M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

Development of GENESIS, a Three-dimensional Heterogeneous Transport Code based on the LEAF Method

Akio Yamamoto, Akinori Giho, Tomohiro Endo

Nagoya University: Furo-cho, Chikusa-ku, Nagoya, Japan, 464-8603
a-yamamoto@nucl.nagoya-u.ac.jp

Abstract - *The present paper describes recent development activities of the GENESIS code, which is a transport code for heterogeneous three-dimensional geometry, focusing on applications to reactor core analysis. For the treatment of anisotropic scattering, concept of the simplified Pn method is introduced in order to reduce storage of flux moments. Accuracy of the present method is verified through a benchmark problem. Next, iteration stability of the GENESIS code for highly voided condition, which would appear in the severe accident conditions, is discussed. Efficiency of the CMFD and GCMR acceleration methods are verified with various stabilization techniques. Use of the effective diffusion coefficient and the artificial grid diffusion (AGD) coefficients are effective to stabilize the acceleration calculation in highly voided conditions.*

I. INTRODUCTION

Significant efforts have been devoted for high fidelity simulation methods of core characteristics. Monte-Carlo and deterministic methods are two distinguished approaches for high fidelity simulations. As the deterministic methods, spatial, angular, energetic, and temporal resolutions are being continuously increased and three-dimensional multi-group transport calculations considering explicit heterogeneous geometry of reactor core are becoming feasible, *e.g.* [1]-[11].

Various approaches can be considered for a three-dimensional multi-group transport calculation with heterogeneous geometry. A straightforward approach to realize this type of calculation is direct application of method of characteristics (MOC) in three-dimensional geometry [9]-[11]. However, it requires large computational resources (both memory and computation time) thus its practical application to large scale geometry, *e.g.*, a commercial light water reactor, would be still difficult. Instead, the planar MOC method is successfully applied for high fidelity core analyses [2]-[8].

In the planar MOC method, neutron transport calculations for radial and axial directions are performed by the conventional MOC and diffusion/low order transport calculation, respectively. In typical commercial reactors, axial heterogeneity is much smaller than that in radial direction, thus different treatments of neutron transport for radial and axial directions are justified and can be applied without significant loss of prediction accuracy. The planar MOC has great advantage on computational efficiency since it utilizes the conventional MOC in two-dimensional geometry.

Recently, high fidelity simulations of core characteristics under severe core conditions, *e.g.* loss of coolant accident (LOCA) or anticipated transient without scram (ATWS), are being required from the viewpoint of safety analysis. In these conditions, highly voided condition should be considered with significant skewed power distribution not only for radial direction but also for axial direction. Since the planar MOC utilizes a diffusion or low order transport method to approximately consider axial leakage, it would pose degradation on prediction accuracy and/or convergent issues in the severe core conditions.

In order to address this issue, the Legendre polynomial Expansion of Angular Flux (LEAF) method is proposed as an extension of the ASMOC3D method [12]-[14]. In the LEAF method, axial leakage is explicitly considered without approximation. Thus, higher accuracy is expected in the severe core conditions including highly voided conditions.

The GENESIS code that is based on the LEAF method is being developed in Nagoya University. The GENESIS code is a multi-group transport code for two- and three-dimensional heterogeneous geometries. The LEAF method and the conventional MOC are used for three- and two-dimensional transport calculations, respectively. The GENESIS code can handle various complicated geometries through the factorial geometry method and the R-function solid modeler [15][16]. Nested geometry can be allowed in any depth. The direct neutron path linking (DNPL) technique is used to reduce computational burden of ray trace in a large repeated geometry such as large power reactors [17]. Two-level GCMR or CMFD method is used as an efficient acceleration method [18][19].

In the present paper, recent developments of the GENESIS code are described.

In section II, fundamental theory of the LEAF method are briefly described. Then in section III, recent developments of the GENESIS code are described especially for treatment of anisotropic scattering using the concept of simplified Pn (SPn) method, and numerical stability of the generalized coarse mesh rebalance (GCMR) and the coarse mesh finite difference (CMFD) acceleration methods for highly voided condition, which appears under design extension condition in LWRs. Finally concluding remarks are provided in section IV.

II. LEAF METHOD

Detail description of the LEAF method can be found elsewhere [13][14], but brief description is provided for readers' understanding.

Concept of the LEAF method is shown in Fig.1. In the conventional "direct" 3D approach of MOC, a three-dimensional geometry is covered by one-dimensional ray traces, which usually require impractical memory storage for large cores such as commercial reactors. In the LEAF method, instead, geometry is covered by planes that is considered as an extension of ray traces drawn in 2D x-y geometry to z-direction. A three-dimensional geometry is covered by sets of parallel planes (characteristics planes) for various azimuthal directions. Since extruded geometry for axial direction is considered, we can assume that a characteristics plane is composed of rectangles as shown in Fig.1. In the case of MOC, neutron transport calculation on a characteristics line, *i.e.*, in one-dimensional geometry, is carried out. Instead, in the LEAF method, neutron transport calculation within the characteristics plane, *i.e.*, in two-dimensional geometry, is carried out. Though any neutron transport method can be used for transport calculation within a two-dimensional characteristics plane, the angular dependent transmission probability (ADTP) method is used in the GENESIS code due to its efficiency [20].

