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Order of Accuracy of Spatial Discretization of Method of Characteristics

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Abstract - *The method of characteristics (MoC) has become an accepted tool for lattice physics calculations. MoC has many advantages such as accurate representations the of the lattice geometry and boundary conditions. The flat source (FS) approximation is most commonly used and the linear source (LS) approximation can improve the accuracy by preserving higher order spatial moments of the neutron source. However, as a non-standard spatial discretization method, the order of accuracy of the spatial discretization is more difficult to obtain, especially for analyzing linear source approximation, because the MoC method utilizes two set of spatial meshes – the FS mesh and the set of characteristic rays that integrate the transport equation over the FS mesh. In this work, we analyze the order of accuracy with spatial resolution in MoC in planar geometry for both FS and LS approximations and verify our predictions with the Method of Manufactured Solutions (MMS). It is shown that the flat source approximation is second order accurate and that the linear source approximation has a fourth order accuracy.*

Keywords: *method of characteristics, order of accuracy, flat source approximation, linear source approximation*

I. INTRODUCTION

The method of characteristics (MoC) has become an accepted tool for lattice physics calculations. MoC has many advantages such as accurate representations the of lattice geometry and boundary conditions. The flat source (FS) approximation is most commonly used. [1,2,3] When improved accuracy is needed, one can employ the linear source (LS) approximation. [4] However, the MoC method utilizes a non-standard spatial discretization method with two sets of spatial meshes – the FS mesh and the set of characteristic rays that integrate the transport equation over the FS mesh. The interaction between the characteristic rays and the spatial mesh is making the error analysis of MoC solution much more complicated. Consequently, the order of accuracy of the spatial discretization of MoC is not well known. In this work, we analyze the order of accuracy with spatial resolution in planar geometry for both FS and LS approximations and verify our predictions with the Method of Manufactured Solutions (MMS). One dimensional geometry bypasses the complexity of ray spacing, enabling us to look at the error convergence rate over spatial grid refinements alone. Being able to obtain the error convergence rate, or the order of accuracy, with the spatial resolution for both FS approximation and LS approximation, is useful for understanding the errors introduced in MoC, which can, in turn, inform the choice of FS mesh size and the ray spacing. Being able to locate and quantify errors can also help develop more accurate MoC schemes. Moreover, knowledge of the theoretical order of accuracy can be used to verify reactor physics codes with code verification methods, such as MMS.

Section II focuses on the theoretical prediction of the order of accuracy. Distributed source and scattering source are analyzed separately. What differentiates this work from previous analysis on spatial discretization [5,6] is that we start from the exact solution along the characteristics and quantitatively track error propagation, making it straightforward to generalize the analysis from FS to LS approximation. Section III gives the numerical results that use MMS to verify the predictions as well as the MoC code, including polynomial and nonpolynomial function forms. Section IV briefly summarizes the conclusions. It is shown that the flat source approximation is second order accurate and that the linear source approximation has a fourth order accuracy.

II. THEORY

In MoC, the angular flux along any characteristics can be integrated analytically with an assumed form of the right-hand-side source. We will represent the theory in one-dimensional geometry for simplicity.

$$\mu\frac{\partial\psi(x,\mu)}{\partial x}+\Sigma_t\psi(x,\mu)=q(x,\mu) \quad (1)$$

Integrating the above equation over a canonical spatial cell j, where $x_{j-1/2}<x<x_{j+1/2}$, will give us the neutron balance

equation within this cell, which in turn can be used to derive the expression for the cell-averaged angular flux $\bar{\psi}_j(\mu)$. To further simplify algebra, the first cell is used to represent the canonical cell with $z'=0$ corresponding to $x_{j-1/2}$ and $z'=z$ corresponding to $x_{j+1/2}$. Operating on Equation (1) with $\frac{1}{z}\int_0^z(\cdot)dz'$ yields

$$\bar{\psi}(\mu)=\frac{\bar{q}(\mu)}{\Sigma_t}+\frac{\mu}{\Sigma_t z}\psi(0,\mu)-\frac{\mu}{\Sigma_t z}\psi(z,\mu) \tag{2}$$

where

$$\begin{aligned}\bar{\psi}(\mu)&=\frac{1}{z}\cdot\int_0^z\psi(z',\mu)dz'\\ \bar{q}(\mu)&=\frac{1}{z}\cdot\int_0^z q(z',\mu)dz'\end{aligned} \tag{3}$$

The exiting angular flux can also be solved analytically with an integration factor $e^{\frac{\Sigma_t z'}{\mu}}$.

$$\psi(z,\mu)=\psi(0,\mu)\cdot e^{-\frac{\Sigma_t z}{\mu}}+\frac{e^{-\frac{\Sigma_t z}{\mu}}}{\mu}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot q(z',\mu)dz' \tag{4}$$

Inserting Equation (4) into Equation (2) yields

$$\bar{\psi}(\mu)=\frac{\bar{q}(\mu)}{\Sigma_t}+\frac{\mu}{\Sigma_t z}\psi(0,\mu)\left(1-e^{-\frac{\Sigma_t z}{\mu}}\right)-\frac{e^{-\frac{\Sigma_t z}{\mu}}}{\Sigma_t z}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot q(z',\mu)dz' \tag{5}$$

The approximating cell-averaged angular flux $\bar{\tilde{\psi}}$ is expressed below, where $\tilde{q}$ approximates q and $\bar{\tilde{q}}$ is the average of this approximation $\tilde{q}$.

$$\bar{\tilde{\psi}}(\mu)=\frac{\bar{\tilde{q}}(\mu)}{\Sigma_t}+\frac{\mu}{\Sigma_t z}\psi(0,\mu)\left(1-e^{-\frac{\Sigma_t z}{\mu}}\right)-\frac{e^{-\frac{\Sigma_t z}{\mu}}}{\Sigma_t z}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\tilde{q}(z',\mu)dz' \tag{6}$$

The error E is defined as the difference between the exact analytical expression of cell averaged angular flux $\bar{\psi}(\mu)$ as in Equation (5) and its approximation $\bar{\tilde{\psi}}(\mu)$ as in Equation (6).

$$\begin{aligned}E&=\bar{\psi}(\mu)-\bar{\tilde{\psi}}(\mu)\\ &=\frac{\bar{q}(\mu)}{\Sigma_t}-\frac{\bar{\tilde{q}}(\mu)}{\Sigma_t}-\frac{e^{-\frac{\Sigma_t z}{\mu}}}{\Sigma_t z}\cdot\left[\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot q(z',\mu)dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\tilde{q}(z',\mu)dz'\right]\end{aligned} \tag{7}$$

This error depends on how well $\tilde{q}(z',\mu)$ approximates the true source shape. Equation (7) is evaluated for both FS and LS approximations and is the basis for error analysis throughout the paper.

