

A Generalized Levermore-Pomraning Closure for Stochastic Media Transport Problems

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Shawn D. Pautz
Brian C. Franke
Sandia National Laboratories
Albuquerque, NM

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Outline

- Summary of research
- LP closure
- Generalized closure
- Discretization
- Results
- Conclusions

Summary of research

- We are interested in improved stochastic media computational techniques, in particular alternatives to the Levermore-Pomraning (LP) closure involving subgrid models.
- We have attempted to create a more general approach to creating closures to the stochastic equations.
- To apply the more general approach we have leveraged previous work on deterministic generation of realizations to construct our closures.

Statistical transport equation

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

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

$\langle \psi_i(\vec{r}, \vec{\Omega}) \rangle$: 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

LP closure

In order to solve the statistical transport equation we must relate $\langle \psi_i(\vec{r}, \vec{\Omega}) \rangle$ and $\langle \psi_{s,i}(\vec{r}, \vec{\Omega}) \rangle$. One way to do that is to make the following assumption (LP closure):

$$\langle \psi_{s,i}(\vec{r}, \vec{\Omega}) \rangle \approx \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle$$

This yields the LP equations:

$$\begin{aligned} & \vec{\Omega} \cdot \nabla \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle + \sigma_{t,i} \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle \\ & = \frac{\sigma_{s,i}}{4\pi} \int d\vec{\Omega}' \langle \psi_i(\vec{r}, \vec{\Omega}') \rangle + \lambda_i^{-1} (\langle \psi_j(\vec{r}, \vec{\Omega}) \rangle - \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle) \end{aligned}$$

Generalized closure

The LP closure may be expressed as:

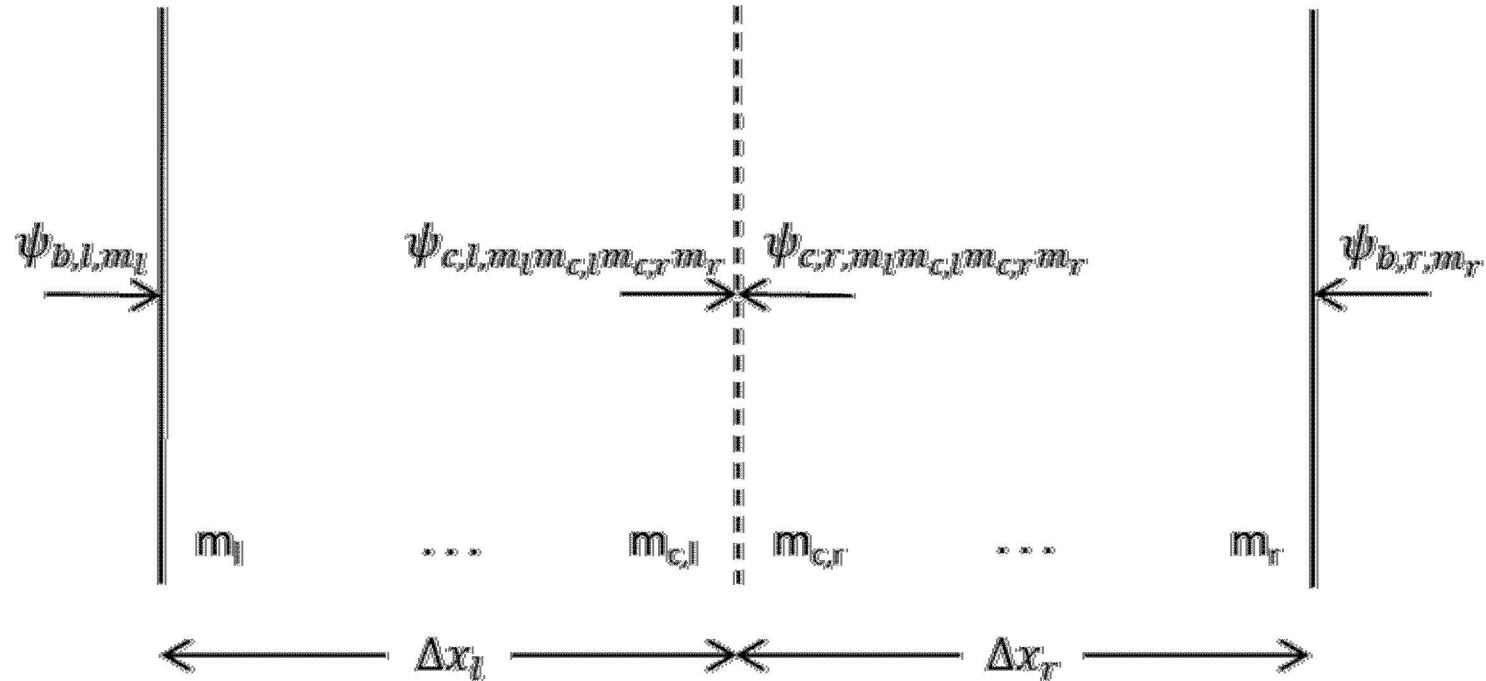
$$[\langle \psi_s(\vec{r}, \vec{\Omega}) \rangle] \approx I[\langle \psi(\vec{r}, \vec{\Omega}) \rangle]$$

