Hybrid Nodal Green's Function Method with SP3 for Pin-by-pin Calculation

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Abstract – In this study, SP_3 pin-by-pin calculation capability was implemented in the in-house developed nodal diffusion code, NuCoT, which was based on the hybrid nodal Green's function method. Event Parity Discontinuity Factor was adopted. A procedure was proposed for obtaining these discontinuity factors. The accuracy of NuCoT was tested by using two benchmark problems, OECD L336 C5G7 and KAIST with reference solutions calculated by MCNP and NEWT respectively. For the C5G7 problem, the RMS of pin power is < 0.9% and maximum error is < 2.6%. The k_{eff} error is < 80 pcm in 2D problem and <160pcm in 3D rodded case. For the KAIST problem, the RMS of pin power error is < 6% and. The k_{eff} error is < 70 pcm for ARI case and < 130 pcm for ARO case.

I. INTRODUCTION

Several approaches have been developed for the next generation method for neutronic analysis of Light Water Reactor (LWR) One is to perform the whole core 3D transport calculation directly^{1,2}, which is straightforward and accurate, but not practical considering current computing capability. Another method is to perform the whole core 3D pin-by-pin calculation³, in which the homogenized cross sections and the discontinuity factors of the pin cells are based on the single-assembly transport calculation. In order to obtain more accurate result, the simplified P_3 (SP₃) method⁴ is proposed to be used for the pin-by-pin calculation to replace the diffusion method. However, without the discontinuity factor, the solution of SP3 calculation is no better than that of the diffusion calculation. The discontinuity factor for the SP₃ calculation has been investigated in many studies⁵⁻⁸. In a 2x2 fuel assembly calculation, the results of SP₃ calculation using appropriate discontinuity factor⁷ were very close to the reference transport results. The maximum pin power error was < 2%. The k_{eff} error was < 50 pcm.

In this study, SP₃ capability was implemented in the inhouse developed nodal diffusion code, NuCoT, based on Hybrid Nodal Green's Function Method (HNGFM)^{9,10}. Event Parity Discontinuity Factor (EPDF)¹¹ was adopted for obtaining the discontinuity factors. A procedure was proposed for obtaining EPDF without modifying the existing transport code. Two benchmark problems, OECD L336 C5G7^{12,13} and KAIST¹⁴, mini cores surrounded by reflectors, were used to verify the accuracy of the SP₃ version of NuCoT.

II. METHODOLOGY

1. Implementation of SP₃ in HNGFM

The typical SP_3 equation of group g of a node is given below.

$$-D_{ng}\nabla^{2}\mathcal{F}_{ng}(\boldsymbol{r}) + \Sigma_{ng}^{r}\mathcal{F}_{ng}(\boldsymbol{r}) = T_{ng}(\boldsymbol{r}), n = 1,2$$

for $\boldsymbol{r} \in \left([-a_{x}, a_{x}], [-a_{y}, a_{y}], [-a_{z}, a_{z}]\right)$ (1)

 $\mathcal{F}_{1g}(r) = \phi_{g0}(r) + 2\phi_{g2}(r)$,

where

$$\mathcal{F}_{2g}(\boldsymbol{r}) = 3\phi_{g2}(\boldsymbol{r}) \,.$$

$$\phi_{g0}(\mathbf{r})$$
 and $\phi_{g2}(\mathbf{r})$ are the flux moments.

$$D_{1g} = \frac{1}{3\Sigma_g^{tr}},$$

$$D_{2g} = \frac{1}{7\Sigma_g^t},$$

$$\Sigma_{1g}^r = \Sigma_g^t - \Sigma_{gg}^s,$$

$$\Sigma_{2g}^r = \Sigma_g^t - \frac{4}{9}\Sigma_{gg}^s,$$

$$T_{1g}(\mathbf{r}) = S_g(\mathbf{r}) + \frac{2}{3}\Sigma_{1g}^r \mathcal{F}_{2g}(\mathbf{r}),$$

$$T_{2g}(\mathbf{r}) = -\frac{2}{3}S_g(\mathbf{r}) + \frac{2}{3}\Sigma_{1g}^r \mathcal{F}_{1g}(\mathbf{r}),$$

$$S_g(\mathbf{r}) = \frac{\chi_g}{k} \sum_{g'}^G \nu \Sigma_{g'}^f \phi_{g'0}(\mathbf{r}) + \sum_{g' \neq g}^G \Sigma_{gg'}^s \phi_{g'0}(\mathbf{r})$$