When different approximations (e.g. FS and LS approximations) are used, the following definition of $\tilde{q}(z')$ is taken, with angular dependence dropped to avoid symbolic entanglements.

$$\tilde{q}(z')=\begin{cases}q^0 & \text{, flat source}\\ q^0-q^1\cdot(z'-z^c), & \text{linear source}\end{cases} \tag{8}$$

where

zeroth source moment,

$$q^0=\frac{1}{z}\cdot\int_0^z q(z')dz'$$

first source moment,

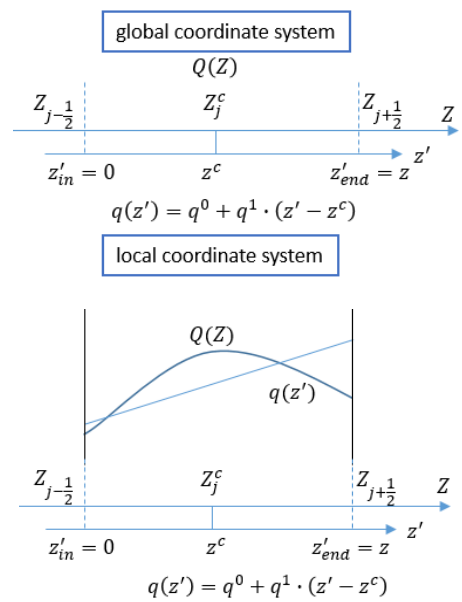
$$\begin{aligned}q^1&=\left[\overline{z'\cdot q(z')}-z^c\cdot\overline{q(z')}\right]\cdot\frac{12}{z^2}\\ &=\left[\frac{1}{z}\cdot\int_0^z z'\cdot q(z')dz'-z^c\cdot\frac{1}{z}\cdot\int_0^z q(z')dz'\right]\cdot\frac{12}{z^2},\end{aligned} \tag{9}$$

cell center location,

$$z^c=\frac{z}{2}$$

Note that the definition q^1 involves a transformation from a global coordinate system to a local one and is briefly illustrated below.

Assume source $Q(Z)$ is the total source in a slab geometry in a global coordinate system $0<Z<Z_{\max}$. The source $Q(Z)$ over a canonical cell $(Z_{j-1/2},Z_{j+1/2})$ is to be linearized as $q^0-q^1\cdot(z'-z^c)$, where z' is the local coordinate in current cell j originated at the left edge of the cell.



Next, we show how to obtain the first spatial source moment q^1 from global quantities $Q(Z)$.

$$Q(Z)\approx\tilde{q}(z')=q^0-q^1\cdot(z'-z^c) \tag{10}$$

Perform operation $\int_0^z[*]\cdot(z'-z^c)dz'$ on the above equation. The right-hand-side (RHS) gives

$$\text{RHS}=\int_0^z\left[q^0-q^1\cdot(z'-z^c)\right]\cdot(z'-z^c)dz'=q^1\cdot\frac{z^2}{12} \tag{11}$$

The left-hand-side (LHS) gives

$$\begin{aligned}\text{LHS} &= \int_0^z \tilde{q}(z')\cdot(z'-z^c)\,dz' \\ &= \int_{Z_{j-1/2}}^{Z_{j+1/2}} Q(Z)\cdot(Z-Z^c)\,d(Z-Z_{j-1/2}) \\ &= \int_{Z_{j-1/2}}^{Z_{j+1/2}} Q(Z)\cdot Z - Q(Z)\cdot Z^c dZ \\ &= \overline{Q(Z)\cdot Z} - Z^c\cdot\overline{Q(Z)}\end{aligned} \tag{12}$$

Therefore, the first spatial source moment can be expressed as

$$q^1 = \left[\overline{Q(Z)\cdot Z} - Z^c\cdot\overline{Q(Z)}\right]\cdot\frac{12}{z^2} \tag{13}$$

For a fixed source problem, the source consists of both scattering and distributed source components as follows.

$$q(z',\mu) = \frac{\Sigma_s}{2}\int_{-1}^{1}\psi(z',\mu)\,d\mu + q_{MMS}(z',\mu) \tag{14}$$

The distributed source is denoted with subscript MMS because MMS is the most common distributed source in the determination of the order of accuracy and code verification practices. Therefore, in this paper, MMS will represent the distributed source with known mathematical forms.

Note that the nature of the scattering source is very different from that of the distributed source. The scattering source changes and updates and resolves its spatial dependence over the source iteration, while the distributed source has a known mathematical form and does not change in this iterative process. Not surprisingly, this distinction makes the error analyses for these two source types very different. This is partially reflected in the *practical expressions* of the zeroth and first source moments of these two source types defined in Equation (15).

zeroth source moment,

$$\begin{aligned} q^{0,(n)}(\mu) &= \frac{\Sigma_s}{2}\left(\sum_{m=1}^{M}\omega_m\cdot\tilde{\bar{\psi}}_m^{(n-1)}\right) + \frac{1}{z}\cdot\int_0^z q_{MMS}(z',\mu)\,dz' \\ &= q^0{}_{scat}(\mu) + q^0{}_{MMS}(\mu),\end{aligned}$$

first source moment,

$$\begin{aligned} q^{1,(n)}(\mu) &= \left[\overline{z'\cdot q(z',\mu)} - z^c\cdot\overline{q(z',\mu)}\right]\cdot\frac{12}{z^2} \\ &= \left[\frac{\Sigma_s}{2}\cdot\left(\sum_{m=1}^{M}\omega_m\cdot\left(\tilde{\hat{\psi}}_m^{(n-1)} - z^c\cdot\tilde{\bar{\psi}}_m^{(n-1)}\right)\right)\right]\cdot\frac{12}{z^2} \\ &\quad + \left[\overline{z'\cdot q_{MMS}(z',\mu)} - z^c\cdot\overline{q_{MMS}(z',\mu)}\right]\cdot\frac{12}{z^2} \\ &= q^1{}_{scat}(\mu) + q^1{}_{MMS}(\mu),\end{aligned} \tag{15}$$

where $\hat{\psi} = \frac{1}{z}\cdot\int_0^z z'\cdot\psi(z',\mu)\,dz'$ is the first spatial moment of the angular flux and $\tilde{\hat{\psi}}$ is its approximation. Note that the superscripts (n) and (n-1) in the above equation are the iteration index and that a quantity with superscript (n) and its counterpart with superscript (n-1) will be equal up to the convergence criteria upon convergence, allowing the superscripts to be dropped.

In the following two subsections, we will look at the distributed source and the scattering source separately due to the different forms of their practical expressions. With the superposition principle, universal for any linear system, the sources here are additive so the final order of accuracy with spatial resolution will be the lower of the two standalone orders of accuracy from each source type. We look at the order of accuracy related to approximating distributed source first.

1. Order of Accuracy related to Approximating Distributed Source

In this subsection, scattering source is assumed to be zero. This happens in a purely absorbing material.

Note that when the distributed source approximation $\tilde{q}(z')$ integrates $q(z')$ exactly, which is usually the case, the first two terms in Equation (7) cancel out, reducing the error to a simpler form

$$E = -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot q(z',\mu)\,dz' - \int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\tilde{q}(z',\mu)\,dz'\right] \tag{16}$$

Now we look at FS and LS approximations respectively.

A. Flat Source (FS) Approximation

FA approximation implies the following

$$\tilde{q}(z') = q^0 \tag{17}$$

Using Equation (16) to evaluate the error introduced into the cell-averaged angular flux due to FS approximation

$$E = -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot q(z',\mu)\,dz' - q^0\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\right] \tag{18}$$

Three cases were examined: constant, linear, and quadratic source shapes. For a constant source shape, the above error is $E=0$. This is verified in our MoC 1D code, showing that the solution is accurate to machine precision regardless of the fineness of the grid.

Second, if the source is linear in space, the flat source approximation introduces an error of second order with the mesh width. Assuming $q(z') = z',\ 0<z'<z$, the error can be evaluated with Equation (18).

$$\begin{aligned} E &= -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot z'dz' - \frac{z}{2}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\right] \\ &= -\frac{\mu}{\Sigma_t{}^2}\frac{e^{-\tau}}{\tau}\cdot\left[\int_0^\tau e^{\tau'}\cdot\tau' d(\tau') - \frac{\tau}{2}\cdot\int_0^\tau e^{\tau'}d(\tau')\right] \\ &= \frac{\mu}{\Sigma_t{}^2}\cdot\left[\left(\frac{1}{\tau}-\frac{1}{2}\right) - \left(\frac{1}{\tau}+\frac{1}{2}\right)\cdot e^{-\tau}\right]\end{aligned} \tag{19}$$

where

$$\tau = \frac{\Sigma_t z}{\mu} \tag{20}$$

which is the optical thickness seen by a neutron flying in the direction characterized by μ.