Where $[\]$ indicates a vector/operator in both angular and material space and I is the identity matrix. For our approach we make the more general ansatz:

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

Here R is a response matrix, which may in general be dense. Our goal is to determine (or approximate) R .

Generalized rod problem



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

Conditional response matrices

Given an ensemble of realizations with particular materials at the boundaries and at a “central” location of interest, we can form the following expression:

$$\begin{bmatrix} \langle \psi_{c,l,m_l m_c, l m_c, r m_r} \rangle \\ \langle \psi_{c,r,m_l m_c, l m_c, r m_r} \rangle \end{bmatrix} = R_{m_l m_c, l m_c, r m_r}(\vec{r}) \begin{bmatrix} \psi_{b,l,m_l} \\ \psi_{b,r,m_r} \end{bmatrix}$$

$R_{m_l m_c, l m_c, r m_r}(\vec{r})$ is a conditional response matrix relating the interior fluxes to the boundary fluxes (conditioned on four different materials).

Conditional response matrices

We form the following conditional averages:

$$\begin{aligned}\langle\psi_{l,1}\rangle &= p_{1111}\langle\psi_{c,l,1111}\rangle + p_{1112}\langle\psi_{c,l,1112}\rangle + p_{1121}\langle\psi_{c,l,1121}\rangle + p_{1122}\langle\psi_{c,l,1122}\rangle + \\ &\quad p_{2111}\langle\psi_{c,l,2111}\rangle + p_{2112}\langle\psi_{c,l,2112}\rangle + p_{2121}\langle\psi_{c,l,2121}\rangle + p_{2122}\langle\psi_{c,l,2122}\rangle \\ \langle\psi_{r,1}\rangle &= p_{1111}\langle\psi_{c,l,1111}\rangle + p_{1112}\langle\psi_{c,l,1112}\rangle + p_{1211}\langle\psi_{c,l,1211}\rangle + p_{1212}\langle\psi_{c,l,1212}\rangle + \\ &\quad p_{2111}\langle\psi_{c,l,2111}\rangle + p_{2112}\langle\psi_{c,l,2112}\rangle + p_{2211}\langle\psi_{c,l,2211}\rangle + p_{2212}\langle\psi_{c,l,2212}\rangle \\ \langle\psi_{l,2}\rangle &= p_{1211}\langle\psi_{c,l,1211}\rangle + p_{1212}\langle\psi_{c,l,1212}\rangle + p_{1221}\langle\psi_{c,l,1221}\rangle + p_{1222}\langle\psi_{c,l,1222}\rangle + \\ &\quad p_{2211}\langle\psi_{c,l,2211}\rangle + p_{2212}\langle\psi_{c,l,2212}\rangle + p_{2221}\langle\psi_{c,l,2221}\rangle + p_{2222}\langle\psi_{c,l,2222}\rangle \\ \langle\psi_{r,2}\rangle &= p_{1121}\langle\psi_{c,l,1121}\rangle + p_{1122}\langle\psi_{c,l,1122}\rangle + p_{1221}\langle\psi_{c,l,1221}\rangle + p_{1222}\langle\psi_{c,l,1222}\rangle + \\ &\quad p_{2121}\langle\psi_{c,l,2121}\rangle + p_{2122}\langle\psi_{c,l,2122}\rangle + p_{2221}\langle\psi_{c,l,2221}\rangle + p_{2222}\langle\psi_{c,l,2222}\rangle\end{aligned}$$