After deriving one-dimensional equation from Eq. (1) and applying the Green's function with Neumaan (or secondtype) boundary condition, the 1D flux in x-direction within a node can be written as:

$$\mathcal{F}_{ngx}(x) = G_{ngx}(x|-a_x)\mathcal{J}_{ngx}(-a_x) - G_{ngx}(x|a_x)\mathcal{J}_{ngx}(a_x) + 2a_x \langle QG_{ngx}(x) \rangle, n = 1,2$$
(2)

where

$$\mathcal{J}_{ngx}(x) = -D_{ng} \frac{d}{dx} \mathcal{F}_{ngx}(x),$$

$$G_{ngx}(x|x_0) = \text{Green's function at } x_0 \text{ with Neumann}$$

boundary condition,

$$\begin{aligned} \langle QG_{ngx}(x)\rangle &\equiv \frac{1}{2a_x} \int_{-a_x}^{a_x} dx_0 \ G_{ngx}(x|x_0) Q_{ngx}(x_0) \\ Q_{ngx}(x) &= T_{ngx}(x) - L_{ngx}(x), \end{aligned}$$

and $L_{nax}(x)$ is the transverse leakage profile.

To evaluate $\langle QG_{ngx}(x) \rangle$ at the surface, two spatial approximations of pseudo fluxes were applied.

$$\mathcal{F}_{ngx}(x) = \sum_{l=0}^{2} \mathcal{F}_{ngxl} P_l\left(\frac{x}{a_x}\right), n = 1,2$$
(3)

where $P_l\left(\frac{x}{a_x}\right)$ is the *l*-th order Legendre polynomial. And the transverse leakage profiles were assumed to be flat. The weighted residual procedure was used to solve \mathcal{F}_{ngxl} using Eq. (2). Then the unsolved term of Eq.(2) at the surface, $\langle QG_{ngx}(\pm a_x) \rangle$, can be obtained.

$$\langle QG_{ngx}(\pm a_x)\rangle = \sum_{l=0}^2 Q_{ngxl} \langle P_l G_{ngx}(\pm a_x)\rangle, n = 1,2 \quad (4)$$

where

$$\langle P_l G_{ngx}(\pm a_x) \rangle \equiv \frac{1}{2a_x} \int_{-a_x}^{a_x} dx \ G_{ngx}(\pm a_x | x) P_l\left(\frac{x}{a_x}\right).$$

The continuity of current and discontinuity of pseudo flux at the interface of two adjacent nodes provide the relationship between the current \mathcal{J}_n and nodal average pseudo flux $\overline{\mathcal{F}}_n$. This relationship can be substituted into the nodal balance equation of node N to obtain Eq. (5).

$$B_{ng}^{N}\bar{\mathcal{F}}_{ng}^{N} - \sum_{u=x,y,z} \left[B_{ngu}^{(N,m-1)} \bar{\mathcal{F}}_{ng}^{(N,m-1)} + B_{ngu}^{(N,m+1)} \bar{\mathcal{F}}_{ng}^{(N,m+1)} \right] \\ = R_{ng}^{N}, n = 1,2$$
(5)

where

m=node index related to the u direction,

$$\begin{split} B_{ng}^{N} &= \Sigma_{ng}^{r,N} \left\{ 1 + \sum_{\substack{u=x,y,z \\ u=x,y,z \\ ngu}} \left[A_{ngu}^{N}(-a_{u}^{N}) + A_{ngu}^{N}(a_{u}^{N}) \right] \right\}, \\ B_{ngu}^{(N,m\pm1)} &= \frac{2a_{u}^{m\pm1}\Sigma_{ng}^{r,m\pm1}\omega_{gu}^{m\pm1}(\mp a_{u}^{m\pm1}|\pm a_{u}^{m\pm1})}{2a_{u}^{N}\Delta\omega_{ngu}^{N}(a_{u}^{N})}, \\ R_{ng}^{N} &= \bar{T}_{ng}^{N} - \sum_{\substack{u=x,y,z \\ u=x,y,z \\ ngu}} \left[C_{ngu}^{N}(-a_{u}^{N}) + C_{ngu}^{N}(a_{u}^{N}) \right], \\ A_{ngu}^{N}(\pm a_{u}^{N}) &= \frac{\omega_{ngu}^{N}(\pm a_{u}^{N}|\mp a_{u}^{N})}{\Delta\omega_{ngu}^{N}(\pm a_{u}^{N})}, \\ C_{ngu}^{N}(\pm a_{u}^{N}) &= \frac{\Delta \langle QG \rangle_{ngu}^{N}(\pm a_{u}^{N}) - \Delta \bar{Q}_{ngu}^{N}(\pm a_{u}^{N})}{2a_{u}^{N}\Delta\omega_{ngu}^{N}(\pm a_{u}^{N})}, \\ \omega_{ngu}^{N}(A|B) &= f_{ngu}^{N}(A)G_{ngu}^{N}(A|B), \\ f_{ngu}^{N}(A) &= \text{discontinuity factor at the location A in u} \\ \text{direction,} \\ \Delta \langle QG \rangle_{ngu}^{N}(\pm a_{u}^{N}) &= 2a_{u}^{N}f_{ngu}^{N}(\pm a_{u}^{N}) \langle QG_{ngu}^{N}(\pm a_{u}^{N}) \rangle \\ &-2a_{u}^{m\pm1}f_{ngu}^{m\pm1}(\mp a_{u}^{m\pm1}) \langle QG_{ngu}^{M}(\mp a_{u}^{m\pm1}) \rangle \end{split}$$

