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Three-Dimensional Discrete Ordinate Transport Code Based on KBA Method

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1. Introduction

Solving the three dimensional(3-D) Boltzmann transport equation in the reactor core calculation and shielding calculation requires vast majority of computational resource such as memory and CPU time. Therefore, it's necessary to develop a massively parallel 3-D transport code for both eigenvalue and shielding calculations.

In this paper, a new parallel S_N code named Hydra is developed. It is a 3-D code based on the Koch-Baker-Alcouffe(KBA) parallel sweeping algorithm[1]. The main features are as follows:

1. The 3-D Cartesian and Cylinder orthogonal structured grids are applied;
2. The domain decomposition parallelism is based on the KBA sweeping algorithm;
3. Both forward and adjoint calculation can be performed;
4. The S_N order can be adjusted for different energy groups;
5. The reflective, vacuum, periodic and rotational boundary conditions are involved;
6. The weighted diamond difference, weighted diamond difference with zero-flux fixed up and theta-weighted diamond[2] difference are involved;
7. The first collision source method is applied for ray effect elimination;
8. The parallel output adopts Silo-hdf5 format.

This paper is organized as follows: Theoretical models are described in Sec. 2. The numerical results of Hydra are shown in Sec. 3. Sec. 4 shows the analysis of parallel efficiency. Concluding remarks are given in Sec. 5.

2. Theoretical model

2.1 Discretization methods

The multi-group steady-state state Boltzmann transport can be written as:

$$\begin{aligned}&\boldsymbol{\Omega}\cdot\nabla\phi_g\left(\boldsymbol{r},\boldsymbol{\Omega}\right)+\Sigma_{t,g}\left(\boldsymbol{r}\right)\phi_g\left(\boldsymbol{r},\boldsymbol{\Omega}\right)\\&=\sum_{g'=1}^{G}\int_{\Omega'}\Sigma_{g'\to g}\left(\boldsymbol{r},\boldsymbol{\Omega}'\to\boldsymbol{\Omega}\right)\phi_{g'}\left(\boldsymbol{r},\boldsymbol{\Omega}'\right)d\boldsymbol{\Omega}'\\&+\frac{\chi_g}{4\pi\cdot k_{eff}}\sum_{g'=1}^{G}\upsilon_{g'}\Sigma_{f,g'}\left(\boldsymbol{r}\right)\psi_{g'}\left(\boldsymbol{r}\right)+Q_e\end{aligned}\qquad(1)$$

Integrating each term of Eq.(1) in a given direction $\Omega_m\left(\mu_m,\xi_m,\eta_m\right)$ and finite volume element (i,j,k), we can get the angularly and spatially discretized transport equation as follows:

$$\begin{aligned}&\frac{\mu_m}{\Delta x_i}\left(\phi_{i+1/2,j,k,m}-\phi_{i-1/2,j,k,m}\right)+\\&\frac{\xi_m}{\Delta y_j}\left(\phi_{i,j+1/2,k,m}-\phi_{i,j-1/2,k,m}\right)+\\&\frac{\eta_m}{\Delta z_k}\left(\phi_{i,j,k+1/2,m}-\phi_{i,j,k-1/2,m}\right)+\\&\Sigma_{i,j,k}\phi_{i,j,k,m}=Q_{i,j,k,m}\end{aligned}\qquad(2)$$

Eq.(2) is the neutron balance equation in XYZ coordinate. For simplicity, the energy group subscript *g* has been ignored. In the R-Theta-Z coordinate, the form is:

$$\begin{aligned}&w_m\mu_m\left[A_{i+\frac{1}{2}}\phi_{m,i+\frac{1}{2}}-A_{i-\frac{1}{2}}\phi_{m,i-\frac{1}{2}}\right]+\\&w_m\xi_m B\left[\phi_{m,j+\frac{1}{2}}-\phi_{m,j-\frac{1}{2}}\right]+\\&w_m\eta_m C\left[\phi_{m,k+\frac{1}{2}}-\phi_{m,k-\frac{1}{2}}\right]-\\&\left[A_{i+\frac{1}{2}}-A_{i-\frac{1}{2}}\right]\left(\alpha_{m+\frac{1}{2}}\phi_{m+\frac{1}{2},i,j,k}-\alpha_{m-\frac{1}{2}}\phi_{m-\frac{1}{2},i,j,k}\right)+\\&w_m\Sigma_{t,i,j,k}\phi_{m,i,j,k}V_{i,j,k}=w_mQ_{m,i,j,k}V_{i,j,k}\end{aligned}\qquad(3)$$

Where,

m: the angular index;
i,j,k: the index of finite volume element;
w_m: the quadrature weight of the angle of *m*;
μ_m,ξ_m,η_m: the cosine value of angle *m*.