$$\begin{bmatrix} \langle\psi_{l,1}\rangle \\ \langle\psi_{r,1}\rangle \\ \langle\psi_{l,2}\rangle \\ \langle\psi_{r,2}\rangle \end{bmatrix} = R_a(\vec{r}) \begin{bmatrix} \psi_{b,l,1} \\ \psi_{b,r,1} \\ \psi_{b,l,2} \\ \psi_{b,r,2} \end{bmatrix}$$

Conditional surface response matrices

We form the following conditional surface/interface averages:

$$\begin{aligned}\langle \psi_{s,l,1} \rangle &= p_{1121} \langle \psi_{c,l,1121} \rangle + p_{1122} \langle \psi_{c,l,1122} \rangle + p_{2121} \langle \psi_{c,l,2121} \rangle + p_{2122} \langle \psi_{c,l,2122} \rangle \\ \langle \psi_{s,r,1} \rangle &= p_{1211} \langle \psi_{c,l,1211} \rangle + p_{1212} \langle \psi_{c,l,1212} \rangle + p_{2211} \langle \psi_{c,l,2211} \rangle + p_{2212} \langle \psi_{c,l,2212} \rangle \\ \langle \psi_{s,l,2} \rangle &= p_{1211} \langle \psi_{c,l,1211} \rangle + p_{1212} \langle \psi_{c,l,1212} \rangle + p_{2211} \langle \psi_{c,l,2211} \rangle + p_{2212} \langle \psi_{c,l,2212} \rangle \\ \langle \psi_{s,r,2} \rangle &= p_{1121} \langle \psi_{c,l,1121} \rangle + p_{1122} \langle \psi_{c,l,1122} \rangle + p_{2121} \langle \psi_{c,l,2121} \rangle + p_{2122} \langle \psi_{c,l,2122} \rangle\end{aligned}$$



$$\begin{bmatrix} \langle \psi_{s,l,1} \rangle \\ \langle \psi_{s,r,1} \rangle \\ \langle \psi_{s,l,2} \rangle \\ \langle \psi_{s,r,2} \rangle \end{bmatrix} = R_s(\vec{r}) \begin{bmatrix} \psi_{b,l,1} \\ \psi_{b,r,1} \\ \psi_{b,l,2} \\ \psi_{b,r,2} \end{bmatrix} = R_s(\vec{r}) R_a^{-1}(\vec{r}) \begin{bmatrix} \langle \psi_{l,1} \rangle \\ \langle \psi_{r,1} \rangle \\ \langle \psi_{l,2} \rangle \\ \langle \psi_{r,2} \rangle \end{bmatrix} \equiv R(\vec{r}) \begin{bmatrix} \langle \psi_{l,1} \rangle \\ \langle \psi_{r,1} \rangle \\ \langle \psi_{l,2} \rangle \\ \langle \psi_{r,2} \rangle \end{bmatrix}$$

Generalized LP equations

We then obtain the generalized form of the LP equations:

$$\begin{aligned}
 & \vec{\Omega} \cdot \nabla \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle + \sigma_{t,i} \langle \psi_i(\vec{r}, \vec{\Omega}) \rangle \\
 & = \frac{\sigma_{s,i}}{4\pi} \int d\vec{\Omega}' \langle \psi_i(\vec{r}, \vec{\Omega}') \rangle + \lambda_i^{-1} \left(\left(R(\vec{r}) \begin{bmatrix} \langle \psi_{l,1} \rangle \\ \langle \psi_{r,1} \rangle \\ \langle \psi_{l,2} \rangle \\ \langle \psi_{r,2} \rangle \end{bmatrix} \right)_{j, \vec{\Omega}} - \left(R(\vec{r}) \begin{bmatrix} \langle \psi_{l,1} \rangle \\ \langle \psi_{r,1} \rangle \\ \langle \psi_{l,2} \rangle \\ \langle \psi_{r,2} \rangle \end{bmatrix} \right)_{i, \vec{\Omega}} \right)
 \end{aligned}$$