$$\Delta \bar{Q}_{ngu}^{N}(\pm a_{u}^{N}) = 2a_{u}^{N} \bar{Q}_{ngu}^{N} \omega_{gu}^{N}(\pm a_{u}^{N} | \mp a_{u}^{N}) -2a_{u}^{m\pm 1} \bar{Q}_{ngu}^{m\pm 1} \omega_{ngu}^{m\pm 1} (\mp a_{u}^{m\pm 1} | \pm a_{u}^{m\pm 1}).$$

and

$$\begin{split} \Delta \omega_{ngu}^N(\pm a_u^N) &= \left[\omega_{ngu}^N(\pm a_u^N) \pm a_u^N) - \omega_{ngu}^N(\pm a_u^N) \mp a_u^N \right] \\ &- \left[\omega_{ngu}^{m\pm 1}(\mp a_u^{m\pm 1}) \pm a_u^{m\pm 1}) - \omega_{ngu}^{m\pm 1}(\mp a_u^{m\pm 1}) \mp a_u^{m\pm 1} \right]. \end{split}$$

The boundary conditions available in SP₃ calculation are albedo or zero flux. The partial moments for the albedo boundary condition are based on the Marshak boundary condition.

$$\begin{cases} \mathcal{J}_{1gu}^{\pm} = \frac{1}{4} \mathcal{F}_{1gu} - \frac{1}{16} \mathcal{F}_{2gu} \pm \frac{1}{2} \mathcal{J}_{1gu} \\ \mathcal{J}_{2gu}^{\pm} = -\frac{1}{16} \mathcal{F}_{1gu} + \frac{7}{48} \mathcal{F}_{2gu} \pm \frac{1}{2} \mathcal{J}_{2gu} \end{cases}$$
(6)

2. Even Parity Discontinuity Factor (EPDF)

In SP₃ calculation, at the pin cell level, the discontinuity factors of two pseudo fluxes cannot be easily generated because the reference 2^{nd} and 3^{rd} flux moments were not available from the widely used transport codes. EPDF was developed for the transport code by Yamamoto⁸. It was unified in the diffusion/SP₃ calculation by Yu⁷. The idea is to make the homogeneous even parity surface flux (not the scalar flux) between two adjacent nodes continuous when the surface net current is the reference solution. After applying EPDF, the homogeneous even parity surface fluxes are made continuous.

EPDF is rewritten as a conventional discontinuity factor form:

$$EPDF = \frac{\Phi^*}{\Phi} \tag{7}$$

where

 Φ^* =averaged homogeneous even parity flux Φ of the right- and left-hand-sides at the surface, and

$$\Phi \cong \frac{1}{4}\phi_0 + \frac{5}{16}\phi_2 = \frac{1}{4}\mathcal{F}_1 - \frac{1}{16}\mathcal{F}_2 \,.$$

In the single assembly transport calculation, using reflective boundary condition represents that the neighboring assemblies are the same. Hence, EPDF on the assembly boundary is one. However, the neighboring fuel assemblies in the core may not be the same, in which case EPDF will not be equal to one. Yu⁷ used the same idea of the conventional discontinuity factor to set Φ^* of Eq. (7) equals to the reference solution Φ^{het} , named Renormalized EPDF (REPDF). The original EPDF definition was named Prime EPDF (PEPDF).

The difficulty was how to obtain the 2nd flux moment $(\mathcal{F}_2 \text{ or } \phi_2)$ and current $(\mathcal{J}_2 \text{ or } 3^{rd} \text{ flux moment})$ for the even parity surface flux. The procedure adopted in this study is to iterate EPDF until it is converged. Following the idea of Kozlowski⁵ (Eq. (28)~(30) of the paper), Eq. (5) can be reduced to solve for $\overline{\mathcal{F}}_2$ which includes EPDF when the reference solution, such as net current, total flux and k_{eff} are known. After \mathcal{F}_2 and \mathcal{J}_2 are calculated, the EPDF can be updated. The process stops when EPDF is converged.