As z (or τ) approaches zero, namely, as we refine the spatial grid, the above error is expanded near $\tau = 0$ as follows,

$$\frac{\Sigma_t^2}{\mu} \cdot E = -\frac{\tau^2}{12} + \frac{\tau^3}{24} - \frac{\tau^4}{80} + O\left(\tau^5\right) \tag{21}$$

Therefore, the error is second order with the mesh size.

Third, if the source is quadratic in space, the flat source approximation will converge to the true solution with third order, which is shown below.

Assuming $q(z') = z'^2,\ 0<z'<z$, the error from Equation (18) can be evaluated

$$\begin{aligned} E &= -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z} \cdot \left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot z'^2 dz' - \frac{z^2}{3} \cdot \int_0^z e^{\frac{\Sigma_t}{\mu}z'} dz' \right] \\ &= -\frac{\mu^2}{\Sigma_t^3} \cdot \frac{e^{-\tau}}{\tau} \cdot \left[\int_0^\tau e^{\tau'} \cdot \tau'^2 d\tau' - \frac{\tau^2}{3} \cdot \int_0^\tau e^{\tau'} d\tau' \right] \\ &= \frac{\mu^2}{\Sigma_t^3} \cdot \left[\left(2 - \frac{2}{3}\tau - \frac{2}{\tau} \right) + \left(\frac{2}{\tau} - \frac{\tau}{3} \right) e^{-\tau} \right] \end{aligned} \tag{22}$$

As τ⟶0, the error approaches zero with third order,

$$\frac{\Sigma_t^3}{\mu^2} \cdot E = -\frac{\tau^3}{12} + \frac{7\tau^4}{180} - \frac{\tau^5}{90} + O\left(\tau^6\right) \tag{23}$$

However, due to the structure and operators in the neutron transport equation, only under special circumstances will we have a singleton quadratic source shape that does not have a linear component. This will cause a degradation in order of accuracy from third order to second order in problems with a quadratic source shape, since the error from the linear component is dominating the error convergence order. Moreover, with induction, it can be shown that generally the flat source approximation can at best be second order accurate in space.

B. Linear Source (LS) Approximation

LS approximation implies the following

$$\tilde{q}(z') = q^0 + q^1 \cdot \left(z' - \frac{z}{2} \right),\ 0 < z' < z \tag{24}$$

Using Equation (16) to evaluate the error introduced into the cell-averaged angular flux via LS approximation

$$\begin{aligned} E &= -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z} \cdot \left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot q(z',\mu) dz' - \int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot \tilde{q}(z',\mu) dz' \right] \\ &= -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z} \cdot \left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot q(z',\mu) dz' - \int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot \left[q^0 - q^1 \cdot \left(z' - \frac{z}{2} \right) \right] dz' \right] \end{aligned} \tag{25}$$

where,

zeroth source moment,

$$q^0_{MMS}(\mu) = \frac{1}{z} \cdot \int_0^z q_{MMS}(z',\mu) dz'$$

first source moment,

$$q^1_{MMS}(\mu) = \left[\overline{z' \cdot q_{MMS}(z',\mu)} - z^c \cdot \overline{q_{MMS}(z',\mu)} \right] \cdot \frac{12}{z^2} \tag{26}$$

It is easy to show that linear source will be able to represent flat source with no error since q^1 will be zero and q^0 can represent the constant source.

Next, we show that linear source approximation can represent linearly distributed source with no error.

Assuming $q(z') = z',\ 0<z'<z$ in q^0 and q^1 defined in Equation (26) gives

$$\begin{aligned} q^0 &= \frac{1}{z} \cdot \int_0^z q(z') dz' = \frac{1}{z} \cdot \int_0^z z' dz' = \frac{z}{2} \\ q^1 &= \left[\overline{z' \cdot q(z')} - z^c \cdot \overline{q(z')} \right] \cdot \frac{12}{z^2} \\ &= \left[\frac{z^2}{3} - \frac{z^2}{4} \right] \cdot \frac{12}{z^2} = 1 \end{aligned} \tag{27}$$

The approximating source shape is exactly the same as the originally manufactured source shape as shown below

$$\begin{aligned} \tilde{q}(z') &= q^0 + q^1 \cdot \left(z' - \frac{z}{2} \right) \\ &= \frac{z}{2} + 1 \cdot \left(z' - \frac{z}{2} \right) = z' = q(z') \end{aligned} \tag{28}$$

Last, if the source shape is quadratic in space as $q(z') = z'^2,\ 0 < z' < z$, we have

$$\begin{aligned} q^0 &= \frac{1}{z} \cdot \int_0^z q(z') dz' = \frac{1}{z} \cdot \int_0^z z'^2 dz' = \frac{z^2}{3} \\ q^1 &= \left[\overline{z' \cdot q(z')} - z^c \cdot \overline{q(z')} \right] \cdot \frac{12}{z^2} \\ &= \left[\frac{z^3}{4} - \frac{z}{2} \cdot \frac{z^2}{3} \right] \cdot \frac{12}{z^2} \\ &= z \end{aligned} \tag{29}$$

Constructing the linear approximation with the zeroth and first source moments gives,

$$\tilde{q}(z') = q^0 + q^1 \cdot \left(z' - \frac{z}{2} \right) = -\frac{z^2}{6} + z \cdot z' \tag{30}$$

The error introduced via linear source (LS) approximation can be evaluated with Equation (25)

$$\begin{aligned} E &= -\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z} \cdot \left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot z'^2 dz' - \int_0^z e^{\frac{\Sigma_t}{\mu}z'} \cdot \left[-\frac{z^2}{6} + z \cdot z' \right] dz' \right] \\ &= -\frac{\mu^2}{\Sigma_t^3} \cdot \frac{e^{-\tau}}{\tau} \cdot \left[\int_0^\tau e^{\tau'} \cdot \tau'^2 d\tau' - \int_0^\tau e^{\tau'} \cdot \left[-\frac{\tau^2}{6} + \tau \cdot \tau' \right] d\tau' \right] \\ &= \frac{\mu^2}{\Sigma_t^3} \cdot \left[\left(1 - \frac{1}{6}\tau - \frac{2}{\tau} \right) + \left(\frac{\tau}{6} + 1 + \frac{2}{\tau} \right) \cdot e^{-\tau} \right] \end{aligned} \tag{31}$$

The error approaches zero with fourth order shown by Taylor expansion near τ=0.

$$\frac{\Sigma_t^3}{\mu^2} \cdot E = -\frac{\tau^4}{360} + \frac{\tau^5}{720} + O\left(\tau^6\right) \tag{32}$$

As mentioned in the flat source section, we normally do not have a standalone quadratic source, rather it usually comes with a linear component. However, with linear source approximation, the linear source can be exactly represented, thus having linear component will not degrade the 4th-order accuracy.

The expected and observed orders of accuracy for the purely absorbing material is summarized in Table 1, which also shows consistency between expectation and observation.

2. Order of Accuracy related to Approximating Scattering Source

This subsection focuses on the error introduced in cell-averaged angular flux due to an error in approximating scattering source with different source approximation schemes, i.e., FS and LS.

