Trivac: A Modular Diffusion Code for Fuel Management and Design Applications

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Abstract

A new three-dimensional neutron diffusion code named TRIVAC was set up using advanced discretization algorithms and improved iteration strategies. The two variable order discretization algorithms used in TRIVAC will be presented. These are based, respectively, on the variational and nodal collocation techniques. These algorithms will be shown to produce reconstructible solutions which are upper and lower limits of the exact solution. The eigenvalue matrix system is solved using an ADI preconditioning of the power method in conjunction with a symmetric variational acceleration technique. Validation results are reported for the IAEA two- and three-dimensional benchmarks, and for a two-dimensional PWR.

Résumé

Un nouveau logiciel tridimensionnel de diffusion neutronique a été conçu en utilisant des algorithmes de discrétisation modernes et des stratégies itératives améliorées. Nous allons présenter les deux algorithmes de discrétisation d'ordre variable utilisées par TRIVAC. Celles-ci sont basées respectivement sur les techniques de collocation variationnelle et nodale. Nous allons montrer que ces algorithmes produisent des solutions interpolables et qui correspondent à des limites supérieure et inférieure de la solution exacte. Le système matriciel aux valeurs propres est résolu à l'aide d'un préconditionnement ADI de la méthode des puissances, en conjonction avec une technique d'accélération variationnelle symétrique. Des résultats de validation sont rapportés pour les cas tests IAEA à deux et trois dimensions ainsi que pour une représentation bidimensionnelle d'un PWR.

Introduction

The primary goal of a discretization algorithm is to transform the differential operators of the diffusion equation into real number matrices adapted to an efficient numerical solution. A review of most common algorithms is presented in reference 1. This list should be updated by appending the variational and nodal discretization techniques presented in this paper [2, 3].

There is no such thing as an 'ideal' discretization algorithm and any choice is the result of a compromise. Some techniques, such as the analytical nodal method (ANM), are very efficient to compute a power map defined over coarse elements, but they lack a straightforward reconstruction technique for the solution [4]. Other algorithms, like the classical finite element approximations, are handicapped by difficulties such as their incompatibility with an ADI preconditioning.

The variational and nodal collocation techniques used in TRIVAC appear to include most desirable properties in spite of the fact that they cannot compete with the efficiency of nodal schemes based on the quadratic leakage approximation. Let us mention the four most interesting properties of the collocation techniques:

1. The numerical solution is reconstructible over each element of the domain. The polynomial nature of the solution greatly simplifies the integration of TRIVAC in applications using the generalized perturbation theory or the quasistatic algorithm of space-time kinetics.
2. The discretization order is variable, being a function of the degree of the polynomials used to represent the neutron flux over each element. High order polynomials (cubic or quartic) are used to model PWR while linear polynomials are used for CANDU reactors. In fact, the linear variational and nodal collocation techniques are respectively equivalent to mesh-corner and mesh-centered finite difference approximations.
3. Collocation techniques are compatible with an ADI preconditioning of the power method [5].
4. Matrices produced as a result of the discretization are real and independent of the eigenvalue. Matrices corresponding to the leakage terms are symmetric, positive definite, and diagonally dominant. Other matrices are diagonal.

The two types of collocation techniques available in TRIVAC will now be presented.

Keywords: reactor physics, diffusion equation, collocation techniques, finite elements, nodal methods.

Definition of the Polynomial Basis

Both variational and nodal collocation techniques rely on a polynomial representation of trial functions. A weighted residual approach is used to find the approximate solution of the diffusion equation over the reactor domain. There is an important distinction in the way the weighted residual formalism is applied to each type of collocation technique, and this distinction affects the choice of the polynomial basis. The variational collocation technique is based on a finite element formalism where the residue, defined over the entire domain, is orthogonal to the entire set of trial functions. In addition, the interface conditions are treated as natural conditions. With the nodal collocation technique, however, the residues are cancelled element by element and the interface conditions are taken into account *a posteriori*. Consequently, the variational collocation technique is constrained to use a polynomial basis with continuous trial functions over the element boundaries. More flexibility is left to the nodal collocation basis, which permits piecewise continuous polynomials to be used.

