Development and Verification of an SP$_3$ Code Using Semi-Analytic Nodal Method for Pin-by-Pin Calculation

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Abstract: SP$_3$ (simplified P$_3$) theory is widely used in LWR (light water reactor) analyses to partly capture the transport effect, especially for pin-by-pin core analysis with pin size homogenization. In this paper, a SP$_3$ code named STELLA is developed and verified at SNERDI (Shanghai Nuclear Engineering Research and Design Institute). For SP$_3$ method, neutron transport equation can be transformed into two coupled equations in the same mathematical form as diffusion equation. In this work, SANM (semi-analytic nodal method) is used to solve diffusion-like equation, due to its easy to handle multi-group problem. Whole core nodal boundary net current coupling is used to improve convergence stability in SANM, instead of solving two-node problem. CMFD (coarse-mesh finite difference) acceleration method is employed for 0-th SP$_3$ equation, which represents the neutron balance relationship. Three benchmarks are used to verify the SP$_3$ code, STELLA. The first one is a self-defined one dimensional problem, which demonstrates SP$_3$ method is extremely accurate, due to no academic approximation in one dimensional for SP$_3$. The second one is a two dimensional one-group problem cited from Larsen’s paper, which is usually used to verify and prove the SP$_3$ code correct and accurate. And the third one is modified from 2D C5G7-MOX benchmark, whose numerical results indicate that STELLA is accurate and efficient in pin size level, compared to diffusion model.

Key words: SP$_3$ method, semi-analytic nodal method, pin-by-pin, CMFD, C5G7-MOX benchmark.

1. Introduction

The current generation LWR (light water reactor) core physics calculation methods are based on the neutron diffusion theory framework, two-group energy structure and the generalized equivalent homogenization theory. The potential deficiencies of current method are as follows. Firstly, two-group energy structure cannot deal with the energy spectrum interference effect very well, such as UO$_2$ and MOX fuel mixed loading problem. Secondly, two-step calculation method which decouples the assembly homogenization and the actual core calculation will induce the depletion historical effect, and usually micro-depletion method is used to improve at the core level in today’s industry nuclear design code. Finally, there exists quite large power distribution error in the region with high leakage or strong absorption, such as core periphery or control rod neighboring fuel assemblies. As the fuel loading pattern of core design becomes more and more complex, it is necessary to improve the existing calculation methods to improve the calculation accuracy.

Considering that diffusion calculation needs many approximation and ordinary transport calculation methods such as MOC or S$_N$ method usually takes more computing resources, isotropic SP$_3$ (simplified P$_3$) method is encouraged to be a middle choice for engineering practice use for whole core pin-by-pin calculation with pin size homogenization [1-4]. For SP$_3$ method, neutron transport equation can be transformed into two coupled equations in the same mathematical form as diffusion equation. Therefore, with the advantage of the SP$_3$ method, all the effective methods for solving the diffusion equation can also be used to deal with the SP$_3$ equation. A next generation nuclear design code system for whole core pin-by-pin calculation with pin homogenization is under development by SNERDI (Shanghai Nuclear
Engineering Research and Design Institute). In this code system, core neutronics engine will intend to employ SP3 method, and will be coupled with sub-channel thermal-hydraulics code for pin size feedback calculation.

In this paper, we will report the development and verification of the SP3 code, STELLA, at SNERDI. There are several numerical methods for solving diffusion-like equation. Nodal method is one of the best choices, specifically for its better performance and superior accuracy. Many kinds of nodal diffusion method have been developed, such as NEM (Nodal Expansion Method), the ANM (Analytic Nodal Method) and the NGFM (Nodal Green’s Function Method), etc. In this work, SANM (Semi-Analytic Nodal Method) will be used to solve diffusion-like equation, due to that it is easy to handle multi-group problem [5]. We use whole core nodal boundary net current coupling to improve convergence stability in SANM, instead of solving two-node problem, which does not need nonlinear iterations. CMFD (Coarse-Mesh Finite Difference) acceleration method is employed for 0-th SP3 equation, which represents the neutron balance relationship. Three benchmarks will be used to verify the SP3 code, STELLA, in this paper. The first one is a self-defined one dimensional problem, which will demonstrate SP3 method is extremely accurate, due to no academic approximation in one dimensional for SP3. The second one is a two dimensional one-group problem cited from Larsen’s paper, which is usually used to verify and prove the SP3 code correct and accurate. And the third one is modified from 2D C5G7-MOX benchmark, whose numerical results indicate that STELLA is accurate and efficient in pin size level, compared to diffusion model.

