The Order of Accuracy Related to the Error from Source Approximation in the Method of Characteristics for Purely Absorbing Materials in Planar Geometry

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Abstract

The method of characteristics (MoC) is a well-established tool for lattice physics calculations, offering advantages such as accurate representations of both lattice geometry and boundary conditions. The flat source (FS) approximation is the most commonly used approach, while the linear source (LS) approximation enhances accuracy by preserving higher-order spatial moments of the neutron source. However, determining the order of accuracy (OoA) for spatial discretization in MoC is challenging, particularly for the LS approximation. This complexity arises because MoC employs two spatial meshes: the fission source region (FSR) mesh and a set of characteristic rays used to integrate the transport equation over the FSR mesh. In this study, we analyze the spatial order of accuracy of MoC in planar geometry for both FS and LS approximations in relation to the distributed source. Our theoretical predictions are consistent with the numerical results using the Method of Manufactured Solutions (MMS). The results demonstrate that the FS approximation achieves second-order accuracy, while the LS approximation attains fourth-order accuracy.

Full Text

Preamble

The order of accuracy related to the error from source approximation in the method of characteristics for purely absorbing materials in planar geometry∗ Ji-Pu Wang,1 Zhen-Wen Wei İD ,1 Can Huang,1 William Martin,2 Brendan Kochunas,2 Qi-Cang Shen,3, † Si-Juan Chen,1, ‡ and Martin Pilch4 1Shenzhen Key Laboratory of Nuclear and Radiation Safety, Institute for Advanced Study

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4MPilchConsulting, 26 Mustang Mesa Trail, Tijeras, NM 87059, USA The method of characteristics (MoC) is a well-established tool for lattice physics calculations, offering ad- vantages such as accurate representation of both lattice geometry and boundary conditions. The flat source (FS) approximation is the most commonly used approach, whereas the linear source (LS) approximation enhances the accuracy by preserving the higher-order spatial moments of the neutron source. However, determining the order of accuracy (OoA) for spatial discretization in the MoC is challenging, particularly for the LS approximation. This complexity arises because MoC employs two spatial meshes: the fission source region (FSR) mesh and a set of characteristic rays used to integrate the transport equation over the FSR mesh. In this study, we analyzed the spatial order of accuracy of the MoC in planar geometry for both FS and LS approximations in relation to the distributed source. Our theoretical predictions are consistent with the numerical results ob- tained using the Method of Manufactured Solutions (MMS). The results demonstrate that the FS approximation achieves second-order accuracy, whereas the LS approximation attains fourth-order accuracy.

Keywords: Method of characteristics, Order of accuracy, Flat source approximation, Linear source approximation, Method of manufactured solutions

INTRODUCTION

The method of characteristics (MoC) is a well-established tool for lattice-physics calculations. More recently, it has been observed in such state-of-the-art deterministic high- fidelity reactor physics codes as MPACT [1], OpenMOC [2], NECP-X [3], and Proteus-MOC [4], offering advantages such as high parallel efficiency and accurate representations of both complex geometry and boundary conditions [5]. The flat source (FS) approximation is the most commonly used approach [6–8], whereas the linear source (LS) approximation is employed when higher accuracy is required [9, 10]. ∗ This work was supported by the Stable Support Plan Program under Shen- zhen Natural Science Fund Contract (No. 20220811012323001), the LingChuang Research Project of China National Nuclear Corporation un- der Contract (No. CNNC-LCKY-202266), the Shenzhen Key Laboratory of Nuclear and Radiation Safety of Shenzhen Science and Technology In- novation Commission under Contract (No. ZDSYS20230626091501002), the Pengcheng Peacock Plan Distinguished Talent project (No.827- 000712), the Shenzhen Science and Technology Innovation Commission Key Technical Project under Contract

(No.s JSGG20220831110607013 and KJZD20231023100200001), the Young Innovative Talent in Guang- dong Province No. 2023KQNCX065, the Teaching Reform Research Programs under Shenzhen University Contract (Nos. JG000066010107, JG000033090185, and JG2022072), and the Teaching Reform Research Program under Guangdong Provincial Department of Education Contract JG2024085). This work was also supported by the Consortium for Advanced Simulation of Light Water Reactors (https://casl.gov/), an Energy Innovation Hub (http://www.energy.gov/hubs) for Modeling and Simulation of Nuclear Reactors, under the U.S. Department of Energy Contract (No. DE-AC05-00OR22725). † Corresponding author, shen_{qicang}@iapcm.ac.cn ‡ Corresponding author, chensijuan@szu.edu.cn While significant attention has been given to implement- ing these numerical methods in reactor physics codes and im- proving their performance, the verification of these codes has received limited research [11]. This study provides a more theoretical and rigorous demonstration. Verification is crucial to ensuring the correctness of both the numerical methods and their implementations. The Consortium for Advanced Simu- lation of Light Water Reactors (CASL) [12] has set a bench- mark in this regard by dedicating substantial efforts to Ver- ification and Validation (V&V) [13] to maintain high code quality and verified methodology. A critical aspect of this process involves analyzing discretization errors in complex methods such as the method of characteristics (MoC) within the MPACT code [14].

