

Cost-accuracy analysis of a variational nodal 2D/1D approach to pin resolved neutron transport

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Abstract: A two-dimensional/one-dimensional (2D/1D) variational nodal approach is presented for pressurized water reactor (PWR) core calculations without fuel-moderator homogenization. It employs diffusion theory in the axial direction combined with two-dimensional transport in the x-y plane. In the x-y direction, finite element trial functions are applied to explicitly model the pin resolved geometry. On the axial interfaces, piece-wise constant trial functions are used to eliminate the interface homogenization that has been a challenge for method of characteristics (MOC) based 2D/1D approximations, and resolve the lack of convergence as the axial mesh is refined. In this paper, the method is tested with the un-rodged C5G7 benchmark case, and the cost-accuracy trade-offs between different angular treatments are analyzed.

Keyword: variational nodal 2D/1D method; eliminating the interface homogenization

1 Introduction

Nowadays substantial neutronics researches have been carried out to develop methods that require no cross-section homogenization. Among them the 2D/1D approximations based on the method of characteristics (MOC) are most widely used, by coupling planar MOC calculations together with 1D axial approximations. However, in these methods, smearing between fuel and coolant at each axial interface usually occurs, leading to lack of convergence as the axial mesh is refined ^{[1][2]}.

As an alternative approach, in this work a 2D/1D variational nodal method (VNM) without spatial homogenization is formulated and implemented in the PANX (Purdue - Argonne - Northwestern - Xi'an) code. We employ diffusion theory in the axial direction combined with two-dimensional transport in the x-y plane. In the x-y direction, finite element trial functions are applied to explicitly model the pin resolved geometry. On the axial interfaces, piece-wise constant trial functions are used to avoid smearing between the fuel and coolant ^[3].

Based on the even-parity form of the transport equation, three different approaches are employed in the angular treatment. First we implement the standard spherical harmonics method ^[4]. To increase accuracy and reduce computational effort, we present two other refinements: First, the even-parity integral method ^[5] within the nodes reduces the computational effort required to form the response matrices. Second, the application of quasi-reflected interface conditions ^[6] reduces the dimension of the resulting response matrices and therefore the CPU time required to solve the matrix equations. The performances of the methods are compared with the two-dimensional and three-dimensional un-rodged C5G7 benchmark problems ^[7].

2 Theory

We start with the even-parity within-group transport equation suitable for implementing a 2D/1D approximation in a variational nodal form:

$$-\hat{\Omega} \cdot \vec{\nabla}_{\perp} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla}_{\perp} \psi^{+} - \hat{\Omega} \cdot \vec{\nabla}_z \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla}_z \phi + \sigma \psi^{+} = \sigma_s \phi + q \quad (1)$$

where ψ^{+} is the even-parity angular flux. Note that the cross derivatives between axial and radial direc-

tions vanish, and the axial leakage is approximated with diffusion theory. The corresponding variational nodal functional is

$$\begin{aligned}
 F_v[\psi^+, \psi^-] = & \\
 & \int_v dV \left\{ \int d\Omega \left[\sigma^{-1} \left(\hat{\Omega} \cdot \vec{\nabla}_\perp \psi^{+2} \right) + \sigma \psi^{+2} \right] \right. \\
 & \left. + D \left(\nabla_z \phi \right)^2 - \sigma_s \phi^2 - 2\phi q \right\} \\
 & + 2 \int_v d\Gamma \int d\Omega \hat{n} \cdot \hat{\Omega} \psi^+ \psi^-
 \end{aligned} \quad (2)$$

where ψ^- is the odd-parity flux along the surface Γ of the node volume V .

To discretize Eq. (2) in a form suitable for PWR computations, special treatments must be made in both spatial and angular variables.

For the spatial approximation, trial functions that are finite element trial functions in x-y and orthogonal polynomials in z within the node are applied. Meanwhile, orthogonal polynomials are used on the lateral interfaces; piecewise constant zones, each corresponding to a finite element, are employed on the axial interfaces. The axial treatment avoids smearing between fuel and coolant regions at the interfaces and guarantees convergence as the axial meshes are refined.

For the angular approximation, three different approaches are employed, which are labeled as below:

- a) In PANX, angular discretization is carried out in the same way as that used in conventional VNM. Even-parity spherical harmonics are adopted within the nodes and the corresponding odd-parity moments are used at the interfaces. In this case, as high order spherical harmonics are employed, CPU times and memory requirements become excessive both in forming the response matrices and in solving the matrix equations.
- b) In PANX-I, the spherical harmonics expansion within the node is substituted by an even-parity integral method^[5], while the spherical harmonics expansion is retained on the x-y interfaces. With this treatment, both the CPU time and memory required to form the response matrices can be greatly reduced. However, the retention of high order spherical harmonics on the interfaces still cause the dimensions of the response matrices to

be large. As a result, the solution time grows rapidly with the P_N order.