We will now present the collocation techniques in the case of a one-speed formalism. Changing over to the multigroup formalism presents no additional difficulty. Moreover, we will limit this study to three dimensional Cartesian domains composed of an assembly of homogeneous parallelepipeds. Under these conditions, the neutron diffusion equation is written

$$-\frac{\partial}{\partial x}D_x(x,y,z)\frac{\partial\phi}{\partial x}-\frac{\partial}{\partial y}D_y(x,y,z)\frac{\partial\phi}{\partial y}-\frac{\partial}{\partial z}D_z(x,y,z)\frac{\partial\phi}{\partial z}+\Sigma_r(x,y,z)\,\phi(x,y,z)=S(x,y,z), \quad (1)$$

with $\phi(x, y, z)$ continuous everywhere in the domain. Currents $-D_x(x, y, z)\,\partial\phi/\partial x$, $-D_y(x, y, z)\,\partial\phi/\partial y$ and $-D_z(x, y, z)\,\partial\phi/\partial z$ are almost continuous, but may present localized discontinuities over lines of singularity [1]. The boundary conditions are either zero flux ($\phi(x, y, z) = 0$) or positive albedo:

$$D_x(x,y,z)\frac{\partial\phi}{\partial x}\pm\frac{1}{2}\frac{1-\beta(x,y,z)}{1+\beta(x,y,z)}\phi(x,y,z)=0; \quad (2a)$$

$$D_y(x,y,z)\frac{\partial\phi}{\partial y}\pm\frac{1}{2}\frac{1-\beta(x,y,z)}{1+\beta(x,y,z)}\phi(x,y,z)=0; \quad (2b)$$

$$D_z(x,y,z)\frac{\partial\phi}{\partial z}\pm\frac{1}{2}\frac{1-\beta(x,y,z)}{1+\beta(x,y,z)}\phi(x,y,z)=0; \quad (2c)$$

where the "−" or "+" sign is used, depending on whether the boundary is to the left of or to the right of the domain in relation to the direction of each axis.

We will now assume that the nuclear properties are uniform over each parallelepiped composing the domain. These parallelepipeds will then be used to support one or more elements. We will designate the value of each nuclear property over element e by D_{xe}, D_{ye}, D_{ze}, and Σ_{re}.

Before introducing the trial functions defined over element e, we will transform Cartesian coordinates (x, y, z) of the element into local coordinates (u, v, w) corresponding to a unitary cube of reference. The Cartesian coordinates are described in Figure 1.

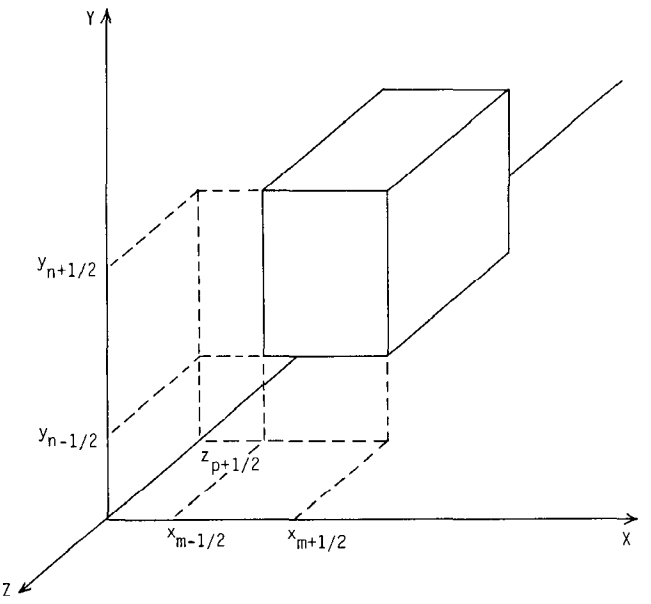

Figure 1: Discretization of a Cartesian domain.

The following variable transformations will be used:

$$u=\frac{1}{\Delta x_e}\left[x-\tfrac{1}{2}(x_{m-\frac{1}{2}}+x_{m+\frac{1}{2}})\right]$$

$$v=\frac{1}{\Delta y_e}\left[y-\tfrac{1}{2}(y_{n-\frac{1}{2}}+y_{n+\frac{1}{2}})\right]$$

$$w=\frac{1}{\Delta z_e}\left[z-\tfrac{1}{2}(z_{p-\frac{1}{2}}+z_{p+\frac{1}{2}})\right], \quad (3)$$