MoC utilizes a non-standard spatial discretization method that involves two sets of spatial meshes: the FSR mesh and a set of characteristic rays used to integrate the transport equa- tion over the FSR mesh. The interaction between the charac- teristic rays and the FSR mesh complicates the error analysis of MoC solutions, making it difficult to determine the order of accuracy (OoA) of MoC' s spatial discretization.

Our preliminary attempt to determine the OoA related to source approximation in one-dimensional (1D) geometry was presented at the M&C 2017 conference [15] and ICONE 30 [16], although they lacked a rigorous proof. In this study, we focused on purely absorbing materials and provided a formal proof of the OoA for spatial resolution in planar geometry for both FS and LS approxima- tions. We verified our predictions using the Method of Manufactured Solutions (MMS) [17], which provides an analytical solution for comparison. The use of 1D geometry eliminates the complexity of ray spacing, allowing us to isolate and analyze the error convergence rate over the FSR mesh refinements.

Understanding the error convergence rate, or the order of accuracy, for both FS and LS approximations is valuable for assessing the errors introduced in the MoC and guiding the selection of the FSR mesh size. Furthermore, quantifying and locating errors can aid in the development of more accurate MoC schemes. Additionally, knowledge of the theoretical or- der of accuracy can be used to verify reactor physics codes through Code Verification methods such as MMS.

Section II presents the theoretical prediction of the order of accuracy, focusing on distributed sources. Unlike previ- ous studies on spatial discretization [18,

19], this study be- gins with the exact solution along the characteristic rays and quantitatively tracks the error propagation, making it easier to generalize the analysis from FS to LS approximations. Sec- tion III provides numerical results [20] that validate our the- oretical predictions using the MMS and the Method of Ex- act Solutions (MES). We also verified the MoC code devel- oped for this study by considering both polynomial and non- polynomial function forms. Additionally, we apply Ganapol's infinite cylinder case [21] using the production code MPACT [1] to confirm the order of accuracy. Section IV summarizes our conclusions, demonstrating that the FS approximation achieves second-order accuracy, while the LS approximation attains fourth-order accuracy.

In the MoC, the angular flux along a characteristic can be analytically integrated using an assumed form of the source term q (x, µ). $\partial\psi$ (x, µ) + Σtψ (x, µ) = q (x, µ) . where µ is the direction cosine, x is the position, ψ (x, µ) is the angular neutron flux, and Σt is the macroscopic total cross-section.

For simplicity, we illustrate the theory in a one-dimensional geometry and apply the following assumptions: homoge- neous materials, isotropic scattering, and energy indepen- dence. The coordinate of this planar model used in our theory is shown in Fig. 1 [Figure 1: see original paper].

Integrating the above equation over a canonical spatial cell j, where xj−1/2 < x < xj+1/2, yields the neutron balance equation within this cell, which in turn can be used to de- rive the expression for the cell-averaged angular flux. To fur- ther simplify the algebra, the first cell is used to represent the canonical cell with z′ = 0 corresponding to x1/2 and z′ = z corresponding to x3/2. Operating on Equation (1) with oper- ation 1 (cid:82) z 0 (•) dz′ yields ¯ψ (µ) = ¯q (µ) ψ (0, µ) − ψ (z, µ) , where ¯ψ (µ) = ¯q (µ) = (cid:90) z ψ (z′, µ) dz′ , (cid:90) z q (z′, µ) dz′.

The exiting angular flux with respect to this cell can also be solved analytically using an integration factor e . Sub- stituting this result back into Eq. (1) provides an explicit so- lution for the angular flux, as follows: ψ (z, µ) =ψ (0, µ) e− Σt e− Σt (cid:90) z q (z′, µ) dz′. ¯q (µ) e− Σt ¯˜q (µ) e− Σt ¯ψ (µ) = ψ (0, µ) (cid:16) 1 − e− Σt µ z(cid:17) (cid:90) z q (z′, µ) dz′.

The approximating cell-averaged angular flux ˜¯ψ is ex- pressed below, where ˜q approximates q and ¯˜q is the average of the approximating source ˜q. ˜¯ψ (µ) = ψ (0, µ) (cid:16) 1 − e− Σt µ z(cid:17) (cid:90) z ˜q (z′, µ) dz′ The error E is defined as the difference between the ana- lytical expression of the cell-averaged angular flux ¯ψ given in Eq. (5) and its approximation ˜¯ψ presented in Eq. (6).

E = ¯ψ (µ) − ˜¯ψ (µ) (cid:90) z ¯q (µ) ¯˜q (µ) e− Σt q (z′, µ) dz′− (cid:90) z ˜q (z′, µ) dz′ II. FORMAL ORDER OF ACCURACY Inserting Eq. (4) into Eq. (2) yields Fig. 1. Global and local coordinate systems This error depends on how well ˜q (z′, µ) approximates the true source distribution. Equation (7) is evaluated for both FS and LS approximations and is the basis for the error analysis throughout the paper.

