Research and Verification of One-Step Resonance and Transport Methods Based on the OpenMOC Code

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Abstract

The one-step method in reactor physics has become one of the important research directions in recent two decades. Based on the open-source OpenMOC code, the following work was carried out. Firstly, the global-local resonance method with multi-group and continuous neutron libraries was researched and established. Next, based on the 2D and 3D MOC solver, the 2D/1D and the MOC/DD transport methods were realized in OpenMOC. Finally, verification of the transport and resonance methods was conducted using the C5G7 macro benchmark and the VERA micro benchmark. The numerical results demonstrated that the average eigenvalue deviation was 44pcm and average maximum pin power distribution deviation was 0.37% in the VERA-2 benchmark, which showed the good accuracy of the resonance method. As for the transport method, 3DMOC method exhibited better accuracy in strong anisotropic cases, but the computational time was 38 times that of the 2D/1D method.

Full Text

Research and Verification of One-Step Resonance and Transport Methods Based on the OpenMOC Code

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ABSTRACT

The one-step method in reactor physics has emerged as an important research direction over the past two decades. Based on the open-source OpenMOC code, this study conducted several key developments. First, a global-local resonance

method was established using both multi-group and continuous-energy neutron libraries. Next, 2D/1D and MOC/DD transport methods were implemented in OpenMOC based on existing 2D and 3D MOC solvers. Finally, verification of both transport and resonance methods was performed using the C5G7 macro benchmark and VERA micro benchmark. Numerical results demonstrated that the VERA-2 benchmark achieved an average eigenvalue deviation of 44 pcm and an average maximum pin power distribution deviation of 0.37%, confirming the good accuracy of the resonance method. For transport methods, the 3DMOC approach exhibited superior accuracy in strongly anisotropic cases, though its computational time was 38 times longer than that of the 2D/1D method.

KEYWORDS: One-step method, Resonance, Transport, OpenMOC

Introduction

In recent years, with continuous advances in computer technology, high-fidelity one-step methods for precise reactor modeling and calculation have become a major focus in reactor physics research. Several high-fidelity codes have been developed worldwide, including DeCART[1], MPACT[2], nTRACER[3], PROTEUS-MOC[4], OpenMOC[5-6], APOLLO-3[7], STREAM[8], NECP-X[9-10], VITAS[11], and ALPHA[12]. Research areas encompass nuclear data libraries, resonance treatment, transport methods, burnup analysis, kinetics, and multi-physics coupling, enabling one-step transport calculations for pressurized water reactors.

OpenMOC is an open-source direct transport code based on the method of characteristics (MOC), developed by the Massachusetts Institute of Technology (MIT). It employs hybrid programming with Python and C++ to balance the computational efficiency of C++ with the user-friendly interface of Python. The code utilizes constructive solid geometry (CSG)[15] and the long characteristic ray method[16] to support arbitrary geometry modeling and calculation capabilities. For large-scale problems, OpenMOC employs spatial domain decomposition parallelism for both memory distribution and computation. Additionally, the code supports coarse mesh finite difference (CMFD) for accelerating iterative convergence and GPU/CPU hybrid computing for MOC calculations.

In this work, a resonance module based on the global-local method was integrated into OpenMOC. Both multi-group and continuous-energy libraries were constructed to support global-local resonance calculations. In the transport module, 2D/1D and MOC/DD solvers were developed based on the existing 2DMOC and 3DMOC solvers. The accuracy and efficiency of these whole-core direct transport methods were subsequently compared.

2. Framework of the OpenMOC Code

The framework of the enhanced OpenMOC code is illustrated in [Figure 1: see original paper]. The input/output module retains its original structure and

logic, employing CSG methods for high-fidelity geometric modeling while incorporating nuclear density information to address realistic microscopic problems. Multi-group and continuous-energy libraries were established for resonance calculations. A global-local resonance calculation module was developed using the global neutron current method and local pseudo-nuclide subgroup method. Inflow transport corrections were then applied to obtain macroscopic cross-sections for each material region. Finally, direct transport calculations were performed using 3DMOC, 2D/1D, and MOC/DD methods, with CMFD and parallel acceleration methods retained from the original OpenMOC code.

