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Discontinuity Factors for Simplified P3 Theory

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1. Introduction

Two concepts of discontinuity factor (DF) for the Simplified P3 (SP3) theory [1][2] are proposed in the present summary.

DF for diffusion theory with the advanced nodal method has been widely used in practical core analysis [3]. In the framework of diffusion theory, freedom of discontinuity for scalar flux is used to satisfy the equivalence of neutron net current (i.e., the 1st moment of angular flux) between heterogeneous and homogeneous geometries. In this context, application of DF for the SP3 method seems to be straightforward since the SP3 and the diffusion equations have similar forms.

However, we should address the following issues to establish a practical implementation of DF for SP3 theory:

- Estimation method of the 2nd and 3rd moments of angular flux (ϕ_2, J_3) from a heterogeneous transport solution is not established since explicit angular flux representation of SP3 equation has not been obvious.
- The value of ϕ_2 could be zero, (e.g., at reflective boundary), which poses a numerical problem in the straightforward application of DF.

Since we can use two DFs in the SP3 theory, we also should address the followings:

- Choice of preserved quantity in addition to the 1st moment (net neutron current).
- Choice of quantity for which additional DF is applied.

Approaches to address the above issues can result various implementation of SP3 DF [4][5].

In section 2, two different implementations of DF (the individual and the unitary DFs) for SP3 is briefly described and their performance is confirmed through benchmark calculations in section 3. Finally concluding remarks are summarized in section 4.

It should be reminded that DF for radial direction is considered in the present paper since treatment of radial heterogeneity is much more important and lattice physics calculation usually carried out in two-dimensional geometry.

2. Theory

2.1 Individual DF

Concept of the individual DF for SP3 is a straightforward extension of that for the diffusion theory. In the diffusion theory, 1st moment of angular flux (i.e., net current, J_1) is preserved and DF is applied to the scalar flux ϕ_0. In the individual DF, 1st and 3rd moments of angular flux (i.e., J_1 and J_3) are preserved and DFs are applied to ϕ_0 and $\Phi = \phi_0 + 2\phi_2$.

As discussed in the previous section, estimation method of ϕ_2 and J_3 from the result of heterogeneous transport calculation has not been well established. In the present study, these quantities are evaluated using the following relations:

$$J_3^x = \frac{8}{7}\left(\phi_0^{x+} - \phi_0^{x-} - \frac{3}{2}J_1^x\right), \tag{1}$$

$$J_3^y = \frac{8}{7}\left(\phi_0^{y+} - \phi_0^{y-} - \frac{3}{2}J_1^y\right), \tag{2}$$

where

$$\phi_0^{x+} \equiv \int_{-\pi/2}^{\pi/2} d\varphi \int_0^{\pi} \sin\theta d\theta \psi(\vec{\Omega}),$$

$$\phi_0^{x-} \equiv \int_{\pi/2}^{3\pi/2} d\varphi \int_0^{\pi} \sin\theta d\theta \psi(\vec{\Omega}),$$

$$\phi_0^{y+} \equiv \int_0^{\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \psi(\vec{\Omega}),$$

$$\phi_0^{y-} \equiv \int_{\pi}^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \psi(\vec{\Omega}),$$

$$J_1^x \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \sin\theta\cos\varphi \psi(\vec{\Omega}),$$

$$J_1^y \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \sin\theta\sin\varphi \psi(\vec{\Omega}).$$

$$\phi_2 = -\frac{16}{5}\left(2J_1^{z+} - \frac{1}{2}\phi_0\right), \tag{3}$$

where

$$J_1^{z+} \equiv \int_0^{2\pi} d\varphi \int_0^{\pi/2} \sin\theta d\theta \cos\theta \psi(\vec{\Omega}),$$

$$J_1^{z-} \equiv \int_0^{2\pi} d\varphi \int_{\pi/2}^{\pi} \sin\theta d\theta \cos\theta \psi(\vec{\Omega}).$$

It should be noted that the following expression is assumed for angular representation of angular flux in the SP3 approximation [6].

$$\psi(\vec{\Omega}) = \frac{1}{4\pi}\begin{pmatrix} P_0(\mu_J)\phi_0 + 3P_1(\mu_J)J_1 \\ +5P_2(\mu_J)\phi_2 + 7P_3(\mu_J)J_3 \end{pmatrix}, \tag{4}$$

where

μ_J :cosine direction to the neutron current vector.

In Eqs.(1) and (2), the "partial scalar flux" is used, which is not commonly used in lattice physics calculations. However, its evaluation in lattice physics code is not difficult since similar calculation procedure with the partial or the net current can be used.