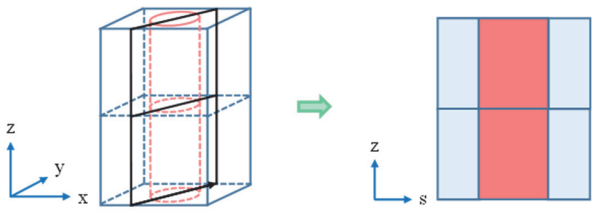

Fig.1 Concept of the LEAF method

In order to reduce spatial discretization error, spatial distributions of incoming and outgoing angular fluxes along faces of a rectangle in a characteristics plane are expanded up to 2nd Legendre polynomials. Similarly, spatial distribution of neutron source in a rectangle is expanded into 1st and 2nd orders in radial and axial directions, respectively.

With the above spatial expansion, outgoing angular fluxes from a rectangle is calculated by:

$$\varphi_i^{out,Right} = \sum_{j=0}^{2} \left(\varphi_j^{in,Left} T_{j,i}(l \to r) + \varphi_j^{in,Bottom} T_{j,i}(b \to r) \right) + q_0 E_{s,0,i}(q \to r) + q_{s,1} E_{s,1,i}(q \to r) + q_{z,1} E_{z,1,i}(q \to r) + q_{z,2} E_{z,2,i}(q \to r), \quad (1)$$

$$\varphi_i^{out,Top} = \sum_{j=0}^{2} \left(\varphi_j^{in,Left} T_{j,i}(l \to t) + \varphi_j^{in,Bottom} T_{j,i}(b \to t) \right) + q_0 E_{s,0,i}(q \to t) + q_{s,1} E_{s,1,i}(q \to t) + q_{z,1} E_{z,1,i}(q \to t) + q_{z,2} E_{z,2,i}(q \to t), \quad (2)$$

where $\varphi_i^{out,Right}$, $\varphi_i^{out,Top}$, $\varphi_j^{in,Left}$, $\varphi_j^{in,Bottom}$ are expansion coefficients of outgoing and incoming angular flux spatial distributions, q_0, $q_{s,1}$, $q_{z,1}$, $q_{z,2}$ are expansion coefficients of neutron source spatial distribution, and:

$T_{j,i}(l \to r)$: angular dependent transmission kernel from *j*-th coefficient of angular flux on the left face to *i*-th coefficient of angular flux on the right face,

$T_{j,i}(b \to r)$: angular dependent transmission kernel from *j*-th coefficient of angular flux on the bottom face to *i*-th coefficient of angular flux on the right face,

$E_{s,k,i}(q \to r)$: angular dependent escape kernel from *k*-th coefficient of neutron source for radial direction to *i*-th coefficient of angular flux on the right face,

$E_{z,k,i}(q \to r)$: angular dependent escape kernel from *k*-th coefficient of neutron source for *z*-direction to *i*-th coefficient of angular flux on the right face.

Note that spatial distribution of neutron angular flux is expanded as:

$$\psi(s) = \sum_{i=0}^{2} \varphi_i \, P_i(s), \quad (3)$$

where $P_i(s)$ is the Legendre polynomials of *i*-th order and *s* is a coordinate along a face of a rectangle normalized from -1 to 1 in an rectangle.

The average angular flux in a rectangle is calculated by:

$$\bar{\psi} = \sum_{j=0}^{2} \left(\varphi_j^{in,Left} C_j(l \to a) + \varphi_j^{in,Bottom} C_j(b \to a) \right) + q_0 C_{s,0}(q \to a) + q_{s,1} C_{s,1}(q \to a) + q_{z,1} C_{z,1}(q \to a) + q_{z,2} C_{z,2}(q \to a), \quad (4)$$

where

$C_j(l \to a)$: angular dependent collision kernel from *j*-th coefficient of angular flux on the left face to average angular flux in the rectangular region,

$C_j(b \to a)$: angular dependent collision kernel from *j*-th coefficient of angular flux on the bottom face to average angular flux in the rectangular region,

$C_{s,k}(q \to a)$: angular dependent collision kernel from *k*-th coefficient of neutron source for radial direction to average angular flux in the rectangular region,

$C_{z,k}(q \to a)$: angular dependent collision kernel from *k*-th coefficient of neutron source for *z*-direction to average angular flux in the rectangular region.

Once average angular flux in a rectangle is obtained, average scalar flux in a flux region can be obtained through integration on phase space (spatial and angular domain), which is essentially the same procedures used in the conventional MOC method.

$$\bar{\phi} = \frac{1}{V}\int \psi dV d\Omega \approx \frac{\sum_m \omega_m \sum_k \delta A_{m,k} \Delta s_{m,k} \Delta z \bar{\psi}_{m,k}}{\sum_m \omega_m \sum_k \delta A_{m,k} \Delta s_{m,k} \Delta z} \quad (5)$$

where

$\bar{\phi}$: average scalar flux in a flux region in three-dimensional geometry,

ω_m: weight of a solid angle quadrature set for direction m,

$\delta A_{m,k}$: ray trace width for direction m, ray trace k,

$\Delta s_{m,k}$: face length of a rectangular region in a characteristics plane for radial direction (direction m, ray trace k), which corresponds to the segment length of ray trace in the conventional 2D MOC,

Δz: face length of a rectangular region in a characteristics plane for axial direction,

$\bar{\psi}_{m,k}$: average angular flux in a rectangular region obtained by Eq. (4) (direction m, ray trace k).