- c) In PANX-IQ_m, the integral treatment is preserved within the node, but the high-order P_N interface conditions are reduced by applying reflected interface conditions to eliminate the high order moments, while retaining lower order moments through up to P_m ^[6].

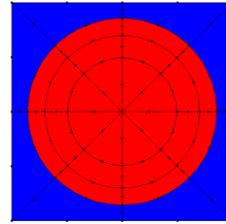


Fig. 1 Quadratic finite element grid for a C5G7 fuel pin cell.

3 Results

3.1 C5G7 Two-dimensional results

In order to examine the order of angular approximation needed to obtain accurate results in the x-y plane, we first tested against the 2D C5G7 benchmark. For each of the pin cells in the four fuel assemblies, the x-y even-parity flux is approximated by 32 quadratic finite elements as shown in Fig. 1. The calculations were performed without parallelization on an Intel Xeon X7560 CPU. The Monte Carlo 2D reference at a 98% confidence interval is $k = 1.18655 \pm 0.00006$. The three different angular treatments illustrated in chapter 2 are compared. Particularly, in the PANX-IQ_m calculations, m value of 1, 3, 5 are adopted to see the impact of increasing the low order moments.

The eigenvalue comparisons for the 2D C5G7 benchmark is shown in Fig. 2. First, with all three approaches, clear convergences toward the reference can be seen by increasing the P_N interface order. Meanwhile, with PANX calculation, the applicable P_N order is strongly limited to achieve adequate accuracy. Second, the integral method seems more accurate than using a P_N expansion within the node because very high order cubature can cheaply be applied to evaluate the angular integrals. Third, in PANX-IQ_m calculations, $m = 1, 3, 5$ come progressively closer to converging to the PANX-I as well as the Monte Carlo reference result as P_N is increased to P_{23} .

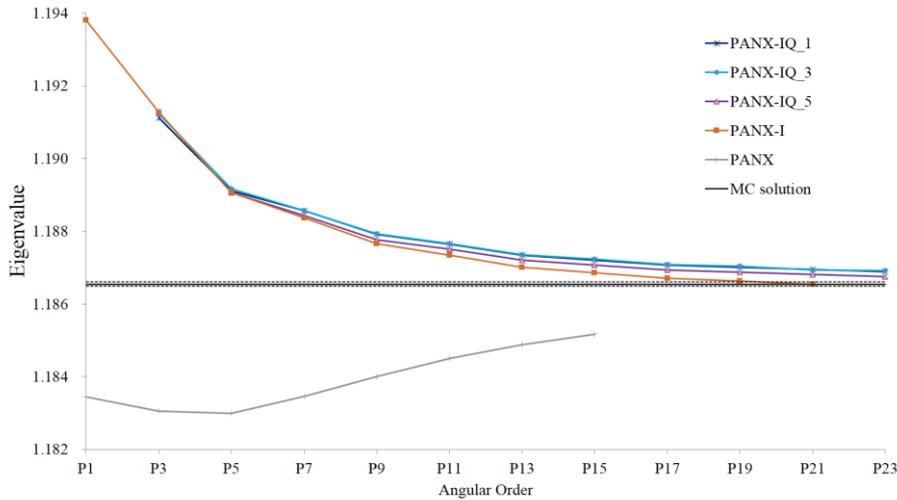


Fig. 2 Eigenvalue vs. P_N approximation for the 2D C5G7 benchmark.

Table 1 lists the eigenvalue accuracy and computational costs of PANX-IQ_1, PANX-IQ_3, PANX-IQ_5 and PANX-I by the P_{21} interface approximation. Table 2 tabulates the percentage pin power error comparisons. It includes the error of the maximum power pin (Max pin), the maximum pin power error (MAX), the average pin power error (AVG) and the root-mean-square error (RMS). Obviously, PANX-I obtains the best accuracy in eigenvalue and pin power distribution as it incorporates the full P_{21} interface approximation. Meanwhile, the PANX-IQ_1 interface condition presents similar eigenvalue accuracy as PANX-IQ_3; however as is shown in Table 2, this advantage does not carry over to the pin power distributions. On the other hand, it is noted that PANX-IQ_3 achieves 60% less computational time and 90% less memory compared to PANX-I, with only negligible loss of accuracy (21 pcm in eigenvalue and 0.04% in RMS pin power). Therefore, for the 2D/1D calculations of the three-dimensional problem, we choose the accuracy of P_{23} and $m = 3$ to be adequate.