The DFs are calculated by:

$$f_0 \equiv \frac{\phi_0^{het,s}}{\phi_0^{hom,s}}, \quad (5)$$

$$f_F \equiv \frac{\Phi^{het,s}}{\Phi^{hom,s}} = \frac{\phi_0^{het,s} + 2\phi_2^{het,s}}{\phi_0^{hom,s} + 2\phi_2^{hom,s}}, \quad (6)$$

where *het*, *hom*, and *s* represent heterogeneous, homogeneous geometries, and surface of homogenized region.

The overall calculation procedures are as follows:

(1)Perform heterogeneous transport calculation (usually by MOC).

(2)Cell-wise homogeneous cross section and cell-surface partial current and partial scalar flux is estimated based on the results of Step (1). ϕ_0 and J_1 are calculated by the common procedure, then ϕ_2 and J_3 are evaluated using Eqs.(1), (2), and (3). Φ is calculated by $\Phi = \phi_0 + 2\phi_2$.

(3)Cell-homogeneous SP3 calculation is carried out in each homogenized cell by forcing J_1 and J_3 obtained in heterogeneous calculation (Step 1) as cell-boundary condition. Note that neutron source is also set from the heterogeneous calculation result.

(4)Surface flux moment of ϕ_0 and ϕ_2 in each homogenized cell are calculated from the calculation result of Step (3) and then Φ is calculated by $\Phi = \phi_0 + 2\phi_2$.

(5)DFs for ϕ_0 and Φ are calculated by the ratio of these values using the results of Steps (2) and (4).

DFs for ϕ_0 and Φ are given in Eqs (5) and (6) and they can be used for the SP3 calculation with the finite-difference method. However, in the numerical solution for SP3 using the advanced nodal method, discontinuity conditions for ϕ_2 and Φ are used. In order to avoid numerical instability, the following relation is used for ϕ_2 in SP3 calculations in this study:

$$f_0^{s+}\phi_2^{hom,s+} = f_0^{s-}\phi_2^{hom,s-} + R, \quad (7)$$

$$R = -\frac{1}{2}\left(f_0^{s-}\Phi^{hom,s-} - f_0^{s+}\Phi^{hom,s+}\right). \quad (8)$$

The value of R in Eq.(8) is updated during iterations of SP3.

2.2 Unitary DF

The individual DF utilizes two different discontinuity factors for ϕ_0 and Φ. In the unitary DF, only one DF is used. The unitary DF has the following conditions:

- J_1 at homogenized (e.g., cell) boundary is preserved.
- Same value of DF is used both for ϕ_0 and Φ except for boundary of geometry.
- Different values of DF are used for ϕ_0 and Φ only at boundary of geometry.
- J_3 is continuous at homogenized region boundary

Since only one DF is used at a surface of homogenized region, memory requirement for storage of DF is smaller than that of the individual DF.

The overall calculation procedures of the unitary DF are as follows:

(1)Perform heterogeneous transport calculation (usually by MOC)

(2)Cell-wise homogeneous cross section and cell-surface partial current and partial scalar flux is estimated based on the results of Step (1). ϕ_0 and J_1 can be calculated by the common procedure, then ϕ_2 can be evaluated using Eq. (3). Φ is calculated by $\Phi = \phi_0 + 2\phi_2$.

(3)Homogeneous SP3 solution forcing the following constraints is carried out: i) J_1 at cell boundary is preserved to that of heterogeneous calculation, ii) DFs for ϕ_0 and Φ is the same except for boundary of geometry, iii) J_1 and J_3 at the boundary of geometry is preserved to that of heterogeneous calculation.

(4)Same as Step (4) for the individual DF

(5) ϕ_0 obtained in Steps (2) and (4) is used to calculate DF, which is used both for ϕ_0 and Φ.

(6) ϕ_0 and Φ obtained in Steps (2) and (4) are used to calculate DFs for ϕ_0 and Φ at geometry boundary.

Equation (7) is also used in the homogeneous SP3 calculation using DF.

3. Calculations and Discussions

Verification calculations of proposed DFs, i.e., the individual and the unitary DFs, are carried out in the color-set geometries consists of UO2 and MOX fuel assemblies defined in the KAIST benchmark problem 2A [7].

The following two verifications are carried out:

- Reproduction of the heterogeneous reference results using a SP3 calculation with the DFs obtained in the color-set configuration.
- Accuracy of SP3 calculation with the DFs obtained in the single assembly calculation.

Figure 1 shows the color-set geometries used in the present verification calculations.

