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Calculation of the C5G7 3-D extension benchmark by ARES transport code

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HIGHLIGHTS

- The ARES code is verified by calculating C5G7 3-D extension benchmark.
- Refinement in spatial and angular domain discretization is investigated.
- The ARES results are in excellent agreement with the reference MCNP calculations.
- Parallel makes ARES possible to conduct large scale neutron transport calculations.

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ABSTRACT

High-fidelity neutron transport calculation is essential to enhance and improve the design of nuclear systems. This paper describes the transport solvers in ARES and presents ARES solutions of the 3-D extension C5G7 benchmark problem, a small LWR core model without spatial homogenization. The transport calculation is paralleled based on spatial-angle domain decomposition and optimal sweeping scheduling algorithm, which makes it possible to conduct neutron transport calculations with fine enough discretization to get high-resolution solutions. The multiplication factor and the normalized pin power are computed and compared with the reference MCNP calculations. Refinement in spatial and angular discretization was investigated and the calculation accuracy is studied via the difference of the multiplication factor from reference value and via the root-mean-square and maximum norm of the error in the pin power. The results were found to be in good agreement with reference, demonstrating that ARES can reach a good accuracy in complex criticality calculations.

1. Introduction

In the nuclear engineering community, neutron transport calculations, especially for large scale problems, are central to predicting core power distribution, determining the criticality state of the reactor and conducting shielding design. Nevertheless, the numerical simulation of the full steady state transport equation (Lewis and Miller, 1993) remains a challenging issue due to the high dimensionality of the phase-space and the heterogeneity in complex geometrical configurations.

In 2003, an extension of the three-dimensional C5G7 benchmark (Smith and Lewis, 2005) was proposed to provide a challenging test to deterministic transport methods. Traditionally, direct transport calculation for the reactor core heterogeneous geometries was not feasible due to the limited capability of computers. However, with the development of computer capability, Cartesian discrete ordinates method has been applied for assembly-level calculations (Pautz, 2005; Schunert and Azmy, 2013) and new discrete ordinate codes, such as PARTISN (Alcouffe et al., 2005; Dahl, 2006), DENOVO (Evans et al., 2010; Davidson et al., 2014), were developed with the ability to conduct large-scale transport calculations.

In order to examine the critical calculation capabilities of the three-dimensional, parallel, discrete ordinates code system ARES (Zhang et al., 2015) for problems with no spatial homogenization, the well-known C5G7 extension benchmark was calculated. To obtain reliable solutions and optimal angular-spatial resolution, refinements in spatial and angular domain are investigated. The results were compared with the reference MCNP solutions.

This paper presents ARES solutions to 3-D extension C5G7 benchmark problems. The remainder of this paper is organized as follows. The transport calculation solvers of ARES, including iteration process and parallel sweeping algorithms, are described in Section 2. The specification and calculation details of benchmark

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problems are presented in Section 3 and the calculation results are given in Section 4. Concluding remarks are in Section 5.

2. Transport solvers in ARES

ARES is a multi-dimensional parallel discrete ordinates neutral particle transport code that uses state-of-the-art solution methods to obtain accurate solutions to the linear Boltzmann transport equation. The steady-state transport equation solved in ARES is

$$\begin{aligned}&\vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E)+\Sigma_t(\vec{r},E)\psi(\vec{r},\vec{\Omega},E)\\&=\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_s(\vec{r},\vec{\Omega}'\to\vec{\Omega},E'\to E)\psi(\vec{r},\vec{\Omega}',E')\\&\quad+\frac{\chi(E)}{4\pi k}\int_0^\infty dE'\nu\Sigma_f(\vec{r},E')\int_{4\pi}d\vec{\Omega}'\psi(\vec{r},\vec{\Omega}',E')\end{aligned}\tag{1}$$

where $\psi(r,\Omega,E)$ is angular neutron flux, and the independent variables are energy E, spatial variables $\vec{r}=(x,y,z)$ and angular variables $\vec{\Omega}=(\theta,\varphi)$. ARES currently provides diamond difference with or without linear fixup, theta-weighted, directional theta-weighted, exponential directional weighted and linear discontinuous finite element spatial discretization schemes. Discrete ordinates differencing in angle and spherical harmonics expansion of the scattering source are adopted. And first collision source method is employed for ray effects mitigation. In the following subsections, we simply write down the iteration strategy and parallel transport sweeping algorithms employed in ARES.

2.1. Iteration strategy

To make the following discussion simple and clear, the steady-state Boltzmann transport equation can be expressed in operator form (Slaybaugh, 2011)

$$\mathbf{L}\psi=\mathbf{MS}\phi+\frac{1}{k}\mathbf{M}\chi\mathbf{f}^T\phi\tag{2}$$

where $\mathbf{L}=\hat{\Omega}\cdot\nabla+\Sigma_t$ is the streaming-plus-collision operator, $\mathbf{M}$ is the operator that converts harmonic moments to discrete angles, $\mathbf{S}$ is the scattering matrix, χ is the block matrix fission spectrum and $\mathbf{f}^T$ is the block matrix of production cross section. Flux moments ϕ and angular flux ψ are related by operator $\mathbf{D}$, which integrates discrete angles into flux moments through quadrature rules,

$$\phi=\mathbf{D}\psi\tag{3}$$

The traditional power iteration (Adams and Larsen, 2002) is adopted to calculate eigenvalues,

$$(\mathbf{I}-\mathbf{DL}^{-1}\mathbf{MS})\phi^{(l+1)}=\frac{1}{k^{(l)}}\mathbf{DL}^{-1}\mathbf{MF}\phi^{(l)}\tag{4}$$

$$k^{(l+1)}=k^{(l)}\frac{\mathbf{f}^T\phi^{(l+1)}}{\mathbf{f}^T\phi^{(l)}}\tag{5}$$