When different approximations (e.g., FS and LS approxi- mations) are used, the following definition of ˜q (z′) is taken, with angular dependence dropped to avoid symbolic entan- glements, ˜q (z′) = (cid:40) q0 + q1 (z′ − zc) flat source linear source where zc refers to the midpoint of local coordinate and we define the zeroth source moment as follows (cid:90) z q (z′) dz′, and the first source moment as follows (cid:21) 12 q (z′) (z′ − zc) dz′ (cid:20) 1 (cid:90) z (cid:104) z′q (z′) − zcq (z′) (cid:20) 1 (cid:105) 12 z′q (z′) dz′ − zc 1 (cid:90) z (cid:90) z q (z′) dz′ (cid:21) 12 Note that the definition of q0 indicates that ¯q = ¯˜q = q0.

In addition, note that the definition q1 involves a transforma- tion from a global coordinate system to a local one, which is briefly illustrated below.

Assume that source Q (x) is the total source in a slab ge- ometry in a global coordinate system 0 < x < xmax. The (cid:1) is to be source Q (x) over a canonical cell (cid:0)xj−1/2, xj+1/2 linearized as q0 + q1 ·(z′ − zc), where z′ is the local coordi- nate in the current cell j originated at the left edge of the cell, as shown in Fig. 2 [Figure 2: see original paper].

Next, we show how to obtain the first spatial source mo- ment q1 from the global quantities Q (x).

Q (x) ˜q (z′) = q0 + q1 (z′ − zc) . (cid:82) z 0 [·] dz′ on the above Eq. (11) Performing operation 1 gives Q (x) = q0. (cid:82) z 0 [·] (z′ − zc) dz′ on Eq. (11). The Perform operation 1 right-hand-side (RHS) gives (cid:90) z RHS = (cid:8)(cid:2)q0 + q1 (z′ − zc)(cid:3) (z′ − zc)(cid:9) dz′ =q1 z2 Fig. 2. Global and local coordinate systems presented with assumed source distribution Therefore, the first spatial source moment can be expressed (cid:104) Q (x) · x − xc ·Q (x) (cid:105) 12 Now, we consider the expression for a fixed source, con- sisting of both scattering and distributed source components, as follows: q (z′, µ) = (cid:90) 1 ψ (z′, µ) dµ + qMMS (z′, µ) .

The left-hand side (LHS) gives LHS = (cid:90) z [˜q (z′) (z′ − zc)] dz′ (cid:90) xj+1/2 [Q (x) (x − xc)] d (cid:0)x − xj−1/2 (cid:1) xj−1/2 (cid:90) xj+1/2 (cid:104) Q (x) x − xcQ (x) xj−1/2 (cid:105) [Q (x) x − Q (x) xc] dx Both scattering and distributed components contribute to the total source term. The distributed source, labeled with the subscript MMS, represents a known math- ematical source commonly used in Code Verification.

The scattering source depends on iterative updates from neutron interactions, which makes it difficult to include in the analytic error analysis. To keep the methodology clear, we consider only the distributed source in this study. With this simplification, the structure of the source can be expressed through its ze- roth spatial source moment, the q0,(n) (µ), and the first spatial source moment, the q1,(n) (µ), defined in MMS (µ) ,

1. Constant Component

Eq. (17): q0,(n) (µ) = (cid:32) M (cid:88) ˜¯ψ(n−1) (cid:33) q1,(n) (µ) = qMMS (z′, µ) dz′ (cid:90) z scat (µ) +q0 (cid:104) z′q (z′, µ) − zcq (z′, µ) (cid:88) ˜ˆψ(n−1) zc ˜¯ψ(n−1) (cid:105) 12 (cid:104) z′qMMS (z′, µ) − zcqMMS (z′, µ) (cid:105) 12 scat (µ) +q1 MMS (µ) , where ˆψ = 1 (cid:82) z 0 z′ψ (z′, µ) dz′ is the first spatial moment of ˜ˆψ is its approximation, ωm is the coef- the angular flux and ficient of Legendre-Gauss quadrature. The superscripts (n) and (n − 1) denote the iteration indices, and once the conver- gence criterion is achieved, these terms become equivalent, allowing the superscripts to be omitted.

Since linear systems obey the superposition principle, the total order of accuracy depends on the worst-case approxi- mation between the distributed and scattering sources. This study focuses on the order of accuracy of the distributed source, assuming the scattering source is zero, which is valid for purely absorbing materials.

When the average of the approximated distributed source ˜q (z′) exactly equals the average of the true source q (z′), the first two terms in the error defined in Eq. (7) cancel out, re- ducing the error to a simplified form:

E = − e− Σt (cid:90) z (cid:90) z q (z′, µ) dz′− ˜q (z′, µ) dz′ Next, we analyze the error behavior for FS and LS approx- imations separately.