Table 1. The eigenvalue errors and computational costs of the 2D C5G7 benchmark by different interface approximations with P_{21}

	Eigenvalue Error-pcm	Total time-h	Storage-MB
PANX-IQ_1	25	0.67	51
PANX-IQ_3	21	0.68	68
PANX-IQ_5	10	0.66	94

It is also noticed in Table 2 that the maximum pin power error with PANX-IQ_m or PANX-I calculations are not as good as the Monte Carlo solution. However, this discrepancy is seen as insignificant. As is illustrated in Fig. 3, the maximum pin power error always occurs at the outer core regions, where the absolute value of pin power is much lower than the core averaged level.

Table 2. The percentage pin power error comparisons of the 2D C5G7 benchmark by different interface approximations with P_{21}

	Max pin	Max	AVG	RMS
Monte Carlo	0.07	0.19	0.14	0.14
PANX-IQ_1	-1.16	3.02	0.72	0.97
PANX-IQ_3	-0.31	0.90	0.23	0.28
PANX-IQ_5	-0.26	0.84	0.21	0.26
PANX-I	-0.26	0.80	0.20	0.24

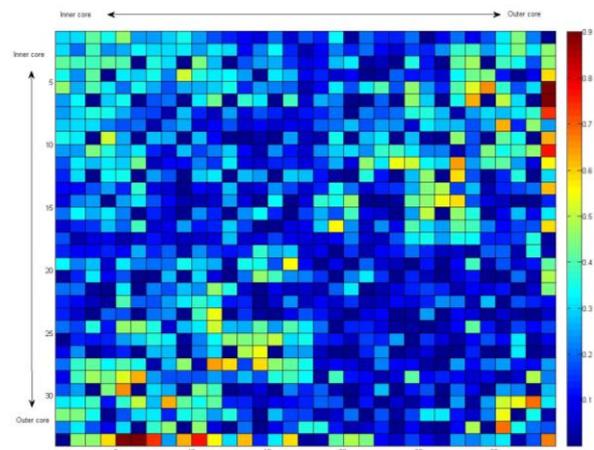


Fig. 3 Pin power error distribution of the 2D C5G7 benchmark by the PANX-IQ_3 calculation.

3.2 C5G7 three-dimensional results

For the 3D C5G7 problem, the domain is divided into 9 axial nodes, with the axial flux distribution within each node represented by a quadratic polynomial. The radial interfaces are approximated with quadratic polynomials and the axial interfaces by 32 piecewise constants.

Table 3. Pin Power comparisons for 3D un-rodged C5G7 Benchmark

		Max Pin-%	Max-%	RMS-%
PANX	P ₁₁	0.12	1.20	0.28
PANX-I	P ₁₅	-0.55	1.12	0.43
PANX-IQ_3	P ₂₃	-0.44	1.00	0.35

The eigenvalue comparisons for the 3D C5G7 un-rodged case are shown in Fig. 4. The Monte Carlo 3D reference is $k = 1.14308 \pm 0.00006$ at 98% confidence interval. Similar to the 2D results, asymptotic convergence can be observed by increasing the P_N angular order with all three different angular treatments. For three-dimensional problems, one may expect some under-estimation from the Monte Carlo reference since the use of diffusion theory in the axial direction is overestimating the axial leakage. Therefore, the eigenvalues keep reducing with increasing the P_N order, and finally achieve the asymptotic convergence when N=23. The PANX-IQ_3 with P₂₃ underestimated the Monte Carlo result by 81 pcm. The

pin power results with the highest applicable P_N order for the three sets of calculations are tabulated in Table 3. PANX-IQ_3 calculation with P₂₃ has a maximum error of 1.00%.

It is illustrated in Fig. 4 that PANX calculations with higher than P₁₁ and PANX-I calculations with higher than P₁₅ are impractical due to the prohibitive computational costs. However, with PANX-IQ_3, we are able to achieve the final asymptotic convergence with an angular order of P₂₃. Figure 5 shows the CPU time comparisons between the three different angular treatments with angular orders up to P₁₁. It can be observed that for PANX and PANX-I, the CPU time increases dramatically as the P_N order at the pin cell lateral boundaries increases. In contrast, the PANX-IQ_3 calculation time remains nearly flat as the P_N order goes up, requiring substantially less solution time because the dimension of the the response matrices are preserved as those of P₃.

The computational time for PANX-IQ_3 with P₂₃ with-in node approximation required only 3.90 hr, with 1.9 hr required for response matrix formation and 2.00 hr for solution. To further reduce the CPU time, we have also implemented a modified form of partitioned matrix acceleration, which reduces the solution time to 0.18 hr. Thus the total time is 2.08 hr.