The following error expression from Equation (7) still holds, except that now $q(z',\mu)$ includes both scattering source $q_{scat}(z',\mu)=\frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\psi(z',\mu)d\mu$ and other distributed sources, e.g., $q_{MMS}(z',\mu)$.

$$\begin{aligned}E&=\frac{\overline{q}(\mu)}{\Sigma_t}-\frac{\overline{\tilde{q}}(\mu)}{\Sigma_t}\\&\quad-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot q(z',\mu)dz'-\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\tilde{q}(z',\mu)dz'\right]\\&=E_1+E_2\end{aligned}\tag{33}$$

Since the previous subsection has studied the order of accuracy related to distributed source, this subsection will focus on the order of accuracy related to approximating scattering source ONLY. The overall order of accuracy will be the lower of the two. With scattering source only, the expression for the zeroth and first spatial source moments can be simplified.

zeroth source moment,

$$q^{0,(n)}(\mu)=\frac{\Sigma_s}{2}\left(\sum_{m=1}^{M}\omega_m\cdot\tilde{\overline{\psi}}_m^{(n-1)}\right)=q^0{}_{scat}(\mu),$$

first source moment,

$$\begin{aligned}q^{1,(n)}(\mu)&=\left[\overline{z'\cdot q(z',\mu)}-z^c\cdot\overline{q(z',\mu)}\right]\cdot\frac{12}{z^2}\\&=\left[\frac{\Sigma_s}{2}\cdot\left(\sum_{m=1}^{M}\omega_m\cdot\left(\tilde{\overline{\psi}}_m^{(n-1)}-z^c\cdot\tilde{\overline{\psi}}_m^{(n-1)}\right)\right)\right]\cdot\frac{12}{z^2}\\&=q^1{}_{scat}(\mu)\end{aligned}\tag{34}$$

The FS approximation is looked at first.

A. Flat Source (FS) Approximation

FS approximation implies the following

$$\tilde{q}(z')=q^0\tag{35}$$

Using the above Equation (33) to evaluate the error introduced into the cell-averaged angular flux due to FS approximation.

The first component E_1 can be evaluated in the following way

$$\begin{aligned}\Sigma_t\cdot E_1&=\overline{q}(\mu)-q^0(\mu)\\&=\frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\left[\frac{1}{z}\int_0^z\psi(z',\mu)dz'\right]d\mu-\frac{\Sigma_s}{2}\cdot\left(\sum_{m=1}^{M}\omega_m\cdot\tilde{\overline{\psi}}_m^{(n-1)}\right)\\&=\frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\overline{\psi}(\mu)d\mu-\frac{\Sigma_s}{2}\cdot\left(\sum_{m=1}^{M}\omega_m\cdot\tilde{\overline{\psi}}_m^{(n-1)}\right)\end{aligned}\tag{36}$$

Assume that the angular flux is isotropic and that the selected quadrature set satisfies $\sum_{m=1}^{M}\omega_m\cdot 1=2$, the above Equation (36) can be further reduced into the following form upon convergence (iteration superscripts dropped)

$$\begin{aligned}\Sigma_t\cdot E_1&=\Sigma_s\cdot\overline{\psi}-\Sigma_s\cdot\tilde{\overline{\psi}}\\&=\Sigma_s\cdot\left(\overline{\psi}-\tilde{\overline{\psi}}\right)=\Sigma_s\cdot E\end{aligned}\tag{37}$$

Therefore,

$$E_1=c\cdot E\tag{38}$$

Next, we look at the second error component using the practical expression from Equation (34),

$$E_2=-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\begin{aligned}&\int_0^z\left[e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(\frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\psi(z',\mu)d\mu\right)\right]dz'\\&-\frac{\Sigma_s}{2}\cdot\left(\sum_{m=1}^{M}\omega_m\cdot\tilde{\overline{\psi}}_m^{(n-1)}\right)\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\end{aligned}\right]\tag{39}$$

Assume isotropic angular flux, the above equation can be further reduced to the following form upon convergence

$$\begin{aligned}E_2&=-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t\cdot z}\cdot\left[\int_0^z\left[e^{\frac{\Sigma_t}{\mu}z'}\cdot\Sigma_s\cdot\psi(z',\mu)\right]dz'-\Sigma_s\cdot\tilde{\overline{\psi}}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\right]\\&=-\frac{c\cdot e^{-\frac{\Sigma_t}{\mu}z}}{z}\cdot\left[\int_0^z\left[e^{\frac{\Sigma_t}{\mu}z'}\cdot\psi(z',\mu)\right]dz'-(\overline{\psi}-E)\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\right]\\&=(1-c)\cdot E\end{aligned}\tag{40}$$

The total error E is solved from the above equation.

$$E=\frac{c\cdot\left[\overline{\psi}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-\int_0^z\left(e^{\frac{\Sigma_t}{\mu}z'}\cdot\psi(z',\mu)\right)dz'\right]}{z\cdot e^{\frac{\Sigma_t}{\mu}z}\cdot(1-c)+c\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'}\tag{41}$$

Similarly, three cases were examined: constant, linear, and quadratic source shapes.

For a constant scattering source shape, the above error is zero. To show this, assume a constant flux shape, which will give a constant scattering source

$$\psi(z',\mu)=\psi_0=1\tag{42}$$

the resulting error from FS approximation can be evaluated using Equation (41)

$$\begin{aligned}E&=\frac{c\cdot\left[\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-\int_0^z\left(e^{\frac{\Sigma_t}{\mu}z'}\right)dz'\right]}{z\cdot e^{\frac{\Sigma_t}{\mu}z}\cdot(1-c)+c\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'}\\&=0\end{aligned}\tag{43}$$

Therefore, the expected error will be zero despite how coarse the mesh is.

Second, if the scattering source is linear in space, the flat source approximation will introduce an error of second order with the spatial mesh width. Assuming the angular flux in the following form

$$\psi(z',\mu)=\psi_1\cdot z'=z' \tag{44}$$

the error introduced from flat source approximation can be evaluated from Equation (41)

$$\begin{aligned} E&=\frac{c\cdot\left[\frac{z}{2}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-\int_0^z\left(e^{\frac{\Sigma_t}{\mu}z'}\cdot z'\right)dz'\right]}{z\cdot e^{\frac{\Sigma_t}{\mu}z}\cdot(1-c)+c\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'}\\ &=\frac{c\mu}{\Sigma_t}\cdot\frac{\left[\frac{\tau}{2}\cdot\int_0^\tau e^{\tau'}d\tau'-\int_0^\tau\left(e^{\tau'}\cdot\tau'\right)d\tau'\right]}{\tau\cdot e^{\tau}\cdot(1-c)+c\cdot\int_0^\tau e^{\tau'}d\tau'}\\ &=\frac{c\mu}{\Sigma_t}\cdot\frac{\left(1-e^{-\tau}\right)-\frac{\tau}{2}\cdot\left(1+e^{-\tau}\right)}{\tau\cdot(1-c)+c\cdot\left(1-e^{-\tau}\right)} \end{aligned} \tag{45}$$

As τ approaches zero, namely, as we refine the spatial grid, the above error can be expanded near τ=0,

$$\frac{\Sigma_t}{c\mu}\cdot E=-\frac{1}{12}\tau^2+\frac{1-c}{24}\tau^3+O\left(\tau^4\right) \tag{46}$$

Therefore, the error is second order with the spatial mesh width.