In Sec. 2, fundamental theory and detailed formulations are described. Numerical results are shown in Sec. 3, followed by conclusions in Sec. 4.

2. Calculation Model

2.1 SP3 Formulation

The SP3 transport equation with isotropic scattering can be written as follow with the standard notation.

\[
-D^2_r \nabla^2 \tilde{\phi}_s^k (r) + \left[ \sigma_{r,0,g}^k \tilde{\phi}_s^k (r) \right] = \left[ \tilde{S}_{r,0,g}^k (r) + 2 \sigma_{r,0,g} \tilde{\phi}_s^k (r) \right]
\]

\[
-D^2_r \nabla^2 \tilde{\phi}_s^k (r) + \left[ \sigma_{r,2,g}^k \tilde{\phi}_s^k (r) \right] = \left[ -\frac{2}{3} \tilde{S}_{r,0,g}^k (r) + \frac{2}{3} \sigma_{r,0,g} \tilde{\phi}_s^k (r) \right]
\]

where

\[
\sigma_{r,0,g}^k = \sigma_{r,g}^k - \sigma_{r,t-g}^k
\]

\[
\sigma_{r,2,g}^k = \frac{5}{3} \sigma_{r,t,g}^k + \frac{4}{3} \sigma_{r,0,g}^k
\]

\[
\tilde{S}_{r,0,g}^k (r) = \sum_{g' \in g}^G \sigma_{g,g'}^{k,g} \left[ \tilde{\phi}_{g,g'}^{r,k} (r) - 2 \tilde{\phi}_{2,g,g'}^{r,k} (r) \right]
\]

\[
+ \frac{1}{k_{eff}} \sum_{g' \in g}^G \nu \sigma_{f,g}^{k,g} \left[ \tilde{\phi}_{g,g'}^{r,k} (r) - 2 \tilde{\phi}_{2,g,g'}^{r,k} (r) \right]
\]

\[
D_{r,2,g}^k = \frac{9}{7} D_{r,0,g}^k
\]

2.2 SANM Formulation

In order to simplify the description, the following one-dimensional sub-diffusion integral equation is given directly.

\[
-D_g^k \frac{d^2 \phi_{g,u}^k (u)}{du^2} + \alpha_g^k \phi_{g,u}^k (u) = \sum_{g' \in g}^G \left( \sigma_{g,g'}^{k,g} + \frac{K_{eff}}{k_{f,g}} \nu \sigma_{f,g}^{k,g} \right) \phi_{g,u}^k (u) - L_{g,u}^k (u)
\]
\[ \phi_{gu}^k(u) = \Phi_g^k + \sum_{i=1}^4 a_{gu}^i P_i\left(\frac{2u}{\Delta u_k}\right) \] (4)

where

\[ p_0(t) = 1 \]
\[ p_1(t) = t \]
\[ p_2(t) = \frac{1}{2}(3t^2 - 1) \]
\[ p_3(t) = \frac{\sinh(\alpha_{gu}^k t) - m_{gu}^{k_0}(\sinh) p_0(t)}{\sinh(\alpha_{gu}^k - m_{gu}^{k_0}(\sinh)} \]
\[ p_4(t) = \frac{\cosh(\alpha_{gu}^k t) - m_{gu}^{k_0}(\cosh) p_0(t) - m_{gu}^{k_2}(\cosh) p_2(t)}{\cosh(\alpha_{gu}^k) - m_{gu}^{k_0}(\cosh) - m_{gu}^{k_2}(\cosh)} \]

(5)

\[ B_{gg}^k = \alpha_{rg}^k \]
\[ B_{kg}^k = -\sum_{g'} \frac{Z_{gg'} \Sigma_{g'}^{k_1}}{k_{g}^{eff}} \]
\[ G_{gu}^k = \frac{\alpha_{gu}^k \sinh(\alpha_{gu}^k) - 3m_{gu}^{k_0}(\cosh)}{\cosh(\alpha_{gu}^k) \cos (m_{gu}^{k_1}(\cosh)) - m_{gu}^{k_2}(\cosh)} \]