A. Flat Source (FS) Approximation FS approximation implies the following ˜q (z′) = q0 .

Using Eq. (18) to evaluate the error introduced into the cell- averaged angular flux due to FS approximation E = − e− Σt (cid:20)(cid:90) z q (z′, µ) dz′ − q0 (cid:90) z (cid:21) To begin with, three low-order monomial cases were examined: constant, linear, and quadratic source distributions.

Based on these cases, the general polynomial case can be re- alized by superposition. Conversely, these low-order cases can be viewed as components of a more general source.

For a constant source distribution, q (z′) = c, 0 < z′ < z, the associated error is E = 0. This result was verified us- ing our MoC 1D code, which demonstrated that the solution maintained machine precision accuracy, irrespective of the grid resolution. This outcome is expected, as q0 precisely represents a constant source. Consequently, the flat source approximation introduced no error. This can be easily proven as follows:

E = − e− Σt e− Σt (cid:20)(cid:90) z (cid:20)(cid:90) z = 0 . q (z′, µ) dz′ − q0 (cid:21) (cid:90) z cdz′ − c (cid:21) (cid:90) z

2. Linear Component

If the source is linear in space, the FS approximation intro- duces an error of second order with the mesh size. Assuming q (z′) = z′, 0 < z′ < z, the error

can be evaluated using Eq. (20). Finally, it is expanded to a Taylor series to obtain the order of accuracy (OoA).

E = − e− Σt (cid:20)(cid:18) 1 (cid:20)(cid:90) z (cid:20)(cid:90) τ where z′dz′ − (cid:21) (cid:90) z (cid:90) τ (cid:19) (cid:21) d (τ ′) (cid:21) τ ′d (τ ′) − (cid:19) (cid:18) 1 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 spa- tial grid, the above error is expanded near τ = 0 as follows, E = − + O (cid:0)τ 5(cid:1) = O (cid:0)τ 2(cid:1) .

Therefore, the error introduced by flat source approxima- tion is second order with respect to the mesh size.

3. Quadratic Component

Therefore, If the source is quadratic in space, the flat source approxi- mation will converge to the true solution to third order, which is shown below.

Assuming q (z′) = z$ ‘2, 0 < *z*’ $ < z, the error from Equa- tion (20) can be evaluated, E = − e− Σt (cid:20)(cid:18) (cid:20)(cid:90) z z$’ 2*dz*’ $ − (cid:20)(cid:90) τ τ $’ 2*d* $ ′ − (cid:19) (cid:18) 2 (cid:90) z (cid:90) τ (cid:21) (cid:21) (cid:19) (cid:21) As τ → 0, the error approaches zero with third order, µ2 E = − + O (cid:0)τ 6(cid:1) = O (cid:0)τ 3(cid:1) .

However, since analytical solutions cannot be obtained di- rectly from pure monomial sources, we instead manufactured corresponding monomial fluxes and generated the source term by substituting them into the left-hand side of Eq. (1).

Owing to the presence of the differential operator in Eq. (1), a quadratic neutron flux inevitably produces a source that con- tains both quadratic and linear components. The inclusion of this linear component leads to a degradation in the observed order of accuracy from third to second order, as the error associated with the linear term dominates the overall error con- vergence.

Moreover, with induction, it can be shown that the flat source approximation is generally second order accurate in space.

4. General Polynomial Component

For any source that can be expressed as q (z′) = z′n, the general form of polynomial sources, we can evaluate the error from Eq. (20) as follows:

E(n) = − e− Σt (cid:90) z z′ndz′− n + 1 (cid:90) z (cid:90) τ n + 1 (cid:19)n eτ ′(cid:18) µ (cid:19)n (cid:90) τ (cid:18) µ (cid:90) τ τ ′nd (cid:19) (cid:19) (cid:18) µ (cid:18) µ τ ′ndτ ′− n + 1 (cid:90) τ (cid:18) µ (cid:19)n+1 . (28) E(n + 1) = − (cid:19)n+2 (cid:18) µ (cid:90) τ τ ′n+1dτ ′− τ n+1 n + 2 (cid:90)

τ Based on the discussions in Sects. II A 2 and II A 3, it can be inferred that the error behaves as E (n) O (cid:0)τ n+1(cid:1).

To prove this, we divide E(n + 1) (Equation (28)) by E(n) (Equation (27)):

E(n + 1) − e−τ (cid:16) µ (cid:17)n+2 − e−τ (cid:16) µ (cid:17)n+1 (cid:90) τ τ ′n+1dτ ′− τ n+1 n + 2 (cid:90) τ (cid:90) τ τ ′ndτ ′− n + 1 (cid:90) τ τ ′n+1dτ ′ − τ n+1 (cid:82) τ 0 eτ ′ (cid:82) τ 0 eτ ′τ ′ndτ ′ − τ n (cid:82) τ 0 eτ ′ (cid:82) τ 0 eτ ′dτ ′ These integrals can be expressed as combinations of the incomplete gamma function and the gamma function, and the behaviors of select incomplete gamma functions as $\tau \to 0$ are illustrated in Fig. 3 [Figure 3: see original paper]: (cid:90) τ (cid:90) τ τ ′n+1dτ ′ = (−1)n+1 [Γ (n + 2) − Γ (n + 2, −τ)] τ ′ndτ ′ = (−1)n [Γ(n + 1) − Γ(n + 1, −τ)] .