The above is a formal expression; we still need to determine each of the conditional response matrices $R_{m_l m_c, l m_c, r m_r}(\vec{r})$.

Properties of generalized closure

- Determination of $R_{m_l m_c, l m_c, r m_r}(\vec{r})$ may still require many transport calculations, but it is an alternative.
- Potential use in subgrid models (we haven't required Δx to be the full problem domain).
- When $\Delta x_l \rightarrow \Delta x_r \rightarrow 0$ we obtain the LP closure.
- We also obtain the LP closure for purely absorbing Markovian materials.

Determination of response matrices

- The various $R_{m_l m_c, l m_c, r m_r}(\vec{r})$ may be obtained by various methods.
- One possible method: Monte Carlo sampling of realizations. Possible problem with correlation.
- Alternative: deterministic generation of realizations (see other presentation in this session). Expensive for large numbers of interfaces, but potentially useful for subgrid models.
- We will use the deterministic approach to the generation of realizations, and also a deterministic transport code (Sceptre) for the solution of each realization.

Results

Response matrix, case 1, 15-point interface quadrature, 15 pseudo-interfaces

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 0.99, \lambda_2 = 0.11$$

Δx	location	
	center	left boundary
0.1	$\begin{bmatrix} 1.00313 & -0.00464 & -0.00306 & 0.00457 \\ -0.00464 & 1.00313 & 0.00457 & -0.00306 \\ -0.02570 & 0.15479 & 1.02536 & -0.15444 \\ 0.15479 & -0.02570 & -0.15444 & 1.02536 \end{bmatrix}$	$\begin{bmatrix} 1.00337 & -0.00009 & -0.00337 & 0.00009 \\ -0.01306 & 1.00307 & 0.01298 & -0.00299 \\ -0.03047 & 0.02769 & 1.03047 & -0.02769 \\ 0.21662 & -0.02785 & -0.21635 & 1.02759 \end{bmatrix}$
1	$\begin{bmatrix} 0.52998 & -0.02478 & 0.66238 & -0.17187 \\ -0.02478 & 0.52998 & -0.17187 & 0.66238 \\ 0.06335 & 0.19044 & 0.75991 & -0.01250 \\ 0.19044 & 0.06335 & -0.01250 & 0.75990 \end{bmatrix}$	$\begin{bmatrix} 1.03240 & -0.00271 & -0.03156 & 0.00190 \\ -0.14695 & 0.46473 & -0.03174 & 0.70810 \\ -0.29650 & 0.10827 & 1.26310 & -0.07598 \\ 0.42104 & 0.07548 & -0.31849 & 0.82529 \end{bmatrix}$
10	$\begin{bmatrix} 0.32325 & -0.03510 & 2.29299 & -1.63250 \\ -0.03510 & 0.32325 & -1.63250 & 2.29299 \\ -0.02831 & 0.25740 & -0.54531 & 1.28868 \\ 0.25740 & -0.02831 & 1.28867 & -0.54530 \end{bmatrix}$	$\begin{bmatrix} 1.04513 & -0.00767 & -0.01727 & -0.01880 \\ -0.23824 & 0.30503 & -1.01312 & 1.88455 \\ -0.35468 & 0.23039 & 0.51859 & 0.56439 \\ 0.82264 & 0.00544 & -0.48904 & 0.67734 \end{bmatrix}$

