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The application of Method of Manufactured Solutions to method of characteristics in planar geometry

Jipu Wang [a,*], William Martin [a], Benjamin Collins [a,b]

[a] University of Michigan, Ann Arbor, MI 48109, USA
[b] Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

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ABSTRACT

The Method of Manufactured Solutions (MMS) is an effective code verification method for assessing the correctness of numerical algorithms and software implementation. It has great flexibility in verifying computational functionalities of a computer code and has seen wide applications in many engineering fields. It has been used for the radiation transport equation but has had limited success in determining whether the observed rate of convergence is consistent with the expected value due to the coupled errors in space and angle. There have also been only limited applications of MMS to eigenvalue problems and very little published research has been performed on applying MMS to multiphysics problems. In this work, MMS is applied to both flat-source and linear-source method of characteristics (MoC) in planar geometry for source problems and eigenvalue problems. A method is developed which allows the angular error to be decoupled from the spatial error, enabling the assessment of the convergence rate with spatial resolution. The angular error removal technique is also applicable to eigenvalue problems. Additionally, two independent approaches to applying MMS to eigenvalue problems are developed, one using an inhomogeneous manufactured source and the other using manufactured cross sections. When the neutronics solver is coupled to a thermal conduction code, MMS is used to investigate the overall order of accuracy of the coupled multiphysics system. Comprehensive tests are devised with a variety of solution structures to verify the theoretical convergence rates. Numerical results show that both the eigenvalue k and the cell-averaged scalar fluxes exhibit orders of accuracy consistent with theoretical predictions, namely, second order for flat-source MoC and fourth order for linear-source MoC. However, for a multiphysics problem coupling neutronics with thermal hydraulics, the overall order of accuracy is limited by the solution field with the slowest rate of convergence.

1. Introduction

Software verification and validation (V&V) are important steps in the standard software development lifecycle. Verification is the process of verifying the correctness of both numerical algorithm and software implementation, distinguished from validation which determines the adequacy of the governing equations for the physical problem being analyzed. As one of the various verification methods, the Method of Manufactured Solutions (MMS) has the advantage of both great flexibility and mathematical rigor, lending itself to wide applications in code verification. (Roache, 2002, 1998)

There have been a few successful applications of MMS to the neutron transport equation (Salari et al., 2000; Pautz, 2001; Schunert and Azmy, 2015) but there has been limited success in determining whether the observed convergence rate of the error is consistent with the expected rate due to the coupled errors in space and angle. There have also been only limited applications of MMS to eigenvalue problems, (Pautz, 2001; Schunert and Azmy, 2015; Wang, 2012) and in those cases, MMS has primarily been used merely as an analytical solution generator rather than a solver verification tool, neither was the method for applying MMS to eigenvalue problems clearly discussed. In our previous work (Wang et al., 2017), we analyzed the theoretical order of accuracy (OoA) with spatial resolution in planar geometry for method of characteristics (MoC), with both flat source (FS) approximation (Askew, 1972; Halsall, 1980; Knott, 1991) and linear source (LS) approximation (Ferrer and Rhodes, 2016), which is the preferred deterministic method to solve neutron transport equation for reactor analysis problems with complicated geometries. It was confirmed that FS is second order and LS is fourth order

* Corresponding author.
E-mail address: jipuwang@umich.edu (J. Wang).

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but a thorough discussion of the angular error removal (AER) technique was not given. Finally, there has been very few published research on applying MMS to a multiphysics system (McClarren and Lowrie, 2008), which turns out to be especially important due to the scarcity of multi-physics validation data.

In this work, the predicted OoAs for MoC with FS and LS approximations are verified with MMS for both fixed source problems and eigenvalue problems. A method is developed allowing the angular error and spatial error to be separated so that the convergence with spatial resolution can be assessed. Additionally, we have developed two independent approaches to apply MMS to eigenvalue problems, one using manufactured source and the other using manufactured cross sections. Finally, the application of MMS to a multiphysics problem has been demonstrated with a source driven sub-critical system coupling neutronics and thermal conduction.

Section 2 of this paper describes the theory and methodology of the angular error separation schemes, the application of MMS to both source problem and eigenvalue problems, and the application of MMS to a multiphysics problem. Section 3 gives the numerical results for both single physics and multiphysics problems using MMS to verify the OoA predictions, with assumed solutions featuring polynomial and nonpolynomial functional forms. Section 4 summarizes the conclusions and implications of this work. As predicted, the flat source approximation is second order accurate in space and the linear source approximation is fourth order accurate after removing the angular error. It is also shown that in a multiphysics system the overall OoA is limited by the solution field with the slowest rate of convergence.