2.2 KBA parallel algorithm

The KBA parallel sweeping algorithm was developed by Koch, Baker and Alcouffe during the 1990's. In the KBA sweeping, the original three-dimensional body is decomposed into two-dimensional sub-domains of size $(\mathrm{I}_b,\mathrm{J}_b,\mathrm{K})$. Each sub-domain is broadcasted on the appointed processor. For each processor, the sub-domain is divided into K/K_b blocks as illustrated in Fig. 1.

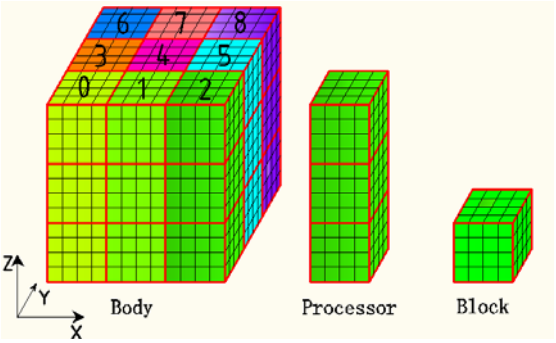


Fig. 1 domain decomposition of KBA method

I_b, J_b, K_b are the size of blocks for each sweeping direction. The sweeping order through blocks is showed in Fig. 2.

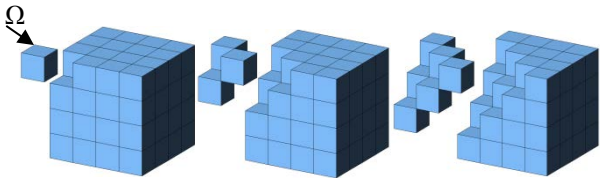


Fig. 2.1 block sweep order in XYZ geometry.

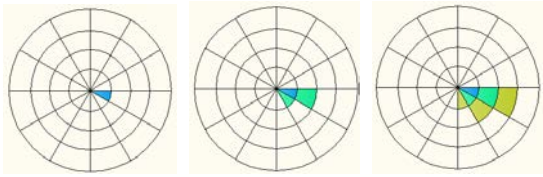


Fig. 2.2 block sweep order in R-Theta-Z geometry.

It should be noted that the angular flux calculation is a serial wavefront solver in each block, as illustrated in Fig. 3. Therefore, the sweeping is extended along the wavefront.

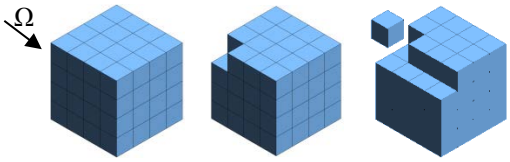


Fig. 3 the wavefront solver in each block

The theoretical parallel efficiency is:

$$\varepsilon = \frac{2MK}{2MK + K_b(\mathrm{I}/\mathrm{I}_b + J/J_b - 2)} \quad (4)$$

Where,

M: the number of angle in one octant;

I,J,K: the size of the body for each direction.

The incoming angular fluxes into each computational block come from boundary conditions or adjacent blocks. The angles are pipelined so that the next angle in the octant is started as soon as the previous angle is finished.

2.3 First collision source method

The first collision source method is derived by splitting the angular flux into the collided and uncollided components[3]:

$$\phi = \phi_u + \phi_c \quad (5)$$

The uncollided angular flux satisfies:

$$\Omega \cdot \nabla \phi^u(r,\Omega) + \sum_t(r)\phi^u(r,\Omega) = S(r,\Omega) \quad (6)$$

For the collided angular flux, the external source is removed:

$$\Omega \cdot \nabla \phi^c(r,\Omega) + \sum_t(r)\phi^c(r,\Omega) = \int_{\Omega'} \Sigma(\boldsymbol{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})[\phi^u(\boldsymbol{r}, \boldsymbol{\Omega}') + \phi^c(\boldsymbol{r}, \boldsymbol{\Omega}')]d\boldsymbol{\Omega}' \quad (7)$$

If the fission material exists, we should add the fission source to the right side of Eq. (7). The uncollied flux has the analytic solution:

$$\phi^u(\Omega) = \delta(\Omega - \Omega_{r \to r_p}) \frac{S}{4\pi} \frac{e^{-\tau(r,r_p)}}{|r - r_p|^2} \quad (8)$$

Where, *p* is the location of the point source.

3. Numerical result

All the numerical calculations were performed on the machine of NECP lab(CPU: Intel Xeon E5620, 2400MHz; Memory: 12GB).

3.1 PWR assembly calculation

This is a 15×15 PWR UO_2 fuel assembly. The configuration is given in Fig. 4. The average enrichment of ^{235}U is 2.4%. The lattice code HELIOS[4] is applied to produce the 4-group homogenized cross sections for each pin.