Generalized LP results

Relative error in reflection, case 7, $x=1$

$$\sigma_1 = \frac{2}{101}, \sigma_2 = \frac{200}{101}, c_1 = 0, c_2 = 1, \lambda_1 = \lambda_2 = 5.05 (P_{avg}=0.396)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01
7	-0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
11	-0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
15	-0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
7	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
11	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
15	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

Generalized LP results

Relative error in transmission, case 7, $\alpha=1$

$$\sigma_1 = \frac{2}{101}, \sigma_2 = \frac{200}{101}, c_1 = 0, c_2 = 1, \lambda_1 = \lambda_2 = 5.05 (P_{avg}=0.396)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.004	0.004	0.004	0.004	0.004	0.004
7	0.004	0.003	0.003	0.003	0.003	0.003
11	0.004	0.003	0.003	0.003	0.003	0.003
15	0.004	0.003	0.003	0.003	0.003	0.003

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.003	0.002	0.002	0.002	0.002	0.002
7	0.002	0.001	< 0.001	< 0.001	< 0.001	< 0.001
11	0.002	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
15	0.002	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001

Generalized LP results

Relative error in reflection, case 4, $x=1$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 9.9, \lambda_2 = 1.1, (P_{avg}=1.01)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.07	-0.07	-0.07	-0.07	-0.07	-0.07
7	-0.06	-0.06	-0.06	-0.05	-0.05	-0.05
11	-0.06	-0.06	-0.05	-0.05	-0.05	-0.05
15	-0.06	-0.05	-0.05	-0.05	-0.05	-0.05

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05
7	-0.04	-0.03	-0.02	-0.02	-0.02	-0.02
11	-0.03	-0.02	-0.01	-0.01	-0.01	-0.01
15	-0.03	-0.02	-0.01	< 0.01	< 0.01	< 0.01

Generalized LP results

Relative error in transmission, case 4, $x=1$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 9.9, \lambda_2 = 1.1, (P_{avg}=1.01)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.010	0.009	0.009	0.009	0.009	0.009
7	0.009	0.008	0.008	0.008	0.008	0.008
11	0.009	0.008	0.007	0.007	0.007	0.007
15	0.008	0.007	0.007	0.007	0.007	0.007

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.008	0.007	0.007	0.006	0.006	0.006
7	0.005	0.004	0.003	0.003	0.003	0.003
11	0.004	0.003	0.002	0.002	0.002	0.002
15	0.004	0.002	0.001	0.001	0.001	0.001

Generalized LP results

Relative error in reflection, case 1, $x=1$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 0.99, \lambda_2 = 0.11, (P_{avg}=10.1)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.004	-0.028	-0.070	-0.316	-0.598	-0.641
7	0.034	0.007	-0.029	-0.263	-0.423	-0.423
11	0.043	0.017	-0.015	-0.215	-0.301	-0.289
15	0.047	0.022	-0.009	-0.188	-0.243	-0.226

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.052	-0.054	-0.186	-0.624	-0.748	-0.763
7	0.104	0.003	-0.116	-0.359	-0.371	-0.366
11	0.116	0.023	-0.080	-0.269	-0.244	-0.230
15	0.121	0.033	-0.064	-0.228	-0.186	-0.169

Generalized LP results

Relative error in transmission, case 1, $x=1$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 0.99, \lambda_2 = 0.11, (P_{avg}=10.1)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.001	0.008	0.021	0.096	0.181	0.194
7	-0.011	-0.002	0.009	0.080	0.128	0.128
11	-0.013	-0.005	0.005	0.065	0.091	0.087
15	-0.014	-0.007	0.003	0.057	0.074	0.068

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.016	0.016	0.056	0.189	0.226	0.231
7	-0.031	< 0.001	0.035	0.109	0.112	0.111
11	-0.035	-0.007	0.024	0.081	0.074	0.070
15	-0.037	-0.010	0.019	0.069	0.056	0.051

Generalized LP results (note instabilities)

Relative error in reflection, case 1, $x=10$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 0.99, \lambda_2 = 0.11, (P_{avg}=101)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.063	0.033	-0.030	-0.840	N/A	N/A
7	0.083	0.047	-0.022	N/A	N/A	N/A
11	0.090	0.052	-0.016	N/A	N/A	N/A
15	0.094	0.056	-0.012	N/A	N/A	N/A