(9)

B. First-order moment equation

\[ a_{gu}^{k_1} - A_{gu}^{k_1} B_{kg}^{k_1} B_{gu}^{k_1} = A_{gu}^{k_1} \left( \sum_{g'} B_{g'g}^{k_1} a_{g'lu}^{k_1} + L_{gu}^{k_1} \right) \]

(10)

\[ A_{gu}^{k_1} = \frac{\sinh(\alpha_{gu}^{k_1}) - m_{gu}^{k_1}(\cosh)}{\sum_{g'} m_{gu}^{k_1}(\sinh)} \]

(11)

C. Second-order moment equation

\[ a_{gu}^{k_2} - C_{gu}^{k_2} B_{kg}^{k_2} B_{gu}^{k_2} = C_{gu}^{k_2} \left( \sum_{g'} B_{g'g}^{k_2} a_{g'lu}^{k_2} + L_{gu}^{k_2} \right) \]

(12)

\[ C_{gu}^{k_2} = \frac{\cosh(\alpha_{gu}^k) - m_{gu}^{k_0}(\cosh) - m_{gu}^{k_2}(\cosh)}{\sum_{g'} m_{gu}^{k_2}(\cosh)} \]

(13)

D. Using transverse neutron flux expansion coefficients to represent the boundary net current

\[ J_{g} = -\frac{2D_g^{k}}{\Delta u_k} (a_{gu}^{k_1} + 3a_{gu}^{k_2} + H_{g}^{k_1} a_{gu}^{k_3} + G_{g}^{k_1} a_{gu}^{k_4}) \]
\[ J_{g} = -\frac{2D_g^{k}}{\Delta u_k} (a_{gu}^{k_1} - 3a_{gu}^{k_2} + H_{g}^{k_1} a_{gu}^{k_3} - G_{g}^{k_1} a_{gu}^{k_4}) \]

(14)

where

\[ H_{g}^{k_1} = \frac{\alpha_{gu}^k \cosh(\alpha_{gu}^k) - m_{gu}^{k_1}(\cosh)}{\sinh(\alpha_{gu}^k) - m_{gu}^{k_1}(\sinh)} \]

(15)
Eqs. (8), (10), (12) and (14) are used to obtain the relationship between nodal average flux and expansion coefficients of transverse integral flux.

\[
\Phi = -\frac{1}{\Delta u \cdot B_{gg}} (J_R - J_L) - \frac{1}{B_{gg}} \left( \sum_{g' \neq} B_{gg'} \Phi_{g'} + L_0 \right)
\]

\[
a_1 = a_{11} (J_R + J_L) + a_{21} \left( \sum_{g' \neq} B_{gg'} a_{g_1} - L_0 \right)
\]

\[
a_2 = a_{22} (J_R - J_L) + a_{22} \left( \sum_{g' \neq} B_{gg'} a_{g_2} - L_2 \right) \quad (16)
\]

\[
a_3 = a_{33} (J_R + J_L) + a_{33} \left( \sum_{g' \neq} B_{gg'} a_{g_3} - L_3 \right)
\]

\[
a_4 = a_{44} (J_R - J_L) + a_{44} \left( \sum_{g' \neq} B_{gg'} a_{g_4} - L_2 \right)
\]

where

\[
a_{11} = -\frac{\Delta u / 4D}{1 + HAB}, \quad a_{22} = \frac{H}{1 + HAB} \cdot A,
\]

\[
a_{21} = -\frac{\Delta u / 4D}{3 + GCB}, \quad a_{22} = \frac{G}{3 + GCB} \cdot C,
\]

\[
a_{33} = -\frac{\Delta u / 4D}{1 + HAB} \cdot AB, \quad a_{44} = -\frac{1}{1 + HAB} \cdot A,
\]

\[
a_{44} = -\frac{\Delta u / 4D}{3 + GCB} \cdot CB, \quad a_{44} = \frac{3}{3 + GCB} \cdot C.
\]

Based on the continuity condition of surface flux after multiplying the discontinuous factors, the following equation is established to represent the boundary net current coupling relationship of neighboring nodes.

