



# A new approach to three-dimensional neutron transport solution based on the method of characteristics and linear axial approximation



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## ARTICLE INFO

### Article history:

Received 9 November 2016  
Received in revised form 12 July 2017  
Accepted 12 August 2017  
Available online 22 August 2017

### Keywords:

3D neutron transport  
Method of characteristics  
Linear axial approximation

## ABSTRACT

A new approach based on the method of characteristics (MOC) is proposed to solve the neutron transport equation. A new three-dimensional (3D) spatial discretization is applied to avoid the instability issue of the transverse leakage iteration of the traditional 2D/1D approach. In this new approach, the axial and radial variables are discretized in two different ways: the linear expansion is performed in the axial direction, then, the 3D solution of the angular flux is transformed to be the planar solution of 2D angular expansion moments, which are solved by the planar MOC sweeping. Based on the boundary and interface continuity conditions, the 2D expansion moment solution is equivalently transformed to be the solution of the axially averaged angular flux. Using the piecewise averaged angular flux at the top and bottom surfaces of 3D meshes, the planes are coupled to give the 3D angular flux distribution. The 3D CMFD linear system is established from the surface net current of every 3D pin-mesh to accelerate the convergence of power iteration. The STREAM code is extended to be capable of handling 3D problems based on the new approach. Several benchmarks are tested to verify its feasibility and accuracy, including the 3D homogeneous benchmarks and heterogeneous benchmarks. The computational sensitivity is discussed. The results show good accuracy in all tests. With the CMFD acceleration, the convergence is stable. In addition, a pin-cell problem with void gap is calculated. This shows the advantage compared to the traditional 2D/1D MOC methods.

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## 1. Introduction

In recent years, the high-fidelity modeling and simulation of nuclear reactors has become more and more attractive based on the fast development of high performance computing (HPC) [1,2]. Solving the three-dimensional (3D) neutron transport equation with pin or sub-pin resolution plays a very important role in the concept of high-fidelity simulation. One of the most popular solutions is to apply the method of characteristics (MOC) in the 3D geometry. The MOC method was proposed by Askew in 1972 [3] and widely accepted in the next few decades for the heterogeneous fuel assembly and reactor core calculations.

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Due to its legacy of success in the past decade, the MOC method based on the 2D/1D computational scheme has brought inspiring achievements by using pin resolution to model real PWRs. This method, known as the 2D/1D fusion method, was firstly proposed by N.Z. Cho [4]. This is a synthetic combination of the MOC method for planar 2D calculation and the  $S_N$ -like method for axial 1D calculation. Later, the DeCART code [5] extended the method by using the axial diffusion approximation and the highly-efficient coarse mesh finite difference (CMFD) method for 3D neutron balance and acceleration. Recently, several improvements have been made by introducing low-order transport approximation and more accurate nodal methods in the axial direction [6]. The massively parallel capability has also been realized for the whole core modeling and simulation [7].

However, the traditional 2D/1D scheme using axial diffusion approximation and homogenized leakage exhibits some instability problems when the neutron leakage for the axial direction is large. This usually arises when the axial mesh is thin or there is a low density region in the reactor. Several years ago, efforts were made to improve the convergence stability [8]. As indicated in the previous work, the CMFD acceleration should be turned off to keep the convergence stable. But for the 3D calculation, turning off the acceleration will cause a huge increase in computational time which makes the method unpractical. More recent works have been proposed to make the 2D/1D iteration more stable and have brought promising solutions. A new equation, the consistent 2D/1D approximation, was derived by Kelley and Larsen to get better iterative stability [9]. An artificial diffusion CMFD method was proposed and compared with other known techniques for stabilizing CMFD, the theoretical analysis and experimental test demonstrated the stability [10].

Another way to further develop the MOC method in the 3D geometry is the direct and full 3D calculation. The full 3D MOC is based on the three-dimensional ray trace [11,12]. The modular ray trace techniques have been proposed to reduce the memory cost. However, it still requires too much memory storage and computational time in the practical modeling of a reactor core.

To solve the problem of computational cost, an alternative approach has been proposed [13]. That approach proposed the concept of a characteristics plane and expanded the axial mesh width to several centimeters to reduce the computational burden. Yamamoto et al. extended this approach and introduced the Legendre Expansion of Angular Flux (LEAF) method [14] to reduce spatial discretization errors. Another advance was made when the linear source approximation and an on-the-fly ray tracing technique in the OpenMOC code were introduced [15]. These methods have shown significant memory reduction with minimal or no computational overhead.

A different way of applying the MOC method was proposed in ANL's work. The MOCFE [16] in the UNIC code was developed based on the fully unstructured 3D geometries. It uses the finite element mesh rather than a combinatorial geometry in the MOC calculation. The linear tetrahedral and quadratic hexahedral finite elements are adopted in three-dimensions. Recently, to reduce the computational burden, a new approach has been proposed in the PROTEUS-MOC code [17]. This approach takes advantage of assuming the 3D model for a typical reactor can be accurately represented by a 2D extruded geometry. Then, the radial and axial dependence of flux is treated with two different approximations. The MOC method is combined with a discontinuous Galerkin method to solve the stability problem in the traditional 2D/1D approach by a fully consistent 3D discretization of the transport equation.

In this paper, we are referring to the works in PROTEUS-MOC and propose a new approach for using the linear approximation in the axial direction, and the traditional planar MOC sweeping radially. In this approach, the 3D flux is expressed into the basis function expansion form of only axial variable  $z$ . Instead of using the finite element method, the basis functions are defined inside the axial mesh and the integration over the axial mesh keeps the neutron balance in each plane. The sweeping scheme is introduced by explicitly using the axial boundary condition and interface condition instead of implicitly using the interface condition to couple each plane. Then, the globally coupled 3D problem can be split into plane-wise individual 2D problems. Then, the plane-wise 2D equations for the expansion coefficients of axial flux are obtained, which have the same form as in the traditional 2D MOC equation. Three benefits are achieved with this new method:

- 1) The equations solved for each plane are reduced by half for the linear approximation, i.e. only one equation must be solved. So, the computational burden is reduced. Based on this equation, the plane-wise calculation is in the same form as the traditional MOC calculation but without the iteration for updating the transverse leakage.
- 2) In the sweeping scheme, the angular dependence is only required while treating the interface coupling of neighboring planes. Therefore, the memory storage is significantly reduced.
- 3) By using the basis function in mesh and axial integration, the neutron balance is preserved, and the coarse mesh finite difference (CMFD) acceleration is easy to establish.

In the following sections, the equations in 3D geometry are derived which are finally transformed into the standard 2D form. The MOC sweeping for the transformed equation is briefly reviewed and then the 3D CMFD equation is established in Section 2. In Section 3, the numerical tests are employed to verify the accuracy of the new approach. Computational sensitivity is discussed based on the pin-cell tests, TAKEDA benchmarks and the C5G7 benchmark problem. Section 4 briefly summarizes the work and makes recommendations for further research.

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