Given µ and Σt are both constant, Eq. (29) can be ex- pressed as E(n + 1) Γ(n + 2) − Γ(n + 2, −τ) − τ n+1 Γ(n + 1, −τ) − nΓ(n) − τ n where Γ (n + 2) is the gamma function, which can be consid- ered a constant. Γ (n + 2, τ) is the incomplete gamma func- tion. When $\tau \to 0$, it can also be viewed as a constant.

Thus Eq. (29) can be viewed as E(n + 1) (n + 2)! − (n + 2)! + τ n+1 eτ −1 (n + 1)! − (n + 1)! + τ n eτ −1 Then Taylor expand this form Eq. (29) at τ = 0 yields, E(n + 1) 6 +O(τ 4) 6 +O(τ 4) Thus the error E (n + 1) associated with a source q (z′) = z′n+1 is one order higher than the error E (n) associated with approaches zero. Applying L' Hôpital' s rule yields E (n + 1) E (n) = lim dE(n+1) dE(n) (cid:90) τ τ ′n+1dτ ′− τ n+1 n + 2 (cid:90) τ (cid:90) τ τ ′ndτ ′− n + 1 (cid:90) τ = lim µ(n + 1)2 Σt (n + 2) n = O(τ) .

From this equation and the fact that E (n = 1) = O (cid:0)τ 2(cid:1), it follows that E(n) = O(τ n+1), n 1 which implies that, in general, for q(z′) = z′n, an nth-order source exhibits (n + 1)th-order accuracy. Consequently, the flat source approximation achieves at most second-order ac- curacy.

B. Linear Source (LS) Approximation LS approximation implies the following ˜q (z′) = q0 + q1 ⋆ (z′ − zc) , 0 < z′ < z.

Using Eq. (18) to evaluate the error introduced into the cell- Fig. 3. Incomplete gamma functions averaged angular flux via LS approximation, a source q (z′) = z′n. By induction, the error follows that E (n) τ n+1, indicating that the flat source approximation is generally second-order accurate in space.

A more systematic method is presented in the following, lending itself to a more consistent way of proof among FS and LS approximations, which will be shown later.

We take the limit of the ratio of E(n+1) in Eq. (29) as τ E = − e− Σt e− Σt (cid:90) z (cid:90) z (cid:90) z (cid:90) z q (z′, µ) dz′− ˜q (z′, µ) dz′ q (z′, µ) dz′− µ z′ (cid:104) q0 + q1 (cid:16) (cid:17)(cid:105) where the zeroth source moment is defined as, MMS (µ) = (cid:90) z qMMS (z′, µ) dz′ , and the first

source moment is defined as, (cid:104) MMS (µ) = (cid:105) 12 The following source cases are the same as Sect. II A. z′qMMS (z′, µ) − zcqMMS (z′, µ)

3. Quadratic Component

It is straightforward to demonstrate that the linear source approximation can represent a flat source without errors.

Since q1 vanishes and q0 exactly represents a constant source, the proof follows directly from Sect. II A 1.

2. Linear Component

Next, we demonstrate that the linear source approximation can exactly represent a linearly distributed source.

Assuming q (z′) = z′, 0 < z′ < z in q0 and q1 defined in Eq. (38) gives (cid:104) (cid:90) z q (z′) dz′ = z′q (z′) − zcq (z′) (cid:20) z2 (cid:21) 12 z2 = 1 (cid:90) z (cid:105) 12 z′dz′ = The approximating source distribution is exactly the same as the originally manufactured source distribution, as shown below ˜q (z′) = q0 + q1 (cid:16) (cid:16) (cid:17) (cid:17) = z′ = q (z′) From Eq. (37), the error E (n = 1) are given by E (n = 1) = − e− Σt e− Σt (cid:90) z (cid:90) z (cid:90) z z q (z′, µ) dz′− ˜q (z′, µ) dz′ z′dz′− z′dz′ Last, if the source distribution is quadratic in space as q (z′) = z$ ‘2, 0 < *z*’ $ < z, we have (cid:104) (cid:90) z q (z′) dz′ = z′q (z′) − zcq (z′) (cid:20) z3 (cid:21) 12 (cid:90) z (cid:105) 12 z$’ 2*dz*’ $ = Constructing the linear approximation with the zeroth and first source moments gives ˜q (z′) = q0 + q1 (cid:16) (cid:17) + zz′ .