Third, if the scattering source is quadratic in space, the FS approximation to scattering source will introduce a third order error, which is negligible compared to the 2nd order error introduced from approximating distributed source. This is shown below. Again, assume the angular flux shape,

$$\psi(z',\mu)=\psi_2\cdot z'^2=z'^2 \tag{47}$$

Then we can evaluate the error introduced by FS approximation to the scattering source with Equation (41).

$$\begin{aligned} E&=\frac{c\cdot\left[\frac{z^2}{3}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-\int_0^z\left(e^{\frac{\Sigma_t}{\mu}z'}\cdot z'^2\right)dz'\right]}{z\cdot e^{\frac{\Sigma_t}{\mu}z}\cdot(1-c)+c\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'}\\ &=\frac{c\cdot\mu^2}{\Sigma_t^2}\cdot\frac{\left[\frac{\tau^2}{3}\cdot\int_0^\tau e^{\tau'}d\tau'-\int_0^\tau\left(e^{\tau'}\cdot\tau'^2\right)d\tau'\right]}{\tau\cdot e^{\tau}\cdot(1-c)+c\cdot\int_0^\tau e^{\tau'}d\tau'}\\ &=\frac{c\cdot\mu^2}{\Sigma_t^2}\cdot\frac{\left(-\frac{2\tau^2}{3}+2\tau-2\right)+\left(2-\frac{\tau^2}{3}\right)\cdot e^{-\tau}}{\tau\cdot(1-c)+c\cdot\left(1-e^{-\tau}\right)} \end{aligned} \tag{48}$$

As τ approaches zero, namely, as we refine the spatial grid, the above error can be expanded near τ=0,

$$\frac{\Sigma_t^2}{c\cdot\mu^2}\cdot E=-\frac{1}{12}\tau^3-\left(\frac{7}{180}-\frac{c}{24}\right)\tau^4+O\left(\tau^5\right) \tag{49}$$

Therefore, the error is third order with the mesh width.

B. Linear Source (LS) Approximation

LS approximation implies the following

$$\tilde{q}(z')=q^0+q^1\cdot\left(z'-\frac{z}{2}\right),\ 0<z'<z \tag{50}$$

Using Equation (33) to evaluate the error introduced into the cell-averaged angular flux due to LS approximation.

The first error component is

$$\begin{aligned} E_1&=\frac{\bar{q}(\mu)}{\Sigma_t}-\frac{\bar{\tilde{q}}(\mu)}{\Sigma_t}\\ &=\frac{\bar{q}(\mu)}{\Sigma_t}-\left(\frac{\overline{q^0}}{\Sigma_t}+\frac{\overline{q^1\cdot\left(z'-\frac{z}{2}\right)}}{\Sigma_t}\right)=\frac{\bar{q}(\mu)}{\Sigma_t}-\frac{\overline{q^0}}{\Sigma_t} \end{aligned} \tag{51}$$

The second error component is

$$\begin{aligned} E_2&=-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\begin{array}{l}\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left[q(z',\mu)\right]dz'\\ \quad-\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left[q^0+q^1\cdot\left(z'-\frac{z}{2}\right)\right]dz'\end{array}\right]\\ &=-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\begin{array}{l}\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left[q(z',\mu)\right]dz'\\ \quad-q^0\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-q^1\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(z'-\frac{z}{2}\right)dz'\end{array}\right] \end{aligned} \tag{52}$$

Assume that the angular flux is isotropic and that the employed quadrature set is chosen such that it satisfies $\sum_{m=1}^{M}\omega_m\cdot 1=2$. Applying the practical definition of the zeroth and first spatial source moments defined in Equation (34), the first error component takes the following form upon convergence.

$$\begin{aligned} E_1&=\frac{\bar{q}(\mu)}{\Sigma_t}-\frac{\overline{q^0}}{\Sigma_t}\\ &=\frac{1}{\Sigma_t}\cdot\left(\Sigma_s\cdot\bar{\psi}(\mu)-\Sigma_s\cdot\tilde{\bar{\psi}}_m^{(n-1)}\right)\\ &=c\cdot\left(\bar{\psi}(\mu)-\tilde{\bar{\psi}}\right)\\ &=c\cdot E \end{aligned} \tag{53}$$

The second error component takes the following form upon convergence.

$$\begin{aligned} E_2&=-\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\Sigma_t z}\cdot\left[\begin{array}{l}\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left[\Sigma_s\cdot\psi(z')\right]dz'\\ \quad-q^0\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-q^1\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(z'-\frac{z}{2}\right)dz'\end{array}\right]\\ &=\frac{c\cdot e^{-\frac{\Sigma_t}{\mu}z}}{z}\cdot\left[\begin{array}{l}-\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\psi(z')dz'+\left(\bar{\psi}-E\right)\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\\ \quad+\left[\frac{12}{z^2}\cdot\left(\left(\hat{\psi}-E_{\hat{\psi}}\right)-\left(\bar{\psi}-E\right)\cdot\frac{z}{2}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(z'-\frac{z}{2}\right)dz'\end{array}\right]\\ &=(1-c)\cdot E \end{aligned} \tag{54}$$

Equation (54) is used to solve for the total error E in cell-averaged angular flux. Move all the terms involving E and $E_{\hat{\psi}}$ to the LHS and solve for the total error E.

$$E=\frac{c\cdot\left[\begin{array}{l}\left[\frac{12}{z^2}\cdot\left(\hat{\psi}-\bar{\psi}\cdot\frac{z}{2}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(z'-\frac{z}{2}\right)dz'\\ \quad+\bar{\psi}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'-\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\psi(z')dz'\end{array}\right]}{\left[\begin{array}{l}(1-c)\cdot ze^{\frac{\Sigma_t}{\mu}z}+c\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}dz'\\ \quad-\left[\frac{12c}{z^2}\cdot\left(\frac{z}{2}-\frac{E_{\hat{\psi}}}{E}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot\left(z'-\frac{z}{2}\right)dz'\end{array}\right]} \tag{55}$$

When the scattering source shape is constant, assuming the angular flux shape as

$$\psi(z',\mu)=\psi_0=1 \tag{56}$$

the resulting scattering source shape and the zeroth and first spatial moments of the angular flux are

$$\begin{aligned} q_{scat}(z') &= \frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\psi(z',\mu)\,d\mu=\Sigma_s \\ \bar{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\,dz'=1 \\ \hat{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\cdot z'dz'=\frac{1}{z}\int_0^z z'dz'=\frac{z}{2} \end{aligned} \tag{57}$$

Equation (55) is evaluated and we conclude that the error introduced due to LS approximation towards scattering source is zero.

$$E=\frac{c\cdot\left[\left[\frac{12c}{z^2}\cdot\left(\frac{z}{2}-1\cdot\frac{z}{2}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz' +1\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot[1]dz'\right]}{\left[(1-c)\cdot ze^{\frac{\Sigma_t z}{\mu}}+c\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz' -\left[\frac{12c}{z^2}\cdot\left(\frac{z}{2}-\frac{E_{\hat{\psi}}}{E}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz'\right]} =0 \tag{58}$$

Next, we show that approximating linear scattering source with LS approximation gives zero error as well.

Assuming the angular flux shape

$$\psi(z',\mu)=\psi_1\cdot z'=z' \tag{59}$$

the resulting scattering source and the zeroth and first spatial moments of the angular flux are

$$\begin{aligned} q(z') &= \frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\psi(z',\mu)\,d\mu=\frac{\Sigma_s}{2}\int_{-1}^{1}z'd\mu=\Sigma_s\cdot z' \\ \bar{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\,dz'=\frac{1}{z}\int_0^z z'dz'=\frac{z}{2} \\ \hat{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\cdot z'dz'=\frac{1}{z}\int_0^z z'\cdot z'dz'=\frac{z^2}{3} \end{aligned} \tag{60}$$

Again, equation (55) is evaluated and we conclude that the error introduced due to LS assumption towards linear scattering source is zero.

$$\begin{aligned} E &= \frac{c\cdot\left[\left[\frac{12}{z^2}\cdot\left(\frac{z^2}{3}-\frac{z}{2}\cdot\frac{z}{2}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz' +\frac{z}{2}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot[z']dz'\right]}{\left[(1-c)\cdot ze^{\frac{\Sigma_t z}{\mu}}+c\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz' -\left[\frac{12c}{z^2}\cdot\left(\frac{z}{2}-\frac{E_{\hat{\psi}}}{E}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz'\right]} \\ &= \frac{c\cdot\left[\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz' +\frac{z}{2}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot z'dz'\right]}{\left[(1-c)\cdot ze^{\frac{\Sigma_t z}{\mu}}+c\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz' -\left[\frac{12c}{z^2}\cdot\left(\frac{z}{2}-\frac{E_{\hat{\psi}}}{E}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz'\right]} \\ &= 0 \end{aligned} \tag{61}$$