with

$$\Delta x_e = x_{m+\frac{1}{2}}-x_{m-\frac{1}{2}}$$

$$\Delta y_e = y_{n+\frac{1}{2}}-y_{n-\frac{1}{2}}$$

$$\Delta z_e = z_{p+\frac{1}{2}}-z_{p-\frac{1}{2}}. \quad (4)$$

Over each element we will assume a tensorial expansion of solution $\phi(x, y, z)$ and of source term $S(x, y, z)$ with the help of low order polynomials, which are denoted $\{P_k(u); k = 0, K\}$. In cases where point (x, y, z) belongs to element V_e, these two expansions take the form

$$\phi(x,y,z)=\phi_e(u,v,w)=\sum_{k_1=0}^{K}\sum_{k_2=0}^{K}\sum_{k_3=0}^{K}\Phi_e^{k_1,k_2,k_3}P_{k_1}(u)P_{k_2}(v)P_{k_3}(w) \quad (5a)$$

and

$$S(x,y,z)=S_e(u,v,w)=\sum_{k_1=0}^{K}\sum_{k_2=0}^{K}\sum_{k_3=0}^{K}S_e^{k_1,k_2,k_3}P_{k_1}(u)P_{k_2}(v)P_{k_3}(w) \quad (5b)$$

The Variational Collocation Method

The classical formalism of the finite element method involves the analytical integration of the terms composing the mass and stiffness matrices. The integrations are trivial insofar as the trial functions are simple polynomials. The mass matrix thus obtained is non-diagonal, which makes the classical approximations incompatible with the ADI preconditioning.

The variational collocation method corresponds to the approximations of the finite element method when the mass and stiffness matrices are numerically integrated in order to diagonalize the mass matrix [2]. This is made possible by expanding the solution in terms of Lagrangian polynomials, whose collocation points are identical to the base points of a Lobatto's quadrature formula. This type of quadrature makes possible the exact integration of the stiffness matrix, which is a necessary condition to ensure the convergence of the variational collocation method. Finally, we note that the linear variational collocation method is identical to the mesh corner finite difference method.

We have already tested the variational collocation method based on linear, quadratic, cubic, and quartic polynomials defined over two- and three-dimensional domains [5]. These approximations use the following trial polynomials:

1. Linear Lagrangian polynomials (K = 1)
   In this case, the collocation points are chosen at abcissa $u_0 = -1/2$ and $u_1 = 1/2$ in local coordinates. The trial polynomials are therefore given as:

$$P_0(u) = -u + \tfrac{1}{2} \tag{6a}$$

   and

$$P_1(u) = u + \tfrac{1}{2}. \tag{6b}$$

2. Quadratic Lagrangian polynomials (K = 2)
   The collocation points are now chosen at abscissa $u_0 = -1/2$, $u_1 = 0$ and $u_2 = 1/2$. The corresponding trial polynomials are

$$P_0(u) = 2u^2 - u, \tag{7a}$$

$$P_1(u) = -4u^2 + 1, \tag{7b}$$

   and

$$P_2(u) = 2u^2 + u. \tag{7c}$$

3. Cubic Lagrangian polynomials (K = 3)
   The collocation points are now chosen at abscissa $u_0 = -1/2$, $u_1 = -1/(2\sqrt{5})$, $u_2 = 1/(2\sqrt{5})$ and $u_3 = 1/2$. Note that the position of points u_1 and u_2 is imposed by the requirement that the set $(u_k;\ k = 0, K)$ correspond to the base points of a Lobatto's quadrature formula. The corresponding trial polynomials are

$$P_0(u) = -5u^3 + \tfrac{5}{2}u^2 + \tfrac{1}{4}u - \tfrac{1}{8}, \tag{8a}$$

$$P_1(u) = 5\sqrt{5}\,u^3 - \tfrac{5}{2}u^2 - \frac{5\sqrt{5}}{4}u + \tfrac{5}{8}, \tag{8b}$$

$$P_2(u) = -5\sqrt{5}\,u^3 - \tfrac{5}{2}u^2 + \frac{5\sqrt{5}}{4}u + \tfrac{5}{8} \tag{8c}$$

   and

$$P_3(u) = 5u^3 + \tfrac{5}{2}u^2 - \tfrac{1}{4}u - \tfrac{1}{8}. \tag{8d}$$

4. Quartic Lagrangian polynomials (K = 4)
   The collocation points are now chosen at abscissa $u_0 = -1/2$, $u_1 = -\sqrt{3/28}$, $u_2 = 0$, $u_3 = \sqrt{3/28}$ and $u_4 = 1/2$. The corresponding trial polynomials are