Verification calculations are carried out with the following procedures:

(1)Heterogeneous transport calculation is carried out in a color-set geometry using MOC to obtain reference result.

(2)Cell-homogenized cross section is obtained using the result of Step (1). Cell average scalar flux and cell-surface average angular flux moment are estimated.

(3)Reference individual and unitary DFs are estimated using the quantities obtained in Step (2) and

calculation procedures described in section 2. These DFs are called as the Ref-individual and the Ref-unitary DFs.

(4)Single assembly calculation with reflective boundary condition is carried out for different types of fuel assembly in the present benchmark calculation using MOC.

(5) Cell-homogenized cross section is obtained using the result of Step (4). Cell average scalar flux and cell-surface average angular flux moment are estimated.

(6) The individual and unitary DFs are estimated using the quantities obtained in Step (5) and calculation procedures described in section 2. These DFs are called as the SA-individual and the SA-unitary DFs, where SA represents single assembly.

(7) SP3 calculations with the Ref-DFs (obtained in Step (3)) or SA-DFs (obtained in Step (6)) are carried out in the color-set configuration. Homogenized cross section obtained in Step (2) is used in the present calculation in order to eliminate errors due to homogenized cross section itself. In other words, error due to DFs is focused in the present study.

(8)Compare k-effective and pin-power (fission rate) distribution obtained in Steps (1) and (7).

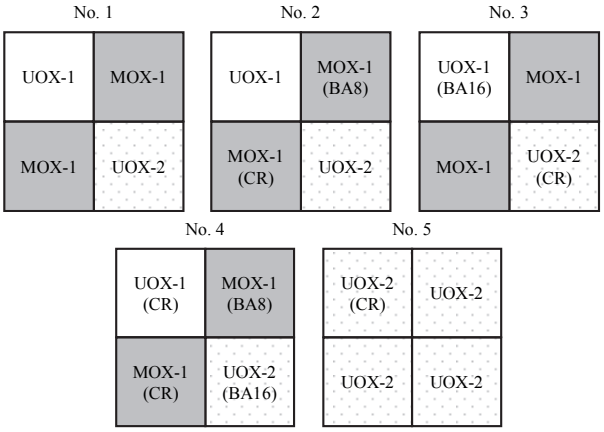

Fig.1 Color-set configuration used in the verification calculation (UOX-1: UO2 2.0 w/o fuel, UOX-2: UO2 3.3 w/o fuel, CR: including Control Rod, BA: including Burnable Absorber)

It should be noted that diffusion calculation is also carried out for comparison. DF for diffusion calculation is obtained through the same procedure described in Steps (4)-(6) above. DF for diffusion calculation is called as Dif DF.

The AEGIS code is used for heterogeneous transport calculation both for color-set and single assembly geometries. [8]

Analytic polynomial nodal method using second-order spatial expansion for source term is used for SP3 and diffusion pin-by-pin calculations in order to practically eliminate spatial discretization errors.

K-effective and pin-power distribution using the Ref-individual, the Ref-unitary DF, and the Ref-Dif DF are summarized in Tables I and II.

Tables I and II indicate that the Ref-DFs reproduce the heterogeneous reference results as expected, which show validity of the theory and implementation of the proposed DFs.

Table I Summary of k-effective and error using Ref-DFs

	keff keff error [%]				
	Color set geometry No.				
Calculation	1	2	3	4	5
reference	1.18185	1.10710	1.03992	0.97237	1.15856
SP3 with Ref-Individual DF	1.18186	1.10711	1.03993	0.97238	1.15857
	0.00	0.00	0.00	0.00	0.00
SP3 with Ref-Unitary DF	1.18186	1.10711	1.03993	0.97238	1.15857
	0.00	0.00	0.00	0.00	0.00
Diffusion with Ref-DifDF	1.18186	1.10711	1.03993	0.97238	1.15857
	0.00	0.00	0.00	0.00	0.00

Table II Summary of maximum and root mean square errors of pin-powers using Ref-DFs

	Pin power RMS error [%] Pin power maximum error [%]				
	Color set geometry No.				
Calculation	1	2	3	4	5
SP3 with	0.00	0.00	0.00	0.00	0.00
Ref-Individual DF	0.01	0.01	0.01	0.01	0.01
SP3 with	0.00	0.00	0.00	0.00	0.00
Ref-Unitary DF	0.01	0.01	0.01	0.01	0.01
Diffusion with	0.00	0.00	0.00	0.00	0.00
Ref-DifDF	0.01	0.01	0.01	0.01	0.01

