Spatial Moments of Continuous Transport Problems Computed on Grids

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Method of Moments

- The method of moments is a well-known technique for determining exact expressions for spatial and angular moments of radiation distributions in infinite, homogeneous media.
- These moments can then be used to calculate other quantities of interest (e.g., the “mean” and “variance” of the radiation distribution).
- The method of moments has also been applied to various numerical techniques in order to investigate their accuracy:
To further describe the method of moments, we consider the following transport problem in an infinite, homogeneous medium:

\[
\mu \frac{\partial \psi}{\partial x} + \Sigma_t \psi = \frac{\Sigma_s}{2} \int_{-1}^{1} \psi(x, \mu') d\mu' + \frac{Q}{2}
\]

\[
\lim_{|x| \to \infty} \psi = 0
\]

Here, we require that \( Q(x) \) vanish rapidly enough as \( |x| \to \infty \) such that the boundary conditions are satisfied but is otherwise arbitrary.

For this problem, we define moments of the scalar flux and the source of the form

\[
\phi_m = \int_{-\infty}^{\infty} x^m \phi(x) dx
\]

\[
Q_m = \int_{-\infty}^{\infty} x^m Q(x) dx
\]
The moments of the scalar flux can be expressed in terms of the moments of the source through a straightforward application of Legendre polynomials and integration by parts (e.g., see Brantley and Larsen, *Nucl. Sci. Eng.*, 2000).

From this process, the first few moments of the scalar flux are

\[
\phi_0 = \frac{1}{\Sigma a} Q_0
\]

\[
\phi_1 = \frac{1}{\Sigma a} Q_1
\]

\[
\phi_2 = \frac{1}{\Sigma a} Q_2 + \frac{2}{3\Sigma t \Sigma a^2} Q_0
\]
If we denote the flux-weighted and source-weighted averages of $x$ by

$$\langle x \rangle_\phi = \frac{\phi_1}{\phi_0}$$

$$\langle x \rangle_Q = \frac{Q_1}{Q_0}$$

then the expressions for $\phi_0$ and $\phi_1$ yield

$$\langle x \rangle_\phi = \langle x \rangle_Q$$

Thus, the flux-weighted average of $x$ is equal to the source-weighted average of $x$. 
Method of Moments (continued)

- Similarly, if we denote the flux-weighted and source-weighted averages of $x^2$ by

$$\langle x^2 \rangle_\phi = \frac{\phi_2}{\phi_0}$$

$$\langle x^2 \rangle_Q = \frac{Q_2}{Q_0}$$

then the expressions for $\phi_0$ and $\phi_2$ yield

$$\langle x^2 \rangle_\phi = \langle x^2 \rangle_Q + 2L^2$$

where $L = 1/\sqrt{3\Sigma_t\Sigma_a}$ is the diffusion length.

- Thus, the flux-weighted average of $x^2$ is greater than the source-weighted average of $x^2$ by $2L^2$. 
Method of Moments on a Grid

- Here, we examine how the method of moments is altered when
  - the underlying transport problem is spatially continuous but involves a grid
  - moments are computed on this grid instead of through integration over the entire domain
- More specifically, we will determine the changes to the expressions for the flux-weighted averages of $x$ and $x^2$ as a result of
  - prescribing a uniform grid consisting of an infinite number of cells
  - replacing our previous moment definitions with

\[
\phi_m = \sum_{j=-\infty}^{\infty} x_j^m \phi_j \Delta x
\]

\[
Q_m = \sum_{j=-\infty}^{\infty} x_j^m Q_j \Delta x
\]
Method of Moments on a Grid (continued)

In these new definitions,
- $\Delta x$ is the cell width
- $x_j$ is the center of cell $j$
- $\phi_j$ and $Q_j$ are the average scalar flux and source in cell $j$, i.e.,

$$
\phi_j = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \phi(x) \, dx
$$

$$
Q_j = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} Q(x) \, dx
$$

where $x_{j-1/2}$ and $x_{j+1/2}$ are the left and right cell edges, respectively.