3. Global-Local Resonance Method

For whole-core resonance calculations, the primary challenge is to accurately simulate various resonance phenomena while maintaining acceptable computational efficiency. The global-local resonance method addresses this by separating resonance phenomena into global and local effects, thereby balancing accuracy and efficiency. This approach has demonstrated good performance in thermal spectrum reactors. The theoretical foundation of the global-local method encompasses three components: libraries, global method, and local method.

3.1. Library

This study employs the classical WIMS-69 group structure. Based on the WIMS library, a new multi-group library was developed to enhance resonance effect calculation capabilities, and a continuous-energy library was constructed to support the global-local resonance method.

Multi-group Library: For thermal spectrum reactors, mainstream one-step calculation codes typically use multi-group library structures with fewer than one hundred groups. The WIMS database is an internationally recognized open-source library, and its 69-group structure is widely used in pressurized water reactor calculations. Based on the WIMS library, improvements were made in several aspects: resonance energy range, resonance nuclides, and resonance integral tables, to create a multi-group database suitable for the global-local resonance method.

Regarding the resonance energy range, the original WIMS resonance range of 4 eV to 9.118 keV cannot account for plutonium nuclide resonance peaks below 4 eV, as shown in [Figure 2: see original paper]. This theoretically introduces deviations in MOX fuel calculations. Furthermore, the ENDF/B-VII.0 evaluated nuclear library provides distinguishable resonance parameters for U-238 above 9.118 keV, which the original resonance energy range division did not consider for resonance self-shielding effects. To address these issues, the multi-group library in this study extends the resonance energy range to 0.625 eV–24.78 keV.

In terms of nuclides, ^{242}Pu exhibits strong resonance effects in the thermal energy region. The WIMS library approximates the resonance self-shielding effect of ^{242}Pu separately for high-enriched and low-enriched MOX assemblies.

The expanded resonance energy range in this study's multi-group library enables explicit and accurate simulation of ^{242}Pu resonance peaks. Additionally, based on the 28 resonance nuclides in the WIMS database, the NJOY program was used to create multi-group databases for Zr, Xe, Sm, Am, Eu, and other nuclides, increasing the total number of resonance nuclides to 66.

Temperature and background cross-section points were also enhanced. The temperature range was extended from 1100 K to 1800 K, and the number of temperature points increased from 4 to 6. The background cross-section points, originally limited to 10 by the NJOY program in the WIMS library, were expanded to 34 points using the RMET21 program to generate resonance integral tables. These improvements enhance the accuracy of resonance integral table interpolation.

Continuous-Energy Library: Since the resonance pseudo-nuclide method requires online solution of neutron moderation equations, an ultra-fine-group continuous library is necessary. Such a library would include ultra-fine energy group cross-sections for various nuclides at multiple temperature points, representing an impractically large data volume for direct storage. Therefore, the continuous-energy library stores only cross-sections. Using the BROADR module of NJOY, energy points, total cross-sections, elastic scattering cross-sections, and fission cross-sections from output files were processed into binary files. A continuous-energy library was created for 66 resonance nuclides at 32 temperature points, with a manageable size of 1.1 GB.

3.2. Global Method

In global calculations for a system with multiple fuel and moderator regions, the neutron balance equation under isotropic approximation can be written as:

Where f is the fuel region index; m is the moderator region index; V is the volume; Σ is the macroscopic cross-section; is the neutron flux density; S is the neutron source; P is the probability of isotropic neutrons produced in region f' undergoing their first collision in fuel region f; and P is the probability of isotropic neutrons produced in moderator region m undergoing their first collision in fuel region f.

By introducing the reciprocity relation, neglecting global resonance interference and temperature distribution effects, and applying the narrow resonance approximation to the moderator region source term, the neutron balance equation simplifies to:

Assuming only absorption (no scattering) in the fuel region with zero source term, the equation further simplifies to:

Introducing the isolated rod approximation, where the fuel rod is placed in an infinite moderator, the escape probability to the moderator equals the collision probability from the fuel. Letting the flux in the isolated rod fuel region be $_0$

and the flux in the original system fuel region be , the gray Dancoff correction factor can be obtained:

To avoid the complexity of energy-dependent gray-Dancoff calculations and reduce computational burden, the black Dancoff factor concept is introduced. Through theoretical derivation of the collision probability, the calculation formula becomes:

Where l is the average chord length of the fuel region, P is the escape probability, and C is the black Dancoff factor. Conservation of the black Dancoff factor for the fuel-moderator system ensures consistency. Therefore, black Dancoff factors must be calculated for each pin cell to establish equivalent one-dimensional models. Using the black body approximation, where the fuel region cross-section is infinitely large, the black Dancoff factor is obtained as:

In practical calculations, corresponding cross-section values are set based on this black body approximation to solve the single-group fixed-source equation globally, obtaining the average flux $_1$ for each fuel rod. For each fuel rod, considering the isolated rod approximation in an infinite moderator, the Carlvik method is used to calculate the first collision probability P_0, denoted as f . This yields the black Dancoff factor for each fuel rod in the global calculation.

3.3. Local Method

Based on gray Dancoff factors from global calculations, an equivalent one-dimensional model is established as shown in [Figure 3: see original paper], enabling conversion of global calculations into local calculations for individual fuel rods.

[Figure 3: see original paper]

First, the moderator radius for each fuel rod in the one-dimensional model is determined based on Dancoff factors. Maintaining constant fuel radius and fuel escape probability P according to Eq.(6), a binary search computes collision probabilities for various moderator radii to find the value matching the pin-cell Dancoff factor.

Next, all resonance nuclides are transformed into a pseudo-nuclide based on nuclear density ratios. Pseudo-nuclide cross-section tables and subgroup probability tables are generated online for each equivalent one-dimensional model. For pseudo-nuclide cross-section tables, total, absorption, and scattering cross-sections at various state points are calculated using a zero-dimensional ultra-fine-energy-group method. Interpolation table inputs include background cross-sections, actual temperatures, average temperatures, and burnup depths, as shown in Eq.(7). For subgroup probability tables, subgroup parameters such as the number of subgroups and subgroup cross-sections are determined using Padé approximation and fitting methods for pseudo-nuclides.

Subsequently, traditional subgroup methods solve each equivalent one-

dimensional model by establishing subgroup fixed-source equations based on subgroup parameters, solving for subgroup flux using collision probability methods, and calculating effective self-shielding cross-sections.

Finally, the SPH factor method addresses multi-group equivalence effects through iterative correction of effective self-shielding cross-sections until convergence of final SPH factors is achieved.

4. Direct Transport Method

For direct one-step transport calculations, the MOC method has become mainstream due to its excellent geometric description capability and computational accuracy. Several techniques have been developed based on MOC, including the 3DMOC method, 2D/1D method, and axial expansion method (MOC/DD).

The 3DMOC method directly extends MOC into three-dimensional space for accurate solutions and is considered the ultimate approach for direct transport calculations. However, it suffers from low computational efficiency and high memory consumption. The 2D/1D method introduces approximations to transform three-dimensional characteristic rays into multi-layer two-dimensional rays, significantly improving computational efficiency but encountering instability and accuracy issues in strongly anisotropic cases. The MOC/DD method also transforms three-dimensional rays into multi-layer two-dimensional rays while introducing differential relationships along the axial direction to eliminate leakage term isotropic approximations.

Based on OpenMOC' s existing 2D MOC calculation module, new modules for the 2D/1D and MOC/DD methods were developed. The existing coarse mesh finite difference (CMFD) acceleration method and spatial domain decomposition parallelization techniques were retained to enhance computational capabilities for direct transport calculations.

5.1. Macro C5G7 Benchmark

The C5G7 benchmark[20] is a standard validation suite for heterogeneous transport calculation codes, including unrodded, half-rodded (rodA), and fully-rodded (rodB) configurations. For the unrodded case, sensitivity analyses of computational parameters were conducted separately for the 2D/1D and 3DMOC methods. Validation calculations for all three methods used consistent parameter sets.

Sensitivity Analysis of Computational Parameters: For the 2D/1D method, parameters analyzed included ray width, azimuthal and polar angle quadrature, reflector and fuel cell flat source region divisions, and axial layer height. Results are presented in . Ray width was examined in cases 1–3, angle quadrature in cases 2, 4, and 5, reflector divisions in cases 4, 6, and 7, fuel flat source region divisions in cases 6, 8, and 9, and axial layer height in cases 8, 10, and 11.

