

## Pin-cell Homogenization for PWR-Core Pin-by-pin P<sub>1</sub> Calculation

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### 1. Introduction

With the development of advanced nuclear reactor, the heterogeneity and neutron leakage of the Pressurized Water Reactor (PWR) core is becoming stronger and stronger. Under this circumstance, the traditional two-step method based on assembly homogenization cannot meet the requirements of the engineering calculation accuracy. Therefore, the pin-by-pin calculation based on pin-cell homogenization has gradually become an important option as the next-generation routine calculation approach.

Most of the pin-by-pin calculation programs introduce diffusion or SP<sub>3</sub> approximation in the neutronics calculation, such as NECP-Bamboo2.0[1], SCOPE2[2], SPHINCS[3] and so on. However, for the whole-core Pin-by-pin SP<sub>3</sub> calculation, its spatial grid can reach tens of millions of orders of magnitude, with at least 4 or even 7 energy groups. The computational cost, including both storage requirements and computing time, still needs to be further reduced.

In the three-dimensional whole-core pin-by-pin calculation, the SP<sub>3</sub> neutronics calculation spends the largest portion of the computational effort. Therefore, the P<sub>1</sub> approximation, which shares the same form with the neutron diffusion equation, is expected to half the calculation cost. Compared with diffusion approximation, the P<sub>1</sub> approximation can also remove the transport correction by retaining the first-order anisotropic scattering source. Therefore, this paper concentrates on the pin-cell homogenization for PWR-core pin-by-pin P<sub>1</sub> calculation.

### 2. Theoretical Models

#### 2.1 The P<sub>1</sub> Equation

The multi-group steady-state neutron transport equation is shown below:

$$\begin{aligned} & \boldsymbol{\Omega} \cdot \nabla \varphi_g(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_{t,g}(\mathbf{r}) \varphi_g(\mathbf{r}, \boldsymbol{\Omega}) \\ &= \sum_{g'=1}^G \int_{4\pi} \Sigma_{s,g' \rightarrow g}(\mathbf{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \varphi_{g'}(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \\ &+ \frac{1}{k_{\text{eff}}} \frac{\chi_g(\mathbf{r})}{4\pi} \sum_{g'=1}^G \int_{4\pi} \nu \Sigma_{f,g'}(\mathbf{r}) \varphi_{g'}(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \end{aligned} \quad (1)$$

where  $\mathbf{r}$  is the spatial location,  $\varphi_g$  is the neutron angular flux of group  $g$  ( $\text{cm}^{-2} \cdot \text{s}^{-1}$ ),  $\boldsymbol{\Omega}$  is the neutron motion direction,  $\Sigma_{t,g}$  and  $\Sigma_{f,g}$  are respectively the total and fission cross-sections of group  $g$  ( $\text{cm}^{-1}$ ),  $\Sigma_{s,g' \rightarrow g}$  is the scattering cross-section from group  $g'$  to group  $g$  ( $\text{cm}^{-1}$ ),  $\chi_g$  is the neutron fission spectrum of group  $g$ ,  $\nu$  is the number of neutrons per fission,  $g=1, 2, \dots, G$  is the

neutron energy group index.

Based on the first-order expansion of angular flux and scattering cross-section in terms of angular, the P<sub>1</sub> equation can be obtained:

$$\nabla \mathbf{J}_g(\mathbf{r}) + \Sigma_{t,g} \phi_g(\mathbf{r}) = \sum_{g'=1}^G \Sigma_{s0,gg'} \phi_{g'}(\mathbf{r}) + \frac{\chi_g}{k_{\text{eff}}} \sum_{g'=1}^G \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}) \quad (2)$$

$$\frac{1}{3} \nabla \phi_g(\mathbf{r}) + \Sigma_{t,g} \mathbf{J}_g(\mathbf{r}) = \sum_{g'=1}^G \Sigma_{s1,gg'} \mathbf{J}_{g'}(\mathbf{r}) \quad (3)$$

where,  $\phi_g$  is the neutron scalar flux of group  $g$  ( $\text{cm}^{-2} \cdot \text{s}^{-1}$ ),  $\mathbf{J}_g$  is the neutron current of group  $g$  ( $\text{cm}^{-2} \cdot \text{s}^{-1}$ ),  $\Sigma_{s1, g' \rightarrow g}$  is the first-order anisotropic scattering cross-section from group  $g'$  to group  $g$  ( $\text{cm}^{-1}$ ).