In the LEAF method, spatial distribution of scalar flux is considered in order to reduce spatial discretization error. Up to 1st (linear) and 2nd (quadratic) spatial distributions are considered for radial and axial directions, respectively. In the radial direction, weighted residual method is used to estimate spatial moments [21]. In the axial direction, average scalar fluxes at the top and bottom mesh surfaces, and average scalar flux in the mesh is used to fit a quadratic scalar flux distribution. The spatial distributions of scalar flux for radial and axial directions are used to evaluate expansion coefficients of spatial neutron source distribution, which are appeared in Eqs.(1), (2), and (4).

As shown in Eqs.(1), (2), and (4), the transmission, escape and collision kernels are used in the LEAF method. These kernels are very frequently evaluated; they correspond to the exponential function appeared in the conventional MOC in two-dimensional geometry. Therefore, their evaluation speed dominates total execution time in actual implementation. In principle, their evaluation can be easily performed by numerical integration using ray traces in a rectangle region appeared in the LEAF calculation. A straightforward approach to estimate these kernels are on-the-fly estimation using numerical integrations with ray traces. However, such approach is equivalent to the direct 3D MOC method, which requires longer computation time. Thus, in the GENESIS code, transmission, escape, and collision kernels are evaluated and tabulated in prior to transport sweeps.

The kernels depend on mesh sizes for radial and axial directions, total cross section, and polar direction. In actual reactor analysis applications, mesh sizes of axial direction can be classified into several types, *e.g.*, core and reflector parts. Similarly, polar directions are discretized into several angles. Therefore, in the GENESIS code, axial mesh size and polar direction are explicitly treated (*i.e.*, not considered as interpolation parameters and tabulated in different table). Only radial mesh size and total cross section are used as interpolation parameters in the pre-tabulated table for the kernels. Significant reduction can be achieved by the tabulation method. However, in the execution time of the GENESIS code, interpolation of the kernel still takes major part.

III. RECENT DEVELOPMENTS AND VERIFICATIONS

1. Treatment of Anisotropic Scattering using the Simplified Pn method

A. Theory

In conventional core analyses, anisotropic scattering has been taken into account through transport correction on total cross section and the assumption of isotropic scattering [22]. However, use of the transport correction would introduces considerable prediction errors especially in highly heterogeneous or high leakage cores. Thus, accurate consideration of anisotropic scattering is being important for high fidelity neutronics simulations.

Treatment of anisotropic scattering has been established with expansion of the real spherical harmonics functions as shown in Eqs.(5) and (6). In this approach, $(L+1)^2$ moments are necessary to represent angular distribution of anisotropic neutron source, where L is the order of anisotropic scattering.

$$S(\boldsymbol{r},\boldsymbol{\Omega}) = \frac{1}{4\pi}\sum_{l=0}(2l+1)\sum_{m=-l}^{l}\Sigma_{sl}(\boldsymbol{r})\phi_{l,m}(\boldsymbol{r})R_{l,m}(\boldsymbol{\Omega}), \quad (5)$$

$$\phi_{l,m}(\boldsymbol{r}) = \int \psi(\boldsymbol{r},\boldsymbol{\Omega})R_{l,m}(\boldsymbol{\Omega})\,d\boldsymbol{\Omega}, \quad (6)$$

where $R_{l,m}(\boldsymbol{\Omega})$ is the real spherical harmonics function.

For example, when anisotropic scattering up to P3 component is taken into account, 16 flux moments are necessary for each flux region in each energy group. Since detail spatial and energetic resolutions are required in precise neutronics simulation, memory requirement for angular moments would be significant especially for a large geometry.

Recently, an explicit angular representation of neutron angular flux/neutron source is proposed for the simplified Pn (SPn) method [23][24]. A great advantage of the SPn method is the smaller number of angular flux moments required for calculation. In the SPn method, (L+1) moments are necessary, which is much smaller than that required in the rigorous treatment using the real spherical harmonics functions.

This concept is introduced in the treatment of anisotropic scattering to reduce computational burden. In addition to the conventional treatment using the spherical harmonics function, the present method is implemented in the GENESIS code. In this approach, angular distribution of neutron source is described by:

$$S(\boldsymbol{r},\boldsymbol{\Omega}) \approx \sum_{l=0} \frac{(2l+1)}{4\pi} \Sigma_{sl}(\boldsymbol{r})\phi_l(\boldsymbol{r})P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega_J}), \quad (7)$$

$$\phi_l(\boldsymbol{r}) = \int \psi(\boldsymbol{r},\boldsymbol{\Omega})P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega_J})\,d\Omega, \quad (8)$$

where $P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega_J})$, $\boldsymbol{\Omega}$, and $\boldsymbol{\Omega_J}$ are the Legendre polynomials, neutron flight direction, and neutron current direction, respectively.

As a more physically intuitive interpretation, we can consider a picture shown in Fig.2. In the concept of SPn method, a "major axis" is considered and angular distribution is assumed to be azimuthally symmetric around the major axis. It is a physical picture of the "locally 1D" model, *i.e.*, we see this angular distribution in a 1D slab geometry. As the major axis, direction of neutron current is used in the GENESIS code.

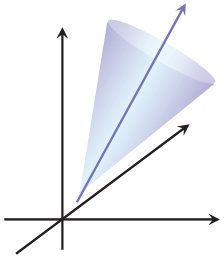

Fig.2 Representation of angular distribution based on the concept of the SPn method

In Eqs.(7) and (8), the value of Legendre polynomial $P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega_J})$ should be evaluated in each mesh since neutron current direction depends on spatial position. It seems to require significant computation time. However, it is reminded that Eq.(8) is used only for a mesh average angular flux, which is obtained after transport sweep for particular angular direction. In this sense, number of evaluations for $P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega_J})$ is limited. Actually, its computation time is negligible in actual implementation of the GENESIS code.