Within each power iterations, solving equation (4) is equivalent to conduct a fixed source calculation as follows,

$$(\mathbf{I}-\mathbf{DL}^{-1}\mathbf{MS})\phi=\mathbf{DL}^{-1}Q\tag{6}$$

where Q represents external fixed source for fixed-source problems and fission source for eigenvalue problems. Actually, Eq. (6) is a serial coupled equation among energy by scattering source. And Gauss Seidel iteration is commonly used over energy groups and can be written as follows,

$$\begin{aligned}&\left(\mathbf{I}-\mathbf{DL}_g^{-1}\mathbf{MS}_{gg}\right)\phi_g^{(l+1)}=\mathbf{DL}_g^{-1}\mathbf{M}\left(\sum_{g'=1}^{g-1}\mathbf{S}_{gg'}\phi_{g'}^{(l+1)}+\sum_{g'=g+1}^{G}\mathbf{S}_{gg'}\phi_{g'}^{(l)}\right)+Q_g\\&\quad g=1,\ldots,G\end{aligned}\tag{7}$$

Regarding Eq. (7), one must solve G within-group equations over angle-space, and they have the general form,

$$\begin{cases}\mathbf{L}_g\psi_g=\mathbf{MS}\phi_g+\bar{Q}_g\\\phi_g=\mathbf{D}\psi_g\end{cases}\tag{8}$$

where $\bar{Q}_g$ involves all sources for group g excluding the within group scattering.

ARES supports two strategies for solving the within-group equation. The default is source iteration,

$$\begin{cases}\mathbf{L}_g\psi_g^{(k+1)}=\mathbf{MS}\phi_g^{(k)}+\bar{Q}_g\\\phi_g^{(k+1)}=\mathbf{D}\psi_g^{(k+1)}\end{cases}\tag{9}$$

However, source iteration will be increasingly inefficient as the problem becomes more scattering dominated. Alternatively, Krylov method (Warsa et al., 2004), which has been demonstrated to have both high efficiency and high robustness, is available in ARES to solve the within-group equation.

$$\left(\mathbf{I}-\mathbf{DL}_g^{-1}\mathbf{MS}_{gg}\right)\phi_g=\mathbf{DL}_g^{-1}\bar{Q}_g\tag{10}$$

Note that the operator $\mathbf{L}_g^{-1}$ is an essential step no matter which method is selected. In ARES, $\mathbf{L}_g^{-1}$ is solved exactly in a transport sweep, which is defined as the calculation of all angular fluxes in the problem given some guess or iterate for the total source. Actually, the transport sweep requires the majority of computational effort in a transport calculation. During a transport sweep, each spatial mesh is solved in a specified order for a single direction in the discrete ordinates. This order is constrained by the fact that a spatial mesh cannot be solved for a particular direction until all its upwind neighbors have been solved. The details about parallelism of transport sweep on structured meshes, the most computational intensive part of a transport calculation, are presented in Section 2.2.

2.2. Parallel algorithm

Parallel is an essential part for the high-fidelity neutron transport calculations, not only to reduce the long calculation times, but also to decompose the excessive memory demand.

Domain decomposition strategy and sweep scheduling algorithm constitute the framework of parallelism in ARES. Without loss of generality, we restricted our attention to problems with reflective boundary conditions at x−, y−, z− directions and vacuum boundary conditions at x+, y+, z+ directions, which can be viewed as one eighth of a fully symmetric three-dimensional problem without reflective boundary conditions.

For spatial domain decomposition, as illustrated in Fig. 1, we consider a $N_x\times N_y\times N_z$ spatial mesh and a virtual processor topology containing $P_x\times P_y\times P_z$ processors. Defining $(A_x,\ A_y,\ A_z)$ as the subdomain number of meshes in each direction and $(\omega_x,\omega_y,\omega_z)$ as overload factors (Adams et al., 2013) in each direction, the spatial decomposition proceeds as follows. The whole spatial domain is decomposed into $\omega_x\times\omega_y\times\omega_z$ blocks. And each block is decomposed into subdomains of size $(A_x,\ A_y,\ A_z)$ on each processor. For presenting conveniently, we have assumed that each subdomain contains the same number of meshes in each direction, which is not a requirement and could otherwise induce load imbalance among processors. Concentrating on the decomposition process, we get

$$A_x=\frac{N_x}{\omega_xP_x},\quad A_y=\frac{N_y}{\omega_yP_y},\quad A_z=\frac{N_z}{\omega_zP_z}\tag{11}$$

For angular domain decomposition, angle aggregation factor, A_m, is defined as the number of directions contained in each angle set. And the A_m directions must be within the same octant.