Defining the diffusion coefficient matrix as:

$$\bar{D} = \frac{1}{3} \left( \bar{\Sigma}_t - \bar{\Sigma}_{s1} \right)^{-1} \quad (4)$$

can transfer the P<sub>1</sub> Eq. into:

$$-\nabla \bar{D} \nabla \phi(\mathbf{r}) + \bar{\Sigma}_t \phi(\mathbf{r}) = \mathcal{S} \quad (5)$$

where,

$$\mathcal{S}_g = \sum_{g'=1}^G \Sigma_{s0,gg'} \phi_{g'}(\mathbf{r}) + \frac{\chi_g}{k_{\text{eff}}} \sum_{g'=1}^G \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}) \quad (6)$$

Eq. (5) is formally identical to the diffusion equation, so the computational efficiency is theoretically the same as the diffusion equation. Meanwhile, due to retaining the first-order anisotropic scattering source and no longer introducing transport correction, the calculation accuracy should be higher than the diffusion equation.

#### 2.2 Finite Difference Solution of the P<sub>1</sub> Equation

Eq. (5) can be discretized by using the finite difference method in three-dimensional Cartesian coordinates:

$$-\frac{\partial}{\partial x} [\bar{D}(x, y, z) \frac{\partial}{\partial x} \phi(x, y, z)] - \frac{\partial}{\partial y} [\bar{D}(x, y, z) \frac{\partial}{\partial y} \phi(x, y, z)] \quad (7)$$

$$-\frac{\partial}{\partial z} [\bar{D}(x, y, z) \frac{\partial}{\partial z} \phi(x, y, z)] + \bar{\Sigma}_t \phi(x, y, z) = \bar{\mathcal{S}}(x, y, z)$$

Defining the flux at the center of the mesh  $(x_i, y_j, z_k)$  as

$\phi_{i,j,k}$  and integrating Eq. (7) in the mesh lead to:

$$\left\{ -\frac{\partial}{\partial x} [\bar{D}(x, y, z) \frac{\partial}{\partial x} \phi(x, y, z)] - \frac{\partial}{\partial y} [\bar{D}(x, y, z) \frac{\partial}{\partial y} \phi(x, y, z)] \right\} \quad (8)$$

$$-\frac{\partial}{\partial z} [\bar{D}(x, y, z) \frac{\partial}{\partial z} \phi(x, y, z)] dx dy dz$$

$$+ \iiint \bar{\Sigma}_t \phi(x, y, z) dx dy dz = \iiint \bar{\mathcal{S}}(x, y, z) dx dy dz$$

Define the leakage of  $u$ -direction as  $L_u$ :

$$L_u = \frac{2}{\Delta u_i \Delta u_i} \bar{D}_u [-\phi_i^u + 2\phi_i - \phi_i^{u+}] \quad (9)$$

By solving the surface flux and substituting it into Eq. (9), the discretized P<sub>1</sub> equation can be obtained:

$$\sum_u^{u=x,y,z} \frac{2}{\Delta u} \left[ \bar{A} \phi_{i-1} + \bar{B} \phi_i + \bar{C} \phi_{i+1} \right] + \bar{\Sigma}_{i,j,k} \phi_{i,j,k} = \bar{\mathcal{S}}_{i,j,k} \quad (10)$$



solver for  $P_1$  equation has been developed. Correspondingly, a cross-sections homogenization program has also been developed based on the PWR-core pin-by-pin analysis code NECP-Bamboo2.0. In order to verify the effectiveness, numerical results are introduced in this session by taking the one-step heterogeneous calculation results provided by Bamboo-Lattice [4] as the reference. The reason for using the Bamboo-Lattice as the reference is firstly that it is a deterministic one-step program, which provides more accurate calculation results. At the same time, it is the program for generating homogenization constants, which can avoid deviations caused by databases and computational models.