B. Numerical Results

Accuracy of the treatment based on the concept of SPn method is verified in a typical pin-cell and 20x20 fuel pin cells array surrounded by thick water reflector. Typical fuel rod type for PWR is assumed. The latter (20x20 fuel pins array) represents an isolated fuel assembly in water. Leakage from the isolated fuel assembly is considered to be very large. Two different fuel materials, *i.e.*, 4.1wt% UO2 and 12wt% Pu-t MOX fuel, are used in the present test calculations since effect of anisotropic scattering effect is especially large in MOX fuel. Anisotropic scattering up to P3 components is considered in 172 energy group and two-dimensional calculations are carried out.

Various treatments on anisotropic scattering are tested:

Tr: isotropic scattering with transport correction. The extended transport approximation, which subtracts sum of out-scattering P1 components from total cross section, is used. Self-scattering cross section is adjusted to preserve cross section balance.

P0: no anisotropic component is taken into account.

P1, P2, P3: Up to P1, P2, P3 components are taken into account with expansion of real spherical harmonics functions (the conventional and rigorous method).

SP2, SP3: Up to P2, P3 component is taken into account with expansion using the SPn concept (present method).

Calculation results are shown in Table I. Table I indicates that the accuracy of anisotropic treatment based on the SPn concept shows reasonable accuracy. The treatment based on the SPn method gives better accuracy than the conventional P1 but worse than the conventional P2 or the P3 case, which utilizes explicit treatment of anisotropic scattering using the real spherical harmonics functions. In one-dimensional slab geometry, the SPn treatment exactly reproduce the reference (conventional) results obtained with real spherical harmonics functions. In this context, when calculation geometry has more "locally 1D" nature, accuracy of the SPn treatment will increase.

The present verification calculations suggest that the present approach on anisotropic scattering treatment would be a useful option for practical core analysis considering anisotropic scattering. In the present verification calculation, application to core analysis is tested. However, the present method can be used in other applications, *e.g.*, shielding analysis. In the shielding analysis, calculation configuration is generally larger and would have "locally 1D" nature, thus accuracy of the present method would be higher.

Table I Calculation results of k-effective with various treatments of anisotropic scattering

Method	Pincell		Small core	
	UO2 4.1wt%	MOX 12wt% Pu-t	UO2 4.1wt%	MOX 12wt% Pu-t
Tr	1.37576	1.19308	0.90434	0.85265
	0.05%	0.22%	-0.19%	-0.39%
P0	1.37531	1.19179	1.01768	0.93840
	0.02%	0.11%	12.32%	9.63%
P1	1.37461	1.18932	0.90222	0.85200
	-0.03%	-0.09%	-0.43%	-0.46%
P2	1.37513	1.19062	0.90639	0.85636
	0.01%	0.01%	0.03%	0.04%
P3	1.37501	1.19045	0.90607	0.85598
	---*)	---	---	---
SP2	1.37476	1.18973	0.904968	0.85479
	-0.02%	-0.06%	-0.12%	-0.14%
SP3	1.37475	1.18969	0.90473	0.85446
	-0.02%	-0.06%	-0.15%	-0.18%

*) Reference value

2. Stability and Efficiency of GCMR/CMFD Acceleration Methods for Highly Voided Condition

A. Outline

In the planar MOC method, axial planes are coupled through axial leakage between axial planes. It would be a cause of numerical instability under specific conditions, *e.g.*, thin axial plane or large leakage for axial direction [25].

After the Fukushima-Daiichi accident, safety analysis for design extension conditions such as ATWS is required in Japan. Application of a precise core analysis method for such extreme conditions will be useful to quantify design margin in safety analyses. However, as described in the above, the planar MOC method would have difficulty for analysis of highly voided conditions since axial leakage becomes extremely large. On the contrary, since the LEAF method does not use any approximation in the treatment of axial leakage, it would not pose instability in highly voided conditions.

For practical core analysis, use of an efficient acceleration method is indispensable. In the GENESIS code, the GCMR or CMFD acceleration method can be used. Efficiency of these methods for typical core conditions have been established, but their applicability to highly voided conditions has not been confirmed.

In the present paper, efficiency and stability of the GCMR and CMFD methods used in the GENESIS code, coupled with various stabilization techniques, are investigated for highly voided conditions in LWR geometries.

B. Theory

The GCMR method is an acceleration method unifying the coarse mesh rebalance (CMR) and the CMFD acceleration methods [18][19]. In the GCMR method, the following equation is used:

$$-\sum_{k\in S}\frac{\alpha_{i,k}^{-}\beta_{i,k}^{+}}{\alpha_{i,k}^{+}+\alpha_{i,k}^{-}}\phi_{j_k}S_k + \left(\sum_{k\in S}\frac{\alpha_{i,k}^{+}\beta_{i,k}^{-}}{\alpha_{i,k}^{+}+\alpha_{i,k}^{-}}S_k+\Sigma_{rem,i}V_i\right)\phi_i = Q_iV_i, \tag{9}$$

where

k	surface index of a mesh,
j_k	neighbor mesh index through surface k,
ϕ_{j_k}	average scalar flux of neighbor mesh adjacent to surface k,
ϕ_i	average scalar flux of region i,
S_k	area of surface k,
$\alpha_{i,k}^{-},\alpha_{i,k}^{+}$	acceleration factor at – and + surface of k,
$\beta_{i,k}^{-},\beta_{i,k}^{+}$,	correction factor at – and + surface of k,
Q_i	neutron source of mesh i,
V_i	volume of mesh i,
$\Sigma_{rem,i}$	removal cross section of mesh i.