$$P_0(u) = 14u^4 - 7u^3 - \tfrac{3}{2}u^2 + \tfrac{3}{4}u, \tag{9a}$$

$$P_1(u) = 49\left\{-\frac{2}{3}u^4 + \frac{1}{\sqrt{21}}u^3 + \frac{1}{6}u^2 - \frac{1}{4\sqrt{21}}u\right\}, \tag{9b}$$

$$P_2(u) = \frac{112}{3}u^4 - \frac{40}{3}u^2 + 1, \tag{9c}$$

$$P_3(u) = 49\left\{-\frac{2}{3}u^4 - \frac{1}{\sqrt{21}}u^3 + \frac{1}{6}u^2 + \frac{1}{4\sqrt{21}}u\right\}, \tag{9d}$$

   and

$$P_4(u) = 14u^4 + 7u^3 - \tfrac{3}{2}u^2 - \tfrac{3}{4}u. \tag{9e}$$

Once the polynomial basis has been defined, the variational collocation method proceeds as any finite element formalism. However, all the linear or bilinear products involving the trial functions should be carried out using a Lobatto's quadrature formula in order to diagonalize the mass matrix.

The Nodal Collocation Method

We have developed a second family of collocation techniques using a nodal formalism. These techniques assume an expansion in Legendre polynomials of the neutron flux over each element, without imposing a C_0 continuity on the interfaces. The absence of a C_0 continuity precludes the use of a variational formulation based on the classical functional of the finite element method [1]. We will show that a nodal formalism makes it possible to bypass this restriction, while satisfying the four conditions previously stated and without having to resort to a numerical integration of the kind used in the variational collocation method.

The nodal collocation method has two features which distinguish it from other polynomial nodal approaches [6]. First, the nodal collocation method does not require the quadratic transverse leakage approximation to generalize in two or three dimensions. Instead, it uses a tensorial expansion of Legendre polynomials, which introduces no further approximation to the one-dimensional case. Second, we will show that the linear nodal collocation method is identical to the mesh centered finite difference method. Until now, only the analytical nodal method (ANM) appeared to be linked to this type of finite difference [4].

The Legendre polynomials used in the nodal collocation method differ somewhat from their classical definition because of the following two constraints:

1. Polynomials $P_k(u)$ must be defined over the interval $(-1/2, 1/2)$ to ensure that the reference cube has a unitary volume.

2. Polynomials $P_k(u)$ must be mutually orthonormal over the reference interval; that is,

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} du\, P_k(u)\, P_l(u) = \delta_{kl} \tag{10}$$

where δ_{kl} is the Kronecker delta function.

We will therefore use the following Legendre polynomials:

$$P_0(u) = 1, \tag{11a}$$

$$P_1(u) = 2\sqrt{3}\,u, \tag{11b}$$

$$P_2(u) = \frac{\sqrt{5}}{2}(12\,u^2 - 1), \tag{11c}$$

and, in general:

$$P_{k+1}(u) = 2\sqrt{\frac{2k+3}{2k+1}}\frac{2k+1}{k+1}\,u\,P_k(u) - \sqrt{\frac{2k+3}{2k-1}}\frac{k}{k+1}P_{k-1}(u), \tag{11d}$$

if $k \geqq 1$.

A weighted residual approach is then applied to these trial functions in order to transform equation (1) into a constant matrix system. The algebra involved with the nodal collocation method is tedious and will be omitted here. A complete description of the method can be found in reference 3.

Matrix Storage Schemes and Resolution Techniques

With a two-group energy formalism, the variational or nodal collocation method is applied group by group to generate the following matrix system:

$$\mathbf{A}_{gg}\vec{\phi}_g = \vec{S}_g \tag{12}$$

with

$$\vec{S}_1 = \frac{1}{K_{eff}}\{\mathbf{B}_{11}\vec{\phi}_1 + \mathbf{B}_{12}\vec{\phi}_2\} \tag{13a}$$

and

$$\vec{S}_2 = \mathbf{A}_{21}\vec{\phi}_1. \tag{13b}$$

Groupwise values of the neutron flux are therefore represented by the polynomial coefficients associated to all the elements. The solution of the overall eigenvalue problem can be found using the preconditioning power method as presented in the reference 5. TRIVAC also offers the possibility to solve a fixed-source eigenvalue problem, which is useful in applications involving the generalized perturbation theory [7, 8, 9] and the improved quasistatic approach in space-time kinetics.