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	0.061	-0.023	-0.153	N/A	N/A	N/A
7	0.123	0.018	-0.227	N/A	N/A	N/A
11	0.145	0.049	-0.153	N/A	N/A	N/A
15	0.156	0.069	-0.094	N/A	N/A	N/A

Generalized LP results (note instabilities)

Relative error in transmission, case 1, $x=10$

$$\sigma_1 = \frac{10}{99}, \sigma_2 = \frac{100}{11}, c_1 = 0, c_2 = 1, \lambda_1 = 0.99, \lambda_2 = 0.11, (P_{avg}=101)$$

Center response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.33	-0.17	0.09	1.0	N/A	N/A
7	-0.43	-0.25	0.05	N/A	N/A	N/A
11	-0.47	-0.27	0.03	N/A	N/A	N/A
15	-0.49	-0.29	0.01	N/A	N/A	N/A

Spatially-varying response matrix:

N	P_{max}					
	1	2	3	7	11	15
3	-0.46	-0.06	0.39	N/A	N/A	N/A
7	-0.68	-0.23	0.48	N/A	N/A	N/A
11	-0.75	-0.33	0.32	N/A	N/A	N/A
15	-0.79	-0.38	0.20	N/A	N/A	N/A

Subgrid results

Relative error of (subgrid) models, $x=1$

Reflection

case	$\Delta x_l + \Delta x_r$		
	0 (LP)	0.1	1
1	-0.084	-0.038	-0.169
2	-0.103	-0.098	0.229
3	-0.091	-0.046	-0.185
4	-0.10	-0.06	< 0.01
5	-0.028	-0.025	< 0.001
6	-0.11	-0.07	< 0.01
7	< 0.01	< 0.01	< 0.01
8	-0.01	-0.01	< 0.01
9	-0.01	< 0.01	< 0.01

Transmission

case	$\Delta x_l + \Delta x_r$		
	0 (LP)	0.1	1
1	0.025	0.012	0.051
2	< 0.001	-0.008	0.365
3	0.024	0.011	0.064
4	0.014	0.008	0.001
5	0.002	0.002	< 0.001
6	0.010	0.006	< 0.001
7	0.003	0.002	< 0.001
8	< 0.01	< 0.01	< 0.01
9	0.004	0.003	< 0.001

Subgrid results

Relative error of (subgrid) models, $x=10$

Reflection

case	$\Delta x_l + \Delta x_r$			
	0 (LP)	0.1	1	10
1	-0.101	-0.076	0.041	---
2	-0.28	-0.28	-0.26	---
3	-0.157	-0.132	-0.033	---
4	-0.24	-0.18	-0.06	-0.17
5	-0.245	-0.244	-0.226	-0.223
6	-0.330	-0.272	-0.141	-0.156
7	-0.113	-0.106	-0.069	-0.017
8	-0.32	-0.31	-0.28	0.04
9	-0.212	-0.200	-0.135	-0.016

Transmission

case	$\Delta x_l + \Delta x_r$			
	0 (LP)	0.1	1	10
1	0.47	0.35	-0.14	---
2	-0.04	-0.11	-0.43	---
3	0.36	0.27	-0.23	---
4	0.29	0.22	0.07	0.19
5	-0.03	-0.03	-0.05	-1.03
6	0.11	0.10	0.08	0.73
7	0.33	0.30	0.20	0.05
8	< 0.01	< 0.01	-0.02	0.15
9	0.19	0.17	0.11	0.11

Conclusions

- We have created a more generalized framework for closures to the statistical transport equations
- The LP closure is a special case/limit of this framework
- We have used a deterministic approach to compute these closures
- These more general closures are more accurate than LP, provided that they are computed with sufficient resolution

Future work

- Improve the theory
- Explore more optimal sizes for subgrid models
- Correct for boundary effects
- Have greater detail near the point of interest and less detail or homogenization far away
- Extend to higher-order angular quadratures and multigroup