The error introduced via linear source (LS) approximation can be evaluated with Eq. (37) (cid:90) z (cid:90) z e− Σt E = − z$’ 2*dz*’ −*z*’ $ (cid:18) (cid:19) + zz′ (cid:20)(cid:18) (cid:19) + 1 + (cid:21) (cid:19) (cid:18) τ The error approaches zero with fourth order as shown by Taylor expansion near $\tau = 0$. µ2 E = − + O (cid:0)τ 6(cid:1) .

As mentioned in Sect. II A 2, we normally do not have a standalone quadratic source; rather, it usually comes with a linear component. Note that the linear component does not affect the accuracy of the linear source approximation, which can be explained by linear superposition. Since the linear source approximation represents the linear component exactly, the error only arises from the higher-order compo- nents.

To illustrate this, assume (cid:101)q (z′) = Cz′ + z$’ 2, 0 < *z*’ $ < z, where C is an arbitrary constant, then we have:

Cz′ + z$’ 2*dz*’ $ = (cid:90) z (cid:20) Cz2 = C + z . (cid:21) Thus, the linear source approximation remains an exact representation of a linear source. (cid:101)q (z′) = (C + z) z′ − Therefore, the linear source approximating form is Now the error associated with this approximation can be be calculated using Eq. (37) as follows:

4. General Polynomial Component

τ ′n+1+ evaluated using Eq. (37). E = − e− Σt e− Σt (cid:90) z (cid:90) z (cid:90) z (cid:90) z q (z′, µ) dz′− µ z′ (cid:16) q0 + q1z′ − q1 z (cid:17) µ z′ (cid:16) Cz′ + z$ ‘2(*cid* : 17)*z*’ $ (cid:18) Cz′ + zz′ − (cid:19) (cid:20)(cid:18) (cid:19) (cid:18) τ + 1 + (cid:19) (cid:21) This equation equals Eq. (44), the error associated with the source distribution q (z′) = z$’ $2. Specifically, when using the LS approximation for a quadratic source, with or without a linear component, the error is 4th order.

Since the mathematical in both Sect. II A 4 and this subsection are consistent, it is reason- able to assume that E = O (τ n+const). From Sect. II B 2, the error can be estimated as forms of the error E = O (cid:0)τ n+2(cid:1) .

To formally prove this result, it is necessary to derive ex- pressions for a general source. For any source expressed as q (z′) = z′n, its zeroth and first spatial moments can be eval- uated using Equation (38) as follows:

E (n) e− Σt (cid:90) z (cid:90) z q (z′, µ) dz′− ˜q (z′, µ) dz′ µne−τ (cid:90) τ τ ′n+ (2n − 2) τ n (n + 1) (n + 2) 6nτ n−1τ ′ (n + 1) (n + 2) dτ ′ .

E(n + 1) can be easily obtained by replacing n with n + 1 in the equation above. Now, we divide E(n + 1) by E(n) and take the limit as $\tau \to 0$. Applying L’ Hôpital’s rule, i.e., taking the derivative of both the numerator and denominator, yields:

E (n + 1) E (n) − µn+1e−τ (cid:82) τ 0 eτ ′ = lim 2nτ n+1 (n + 2) (n + 3) 6 (n + 1) τ nτ ′ (n + 2) (n + 3) τ ′n+ − µne−τ (cid:82) τ 0 eτ ′ (2n − 2) τ n (n + 1) (n + 2) 6nτ n−1τ ′ (n + 1) (n + 2) (cid:82) τ 0 eτ ′ (cid:104) 0 eτ ′ (cid:104) (cid:82) τ τ ′n+1 + 2nτ n+1−6(n+1)τ nτ ′ (cid:105) τ ′n + (2n−2)τ n−6nτ n−1τ ′ (n+2)(n+3) (n+1)(n+2) (cid:105) µ(n + 1)2 Σt (n − 1) (n + 3) q0 (n) = q1 (n) = (cid:90) z z′ndz′ n + 1 (cid:104) z′q (z′) − zcq (z′) (cid:20) zn+1 n + 2 6nzn−1 n2 + 3n + 2 2(n + 1) (cid:105) 12 (cid:21) 12 LS approximation of q (z′) = z′n presents ˜q (z′, n) = q0 + q1 (z′ − zc) n + 1 (2 − 2n) zn + 6nzn−1z′ n2 + 3n + 2 6nzn−1 n2 + 3n + 2 (cid:16) Thus, the error associated with the LS approximation can = O (τ) .

From this equation and E (n = 2) = O (cid:0)τ 4(cid:1), we can easily conclude E (n) = O (cid:0)τ n+2(cid:1) , n 2.

This result implies that, in general, for q(z′) = z′n, an nth- order source exhibits (n + 2)th-order accuracy. At least, the linear source approximation achieves fourth-order accuracy. (cid:17) III. VERIFICATION TESTING RESULTS Using the Method of Manufactured Solutions (MMS), we have developed a one-dimensional (1D) MoC code in MAT- LAB to verify the conclusions presented in Sect. II. The cor- responding results are provided in Sect. III A. Additionally, The zeroth and first spatial moments of the MMS source are calculated using the following equation: j = q (x) (cid:104) q (x) ⋆x − xc (cid:105) j ⋆q (x)

2. Testing Purely Absorbing Materials

To test the distributed source only, we chose purely absorb- ing materials, whose scattering cross section was set to zero.