Convergence of the preconditioned power method is very slow in cases where the solution corresponds to a flattened neutron flux. This difficulty was resolved in TRIVAC using the symmetric variational acceleration technique (SVAT), as pointed out in reference 10. This approach offers some similarities with a conjugate gradient technique applied to the eigenvalue problem.

The preconditioning matrix used in TRIVAC is equivalent to an ADI splitting of the matrices $\mathbf{A}_{gg}$. This approach will be effective only insofar as the matrices $\mathbf{A}_{gg}$ may be split according to the equation

$$\mathbf{A}_{gg} = \mathbf{U}_{gg} + \mathbf{X}_{gg} + \mathbf{P}_y\mathbf{Y}_{gg}\mathbf{P}_y^T + \mathbf{P}_z\mathbf{Z}_{gg}\mathbf{P}_z^T, \tag{14}$$

where $\mathbf{U}_{gg}$ = matrix containing the diagonal elements of $\mathbf{A}_{gg}$; $\mathbf{X}_{gg}$, $\mathbf{Y}_{gg}$, $\mathbf{Z}_{gg}$ = symmetrical matrices containing the non-diagonal elements of $\mathbf{A}_{gg}$ corresponding to x, y, and z couplings, respectively; $\mathbf{P}_y$, $\mathbf{P}_z$ = permutation matrices which ensure a minimum band width for matrices $\mathbf{Y}_{gg}$ and $\mathbf{Z}_{gg}$.

This type of splitting capitalizes on the possibility of numbering the unknowns in such a way that matrices $\mathbf{X}_{gg}$, $\mathbf{Y}_{gg}$, and $\mathbf{Z}_{gg}$ appear with a diagonal banded structure. An important characteristic of the variational and nodal collocation methods allows a maximum band width, respectively equal to K + 1 and 2K for a given order of discretization.

Numerical Results

The variational and nodal collocation methods were programmed and included in the TRIVAC computer code. The two kinds of discretization share the same computer environment and use the same numerical analysis techniques for the solution of matrix systems.

The TRIVAC computer code is written in FORTRAN-77 and compiled by FORTRAN-VS (IBM) at level two optimization. All vectors and matrices are declared in single-precision (1 word = 32 bits) and are dynamically allocated by a subroutine written in assembler. Certain accumulators assigned to bilinear product calculations are declared in double-precision, in order to minimize round-off error. Numerical tests were carried out on an IBM-4381 (group two) computer and are therefore typical of a scalar computer.

It is useful to mention the main numerical techniques and the calculation options used in this study:

1. The neutron diffusion equation (1) is discretized using the variational or nodal collocation method. The order K of discretization is equal to three (cubic polynomials) or four (quartic polynomials). In all cases, the reactor radial plane is partitioned using one and only one element per assembly.
2. The fundamental solution of the eigenvalue system (12) and (13) is obtained by the preconditioned power method, with a two-parameter variational acceleration [5, 10].
3. A preconditioning is applied by carrying out one or two ADI iterations per outer iteration of the power method [5].
4. The power method is initialized by a uniform estimate of the solution ($\phi_i = 1.0$). The iterations are interrupted when the following convergence criterion is satisfied:

$$\frac{\max_i |\phi_i^{(k-1)} - \Phi_i^{(k)}|}{\max_i |\phi_i^{(k)}|} \leq 10^{-4}, \tag{15}$$

Table 1: IAEA-2D Benchmark Calculations

	Polynomial order	*Bandwidth*	K^a_{tot}	K^b_{eff}	ϵ_{max} (%)	$\bar{\epsilon}$ (%)	*CPU time (s)*	*Outer iterations*	*Inner / outer*
Variational collocation	3[c]	4	568	1.029786	5.8	2.2	4.8	51	1
	3	4	568	1.029785	5.8	2.2	6.4	39	2
	4	5	1033	1.029596	0.93	0.34	15.9	87	1
	4	5	1033	1.029592	0.93	0.34	14.3	45	2
Nodal collocation	3[d]	6	621	1.029370	4.9	1.8	4.8	39	1
	3	6	621	1.029374	5.0	1.8	7.1	33	2
	4	8	1104	1.029590	0.78	0.26	15.1	63	1
	4	8	1104	1.029582	0.77	0.26	16.7	39	2

[a]The number of unknowns per energy group.
[b]The reference solution was obtained by a nodal analytic calculation with a mesh of 34 × 34. The corresponding effective multiplication factor is K_{eff} = 1.029585.
[c]See Figure 2 for an illustration of thermal flux distribution.
[d]See Figure 3 for an illustration of thermal flux distribution.