The correction factor in the GCMR method ($\beta_{i,k}^{-},\beta_{i,k}^{+}$), are calculated by:

$$\beta_{i,k}^{-}=\frac{\left(J_{i\to j_k}-J_{j_k\to i}\right)+2\alpha_{i,k}^{-}\left(J_{i\to j_k}+J_{j_k\to i}\right)}{\phi_i},$$
$$\beta_{i,k}^{+}=\frac{\left(J_{j_k\to i}-J_{i\to j_k}\right)+2\alpha_{i,k}^{+}\left(J_{i\to j_k}+J_{j_k\to i}\right)}{\phi_i}, \tag{10}$$

where

$J_{i\to j_k}$	partial current from mesh i to j_k,
$J_{j_k\to i}$	partial current from mesh j_k to i,
$\alpha_{i,k}^{-}$	acceleration factor at – side of surface k,
$\alpha_{i,k}^{+}$	acceleration factor at – side of surface k.

When $\alpha_{i,k}^{-}$ and $\alpha_{i,k}^{+}$ are set to be $D_i/\Delta x_{i,k}$, the GCMR method is equivalent to the one-node type CMFD method. By adjusting $\alpha_{i,k}^{-}$ and $\alpha_{i,k}^{+}$, stability of the GCMR method can be controlled as shown in the numerical results.

The CMFD acceleration method is a well-known and successful acceleration method applied to various iteration method. The following balance equation is used in the CMFD method:

$$-\sum_{k\in S}\left(\widehat{D}_{i,k}+\widetilde{D}_{i,k}\right)\phi_{j_k}S_k + \left(\sum_{k\in S}\left(\widehat{D}_{i,k}-\widetilde{D}_{i,k}\right)S_k+\Sigma_{rem,i}V_i\right)\phi_i = Q_iV_i, \tag{10}$$

where

$$\widehat{D}_{i,k}=\frac{\alpha_{i,k}^{+}\alpha_{i,k}^{-}}{\alpha_{i,k}^{+}+\alpha_{i,k}^{-}},$$
$$\widetilde{D}_{i,k}=-\frac{\left(J_{i\to j_k}-J_{j_k\to i}\right)+\widehat{D}_{i,k}\left(\phi_{j_k}-\phi_i\right)}{\phi_{j_k}+\phi_i},$$
$$\alpha_{i,k}^{-}=D_i/\Delta x_{i,k},$$
$$\alpha_{i,k}^{+}=D_{j_k}/\Delta x_{j_k,k}.$$

Note that $\widetilde{D}_{i,k}$ is generally called the current correction factor.

The CMFD and GCMR acceleration methods are very effective to reduce iteration number of transport sweep. However, they would show numerical instability when mesh size used in acceleration is optically large. In the GCMR method, numerical instability can be avoided by adjusting the acceleration parameters ($\alpha_{i,k}^{-},\alpha_{i,k}^{+}$) but convergent efficiency is degraded.

In the LEAF method, spatial distribution inside a mesh is considered. The spatial distributions are treated as relative shape to mesh average scalar flux. When the CMFD and GCMR acceleration methods are applied, only mesh average scalar flux (flat distribution) is corrected with rebalance factor. Higher order spatial moments are not directly accelerated.

In order to increase convergence stability of the CMFD method, various methods have been investigated [25]. In the present study, the following stability techniques are used and tested.

(1)Effective diffusion coefficient (Deff)

(2)Damping factor for current correction factor in CMFD ($\widetilde{D}_{i,k}$) or correction factor in GCMR ($\beta_{i,k}^{-}, \beta_{i,k}^{+}$) (Damping)
(3)Correction of diffusion coefficient by additional constant, which is the artificial grid diffusion (AGD) coefficient
(4)Correction of diffusion coefficient by multiplicative constant, which is used in the GCMR method
(5)Increase number of inner iterations of MOC

C. Numerical Results

The C5G7 2D and 3D benchmark problems are used for calculations [26]. In the original C5G7 2D/3D benchmark problem, UO2-MOX color-set fuel assemblies are surrounded by water reflector. In the present calculation, in addition to the original benchmark problem, moderator in two MOX fuel assemblies is voided to 99.9%.

Calculation conditions used in the GENESIS code are summarized as follows:

(2D case)
- Number of Azimuthal Angle: $48/2\pi$
- Number of Polar Angle: $8/\pi$ (Gauss Legendre)
- Track Spacing: 0.1cm

(3D case)
- Number of Azimuthal Angle: $8/2\pi$
- Number of Polar Angle: $4/\pi$ (Gauss Legendre)
- Track Spacing: 0.2cm
- Acceleration mesh size for axial direction 3.0cm

(2D & 3D cases)
- Convergence for k-effective 5.0E-6
- Convergence for scalar flux 1.0E-5
- Axial mesh size for 3D case 3.0cm
- Acceleration mesh size for radial direction 1x1/pin cell
- 1 or 2 transport sweep(s) (per inner iteration)

The above calculation conditions would not be sufficient to obtain fully converged (accurate) results, but are sufficient to verify numerical stability of the acceleration methods. Note that prediction accuracy of the GENESIS code in these benchmark problems were confirmed through comparison with the Monte-Carlo code [14].