For simplicity, we will also assume that the source is piecewise constant such that $Q_j$ is the value of the source in cell $j$, although the work that follows can certainly be adapted to other spatial dependencies.
This modification to the method of moments is of interest, for example, in the Monte Carlo simulation of radiative transfer, where:

- some quantities are treated as spatially continuous (i.e., the radiation intensity)
- some quantities are treated as spatially discrete (i.e., the material temperature)

Under these conditions, it is not straightforward to generate expressions for moments that are defined by integrals over the entire domain.

With this modification, the method of moments can be employed to investigate the accuracy of these types of calculations and develop improved spatial discretizations.
Singular Eigenfunction Solution

- We first develop expressions for the flux-weighted averages of $x$ and $x^2$ corresponding to the new moment definitions using the singular eigenfunction method.
- From this method, the angular flux within cell $j$ is of the form

$$\psi(x, \mu) = a_j \phi_+(\mu) e^{-\Sigma_t(x-x_{j-1}/2)/\nu_0} + b_j \phi_-(\mu) e^{\Sigma_t(x-x_{j-1}/2)/\nu_0}$$

$$+ \int_{-1}^{1} A_j(\nu) \phi_{\nu}(\mu) e^{-\Sigma_t(x-x_{j-1}/2)/\nu} d\nu + \frac{Q_j}{2\Sigma_a}$$

- Here,
  - $\phi_+(\mu)$ and $\phi_-(\mu)$ are the discrete eigenfunctions
  - $\phi_{\nu}(\mu)$ is the continuum eigenfunction
  - $\nu_0$ is the (positive) discrete eigenvalue
  - $a_j$, $b_j$, and $A_j(\nu)$ are coefficients yet to be determined
The average scalar flux in cell $j$ is then

$$
\phi_j = \frac{1}{\Sigma_t \Delta x} \left[ a_j \nu_0 \left( 1 - e^{-\Sigma_t \Delta x / \nu_0} \right) - b_j \nu_0 \left( 1 - e^{\Sigma_t \Delta x / \nu_0} \right) 
+ \int_{-1}^{1} A_j(\nu) \nu \left( 1 - e^{-\Sigma_t \Delta x / \nu} \right) d\nu \right] + \frac{Q_j}{\Sigma_a}
$$
Singular Eigenfunction Solution (continued)

In addition, continuity of the angular flux at cell edges and orthogonality of the eigenfunctions yield

\[ a_j N_0 e^{-\Sigma t \Delta/\nu_0} + \frac{\nu_0 Q_j}{2\Sigma_t} = a_{j+1} N_0 + \frac{\nu_0 Q_{j+1}}{2\Sigma_t} \]

\[ b_j N_0 e^{\Sigma t \Delta/\nu_0} + \frac{\nu_0 Q_j}{2\Sigma_t} = b_{j+1} N_0 + \frac{\nu_0 Q_{j+1}}{2\Sigma_t} \]

\[ A_j(\nu) N(\nu) e^{-\Sigma t \Delta/\nu} + \frac{\nu Q_j}{2\Sigma_t} = A_{j+1}(\nu) N(\nu) + \frac{\nu Q_{j+1}}{2\Sigma_t} \]

where \( N_0 \) and \( N(\nu) \) are the discrete and continuum full-range normalization constants, respectively.
Multiplying these equations for $a_j$, $b_j$, and $A_j(\nu)$ by 1, $x_j$, and $x_j^2$, summing over all cells, and using the results with the expression for $\phi_j$ allows us to write

\[
\phi_0 = \frac{1}{\Sigma_a} Q_0
\]

\[
\phi_1 = \frac{1}{\Sigma_a} Q_1
\]

\[
\phi_2 = \frac{1}{\Sigma_a} Q_2 + \frac{\Delta x}{\Sigma_t^2} \left[ \frac{\nu_0^2}{N_0} \coth \left( \frac{\Sigma_t \Delta x}{2\nu_0} \right) + \int_0^1 \frac{\nu^2}{N(\nu)} \coth \left( \frac{\Sigma_t \Delta x}{2\nu} \right) d\nu \right] Q_0
\]
Thus, the flux-weighted average of $x$ is still equal to the source-weighted average of $x$,