III. NUMERICAL RESULTS

Two benchmark problems, OECD-L336 C5G7 and KAIST, were selected to verify the accuracy of NuCoT. Root-Mean-Square (RMS) error was used for the pin power comparison.

$$RMS(\%) = \frac{\sqrt{\Sigma(P - P^{ref})^2/N}}{\Sigma^{P^{ref}/N}} \times 100$$
(8)

where

N = total number of fuel pins,

P = pin power, and

 P^{ref} = pin power of reference solution.

In case "PEPDF", PEPDF were applied to all surfaces of the pin cells. In case "REPDF", REPDF were applied to the surfaces of the pin cells on the assembly/reflector boundary and PEPDF were applied to the rest of the surfaces.

1. OECD-L336 C5G7 Benchmark Problem

C5G7 benchmark problem is a mini quarter PWR core containing UO_2 and MOX 17x17 fuel assemblies, surrounded by reflectors. This benchmark problem includes one 2D case and three 3D cases, Unrodded, RoddedA and RoddedB. The fuel patterns of 3D cases are the same as the 2D case.

The reference solution for EPDF iteration and homogenized pin-cell cross sections of the fuel assembly were obtained by the assembly calculation using NEWT¹⁵ using S_{16} angular quadrature set. The convergence criteria for k_{eff} , flux and source were 10^{-5} . The seven-group macroscopic cross section set, including the transport-corrected total and scattering cross sections, were provided by the benchmark problem^{12,13}.

Two pin-cell discontinuity factor cases, PEPDF and REPDF were used in NuCoT. The PEPDF and REPDF of pin cells in the fuel assembly were obtained by the single assembly calculation. The reflector of the 2D problem was divided into 17x17 cells as the fuel assembly. Since the reflector is homogeneous, the pin-cell discontinuity factor in the reflector was set to one, except the one at the reflector boundary adjacent to the heterogeneous fuel assembly. In the pin-by-pin core calculation, the effect of using different reflector discontinuity factors, NoRefDF, RefDF1 and RefDF2, were investigated. The two discontinuity factors at the surface between the fuel and reflector can be obtained from the reflector-model transport calculation. In Case NoRefDF, the discontinuity factors on the reflector side were set to one. In Case RefDF1, only the above discontinuity factor on the reflector side was used. In Case RefDF2, the above two discontinuity factors were used for both sides of the surface between the fuel and reflector. Case RefDF2 is used only in PEPDF condition, not in **REPDF** condition.

The reference solution of C5G7 2D problem was obtained from MCNP¹⁶ calculation using the seven-group macro cross section set provided by the benchmark problem^{12,13}. The statistic error of k_{eff} was 7 pcm and of pin power was < 0.5%.

The accuracy of NuCoT is shown in Table I. The convergence criteria of NuCoT for k_{eff} , flux and power were all 10⁻⁵. Unlike the situation in diffusion calculation, the SP₃ results were not sensitive to the discontinuity factors used for the reflector. The SP₃ method gives more accurate pin power results than the diffusion method. In SP₃ calculation using PEPDF gives more accurate results than using REPDF. The RMS of pin power is < 0.8% and maximum error is < 2.6%. The k_{eff} error is < 80 pcm.

Table I. The NuCoT Result of C5G7 2D Benchmark Problem

Reference k _{eff} =1.18645			k _{eff}	Pin Power Error(%)				
			Error (pcm)	MOX	inner UO2	outer UO2	All	
iffusion	DF	NoRefDF	-137.0	0.89^{a} 4.26^{b}	0.34 0.76	1.49 -4.12	0.71 4.26	
	REH	RefDF1	-45.9	0.88 4.62	0.36 -0.67	1.10 4.01	0.66 4.62	
	PEPDF	NoRefDF	-153.7	1.32 6.94	0.40 -1.65	1.68 4.76	0.95 6.94	
D		RefDF1	-75.3	1.28 6.35	0.77 -1.70	1.33 4.90	1.08 6.35	
		RefDF2	-4.3	1.33 5.67	1.14 -1.98	1.51 4.93	1.36 5.67	
	DF	NoRefDF	39.0	0.71 -3.11	0.62 1.08	0.85 -4.06	0.74 -4.06	
	REH	RefDF1	51.1	0.68 -3.01	0.54 1.02	0.78 -3.76	0.67 -3.76	
SP ₃	PEPDF	NoRefDF	32.9	0.51 2.53	0.24 -0.91	0.76 2.39	0.42 2.53	
		RefDF1	54.8	0.49 2.41	0.19 -0.91	0.72 2.42	0.38 2.42	
		RefDF2	76.2	0.49 2.29	0.22 -0.92	0.75 2.46	0.40 2.46	