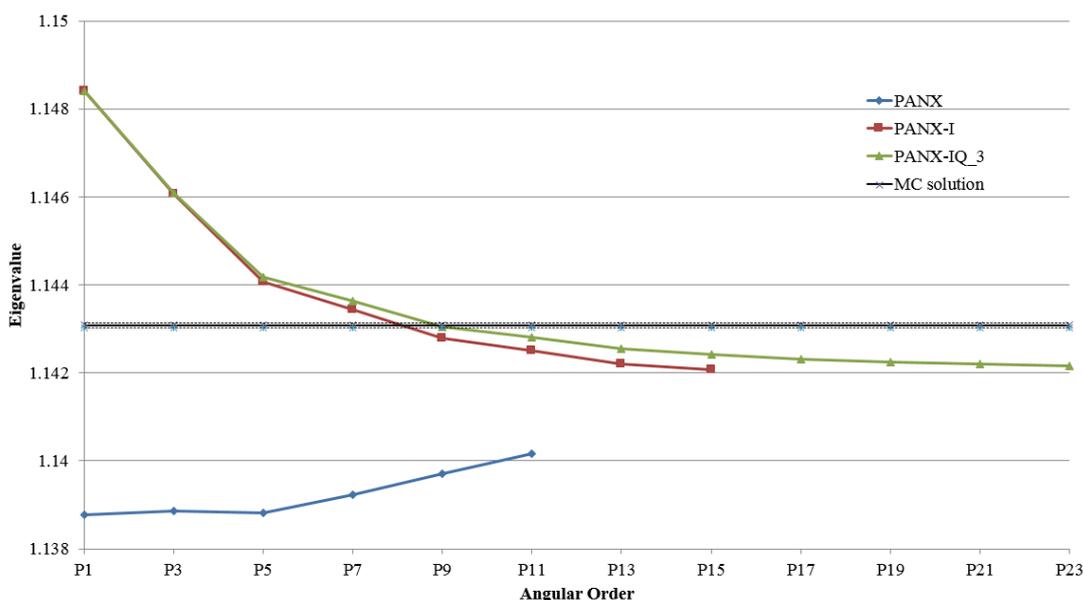


Fig. 4 Eigenvalue pcm Error vs. P_N Order for the 3D un-rodged C5G7 benchmark.

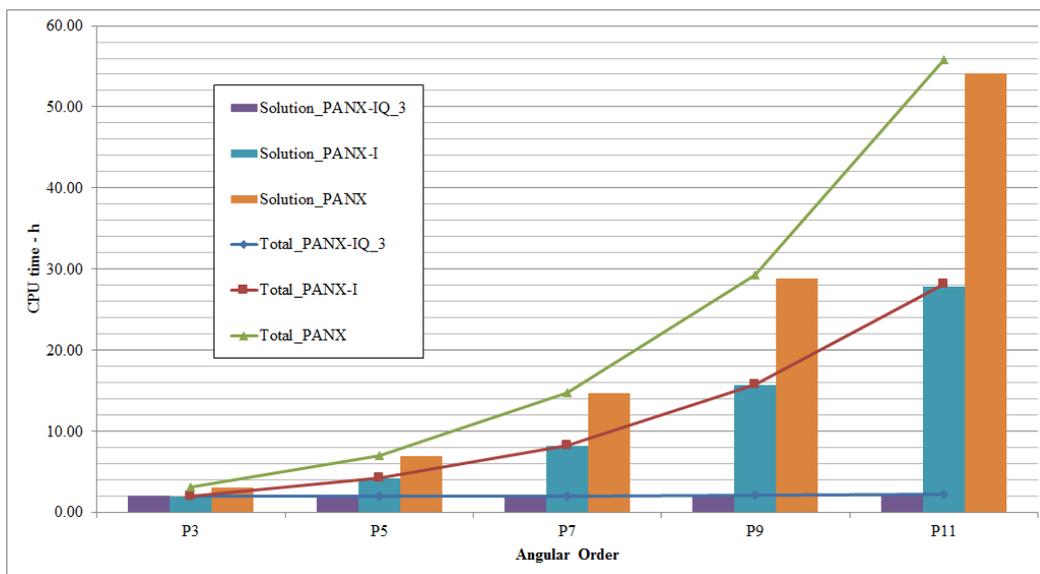


Fig. 5 The CPU time comparisons for the 3D un-rodged C5G7 benchmark.

4 Future work

Efforts to increase accuracy are being focused on implementing a P_N axial approximation to improve upon the present P_1 approximation. Efforts will also be undertaken to reduce the CPU time required to form the response matrices. Acceleration of the fission source iteration will also be considered.

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