The sensitivity analyses revealed relatively small parameter influence, with maximum deviation from the reference solution of only 63 pcm in case 10. Input parameters, particularly reflector flat source region division, significantly impacted pin power distribution results. Refinement of reflector flat source regions improved the maximum pin power difference from 4.30% to 2.96% between cases 4 and 6.

Based on these analyses, default parameters for subsequent calculations were set to: 0.03 cm ray width, 32 azimuthal and 6 polar angles, 100 and 32 flat source regions for moderator and fuel pin cells respectively, and 3.57 cm axial height.

For the 3DMOC method, sensitivity analyses were conducted based on 2D/1D default parameters, examining polar ray spacing, axial layer height, linear source method, and angle quadrature. Results are shown in . Polar ray spacing of 0.75 cm was used in cases 1–3, axial height less than 1.428 cm in cases 3–5, and angle quadrature showed minimal influence in cases 2 and 7. Default 3DMOC parameters were therefore set to: 0.75 cm polar ray spacing, 0.714 cm axial height, with linear source method enabled.

Benchmark Results: Using the optimized parameters, the C5G7 benchmark was calculated with all three methods using 162 CPUs. Results are presented in .

For unrodded and rodA cases, all methods showed similar eigenvalue and pin power differences, with eigenvalue deviations below 50 pcm and maximum pin power differences below 3%. For the strongly anisotropic rodB case, 3DMOC demonstrated superior accuracy, reducing the maximum pin power difference from 2.27% to 1.71%.

Regarding computational efficiency, 3DMOC required an average of 11,331 seconds—38 times longer than the 2D/1D method (298 seconds) and 8.7 times longer than MOC/DD (1,298 seconds). The 2D/1D method required 2.50 times more outer iterations than 3DMOC and 1.77 times more than MOC/DD, indicating poorer convergence due to its 2D and 1D iteration procedure.

5.2. Micro VERA-1 Benchmark

The VERA benchmark problems are based on the Watts Bar pressurized water reactor. VERA-1 consists of five pin-cell cases used to validate the global-local resonance module in OpenMOC. Calculation parameters included 0.01 cm ray spacing, 64 azimuthal angles, and 6 polar angles. Eigenvalue results are shown in .

5.3. Micro VERA-2 Benchmark

VERA-2 comprises lattice benchmark cases 2A–2Q. Descriptions and OpenMOC results are presented in . Ray spacing was set to 0.03 cm for all cases except

IFBA cases (0.01 cm). The VERA-2 benchmark achieved an average eigenvalue difference of 44 pcm, with average maximum and RMS pin power differences of 0.37% and 0.10% respectively. Except for case 2H with 24 B_4C absorber rods, all eigenvalue differences were below 120 pcm. Except for cases 2O and 2P with Gd absorber rods, maximum pin power differences were below 0.6%. These results demonstrate good accuracy of the newly developed global-local resonance module in OpenMOC.

To investigate larger eigenvalue and pin power differences in B_4C and Gd absorber cases, results for cases 2O and 2P with Gd absorbers were analyzed. Geometry modeling for these cases is shown in [Figure 4: see original paper], where red rods indicate burnable absorbers. Detailed pin power differences are presented in [Figure 5: see original paper] and [Figure 6: see original paper]. The analysis indicates that the global-local resonance method underestimates pin power in burnable absorber rods, requiring further algorithmic investigation.

[Figure 4: see original paper]
[Figure 5: see original paper]
[Figure 6: see original paper]

6. Conclusion

Based on the open-source OpenMOC MOC transport code, this work developed global-local resonance and direct transport methods. A resonance calculation module with multi-group and continuous-energy libraries was created to provide multi-group cross-sections, and a direct transport module implementing 3DMOC, 2D/1D, and MOC/DD methods was developed to offer multiple calculation options. Validation and performance comparisons were conducted using the macro C5G7 and micro VERA benchmarks.

For the C5G7 macro benchmark, three direct transport methods were compared for accuracy and efficiency. Numerical results showed 3DMOC provided better accuracy in strongly anisotropic cases but required 38 times more computation time than 2D/1D. For the VERA micro benchmark, the resonance method achieved average eigenvalue and maximum pin power differences of 44 pcm and 0.37%, respectively, demonstrating its capability to provide accurate multi-group cross-sections for OpenMOC' s direct transport solvers.

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