Figures 4, 5, 6, 7 present the grid refinement results for four cases, each corresponding to a constant, linear, quadratic, or non-polynomial manufactured source. • Figure 4 [Figure 4: see original paper] (Constant Source): The FS-MoC solution is exactly zero, as indicated by the absence of blue stars in the log-log scale plot. The LS-MoC solution, represented by or- ange stars, also exhibits near-zero errors for this case. • Figure 5 [Figure 5: see original paper] (Linearly Distributed Source): The FS-MoC method demonstrates second-order accuracy, with the numer- ical results converging along the green line corresponding to the expected second-order convergence rate. The LS-MoC solution exhibits near-zero errors within machine precision, as it exactly represents the linear source distribution. • Figure 6 [Figure 6: see original paper] (Quadratically Distributed Source): FS-MoC maintains second-order accuracy, while LS-MoC achieves fourth-order accuracy. • Figure 7 [Figure 7: see original paper] (Non-Polynomial Source): Results indicate that FS-MoC and LS-MoC methods maintain second-order and fourth-order accuracy, respectively. our previous research using the Method of Exact Solutions (MES) for the Ganapol case supports that our theoretical pre- diction can be generalized to 2D, which is documented in Sect. III B.

A. Verification Testing Using the Method of Manufactured Solutions The MMS is a widely used verification technique for as- sessing the correctness of numerical algorithms in scien- tific computing. Unlike traditional benchmark comparisons, MMS involves prescribing an exact analytical solution by introducing a manufactured source term into the governing equations. This approach enables the systematic testing of numerical methods by isolating discretization errors, ensur- ing consistency, and verifying the accuracy of computational models. MMS is particularly useful in complex multi-physics simulations, including neutron transport, fluid dynamics, and heat transfer, where analytical solutions are otherwise diffi- cult to obtain.

1. Testing Suite

The 1D MoC code we developed has tested the formal or- der of accuracy for FS and LS approximations. Four test cases were devised, each based on an assumed flux shape and its corresponding manufactured source, both defined in the global coordinate system.

Test listings: Case 1: constant source distribution ψ (x, µ) = \$ \$0 qMMS (x, µ) = \$ 0(\$t − Σs) Case 2: linear source distribution ψ (x, µ) = \$ \$0 + \$ \$1eµx qMMS (x, µ) = \$ 0(\$t − Σs) + \$ \$1µeµ (cid:20) Σteµ − (cid:0)e − e−1(cid:1) (cid:21) Case 3: quadratic source distribution ψ (x, µ) = \$ \$0 + \$ \$2eµx2 qMMS (x, µ) = \$ 0(\$t − Σs) + 2\$ \$2µeµx (cid:20) Σteµ − (cid:0)e1 − e−1(cid:1) (cid:21) Fig. 4. Order of accuracy with constant manufactured source (FS: exact, LS:

exact) Case 4: non-polynomial source distribution ψ (x, μ) = x + 1 qMMS (x, μ) = x + 1 + (Σt − Σs) x + 1 All experimental results align with analytical predictions, as summarized in Table 1 , where the observed order of ac- curacy is presented alongside the formal order of accuracy in the format.

Fig. 5. Order of accuracy with linear manufactured source (FS: 2nd order, LS: exact) Fig. 7. Order of accuracy with non-polynomial manufactured source (FS: 2nd order, LS: 4th order) B. Verification Testing Using the Method of Exact Solutions The Method of Exact Solutions (MES) verifies numeri- cal solutions by comparing them to known analytical expres- sions, typically sourced from the existing literature. These ex- act solutions provide precise values across all spatial and tem- poral points, enabling direct verification of numerical meth- ods. If discrepancies remain within acceptable limits (e.g., round-off errors), the code is considered verified. Addition- ally, grid refinement studies can be conducted to analyze con- vergence behavior, either confirming theoretical expectations or establishing new benchmarks where none exist. Notably, the findings presented in this section originate from our pre- vious work [20].

1. Ganapol benchmark

Benchmark Problem 3.4 from Ganapol' s analytical bench- mark book [21] is a robust verification test case that can be implemented in MPACT [1] without special modifications to the code. This benchmark enables the verification of both our order-of-accuracy predictions and the accuracy of the MPACT code itself, as previously published in [15]. It also supports the broader code and solution verification activities for MPACT.

This case is presented again to confirm that the spatial con- vergence rate es- tablished in 1D extends to 2D problems. Be- low, we restate the problem con- figuration.

The Ganapol benchmark problem is an analytic, or "semi- analytic," benchmark based on the exact solution of the singu- lar integral equation that describes the single-group cylindri- cal transport problem. This solution methodology is a com- plex sequence of steps, which are described in detail in the book [21].

