\ \hat{\psi}_{s,2,l} \\ \hat{\psi}_{s,2,r} \end{bmatrix} = R_s \begin{bmatrix} \psi_{1,l} \\ \psi_{1,r} \\ \psi_{2,l} \\ \psi_{2,r} \end{bmatrix} \longrightarrow \begin{bmatrix} \hat{\psi}_{s,1,l} \\ \hat{\psi}_{s,1,r} \\ \hat{\psi}_{s,2,l} \\ \hat{\psi}_{s,2,r} \end{bmatrix} = R_s {R_i}^{-1} \begin{bmatrix} \psi_{1,l} \\ \psi_{1,r} \\ \psi_{2,l} \\ \psi_{2,r} \end{bmatrix}$$

Improvements to LP

- We have calculated some of the response matrices via Monte Carlo sampling of realizations and implemented in an LP code.
- Mixed results
  - Combined response matrix seems sensitive to statistical noise
  - Preliminary results do seem better than standard LP
- Deterministic selection of realizations may be helpful
  - Correlated selection of realizations
  - Fewer realizations for small number of interfaces
- Ultimate goal: Perform *local* calculation of response matrices: either ignore problem outside some radius of influence or homogenize the materials

Future work

- Condensed calculations
- Sparse-grid quadratures
- Apply to subgrid modeling (e.g. Levermore-Pomraning improvements)

Conclusions

- Quadrature generation/integration of realizations is computationally efficient when the number of pseudo-interfaces is small
- Approach quickly becomes expensive as the number of pseudo-interfaces grows
- Demonstrated in 1D, but easily extended to multi-D
- There may be practical applications, e.g. local models
- Bigger picture – examine stochastic problems from a stratified perspective