2. Theory and methodology

2.1. Method of Manufactured Solutions

The essential idea of MMS is that instead of solving a specified problem with prescribed boundary and initial conditions, one can assume a solution beforehand and substitute it into the governing equation that the software intends to solve. The equation is then balanced by evaluating the resultant manufactured source. The boundary and initial conditions can be obtained by evaluating the manufactured solution at the boundary and at the initial time. The software is then used to solve the system with the manufactured source and boundary and initial conditions. By comparing the numerical solution with the manufactured solution and observing the expected rate of convergence of the error with systematic grid refinements, the computer code can be verified.

2.2. Application of MMS to a fixed source problem

The neutron Boltzmann transport equation with a fixed source can be presented as:

$$(L+T)\psi = S\psi + Q \tag{1}$$

where L, T, S, Q respectively represent leakage, collision, in-scattering and external source operators and ψ is the neutron angular flux.

The application of MMS to a fixed source problem is straightforward. Start with an assumed solution ψ_{MMS}, and evaluate the manufactured source and boundary conditions:

$$\begin{aligned} Q_{\text{MMS}} &= (L+T-S)\psi_{\text{MMS}} \\ \psi_{\text{Bndy}} &= \psi_{\text{MMS}}|_{\text{Bndy}}, \text{ for incoming directions} \end{aligned} \tag{2}$$

The above continuous source and boundary conditions can be discretized by cell-averaging over a spatial cell and evaluating at angles defined in the applied quadrature set.

For example, in planar geometry discretized into J slab intervals $x_{j-1/2} < x < x_{j+1/2}$, $j = 1, \ldots, J$ as shown in Fig. 1,

the discretized source (for flat source approximation) and boundary conditions can be expressed as:

$$\begin{aligned} Q_{\text{MMS},j,n} &= \tfrac{1}{\Delta x_j}\int_{x_{j-1/2}}^{x_{j+1/2}} Q_{\text{MMS}}(x,\mu_n)dx \\ \psi_{\text{LB},n} &= \psi_{\text{MMS}}(x=0,\mu_n), \;\; \mu_n > 0 \\ \psi_{\text{RB},n} &= \psi_{\text{MMS}}(x=X,\mu_n), \;\; \mu_n < 0 \end{aligned} \tag{3}$$

where μ_n is from the applied quadrature set (μ_n, ω_n), $n \in [1, \ldots, N]$.

More details about MMS in linear source MoC can be found in (Wang et al., 2017, 2018).

This problem is then modeled and solved with a series of refined grids. The RMS error is defined as:

$$E_{\text{RMS}} = \sqrt{\frac{1}{J}\cdot\sum_{j=1}^{J}(E_j)^2} = \sqrt{\frac{1}{J}\cdot\sum_{j=1}^{J}\left(\phi_j - \phi_{\text{MMS},j}\right)^2} \tag{4}$$

where ϕ_j is the cell-averaged scalar flux and $\phi_{\text{MMS}}(x)$ is the corresponding manufactured scalar flux:

$$\phi_{\text{MMS},j} = \frac{1}{\Delta V_j}\int_{V_j}\int_{4\pi}\psi_{\text{MMS}}\left(\underline{r},\hat{\Omega}\right)d\Omega dV \tag{5}$$

The order of accuracy (OoA), or rate of convergence, measures the rate of error reduction with refined grids and can be calculated as:

$$p = \frac{\log\left(\frac{E_{\text{grid1}}}{E_{\text{grid2}}}\right)}{\log(r)} \tag{6}$$

where r is the ratio of the mesh size of grid 1 to that of grid 2, known as the grid refinement ratio.

2.3. Procedure to remove the angular error

When equations with more than one independent variable are discretized, discretization errors propagate and interact through the numerical algorithm, concealing the expected rate of convergence with respect to one variable when its grid is refined. To reveal this rate of convergence, it is possible to use the assumed solution to remove the error components of the other variables, such as the angular variable μ when assessing the spatial convergence rate. This will avoid error contamination and help reveal the rate of convergence during grid refinements in the selected variable.

The following quantities represent the angular and spatial error components.

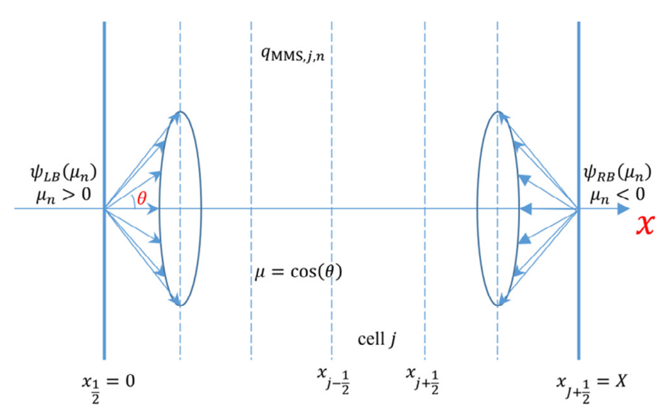

Fig. 1. Planar geometry with azimuthal symmetry.