\[
\left[ (C_1 - C_2) \cdot f_{\phi,0} \right] f_{\phi} + \left[ (C_1 + C_2) \cdot f_{\phi} + (C_{11} + C_{22}) \cdot f_{\phi} \right] f_{\phi} =
\]

\[
\left[ (C_3 - C_4) \cdot f_{\phi} \right] f_{\phi} =
\]

\[
\left[ (S_1 - L_1) \cdot B_{gg} \cdot C_3, (S_2 - L_2) \cdot B_{gg} \cdot C_4 \right] f_{\phi} =
\]

\[
\left[ (S_1 - L_1) \cdot B_{gg} \cdot C_3, (S_2 - L_2) \cdot B_{gg} \cdot C_4 \right] f_{\phi}
\]

where

\[
C_1 = a_{11} + a_{1}, \quad C_2 = a_{21} + a_{41} = \frac{1}{\Delta u B_{gg}}, \quad C_3 = a_{12} + a_{22}, \quad C_4 = a_{22} + a_{42}.
\]

Once the boundary net current is obtained, the nodal average flux can be calculated by using the nodal neutron balance equation. And then the neutron source term can be updated and the iterative process can be established.

### 2.3 CMFD Acceleration for SP3 Formulation

CMFD (Coarse-Mesh Finite Difference) is an effective acceleration convergence technique, which is widely used in the field of three dimensional diffusion calculation and heterogeneous transport calculation. In this paper, we have developed a CMFD acceleration method for the SP3 equation with reference to recent research progress, and obtained a good acceleration effect.

\[
-D_{g} \nabla^{2} \Phi_{g} (r) + \sigma_{g} \Phi_{g} (r)
\]

\[
= \sum_{g' \neq} \left[ \sigma_{g'g} + \frac{\chi_{g}}{k_{eff}} \cdot \sigma_{g'g} \right] \Phi_{g} (r) \quad (20a)
\]

\[
-D_{0g} \nabla^{2} \left[ \phi_{g} (r) + 2 \phi_{g} (r) \right] + \sigma_{g} \phi_{g} (r)
\]

\[
= \sum_{g' \neq} \left[ \sigma_{0,g'} + \frac{\chi_{g}}{k_{eff}} \cdot \sigma_{0,g'} \right] \phi_{g'} (r) \quad (20b)
\]

Eq. (20a) is the neutron diffusion equation, and Eq. (20b) is the 0-th equation of SP3. Comparing Eqs. (20a) and (20b), the remaining items are identical except for the first item on the left side. Therefore, as long as keeping the first term of Eq. (20a) same as Eq. (20b), the flux and k-effective of Eq. (20a) can converge to the flux and k-effective of 0-th equation of SP3. Furthermore, it is found that the 2-th flux of SP3 equation is usually about 1 to 2 orders of magnitude smaller than the 0-th flux. Therefore, the convergence of the 0-th flux of the SP3 equation is dominated by the solution of the SP3 equation. In this paper, the CMFD equation is proposed to accelerate the convergence of 0-th flux of the SP3 equation, and this practice enhances the stability of the CMFD acceleration. The formula is as follows.
The nodal coupling correction factor is updated according to Eq. (22), in the iterative process of solving the SP3 SANM equations. The remaining process is identical to the conventional CMFD acceleration for the nodal diffusion method, which is omitted for simplicity.

\[
J_{g+}^{k,SP3-0th} = -D_{g+}^{k,FDM} \left( \Phi_{g}^{k+1} - \Phi_{g}^{k} \right) - D_{g+}^{k,SP3} \left( \Phi_{g}^{k+1} + \Phi_{g}^{k} \right) \tag{21}
\]

2.4 Iteration Process

The STELLA code is written in the Fortran-95 standard. The source iterative method is used to solve the SP3 equations. Firstly, given the initial source, 0-th SP3 equation with CMFD acceleration is solved, where the number of iterations should be fixed (usually 5 to 8). Secondly, using the 0-th flux to update the source term of 2-th SP3 equation, and then drive the SANM to solve the 2-th SP3 equation. Finally, taking both 0-th and 2-th flux contribution into account, update the k-effective and source term until the iterations are reached to convergence.