The last case evaluates the error introduced due to inaccuracy in approximating quadratic scattering source with LS approximation. Assuming $\psi(z',\mu)=\psi_2\cdot z'^2=z'^2$, the scattering source and the zeroth and first spatial moments of the angular flux are

$$\begin{aligned} q(z') &= \frac{\Sigma_s}{2}\cdot\int_{-1}^{1}\psi(z',\mu)\,d\mu=\frac{\Sigma_s}{2}\cdot\int_{-1}^{1}z'^2d\mu=\Sigma_s\cdot z'^2 \\ \bar{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\,dz'=\frac{1}{z}\int_0^z z'^2dz'=\frac{z^2}{3} \\ \hat{\psi} &= \frac{1}{z}\int_0^z \psi(z',\mu)\cdot z'dz'=\frac{1}{z}\int_0^z z'^2\cdot z'dz'=\frac{z^3}{4} \end{aligned} \tag{62}$$

Once again, Equation (55) is used to evaluate the error from LS approximation. Note that the ratio $E_{\hat{\psi}}/E$ is dropped in the formulation for having a higher order than $O(z)$, which will be shown later.

$$\begin{aligned} E &= \frac{c\cdot\left[\left[\frac{12}{z^2}\cdot\left(\frac{z^3}{4}-\frac{z^2}{3}\cdot\frac{z}{2}\right)\right]\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz' +\frac{z^2}{3}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left[z'^2\right]dz'\right]}{\left[(1-c)\cdot ze^{\frac{\Sigma_t z}{\mu}}+c\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\frac{6c}{z}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot\left(z'-\frac{z}{2}\right)dz'\right]} \\ &= c\cdot\frac{\left[-\frac{z^2}{6}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'+z\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot z'dz'-\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot z'^2dz'\right]}{\left[(1-c)\cdot ze^{\frac{\Sigma_t z}{\mu}}+4c\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}dz'-\frac{6c}{z}\cdot\int_0^z e^{\frac{\Sigma_t z'}{\mu}}\cdot z'dz'\right]} \\ &= \frac{c\mu^2}{\Sigma_t^2}\cdot\frac{\left[-\frac{\tau^2}{6}\cdot\int_0^\tau e^{\tau'}d\tau'+\tau\cdot\int_0^\tau e^{\tau'}\cdot\tau'd\tau'-\int_0^\tau e^{\tau'}\cdot\tau'^2d\tau'\right]}{\left[(1-c)\cdot\tau e^{\tau}+4c\cdot\int_0^\tau e^{\tau'}d\tau'-\frac{6c}{\tau}\cdot\int_0^\tau e^{\tau'}\cdot\tau'd\tau'\right]} \\ &= \frac{c\mu^2}{\Sigma_t^2}\cdot\frac{\left(-\frac{\tau}{6}+1-\frac{2}{\tau}\right)+\left(\frac{\tau}{6}+1+\frac{2}{\tau}\right)\cdot e^{-\tau}}{1-c-\frac{2c}{\tau}+\frac{6c}{\tau^2}-\left(\frac{4c}{\tau}+\frac{6c}{\tau^2}\right)\cdot e^{-\tau}} \end{aligned} \tag{63}$$

The error introduced by LS approximation towards quadratic scattering source is 4th order by expanding the above error near τ=0.

$$\frac{\Sigma_t^{\,2}}{c\mu^2}\cdot E=-\frac{\tau^4}{360}+\frac{1-2c}{720}\tau^5+O\left(\tau^6\right) \tag{64}$$

Therefore, the order of accuracy is the same as that related to approximating distributed source.

C. Assessing Error in $E_{\hat{\psi}}$

In this subsection, we give an error assessment for $E_{\hat{\psi}}$, denoting the error in the first spatial moment of the angular flux. It is shown that its order is higher than that of the total error E.

The first spatial moment of the angular flux over the canonical cell is defined as

$$\hat{\psi}(\mu)=\frac{1}{z}\int_0^z z'\cdot\psi(z',\mu)\,dz' \tag{65}$$

where

$$\psi(z,\mu)=\psi(0,\mu)\cdot e^{-\frac{\Sigma_t}{\mu}z}+\frac{e^{-\frac{\Sigma_t}{\mu}z}}{\mu}\cdot\int_0^z e^{\frac{\Sigma_t}{\mu}z'}\cdot q(z',\mu)\,dz' \tag{66}$$

Therefore,

$$\begin{aligned}\hat{\psi}(\mu)&=\frac{1}{z}\int_0^z z'\cdot\psi(z',\mu)\,dz'\\&=\frac{1}{z}\int_0^z z'\cdot\left[\psi(0,\mu)\cdot e^{-\frac{\Sigma_t}{\mu}z'}+\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot q(z'',\mu)\,dz''\right]dz'\\&=\psi(0,\mu)\cdot\frac{1}{z}\int_0^z z'\cdot e^{-\frac{\Sigma_t}{\mu}z'}dz'+\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot q(z'',\mu)\,dz''\right]dz'\end{aligned} \tag{67}$$

The approximation for $\hat{\psi}(\mu)$ is

$$\begin{aligned}\tilde{\hat{\psi}}(\mu)&=\psi(0,\mu)\cdot\frac{1}{z}\int_0^z z'\cdot e^{-\frac{\Sigma_t}{\mu}z'}dz'\\&\quad+\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot\tilde{q}(z'',\mu)\,dz''\right]dz'\end{aligned} \tag{68}$$

$E_{\hat{\psi}}$ is defined as the difference between the analytical expression $\hat{\psi}$ and its approximation $\tilde{\hat{\psi}}$, which is determined by how well $\tilde{q}(z',\mu)$ approximates the true source shape $q(z',\mu)$.

$$\begin{aligned}E_{\hat{\psi}}&=\hat{\psi}-\tilde{\hat{\psi}}\\&=\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot\left(\frac{\Sigma_s}{2}\int_{-1}^{1}\psi(z'',\mu)\,d\mu\right)dz''\right]dz'\\&\quad-\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot\left(q^0+q^1\cdot\left(z''-\frac{z}{2}\right)\right)dz''\right]dz'\end{aligned} \tag{69}$$

where upon convergence

$$\begin{aligned}q^0(\mu)&=\Sigma_s\cdot(\bar{\psi}-E)\\q^1(\mu)&=\left[\Sigma_s\cdot\left(\left(\hat{\psi}-E_{\hat{\psi}}\right)-z^c\cdot(\bar{\psi}-E)\right)\right]\cdot\frac{12}{z^2}\end{aligned} \tag{70}$$

In case of a quadratic spatial angular flux, (or quadratic scattering source), the error defined in Equation (69) is evaluated

$$\begin{aligned}E_{\hat{\psi}}&=\Sigma_s\cdot\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot z''^2\,dz''\right]dz'\\&\quad-\left(q^0\right)\cdot\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}dz''\right]dz'\\&\quad-\left(q^1\right)\cdot\frac{1}{z}\int_0^z z'\cdot\left[\frac{e^{-\frac{\Sigma_t}{\mu}z'}}{\mu}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot\left(z''-\frac{z}{2}\right)dz''\right]dz'\end{aligned} \tag{71}$$