^aRoot-Mean-Square

^bMaximum Error

In C5G7 3D problem, for simplicity, the top reflector was assumed to be pure reflector without control rods or holes. The DFs in the top reflector were set to one. RefDF1 of PEPDF was adopted. The axial nodal size was 7.14 cm. The reference solution of C5G7 3D problems were also obtained from MCNP calculation. The statistic errors of k_{eff} in three cases were 3 pcm and of nodal pin power were all < 1.0%. The convergence criteria of NuCoT for 3D problems were the same as those of 2D problem.

The results of C5G7 3D problem by SP_3 method in NuCoT are shown in Table II. The pin power error is small and good. The RMS of pin power is < 0.9% and maximum

error is < 2.5%. The k_{eff} error is ~ 60 pcm for unrodded condition, and ~ 1.6 mk for rodded case.

Table	II.	The	NuCoT	Result	of	C5G7	3D	Benchmark
Proble	m							

l Pin	Whole Pin
2.47 ^b	0.59 / 2.24
-2.39	0.41 / -2.28
-2.22	0.46 / -2.10
	-2.39 -2.22

^aRoot-Mean-Square

^bMaximum Error

2. KAIST Benchmark Problem

KAIST benchmark problem is a small 2D quarter PWR core consists of three types of UO_2 fuel assembly and two types of zoned MOX 17x17 fuel assembly. There are two core conditions, all rod out (ARO) and all rod in (ARI). The seven-group macro cross sections set including anisotropic scattering cross sections were provided by the KAIST 2A benchmark problem¹⁴.

NEWT calculation was performed to obtain the pin-cell homogenized cross sections as well as the reference solution The angular quadrature and the convergent criteria were the same as those used in the calculation of C5G7 problem. Two types of pin-cell discontinuity factor (PEPDF and REPDF) and three types of reflector discontinuity factor (NoRefDF, RefDF1 and RefDF2) were used.

The benchmark results are listed in Table III. The results are insensitive to the choice of the type of reflector discontinuity factor. The PEPDF results are better than the REPDF results. The SP₃ results are better than the diffusion results. In SP₃ calculation using PEPDF discontinuity factor, the maximum pin power error is < 6% and the RMS of pin power error is ~1%. The k_{eff} error is < 70 pcm for ARI case and < 130 pcm for ARO case.

IV. CONCLUSION

The SP₃ pin-by-pin calculation capability incorporated in NuCoT provides quite satisfactory result for LWR benchmark problems. The SP₃ method gives more accurate pin power results than the diffusion method. Using PEPDF gives more accurate results than using REPDF. The SP₃ results were not sensitive to the discontinuity factors used for the reflector. For C5G7 problem, compared with MCNP result, the k_{eff} error is < 160 pcm and the RMS of pin power is < 0.9%. In KAIST problem, compared with NEWT result, the k_{eff} error is < 130 pcm and the RMS is ~ 1%.

Table	III.	The	NuCoT	Result	of	KAIST	Benchmark
Proble	m						

Case			ARO, Ref =1.13	Ference k _{eff} 36577	ARI, Reference k _{eff} =0.983737			
			keff Error	Pin Power	keff Error	Pin Power		
			(pcm)	Error(%)	(pcm)	Error(%)		
Diffusion	DF	NoRefDF	-208.8	1.06 ^a / 4.01 ^b	-347.0	2.47 / 3.73		
	REI	RefDF1	-190.8	1.15 / 5.46	-314.1	2.49 / 5.28		
	Ρ	NoRefDF	-182.7	0.82 / 4.08	-241.3	1.72 / 3.89		
	EPD	RefDF1	-196.0	0.97 / 5.07	-229.2	1.73 / 4.34		
	ď	RefDF2	-188.4	1.01 / 5.54	-217.3	1.75 / 4.81		
SP_3	PDF	NoRefDF	-134.4	0.68 / 5.14	-134.2	1.51 / 5.47		
	RE	RefDF1	-142.7	1.05 / 4.75	-140.3	1.47 / 5.03		
	F	NoRefDF	-129.8	0.80 / 5.78	-66.9	1.13 / 5.97		
	EPD	RefDF1	-129.8	0.78 / 5.46	-67.8	1.10 / 5.56		
	P	RefDF2	-130.8	0.77 / 5.06	-68.8	1.06 / 5.19		
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^aRoot-Mean-Square

^bMaximum Error

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