3. Numerical Results

3.1 Self-defined 1D Problem

A one dimensional 7-group benchmark problem is self-defined. Fig. 1 shows the layout of this problem. Materials from the left side to right are H₂O, UO₂, 4.3% MOX, 7.0% MOX and 8.7% MOX. The cross-section parameters of materials are from the 2D C5G7-MOX benchmark [6]. The left side is the vacuum boundary condition, and the right side is the reflective boundary condition. The width for each material is 20 cm shown in Fig. 1. Due to the large differences in energy spectrum among the various materials and the strong leakage, it's a good case for code STELLA accuracy verification.

The reference solution including k-effective and power distribution of the problem is given by the Monte Carlo program MCMG [7]. In order to obtain a reliable reference result, we use 1,000 cycles (including 50 inactive cycles) with 100,000 sampling for each cycle. The result of STELLA is given by the SANM-SP3 module and the mesh is divided into 1 cm per mesh. Table 1 shows the results comparison of the STELLA and MCMG. Since there is no academic approximation in one dimensional for SP3 theory, the difference should be very small. It can be seen from Table 1 that STELLA is very accurate, with k-effective error of only -1 pcm and the maximum power error of -0.15%.

3.2 Larsen’s One-Group Problem

Brantley and Larsen [1] have established a two dimensional one-group isotropic problem. Fig. 2 shows the layout of the problem, and Table 2 gives the cross-section parameters. Boundary condition and geometry size are also shown in Fig. 2.

![Fig. 1 Layout of the self-defined 1D problem.](image)
The benchmark reference solution is established by the two dimensional $S_N$ transport code TWODANT, with the quadrature group $S_{16}$ and the $150 \times 150$ meshes. In reference paper only provides k-effective and does not provide power distribution. In order to further evaluate the benchmark problem, a two dimensional MOC transport code PEACH [8] is used to provide the detailed power distribution; PEACH uses $150 \times 150$ meshes and 0.01 cm ray spacing, with 32 azimuthal angles and 2 optimal polar angles in an octant. STELLA $P_1$ and SP$_3$ model uses the same $10 \times 10$ meshes division.

According to Table 3, we can see that the corresponding deviations of STELLA-$P_1$ and STELLA-SP$_3$ are 35.6 pcm and 51.3 pcm respectively. We also find that the k-effective error is only 2.8 pcm between reference and PEACH-MOC, so the results from PEACH-MOC are reliable and the power distribution of PEACH-MOC can be used as the benchmark reference. The maximum power error is 1.38% between PEACH-MOC and STELLA SP$_3$ according to Fig. 3. Compared with those reference results, the quite small deviation can prove that the theoretical derivation and code development are correct in this paper.

### 3.3 2D C5G7-MOX Problem

A 2D C5G7-MOX homogenized pin problem is generated from original C5G7 benchmark [6]. For the homogenized pin problem, the reference solution is obtained by a two dimensional MOC code PEACH, in which the single pin is subdivided with $5 \times 5$ meshes, and the ray spacing is about 0.04 cm. Fig. 4 is the layout of this problem. STELLA has two modules of neutronics solution, one is diffusion calculation module with SANM (named STELLA $P_1$), and the other is SP$_3$ module introduced in Sec. 2.

In this paper, the problem of the 2D C5G7-MOX homogenized pin problem is solved by using both STELLA $P_1$ model and SP$_3$ model. The single fuel pin mesh is not subdivided, and still uses original $1\times1$ mesh.
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Table 4  K-effective difference and performance comparison.

|                | keff  | Err. /pcm | Time /s | CMFD |
|----------------|-------|-----------|---------|------|
| PEACH          | 1.18716 | Reference |         |      |
| STELLA -P₁     | 1.18426 | -290      | 5.34    | No   |
| STELLA -P₁     | 1.18426 | -290      | 2.56    | Yes  |
| STELLA -SP₃    | 1.18561 | -155      | 39.73   | No   |
| STELLA -SP₃    | 1.18561 | -155      | 15.76   | Yes  |

Table 5  Power distribution difference comparison between STELLA P₁ and SP₃.

|                | STELLA-P₁ | STELLA-SP₃ |
|----------------|-----------|------------|
| Assembly power err. /% | Inner UO₂ | -0.18      | 0.05      |
|                  | MOX       | 0.35       | -0.06     |
|                  | Outer UO₂ | -0.59      | 0.03      |
| Fuel pin power err. /% | Max. power pin | -0.29 (2.368)¹ | 0.14 (2.368)¹ |
|                  | Max.      | 3.18 (0.660)¹ | -0.74 (0.557)¹ |
|                  | RMS       | 0.88       | 0.19      |

¹ Number in parentheses stands for normalized power.