Multiplying both sides by $\frac{\mu}{\Sigma_s}$ gives

$$\begin{aligned}\mu\frac{E_{\hat{\psi}}}{\Sigma_s}&=\frac{1}{z}\int_0^z z'\cdot\left[e^{-\frac{\Sigma_t}{\mu}z'}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot z''^2\,dz''\right]dz'\\&\quad-\left(\frac{q^0}{\Sigma_s}\right)\cdot\frac{1}{z}\int_0^z z'\cdot\left[e^{-\frac{\Sigma_t}{\mu}z'}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}dz''\right]dz'\\&\quad-\left(\frac{q^1}{\Sigma_s}\right)\cdot\frac{1}{z}\int_0^z z'\cdot\left[e^{-\frac{\Sigma_t}{\mu}z'}\cdot\left(\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}\cdot z''dz''-\frac{z}{2}\cdot\int_0^{z'}e^{\frac{\Sigma_t}{\mu}z''}dz''\right)\right]dz'\\&=\frac{1}{\rho^4}\cdot\frac{1}{\tau}\int_0^\tau\tau'\cdot\left[e^{-\tau'}\cdot\int_0^{\tau'}e^{\tau''}\cdot\tau''^2\,d\tau''\right]d\tau'\\&\quad-\frac{1}{\rho^2}\cdot\left(\frac{q^0}{\Sigma_s}\right)\cdot\frac{1}{\tau}\int_0^\tau\tau'\cdot\left[e^{-\tau'}\cdot\int_0^{\tau'}e^{\tau''}d\tau''\right]d\tau'\\&\quad-\frac{1}{\rho^3}\cdot\left(\frac{q^1}{\Sigma_s}\right)\cdot\frac{1}{\tau}\int_0^\tau\tau'\cdot\left[e^{-\tau'}\cdot\left(\int_0^{\tau'}e^{\tau''}\cdot\tau''d\tau''-\frac{\tau}{2}\cdot\int_0^{\tau'}e^{\tau''}d\tau''\right)\right]d\tau'\\&=\frac{1}{\rho^4}\cdot\left[\left(\frac{\tau^3}{4}-\frac{2\tau^2}{3}+\tau-\frac{2}{\tau}\right)+\left(2+\frac{2}{\tau}\right)\cdot e^{-\tau}\right]\\&\quad-\frac{1}{\rho^2}\cdot\left(\frac{q^0}{\Sigma_s}\right)\cdot\left[\frac{\tau}{2}-\frac{1}{\tau}+\left(1+\frac{1}{\tau}\right)\cdot e^{-\tau}\right]\\&\quad-\frac{1}{\rho^3}\cdot\left(\frac{q^1}{\Sigma_s}\right)\cdot\left[\frac{\tau^2}{12}-\frac{\tau}{2}+\frac{1}{2}+\frac{1}{\tau}-\left(\frac{\tau}{2}+\frac{1}{\tau}+\frac{3}{2}\right)\cdot e^{-\tau}\right]\end{aligned} \tag{72}$$

where $\rho=\Sigma_t/\mu$.

Inserting the practical expressions of the q^0 and q^1 defined in Equation (70) into Equation (72) and then solve for $E_{\hat{\psi}}$.

$$\begin{aligned}E_{\hat{\psi}}&=\frac{\left[\begin{array}{l}\frac{1}{\rho^4}\cdot\left[\frac{\tau^3}{4}-\frac{2\tau^2}{3}+\tau-\frac{2-2\cdot e^{-\tau}(\tau+1)}{\tau}\right]\\-\frac{1}{\rho^4}\cdot\left(\frac{\tau^2}{3}\right)\cdot\left[\frac{\tau}{2}-\frac{1-e^{-\tau}(\tau+1)}{\rho z}\right]\\-\frac{1}{2\rho^4}\cdot(\tau)\cdot\left[1-3e^{-\tau}+\frac{\tau^2}{6}+\frac{2\left(1-e^{-\tau}\right)}{\tau}-\tau\left(1+e^{-\tau}\right)\right]\end{array}\right]}{\frac{1}{\rho c}+\frac{1}{2\rho}\cdot\left(-\frac{12}{\tau^2}\right)\cdot\left[1-3e^{-\tau}+\frac{\tau^2}{6}+\frac{2\left(1-e^{-\tau}\right)}{\tau}-\tau\left(1+e^{-\tau}\right)\right]}\\&\quad+\frac{\left[\begin{array}{l}-\frac{1}{\rho^2}\cdot(-1)\cdot\left[\frac{\tau}{2}-\frac{1-e^{-\tau}(\tau+1)}{\tau}\right]\\-\frac{1}{2\rho^2}\cdot\left(\frac{6}{\tau}\right)\cdot\left[1-3e^{-\tau}+\frac{\tau^2}{6}+\frac{2\left(1-e^{-\tau}\right)}{\tau}-\tau\left(1+e^{-\tau}\right)\right]\end{array}\right]}{\frac{1}{\rho c}+\frac{1}{2\rho}\cdot\left(-\frac{12}{\tau^2}\right)\cdot\left[1-3e^{-\tau}+\frac{\tau^2}{6}+\frac{2\left(1-e^{-\tau}\right)}{\tau}-\tau\left(1+e^{-\tau}\right)\right]}\cdot E\end{aligned} \tag{73}$$

As $\tau\to 0$, the error is expanded near τ=0.

$$\begin{aligned}E_{\hat{\psi}}&=-\frac{1}{2\rho^4}\cdot\frac{\frac{1}{180}\tau^4-\frac{1}{360}\tau^5+O\left(\tau^6\right)}{\frac{1}{\rho c}-\frac{1}{\rho}\cdot\left(-\frac{1}{2}\tau+\frac{7}{20}\tau^2-\frac{7}{60}\tau^3+O\left(\tau^4\right)\right)}\\&\quad+\frac{\frac{7}{12}\tau^2-\frac{3}{10}\tau^3+O\left(\tau^4\right)}{\frac{1}{\rho c}-\frac{1}{\rho}\cdot\left(-\frac{1}{2}\tau+\frac{7}{20}\tau^2-\frac{7}{60}\tau^3+O\left(\tau^4\right)\right)}\cdot\frac{1}{\rho^2}\cdot E\\&=-\frac{c}{2\rho^3}\cdot\left(\frac{1}{180}\tau^4-\frac{1}{360}\tau^5+O\left(\tau^6\right)\right)\\&\quad+\left(\frac{7}{12}\tau^2-\frac{3}{10}\tau^3+O\left(\tau^4\right)\right)\cdot\frac{c}{\rho}\cdot E\end{aligned} \tag{74}$$

In a shorter expression, it is of the following form,

$$E_{\hat{\psi}}=O\left(\tau^4\right)+O\left(\tau^2\right)\cdot E \tag{75}$$

Therefore $E_{\hat{\psi}}$ will be at least two orders higher than E or is $O(z^4)$. Either way, the ratio $E_{\hat{\psi}}/E$ is negligible compared to z/2, validating the dropping of this ratio when evaluating Equation (61) for a quadratic scattering source case.

III. EXPERIMENTAL RESULT

MoC 1D code is developed for testing the predictions of the order of accuracy for FS and LS approximations.

Four test problems are devised for the tests, each of which consists of an assumed flux shape and the corresponding manufactured sources listed below.