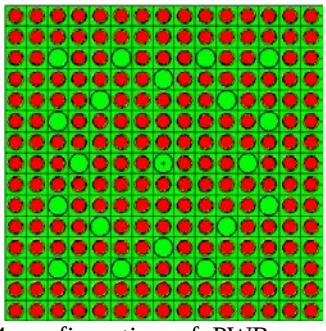


Fig 4 configuration of PWR assembly

In this problem, the K_{inf} and power distribution by Hydra with homogenized cross sections are compared with the reference results from HELIOS. The results are given in Table 1 and Fig. 5.

Table 1 the K_{inf} result of HELIOS and Hydra

	HELIOS	Hydra	error/pcm
Kinf	1.28429	1.28549	120

The relative error of K_{inf} is less than 0.1% and the maximum error of relative pin power error is less than 0.8%. The results of Hydra and HELIOS are in good agreement.

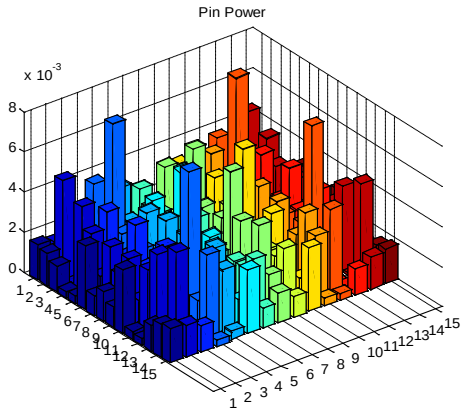


Fig 5 the relative error of power distribution of Hydra compared with HELIOS

3.2 PWR core calculation

This is a 1/4 PWR core problem, as illustrated in Fig. 6. There are 6 kinds of assemblies in the core, which are given in Fig. 7. The UO_2 enrichment are 3.1%, 2.4% and 1.8%, respectively. Half of the assemblies are loaded with control rods. The SRAC is applied to produce the 4-group homogenized cross sections. The reference results come from MCNP code[5] in multi-group mode. The K_{eff} result is shown in Table 2. Figure 8 gives the flux distribution of each group.

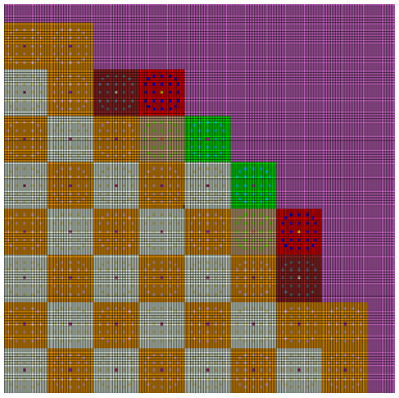
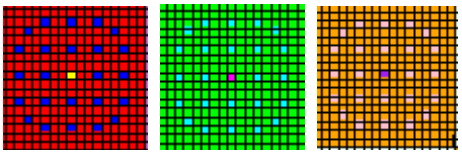
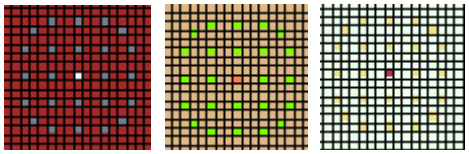


Fig 6 1/4 PWR core



UO_2 3.1wt% UO_2 2.4wt% UO_2 1.8wt%

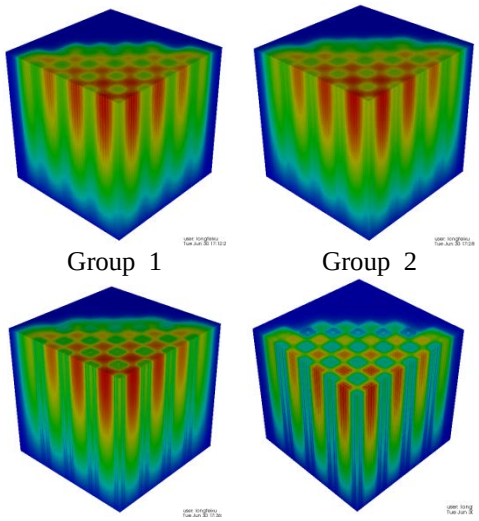


UO_2 3.1wt% (black rod) UO_2 2.4wt% (black rod) UO_2 1.8wt% (black rod)

Fig 7 six kinds of lattice type

Table 2 the K_{eff} result of MCNP and Hydra

	MCNP	Hydra	error/pcm
K_{eff}	0.94104	0.93965	139



Group 1 Group 2 Group 3 Group 4

Fig 8 Flux distribution of each group

3.3 Three dimensional cylinder problem

This is a designed 3-D cylinder core to verify the accuracy of Hydra in R-Theta-Z geometry. The configuration of cylinder core is given in Fig. 9.