### 3.1 Single-Assembly Case

A single fuel assembly case is designed, whose diagram is shown in Fig. 2. The reference solution is obtained by Bamboo-Lattice with  $P_2$  scattering. For comparison, in addition to using  $P_1$  approximation for calculation, this paper also uses diffusion approximation and  $SP_3$  approximation calculated by the Exponential Function Expansion Nodal method (EFEN) [5, 6]. The homogenized area is based on the pin-scale. Therefore, in order to ensure the consistency in the calculation area before and after homogenization, all the calculated meshes of the various homogenized calculation method are pin-scale.

As shown in Table I, all  $k_{eff}$  obtained by different homogenized calculation are in good agreement with the reference, with the deviations less than 50 pcm. As for the distribution quantities, the bias of the fission rates are shown in Table II and Fig. 3. It can be found that the bias of diffusion approximation is the largest (max 1.39% and the root mean square 0.60%). In contrast, the bias for  $P_1$  and the  $SP_3$  are very close, 0.69% for the max while 0.30% for the RMS. Overall, the deviations of all three methods are acceptable for this example, none of which exceed 1.5%.

According to the traditional homogenization theory, the calculation results should be consistent when the boundary conditions are the same. For this case, due to the reference using  $P_2$  scattering for calculation, and none of three methods can consider such high-order scattering, resulting in a certain deviation.

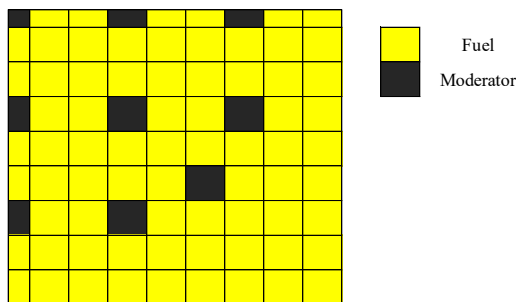
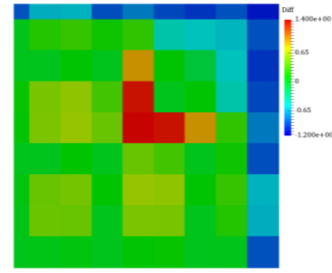
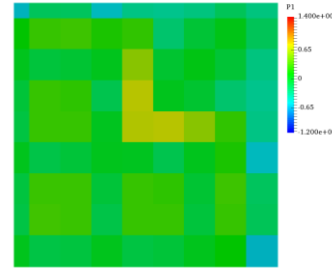


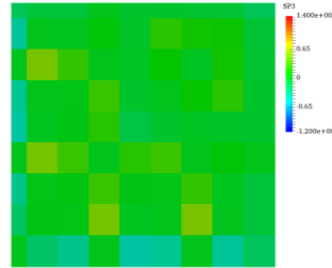
Fig. 2. The material and geometry diagram of the single assembly case.



(a) Diffusion approximation



(b)  $P_1$  approximation



(c)  $SP_3$  approximation

Fig. 3. The bias of fission rate distributions.

Table I:  $k_{eff}$  of various methods

	Ref.	Diff.	$P_1$	$SP_3$
$k_{eff}$	1.22925	1.22974	1.22894	1.22942
Bias/pcm	-	49	-31	17

Table II: The bias of fission rates

	Diff.	$P_1$	$SP_3$
MAX/%	1.39	0.69	0.50
RMS/%	0.60	0.30	0.22

### 3.2 Multi-Assemblies Case

For the further verification, a multi-assembly case diagram is shown in Fig. 4. The  $k_{eff}$  results are shown in Table III. All  $k_{eff}$  results obtained by different homogenized calculation are in good agreement with the reference, with the deviations not exceeding 150 pcm. Among them, the bias of the diffusion approximation is the largest, and the bias of  $P_1$  and  $SP_3$  approximation are very close.