Case 1: constant source shape

$$\psi(z',\mu)=\psi_0,$$

$$q_{MMS}(z',\mu)=\psi_0\cdot(\Sigma_t-\Sigma_s) \quad (76)$$

Case 2: linear source shape

$$\psi(z',\mu)=\psi_0+\psi_1 e^{\mu}\cdot z',$$

$$q_{MMS}(z',\mu)=\psi_0\cdot(\Sigma_t-\Sigma_s)+\psi_1\cdot\mu e^{\mu} +\left[\psi_1\cdot\Sigma_t e^{\mu}-\psi_1\cdot\frac{\Sigma_s}{2}\left(e-e^{-1}\right)\right]\cdot z' \quad (77)$$

Case 3: quadratic source shape

$$\psi(z',\mu)=\psi_0+\psi_2 e^{\mu}\cdot z'^2$$

$$q_{MMS}(z',\mu)=\psi_0\cdot(\Sigma_t-\Sigma_s)+2\psi_2\mu e^{\mu}\cdot z' +\psi_2\left[\Sigma_t e^{\mu}-\frac{\Sigma_s}{2}\left(e^{1}-e^{-1}\right)\right]\cdot z'^2 \quad (78)$$

Case 4: non-polynomial source shape

$$\psi(z',\mu)=\sqrt{z'}$$

$$q_{MMS}(z',\mu)=\frac{\mu}{2\sqrt{z'+1}}+(\Sigma_t-\Sigma_s)\cdot\sqrt{z'+1} \quad (79)$$

1. Testing Purely Absorbing Materials

For purely absorbing materials, the scattering cross section is set to be zero. Case 1 gives machine-precision results for both FS and LS approximation for all mesh sizes.

The following Figure 1, Figure 2 and Figure 3 show the grid refinement results for Case 2, Case 3 and Case 4 (without scattering source) involving linear, quadratic and a non-polynomial manufactured source.

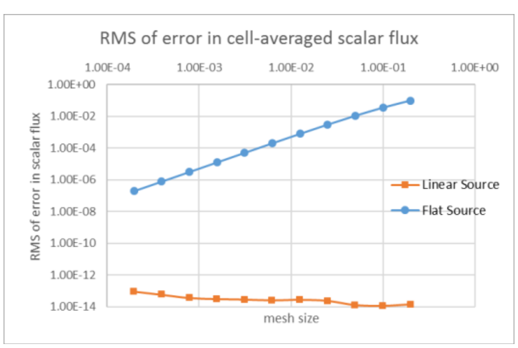


Figure 1. Order of accuracy with linear manufactured source (FS: 2nd order, LS: exact)

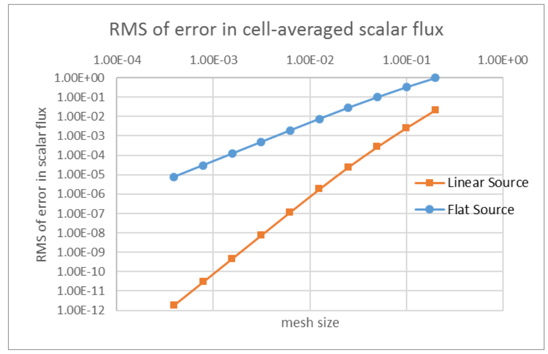


Figure 2. Order of accuracy with quadratic manufactured source (FS: 2nd order, LS: 4th order)

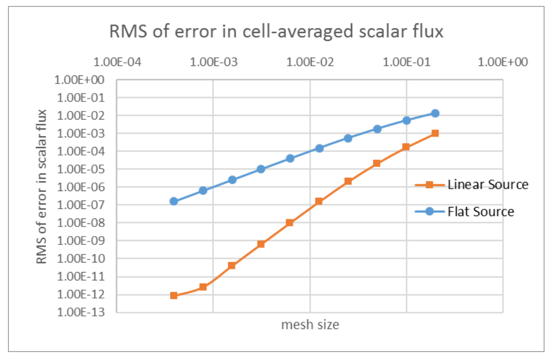


Figure 3. Order of accuracy with non-polynomial manufactured source (FS: 2nd order, LS: 4th order)

All the experimental results agree with the analytical predictions and are listed in Table 1. The number before the slash is the observed order of accuracy and the one after the slash is the predicted order of accuracy, i.e., in a form of (observation/prediction).

Table 1. Observed and Predicted Order of Accuracy (purely absorbing)

Approx.	Constant	Linear	Quadratic
FS	exact / exact	2nd / 2nd	2nd / 3rd →2nd*
LS	exact / exact	exact / exact	4th / 4th

* The arrow indicates the aforementioned order degradation

Angular error from the numerical result is removed from the overall error with the error removal technique developed in previous work. [7].

2. Testing Scattering Materials

The expected order of accuracy related to approximating scattering source with FS and LS approximations are tabulated in Table 2.

Table 2. Predicted Order of Accuracy (scattering source only)

Approx.	Constant	Linear	Quadratic
FS	exact	2^{nd}	3^{rd}
LS	exact	exact	4^{th}

As mentioned before, compiling the results from Table 1 and Table 2 by taking the lower order gives the expected order of accuracy for cases with both scattering source and distributed source, which is listed in Table 3.

Table 3. Observed and Predicted Order of Accuracy (scattering source plus distributed source)

Approx.	Constant	Linear	Quadratic
FS	exact / exact	2^{nd} / 2^{nd}	2^{nd} / 2^{nd}
LS	exact / exact	exact / exact	4^{th} / 4^{th}

The following Figure 4, Figure 5 and Figure 6 show the grid refinement results for Case 2, Case 3 and Case 4 (with scattering source) involving linear and quadratic manufactured source.

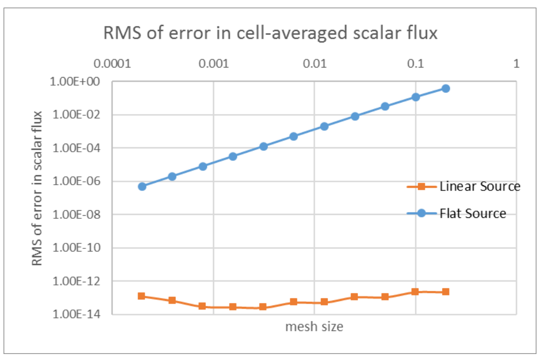


Figure 4. Order of accuracy with linear manufactured source (FS: 2^{nd} order, LS: exact)

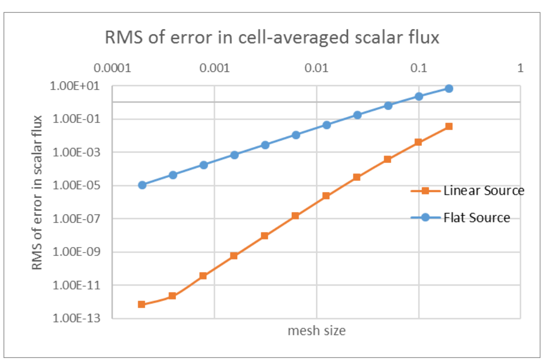


Figure 5. Order of accuracy with quadratic manufactured source (FS: 2^{nd} order, LS: 4^{th} order)

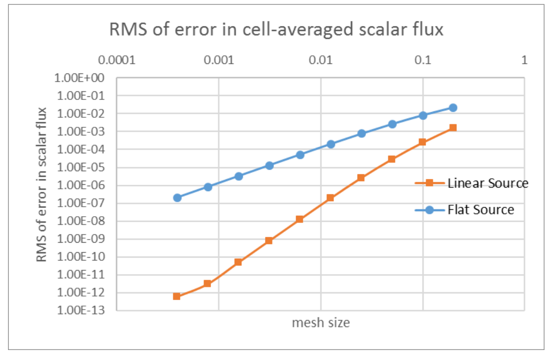


Figure 6. Order of accuracy with quadratic manufactured source (FS: 2^{nd} order, LS: 4^{th} order)

All the experimental results agree with the analytical predictions and are listed in Table 3.

IV. CONCLUSIONS

A systematic analysis of the order of accuracy for spatial discretization of MoC method in a slab geometry has been performed for both flat source approximation and linear source approximation. It is shown that including scattering source does not degrade the order of accuracy and that the order of the error of the first spatial moments of the angular flux is two orders higher than that of the zeroth spatial moments of the angular flux. Both theoretical prediction and experimental results show that flat source approximation is second order accurate and that linear source approximation has a fourth order accuracy.

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