Number of outer iterations required for convergence is shown in Figs. 3, 4, 5, and 6. The legends "ite 1" and "ite 2 indicate number of inner iterations.

From Figs. 3 and 4, the following observations are obtained for two-dimensional calculation results:

- Numbers of outer iterations are similar both in original (non-voided) and voided benchmark problems. The results indicate that the GCMR and CMFD acceleration method can be directly applied to highly voided condition in two-dimensional geometry.
- By increasing number of inner iterations from 1 to 2, stability of acceleration calculation is increased.
- When no stabilization technique is applied ("none" in these figures), acceleration calculation shows divergence. Thus, stabilization technique(s) are necessary to obtain converged results in this benchmark problem with an acceleration calculation.
- No significant difference from the viewpoint of efficiency is observed among stabilization techniques when appropriate parameters in these methods are chosen.
- GCMR and CMFD methods show similar convergent behavior but GCMR shows slightly more stable trend.

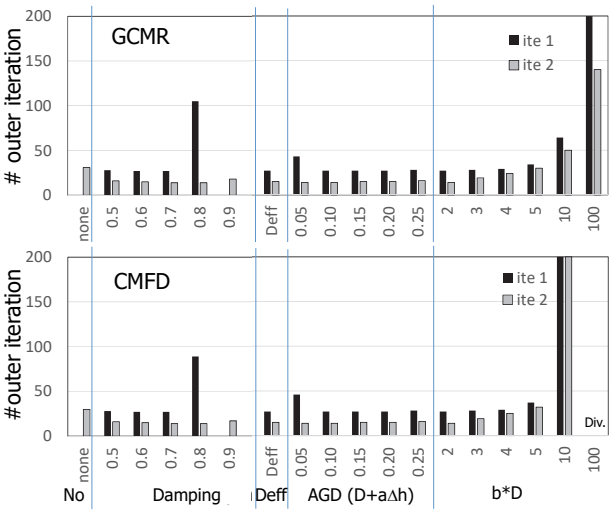

Fig. 3 Number of outer iterations (2D C5G7 original benchmark problem)

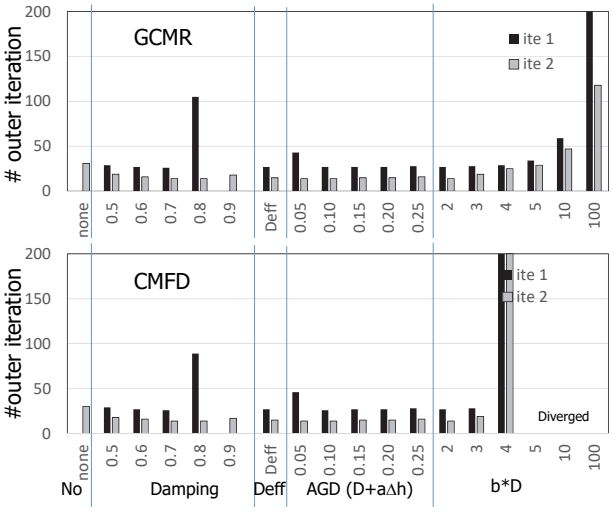

Fig. 4 Number of outer iterations (2D C5G7 voided benchmark problem)

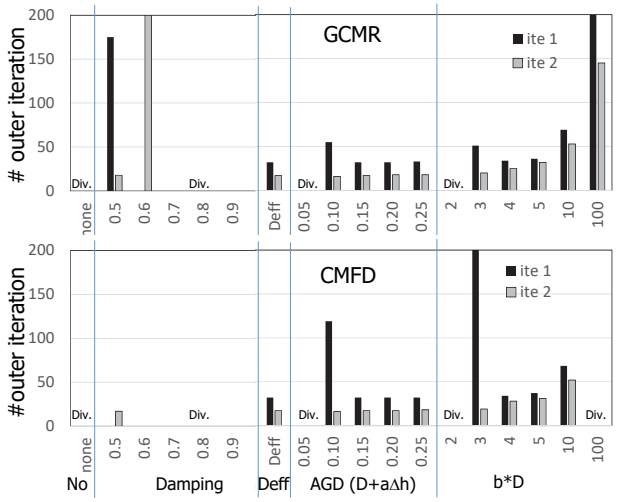

Fig. 5 Number of outer iteration (3D C5G7 original benchmark problem, un-rodded)

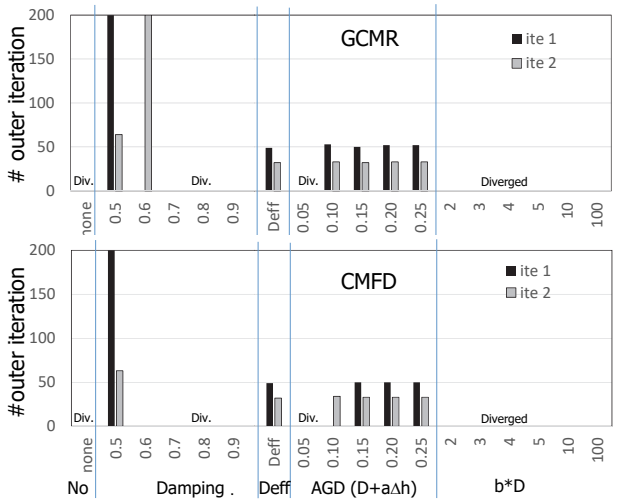

Fig. 6 Number of outer iteration (3D C5G7 voided benchmark problem, un-rodded)