Meanwhile, in order to compare the distribution, this paper compared the bias between the fission rates of different methods and the reference, as shown in Table IV and Fig. 5. For different methods, the bias of the diffusion approximation is the largest, whose max bias is 9.39% and the root mean square bias is 3.98%. In

addition, the  $P_1$  and the  $SP_3$  approximation are very close, both have comparable accuracy. From the Fig. 5, only at the interfaces of the assembly, the bias will be relatively high, and the bias inside the assembly will be minimal, not exceeding 1% for the  $P_1$  and the  $SP_3$  approximation. However, there may also be significant bias inside the assembly for the diffusion approximation.

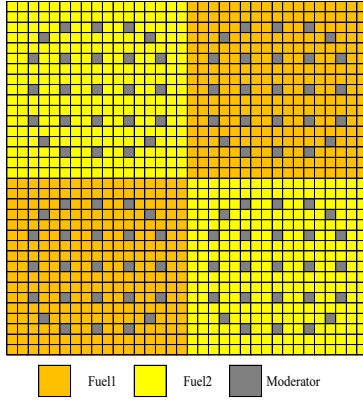


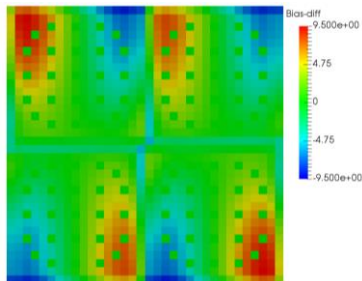
Fig. 4. The diagram of the multi-assembly case.

Table III: The  $k_{eff}$  results of various methods

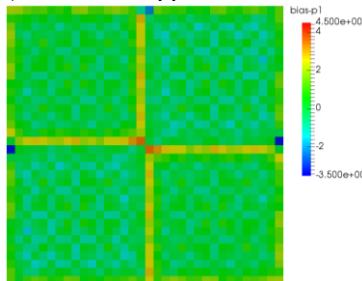
	Ref.	Diff.	$P_1$	$SP_3$
$k_{eff}$	1.08011	1.08123	1.07937	1.08078
Bias/pcm	-	112	-74	67

Table IV: The bias of fission rates

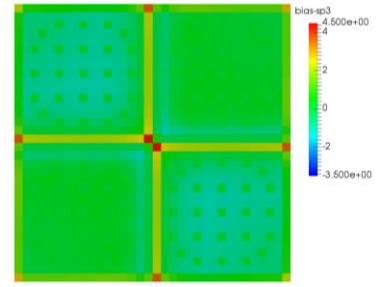
	Diff.	$P_1$	$SP_3$
MAX/%	9.39	3.48	4.26
RMS/%	3.98	0.92	0.88



(a) Diffusion approximation



(b)  $P_1$  approximation



(c)  $SP_3$  approximation

Fig. 5. The bias of fission rate distributions for different method compared with the reference.

## 4. Conclusions

In order to further improve the efficiency of PWR-core pin-by-pin calculation, this paper proposes a new homogenization and numerical calculation method based on the  $P_1$  equation.

Numerical results indicate that the method has higher accuracy compared to diffusion approximation and is comparable in accuracy to  $SP_3$  approximation. For single assembly case,  $P_1$  method can reduce the deviation to less than 1%. For multi-assemblies case, the deviations of the  $P_1$  method is significantly lower than the diffusion approximation, and this method can reduce the deviation from nearly 10% to 3.5%. Therefore, the new method provides a theoretical basis for the whole-core pin-by-pin calculation, which is expected have practical applications in the future.

The  $P_1$  equation solved in this paper only have one equation, which theoretically has a higher computational efficiency than the two coupled equations of  $SP_3$  approximation.

## REFERENCES

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