Pin power error: (Homo. – reference) / reference
RMS: Root mean square

Tables III and IV show error of k-effective and pin-powers using SA-DFs. From Tables III and IV, the following observations are obtained:

- SA-DF can significantly decrease cell-homogenization errors both for SP3 and diffusion calculations.
- Comparison of Case C and D shows reduction of homogenization error is comparable for the SA-individual and the SA unitary DFs. The present result indicates that preservation of J_1 at homogenized region boundary dominates prediction accuracy in the homogenized SPn calculation. Furthermore, the present results also implies that the unitary DF can work well for higher order SPn calculations since contribution of higher order moment would not be very large.
- Comparison of Cases C, D and Case G indicates that SP3 calculation with SA-DF shows higher accuracy than that of diffusion calculation with SA-DF.[6][9] It also noted that SP3 without DF shows worse result than that of diffusion with SA-DF. It shows the significance of DF in cell-homogenized calculations.
- Comparison of Case D and Case E indicates that the freedom of DF at geometry boundary is important for the unitary DF.

The present verification results shows the validity of the proposed DFs (the individual and the unitary DFs) for SP3 calculations. Since practical calculation procedure for actual implementation is also established,

the proposed DFs will be a good candidate for core analysis with the SP3 theory.

Table III Summary of k-effective and error using SA-DFs

		keff keff error [%]				
		Color set geometry No.				
Case	Calculation	1	2	3	4	5
A	reference	1.18185	1.10710	1.03992	0.97237	1.15856
B	SP3 with	1.18163	1.10329	1.02837	0.95775	1.15268
	no DF	-0.02	-0.34	-1.11	-1.50	-0.51
C	SP3 with	1.18173	1.10704	1.03955	0.97220	1.15879
	SA-Individual DF	-0.01	-0.01	-0.04	-0.02	0.02
D	SP3 with	1.18172	1.10702	1.03950	0.97205	1.15868
	SA-Unitary DF	-0.01	-0.01	-0.04	-0.03	0.01
E	SP3 with	1.18160	1.10717	1.03885	0.97163	1.15885
	SA-Unitary DF(*)	-0.02	0.01	-0.10	-0.08	0.02
F	Diffusion with	1.18156	1.10026	1.01881	0.94604	1.14679
	no DF	-0.02	-0.62	-2.03	-2.71	-1.02
G	Diffusion	1.18138	1.10679	1.03775	0.97010	1.15797
	with SA-DifDF	-0.04	-0.03	-0.21	-0.23	-0.05

(*) DF for Φ is identical to that for ϕ_0 at boundary surfaces of the fuel assemblies, i.e., Eq.(5) is used for DF for Φ.

Table IV Summary of maximum and root mean square errors of pin-powers using SA-DFs

		Pin power RMS error [%] Pin power maximum error [%]				
		Color set geometry No.				
Case	Calculation	1	2	3	4	5
B	SP3 with	0.48	1.14	2.42	2.69	2.63
	no DF	2.01	3.76	6.71	7.51	8.11
C	SP3 with	0.55	0.60	0.51	0.55	0.16
	SA-Individual DF	1.45	1.56	1.32	1.42	0.40
D	SP3 with	0.53	0.56	0.49	0.50	0.09
	SA-Unitary DF	1.47	1.58	1.29	1.37	0.23
E	SP3 with	1.19	1.25	1.09	1.12	0.18
	SA-Unitary DF(*)	2.65	2.64	2.78	2.62	0.45
F	Diffusion with	1.15	1.50	3.00	2.93	3.00
	no DF	3.36	3.63	11.41	9.48	9.81
G	Diffusion	1.02	1.08	1.19	1.42	0.48
	with SA-DifDF	1.98	2.20	2.14	3.21	1.55

(*) DF for Φ is identical to that for ϕ_0 at boundary surfaces of the fuel assemblies, i.e., Eq.(5) is used for DF for Φ.

4. Summary

New discontinuity factors (DFs) for SP3 theory, i.e., the individual and the unitary DFs are proposed. In the individual DFs, different values of DF are assigned for Φ and ϕ_0 of SP3 at the surface of homogenized region. On the contrary, the same value of DF are assigned for Φ and ϕ_0 in the unitary DF. Theoretical derivation for these DFs are described and then actual estimation procedure of these DFs are explained.

Verification results using the color-set geometry consists of UO2 and MOX fuel assemblies indicate the validity of the present method. Errors of k-effective and pin-power distribution are significantly reduced by using these DFs.

The proposed DFs can be used for practical core analysis using the SP3 theory.

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