From Figs. 5 and 6, the following observations are obtained for three-dimensional calculation results:

- In comparison to two-dimensional case, acceleration calculations tend to unstable. If no stabilization technique (except for increasing number of inner iterations) is used, acceleration calculation diverges both for the original (non-voided) and the voided cases.
- Application of the damping factor method for correction factor, which is an effective approach in two-dimensional geometry, is not very efficient in the present results. The present results seem to be inconsistent with the previous results in which the CMFD acceleration methods are applied to three-dimensional transport calculation [25]. The difference between the previous and the present studies are the transport method used in three-dimensional calculation. In the previous study, the planar MOC method is used in which axial planes are coupled through diffusion or low order transport theory. On the other hand, the GENESIS code utilizes the LEAF method that explicitly treat angular flux propagation between axial planes. The LEAF method performs an explicit transport calculation not only for radial direction, but also for axial direction. This difference would have impact on stability of acceleration method. It should be reminded that axial mesh size for acceleration is 3 cm, which is much larger than that for radial direction (~1 cm). The GCMR and CMFD acceleration methods tend to become unstable for optically thick (large) meshes. The large mesh size for axial direction would also contribute to decrease stability of the acceleration in the GENESIS code.
- In contrast to two-dimensional geometry, numbers of iterations increase for voided condition. This trend would be also caused by the nature of the LEAF method used in the GENESIS code.

Throughout Figs.3, 4, 5, and 6, use of effective diffusion coefficient (Deff) and the artificial grid diffusion (AGD) coefficient with a=0.25 show stable convergence. Figure 7 show ratio of adjusted (corrected) diffusion coefficient over the unadjusted (original) diffusion coefficient. As shown in Fig.7, Deff and AGD with a=0.25 show similar trends for small (h=0.63cm) and large (h=10cm) meshes. This is the root cause of stable acceleration with these stabilization techniques.

Through the present benchmark calculations, capability to treat highly voided condition of the GENESIS code is confirmed and calculation conditions to realize stable acceleration are clarified.

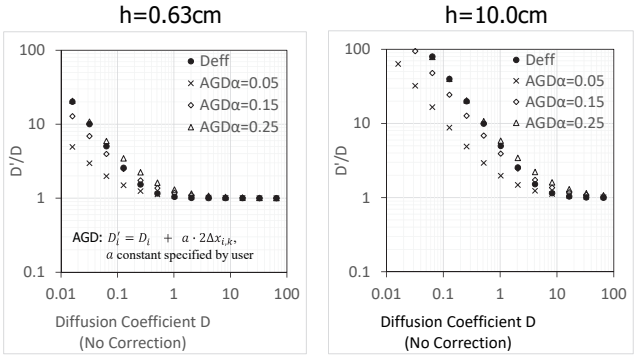

Fig.7 Ratio of diffusion coefficients (adjusted/unadjusted) in effective diffusion coefficient (Deff) and artificial grid diffusion (AGD) coefficient

IV. SUMMARY

A three-dimensional transport code for heterogeneous geometry using the Legendre polynomial Expansion of Angular Flux (LEAF) method, GENESIS, is being developed in Nagoya University. In the present paper, the LEAF method and overview of the GENESIS code are briefly reviewed. As the recent developments of the GENESIS code, application of the simplified Pn (SPn) concept for the treatment of

anisotropic scattering and numerical stability of the CMFD/GCMR acceleration methods for highly voided conditions are discussed.

Use of SPn concept would be useful to reduce memory storage burden especially for multi-group and large scale problems since the present method can significantly reduce number of flux moments required for anisotropic scattering. The verification results show reasonable accuracy in comparison with the conventional treatment using the real spherical harmonics.

Stability of the GENESIS code for highly voided condition is verified using the special version of C5G7 benchmark problem containing fully voided assemblies. Iteration stability for three-dimensional geometry is lower than that for two-dimensional geometry, but stable iteration can be achieved using the effective diffusion coefficient or the artificial grid diffusion (AGD) coefficient in CMFD/GCMR acceleration method.

ACKNOWLEDGMENTS

This work was supported in part by JSPS KAKENHI, Grant-in-Aid for Scientific Research (C) (16K06956).