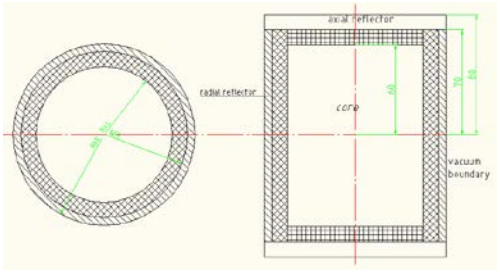


Fig 9 the configuration of cylinder core

The outside diameter of the core is 120cm, and the height is 160cm. The results are compared with the references form TORT[6] calculation, in which the mesh amount is set to 120×10×160. The number of energy group is 4, and the S_N order is 8. The comparison of flux error, computational time and parallel efficiency are showed in Table 3.

Table 3 Comparison of TORT and Hydra

mesh	**120×10×160**	**120×120×160**
Time	TORT: 849 s Hydra 6 s	serial: 16124 s 100cpu 183 s
Max error of flux	1.37e-04	~
Parallel efficiency	~	88.15%

The results of Hydra and TORT are in very good agreement. The parallel efficiency of Hydra is approximately 90% under the condition of 100 processors.

4. Parallel efficiency test

In order to test the parallel efficiency of Hydra, the Kobayashi problem is calculated. The Kobayashi problem is composed of three regions: source region, vacuum region and shielding region, as illustrated in Fig. 10. The scattering cross section is 50% of the total cross section for the shielding material[7]. S16 considering isotropic scattering is applied in the calculation, and 0.25cm spatial resolution is adopted with 400×400×400 meshes. The parallel efficiency with 4, 16, 25, 64 and 100 processors is given as shown in Fig. 11.

The theoretical parallel efficiency has ignored the time spent communicating. The practical parallel efficiency should be[8]:

$$\varepsilon = [\frac{2MK}{2MK + K_b(\mathrm{I}/\mathrm{I}_b + \mathrm{J}/\mathrm{J}_b - 2)}][\frac{T_{task}}{T_{task} + T_{comm}}] \quad (9)$$

Where,

T_{task} : amount of time spent calculating a single block in a given angular direction;

T_{comm} : time spent communicating the data exiting to the two neighboring blocks.

Considering the time spent communicating, the practical and theoretical parallel efficiency are in good agreement for 4 to 100 processors.

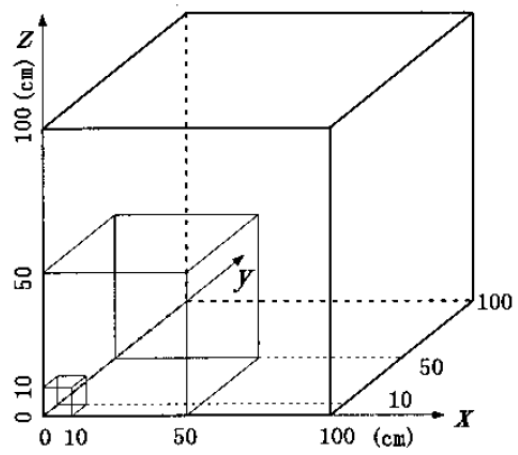


Fig 10 The configuration of Kobayashi problem

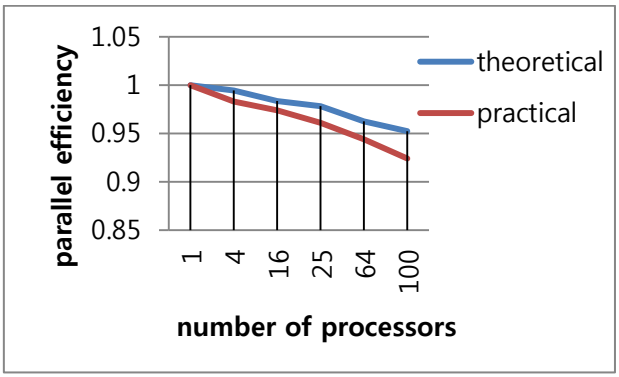


Fig 11 Parallel efficiency test of Hydra

5. Conclusions

A new S_N transport code Hydra is developed based on the KBA sweeping algorithm. Both the X-Y-Z orthogonal mesh and R-Theta-Z orthogonal mesh are involved. Several calculations prove that the results of Hydra are in good agreement with other codes such as TORT, MCNP(multi-group) and HELIOS. In additions, Hydra has very good parallel efficiency on O(100) processors.

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