$$\langle x \rangle_\phi = \langle x \rangle_Q$$

However, the flux-weighted average of $x^2$ is now

$$\langle x^2 \rangle_\phi = \langle x^2 \rangle_Q$$

$$+ \frac{(1 - c)\Delta x}{\Sigma_t} \left[ \frac{\nu_0}{N_0} \coth \left( \frac{\Sigma_t \Delta x}{2\nu_0} \right) + \int_0^1 \frac{\nu^2}{N(\nu)} \coth \left( \frac{\Sigma_t \Delta x}{2\nu} \right) d\nu \right]$$

where $c = \Sigma_s / \Sigma_t$ is the scattering ratio.
We can simplify this expression somewhat through the singular eigenfunction expansions of 1 and \( \mu^2 \), which yield the following identity:

\[
1 = \int_{-1}^{1} \left[ \frac{c}{2} \right]^{1} + \frac{3(1 - c)}{2} \mu^2 \right) d\mu \\
= 3(1 - c)^2 \left[ \frac{\nu^3}{N_0} + \int_{0}^{1} \frac{\nu^3}{N(\nu)} d\nu \right]
\]
We then have

\[ \langle x^2 \rangle_\phi = \langle x^2 \rangle_Q + 2L^2 + E \]

Here, the error term \( E \) is defined by

\[
E = \frac{1 - c}{\sum_t^2} \left\{ \frac{2\nu_0^3}{N_0} \left[ \frac{\Sigma_t \Delta x}{2\nu_0} \coth \left( \frac{\Sigma_t \Delta x}{2\nu_0} \right) - 1 \right] + \int_0^1 \frac{2\nu^3}{N(\nu)} \left[ \frac{\Sigma_t \Delta x}{2\nu} \coth \left( \frac{\Sigma_t \Delta x}{2\nu} \right) - 1 \right] d\nu \right\}
\]
Singular Eigenfunction Solution (continued)
Fourier Transform Solution

- As an alternative to the above procedure, we can also develop an expression for $E$ via Fourier transform.
- We first represent the piecewise-constant source for all values of $x$ using

$$Q(x) = \sum_{j=-\infty}^{\infty} H(x - x_{j-1/2})(Q_j - Q_{j-1})$$

where $H(x - x_{j-1/2})$ is the Heaviside step function shifted to the cell edge $x_{j-1/2}$.
- The Fourier transform of the scalar flux is then

$$\hat{\phi}(k) = \frac{1}{ik} \frac{\tan^{-1}(k/\Sigma_t)}{k - \Sigma_s \tan^{-1}(k/\Sigma_t)} \sum_{j=-\infty}^{\infty} \left( e^{-ikx_{j-1/2}} - e^{-ikx_{j+1/2}} \right) Q_j$$
Fourier Transform Solution (continued)

- In addition, we have from the definition of the inverse Fourier transform

\[ \phi_j = \frac{1}{2\pi\Delta x} \int_{-\infty}^{\infty} \frac{e^{ikx_{j+1/2}} - e^{ikx_{j-1/2}}}{ik} \hat{\phi}(k) dk \]

- Combining these expressions for \( \hat{\phi}(k) \) and \( \phi_j \) yields

\[ \phi_j = \frac{2}{\pi\Delta x} \int_{-\infty}^{\infty} \frac{\sin^2 \left( k \Delta x / 2 \right)}{k^2} \frac{\tan^{-1} \left( k / \Sigma_t \right)}{k - \Sigma_s \tan^{-1} \left( k / \Sigma_t \right)} \times \sum_{j'=-\infty}^{\infty} \cos \left[ (j - j') k \Delta x \right] Q_{j'} dk \]
The moments of the scalar flux are then given by

$$\phi_m = \frac{2}{\pi} \int_{-\infty}^{\infty} \frac{\sin^2 (k\Delta x/2)}{k^2} \frac{\tan^{-1} (k/\Sigma_t)}{k - \Sigma_s \tan^{-1} (k/\Sigma_t)} \times \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} x_j^m \cos [(j - j')k\Delta x] Q_{j'} dk$$
Fourier Transform Solution (continued)