Fig. 3  Comparison of power distribution between PEACH-MOC and STELLA SP₃.

Fig. 4  Layout of the 2D C5G7-MOX homogenized pin problem.

Fig. 5  Pin power error (%) distribution of STELLA diffusion calculation module.

Fig. 6  Pin power error (%) distribution of STELLA SP₃ calculation module.
Table 4 gives the results of the 2D C5G7-MOX benchmarks k-effective calculation. The results show k-effective difference and performance comparison. We can see that the STELLA P₁ model k-effective error is 290 pcm and the STELLA SP₃ model is 155 pcm. We also find that CMFD can significantly accelerate the convergence rate and greatly reduce the computation time without affecting the calculation results. Table 5 shows the power distribution difference comparison between STELLA P₁ and SP₃. For the assembly power error and fuel pin power error, the result of STELLA SP₃ is more accurate compared with P₁, with maximum error in assembly power of -0.06% and RMS error in pin power of 0.19%.

Fig. 5 shows pin power error distribution of STELLA P₁ module compared with reference. Fig. 6 gives pin power error distribution of STELLA SP₃ module. The results of these two figures show that the diffusion model has a large error at the interface of fuel-reflector and UO₂-MOX fuel cell, and the SP₃ model can obtain perfect results, which shows that the SP₃ model is better than the diffusion model in accuracy.

4. Conclusions

In this paper, we report the development and verification of the SP₃ code, STELLA, at SNERDI. We use SANM with CMFD acceleration to solve the diffusion-like SP₃ equations. Numerical results of several benchmarks demonstrate that STELLA SP₃ module is accurate at pin-by-pin level, compared to diffusion model. In the future, we will extend the code for whole core pin-by-pin calculation.

Acknowledgments

The author would like to express his sincere gratitude to Dr. Y. A. Chao for invaluable discussions.

References

[1] Brantley, P. S., and Larsen, E. W. 2000. “The Simplified Approximation.” Nuclear Science and Engineering 134: 1-21.
[2] TATSUMI, M., and YAMAMOTO, A. 2003. “Advanced PWR Core Calculation Based on Multi-group Nodal-transport Method in Three-dimensional Pin-by-Pin Geometry.” Journal of Nuclear Science and Technology 40 (6): 376-87.
[3] Lee, C. H., and Downar, T. J. 2004. “A Hybrid Nodal Diffusion/SP₁ Method Using One-Node Coarse-Mesh finite Difference Formulation.” Nuclear Science and Engineering 146: 176-87.
[4] Beckert, C., and Grundmann, U. 2008. “Development and Verification of a Nodal Approach for Solving the Multigroup SP₃ Equations.” Annals of Nuclear Energy 35: 75-86.
[5] Zimin, V. G., Ninokata, H., and Pogosbekyan, L. R. 1998. “Polynomial and Semi-Analytic Nodal Methods for Nonlinear Iteration Procedure.” Proceedings of the International Conference on the Physics of Nuclear Science and Technology 2: 994-1002.
[6] Lewis, E. E., Smith, M. A., Tsoulfanidis, N., et al. 2001. Benchmark Specification for Deterministic 2-D/3-D MOX Fuel Assembly Transport Calculations without Spatial Homogenisation (C5G7 MOX). OECD/NEA report, NEA/NCS/DOC(2001)4.
[7] Deng, L., Xie, Z. S., and Zhang, J. M. 2000. “A 3-D Multi-group P-3 Monte Carlo Code and Its Benchmarks.” J. Nucl. Sci. Technol. 37: 608-14.
[8] Tang, C. T., and Zhang, S. H. 2009. “Development and Verification of an MOC Code Employing Assembly Modular Ray Tracing and Efficient Acceleration Techniques.” Annals of Nuclear Energy 36: 1013-20.