REFERENCES

1. R. SANCHEZ, “Prospects in Deterministic Three-dimensional Whole-Core Transport Calculations,” Nucl. Eng. and Technol., 44, 113 (2012).
2. J. Y. CHO, H. G. JOO, K. S. KIM, S. Q. ZEE, M. H. CHANG, “Three-dimensional Heterogeneous Whole Core Transport Calculation Employing Planar MOC Solutions,” Trans. Am. Nucl. Soc., 87, 234 (2002).
3. S. KOSAKA, T. TAKEDA, “Verification of 3D Heterogeneous Core Transport Calculation utilizing Non-linear Iteration Technique,” J. Nucl. Sci. Technol., 41, pp. 645-654 (2004).
4. H. G. JOO, J. Y. CHO, K. S. KIM, C. C. LEE, AND S. Q. ZEE, “Methods and Performance of a Three-Dimensional Whole-Core Transport Code DeCART,” Proc. PHYSOR2004, Apr. 25-29 (2004). [CD-ROM]
5. B. KOCHUNAS, B. COLLINS, D. JABAAY, T. J. DOWNAR, W. R. MARTIN, “Overview of Development and Design of MPACT: Michigan Parallel Characteristics Transport Code”, Proc. M&C2013, Sun Valley, Idaho, May 5-9, 2013, (2013), [CD-ROM].
6. Y. S. JUNG, C. B. SHIM, C. H. LIM, H. G. JOO, “Practical Numerical Reactor Employing Direct Whole Core Neutron Transport and Subchannel Thermal/hydraulic Solvers”, Ann. Nucl. Energy, 62, pp.357-374, (2013).
7. M. RYU, Y. S. JUNGA, H. H. CHO, H. G. JOO, “Solution of the BEAVRS Benchmark using the nTRACER Direct Whole Core Calculation Code,” J. Nucl. Sci. Technol., 52, pp.961-969 (2015).
8. M. HURSIN, Full Core, Heterogeneous, Time Dependent Neutron Transport Calculations with the 3D Code DeCart, Ph. D. Thesis, UC Berkeley (2010).
9. J. B. TAYLOR, D. KNOTT, A.J. BARATTA, "A Method of Characteristics Solution to the OECD/NEA 3D Neutron Transport Benchmark Problem", Proc. M&C + SNA 2007, Monterey, CA, (2007).
10. Z. LIU, H. WU, L. CAO, Q. CHEN, Y. LI, “A New Three-dimensional Method of Characteristics for Neutron Transport Calculation,” Ann. Nucl. Energy, 38, 447 (2011).
11. B. KOCHUNAS, T. J. DOWNAR, Z. LIU, “Parallel 3-D Method of Characteristics in MPACT”, Proc. M&C2013, Sun Valley, Idaho, May 5-9, 2013, (2013), [CD-ROM].
12. A GIHO, K SAKAI, Y, IMAMURA, H. SAKURAI, K. MIYAWAKI, “Development of Axially Simplified Method of Characteristics in Three-Dimensional Geometry”, J. Nucl. Sci. Technol., 45, 985 (2003).
13. Y. KATO, T. ENDO, A. YAMAMOTO, “Development of Legendre Expansion of Angular Flux Method for 3D MOC Calculation” Proc. PHYSOR2014, JAEA-Conf 2014-003, Japan Atomic Energy Agency (2014).
14. A. YAMAMOTO, A GIHO, Y. KATO, T. ENDO, “GENESIS – A Three-dimensional Heterogeneous Transport Solver based on the Legendre Polynomial Expansion of Angular Flux Method,” accepted in Nucl. Sci. Eng.
15. Z. WEISS, G. BALL, “Ray-Tracing in Complicated Geometries,” Ann. Nucl. Energy, 18, 483 (1991).
16. T. JEVREMOVIC, J. VUJIC, AND K. TSUDA, “ANEMONA—A Neutron Transport Code for General Geometry Reactor Assemblies Based on the Method of Characteristics and R-Function Solid Modeler,” Ann. Nucl. Energy, 28,125 (2001).
17. S. KOSAKA, E. SAJI, “Transport Theory Calculation for a Heterogeneous Multi-Assembly Problem by Characteristics Method with Direct Neutron Path Linking Technique,” J. Nucl. Sci. Technol., 37, 1015 (2000).
18. K. SMITH AND J. D. RHODES, “Full-Core, 2-D, LWR Core Calculations with CASMO-4E,” Proceedings of PHYSOR, Seoul, South Korea (2002). [CD-ROM]
19. A. YAMAMOTO, “Generalized Coarse-Mesh Rebalance Method for Acceleration of Neutron Transport Calculations,” Nucl. Sci. Eng., 151, 274 (2005).
20. A. YAMAMOTO, K. KIRIMURA, Y. KAMIYAMA, K. YAMAJI, S. KOSAKA, H. MATSUMOTO, "Angular Dependent Transmission Probability Method for Fast Reactor Core Transport Analysis," Trans. Am. Nucl. Soc., 112, 736 (2015).
21 K. S. SMITH, R. FERRER, J. D. RHODES, “Linear Source Approximation in CASMO5,” Proc. PHYSOR2012, Knoxville Tennessee, USA, April 15-20, (2012), [CD-ROM].
22. Z. LIU, K. SMITH, B. FORGET, “A Cumulative Migration Method for Computing Rigorous Transport Cross Sections and Diffusion Coefficients for LWR

Lattices with Monte Carlo," Proc. PHYSOR2016, Sun Valley, ID. May 1-5, 2016 (2016). [USB-DRIVE]
23. Y. A. CHAO, "A New SPN Theory Formulation with Self-consistent Physical Assumptions on Angular Flux," Ann. Nucl. Energy, 87, 137 (2016).
24. Y. A. CHAO, A. YAMAMOTO, "The Explicit Representation for the Angular Flux Solution in Simplified PN (SPN) Theory," Proc. PHYSOR2012, Knoxville, Tennessee, Apr. 15-20 (2012). [CD-ROM]
25. M. JARRETT, B. KOCHUNAS, A. ZHU, T. DOWNAR, "Analysis of Stabilization Techniques for CMFD Acceleration of Neutron Transport Problems," *Nucl. Sci. Eng.*, **184**, 208 (2016).
26. OECD/NEA, Benchmark on Deterministic Transport Calculations Without Spatial Homogenisation - MOX Fuel Assembly 3-D Extension Case, NEA/NSC/DOC(2005)16, (2005).