- This expression contains the series

\[
\sum_{j=-\infty}^{\infty} x_j^m \cos [(j - j')k\Delta x] =
\begin{cases}
1 + 2 \sum_{n=1}^{\infty} \cos (nk\Delta x) , & m = 0 \\
x_j \left[ 1 + 2 \sum_{n=1}^{\infty} \cos (nk\Delta x) \right] , & m = 1 \\
\left( x_j'^2 - \frac{d^2}{dk^2} \right) \left[ 1 + 2 \sum_{n=1}^{\infty} \cos (nk\Delta x) \right] , & m = 2
\end{cases}
\]
Fourier Transform Solution (continued)

- We can use these alternate forms of the series to express $\phi_0$, $\phi_1$, and $\phi_2$, in terms of $Q_0$, $Q_1$, and $Q_2$.
- However, the resulting equations are rather complicated as they involve integrals over the transform variable $k$.
- Fortunately, these equations also involve the following Fourier series,

$$1 + 2 \sum_{n=1}^{\infty} \cos (nk \Delta x) = \frac{2\pi}{\Delta x} \sum_{n=-\infty}^{\infty} \delta \left( k - \frac{2\pi n}{\Delta x} \right)$$

which, because it represents a sequence of Dirac delta functions, facilitates a straightforward evaluation of these integrals.
We then obtain the previously developed expressions for $\phi_0$, $\phi_1$, and consequently the flux-weighted average of $x$.

However, we now have

$$\phi_2 = \frac{1}{\Sigma_a} Q_2$$

$$+ \frac{1}{\Sigma_a} \left[ 2L^2 + \frac{\Delta x^2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{2\pi n/\sum \Delta x - \tan^{-1} (2\pi n/\sum \Delta x)}{2\pi n/\sum \Delta x - c \tan^{-1} (2\pi n/\sum \Delta x)} \right] Q_0$$

The corresponding error term in the equation for the flux-weighted average of $x^2$ is

$$E = \frac{\Delta x^2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{2\pi n/\sum \Delta x - \tan^{-1} (2\pi n/\sum \Delta x)}{2\pi n/\sum \Delta x - c \tan^{-1} (2\pi n/\sum \Delta x)}$$
Equivalence of the Two Approaches

To demonstrate that the two expressions for $E$ are equivalent, we use a technique for replacing summations with contour integrals based on the following properties of $\pi \cot (\pi z)$:
- the poles are at integer values of $z$
- the corresponding residues are one
- see F. Bornemann, *et al.*, *The SIAM 100-Digit Challenge*

Thus, we can rewrite the equation for $E$ developed via Fourier transform as

$$ E = \lim_{N \to \infty} \frac{1}{2\pi i} \frac{\Delta x^2}{\pi^2} \int_{C_N} \frac{\pi \cot (\pi z)}{z^2} \frac{2\pi z/\Sigma_t \Delta x - \tan^{-1} (2\pi z/\Sigma_t \Delta x)}{2\pi z/\Sigma_t \Delta x - c \tan^{-1} (2\pi z/\Sigma_t \Delta x)} \, dz $$

where the contour $C_N$ contains all of the positive integers up to and including $N$.  

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Equivalence of the Two Approaches (continued)
Equivalence of the Two Approaches (continued)

- As $N \to \infty$, we are able to evaluate this integral from
  - the poles at 0 and $\pm i\Sigma_t \Delta x/2\pi \nu_0$
  - the portions of the contour along the branch cut, i.e.,
    $i\Sigma_t \Delta x/2\pi < z < i\infty$ and $-i\infty < z < -i\Sigma_t \Delta x/2\pi$

- A lengthy algebraic manipulation shows that the resulting expression for $E$ is equivalent to the one developed using the singular eigenfunction method.
Conclusions

- We have examined how the method of moments is altered when
  - the transport problem of interest is spatially continuous but involves a grid
  - moments are computed on this grid instead of through integration over the entire domain
- For the problem we considered, we found, through both singular eigenfunction and Fourier transform approaches, that when moments are evaluated in this manner
  - the flux-weighted average $x$ remains equal to the source-weighted average of $x$
  - the flux-weighted average of $x^2$ differs from the source-weighted average of $x^2$ by an additional error term
- We have also demonstrated that the two resulting expressions for this error term are equivalent.
Conclusions (continued)

- In future work, we plan on
  - extending our modification of the method of moments to time-dependent problems
  - applying this extension to the analysis and improvement of Monte Carlo methods for simulating radiative transfer