Fig. 6. Order of accuracy with quadratic manufactured source (FS: 2nd order, LS: 4th order) TABLE 1. Observed and formal order of accuracy Approx.

FS Pr. FS Ob. exact LS Pr. exact LS Ob. * The arrow indicates the aforemen- tioned order degradation.

Quad. 3rd$→$2nd* Const. exact exact exact exact Non-poly.

The angular errors inherent in the numerical results were isolated using an error removal technique developed in a pre- vious study [22].

The benchmark considers a homogeneous right circular cylinder of infinite height (Fig. 8 [Figure 8: see original paper]), characterized by: its boundaries. On

the other hand, the addition of a bound- ing box transforms the 1D cylinder configuration into a 2D fuel-pin problem.

Fig. 8. Infinite homogeneous cylinder • Radius: r = R (measured in mean free paths) • Physical Radius: r/Σt • Height: h → ∞ • Total cross section: Σt • Scattering cross section: Σs • Fission cross section: Σf • Secondary neutrons per collision: c, where c = (Σs + νΣf) /Σt, ν is average of fission neutrons per fission.

The benchmark results are provided for several cases: (a) Uniform isotropic source - the scalar flux ϕ (r) is tabu- lated for selected values of c < 1; (b) Critical rod - the critical radius is tabulated as a function of c > 1; (c) Critical rod - the scalar flux ϕ (r) is depicted for critical rods as a function of c > 1.

Table 2 , sourced from Ganapol [21], provides the bench- mark results for the critical rod problem, listing the critical rod radius as a function of c. The values are accurate to the last known significant digit (within eight decimal points).

This table also confirms agreement with previously published benchmarks (i.e. [23, 24]), with discrepancies highlighted in bold results.

2. MPACT results

For MPACT verification, critical rod problems (b) in Sect. III B 1 are chosen as benchmarks because they exercise both the 2D MoC solver and the eigenvalue solver.

Because MPACT was used for LWR lattices, special input processing in the code is required to model the isolated cylin- der. To avoid this, the benchmark is adapted by modeling the cylinder as a fuel pin within a non-scattering square bound- ing box (Fig. 9 [Figure 9: see original paper]). On the one hand, this approximation en- sures the incoming angular flux remains zero outside the rod, with scattering and fission sources contributing only within Fig. 9. The material of the cylinder TABLE 2. Critical rod radii in MPACT from Table 3 .4.3(a) [21] R [24] MPACT determines the eigenvalue k based on the critical rod radii listed in Table 2. Each case should yield k = 1 to high precision, verifying the accuracy of the transport solu- tion. The radial mesh was refined by increasing the number of rings.

All cases were run with the following phase space dis- cretization parameters:

Bounding box side length = 30 cm Ray spacing = 0.0005 cm Number of radial rings = [10,160] by increment of 10 Number of azimuthal slices = 32 Quadrature set = CHEBYSHEV GAUSS 32 24 Convergence criterion = 10−7 for both k and RMS error of Table 3 presents the eigenvalues computed by MPACT, all within a few pcm of criticality. This confirms strong agree- ment with analytical solutions, reinforcing the reliability of MPACT.

TABLE 3. MPACT' s keff and error R (mfp) Error(pcm)

3. Mesh convergence analysis

A radial mesh refinement study was conducted using the c = 1.01 case. The convergence curve in Fig. 10 [Figure 10: see original paper] demon- strates that MPACT achieves second-order accuracy in the ra- dial direction, which is consistent with the FS-MoC expecta- tions.

IV. CONCLUSIONS A comprehensive analysis of the order of accuracy related to spatial discretization in the MoC for slab geometry has been conducted, focusing on the flat source (FS) and linear source (LS) approximation of the distributed source. The study develops an analytical approach that integrates the an- gular flux using an assumed source term, yielding explicit ex- pressions for the error in cell-averaged flux from source ap- proximations, demonstrating that FS achieves at least second- order accuracy, whereas LS is expected to achieve fourth- order accuracy. These theoretical predictions were verified through numerical tests using the method of manufactured solutions (MMS) using a test suite that included constant, lin- ear, quadratic, and non-polynomial solutions. The method of exact solutions (MES), utilizing the Ganapol critical rod problems, was also implemented using MPACT. The numeri- cal results further verify the theoretical order of accuracy for the FS approximation in 2D.

These findings provide a rigorous foundation for assess- ing spatial discretization errors in MoC-based neutron trans- port. Future work will extend this analysis to the convergence behavior related to approximating the scattering source, ultimately helping determine the overall order of accuracy for spatial discretization in MoC.

V. CONTRIBUTION All authors contributed to the study conception and design.

Material preparation, data collection and analysis were per- formed by Jipu Wang, Zhenwen Wei and Can Huang. The first draft of the manuscript was written by Jipu Wang, Zhen- wen Wei and Can Huang, and all authors commented on pre- vious versions of the manuscript. All authors read and approved the final manuscript.

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Note: Figure translations are in progress. See original paper for figures.