Table 2: Tihange Test Problem Calculations

	Polynomial order	*Bandwidth*	K_{tot}	K^a_{eff}	ϵ_{max} (%)	$\bar{\epsilon}$ (%)	*CPU time (s)*	*Outer iterations*	*Inner / outer*
Variational collocation	3	4	1888	1.000312	4.2	1.9	18.8	45	1
	3	4	1888	1.000312	4.3	1.9	24.7	33	2
	4	5	3401	1.000707	1.1	0.45	55.6	69	1
	4	5	3401	1.000704	1.1	0.46	57.9	39	2
Nodal collocation	3	6	1989	1.001300	4.1	1.7	35.4	63	1
	3	6	1989	1.001303	4.1	1.7	52.2	51	2
	4	8	3536	1.000971	1.1	0.43	128.1	111	1
	4	8	3536	1.000961	1.1	0.43	162.9	75	2

[a]The reference solution was obtained by a nodal analytic calculation with a mesh of 51 × 51. The corresponding effective multiplication factor is K_{eff} = 1.000823.

Table 3: IAEA-3D[a] Benchmark Calculations

	Polynomial order	*Bandwidth*	K_{tot}	K^b_{eff}	ϵ_{max} (%)	$\bar{\epsilon}$ (%)	*CPU time (s)*	*Outer iterations*	*Inner / outer*
Variational collocation	3	4	9088	1.029313	6.8	2.3	240.8	87	1
	3	4	9088	1.029315	6.8	2.3	258.2	51	2
	4	5	21693	1.029117	1.2	0.36	1012.0	141	1
	4	5	21693	1.029113	1.2	0.36	1128.0	87	2
Nodal collocation	3	6	9315	1.028810	5.3	2.0	223.9	75	1
	3	6	9315	1.028812	5.2	2.0	247.3	45	2
	4	8	22080	1.029045	0.97	0.34	815.5	99	1
	4	8	22080	1.029037	0.97	0.34	1144.0	75	2

[a]All TRIVAC calculations are based on a mesh of 9 × 9 × 5 with axial mesh lines at 0., 20., 150., 280., 360. and 380. cm.
[b]The reference solution was obtained by a nodal analytic calculation with a mesh 26 × 26 × 18. The corresponding effective multiplication factor is K_{eff} = 1.029060.

where $\phi_i^{(k)}$ is the i-th flux component after k iterations. This criterion makes possible a convergence precision better than 0.05% over the zonal powers.

5. The solutions thus obtained are compared to the reference calculations carried out with the analytic nodal method [4]. The maximum and average errors over zonal powers ϵ_{max} and $\bar{\epsilon}$ are calculated as in reference 1.

Tables 1 to 3 give the numerical results for three specific cases: the two-dimensional (2D) and three-dimensional (3D) IAEA benchmarks [11] and the two-dimensional Tihange test problem, which represents a complete configuration of a pressurized water reactor (PWR) at the beginning of the second cycle [12].

The overall numerical results reveal two interesting

Table 4: Bounding Effect of Zonal Powers[a]

e	*Variational collocation (%)*	*Nodal collocation (%)*
1	−0.09	0.12
2	−0.51	0.30
3	−0.36	0.25
4	−0.42	0.34
5	0.14	−0.05
6	−0.14	0.16
7	0.18	−0.09
8	0.56	−0.42
9	−0.39	0.25
10	−0.34	0.23
11	−0.30	0.23
12	−0.30	0.21
13	−0.02	0.05
14	0.21	0.14
15	0.57	−0.46
16	−0.29	0.22
17	−0.24	0.19
18	−0.13	0.14
19	0.05	−0.01
20	0.23	−0.17
21	0.93	−0.77
22	−0.21	0.18
23	−0.19	0.21
24	0.11	−0.07
25	0.61	−0.48
26	0.37	−0.32
27	0.06	−0.04
28	0.89	−0.77
29	0.91	−0.77

[a]IAEA-2D benchmark calculations discretized by a quartic collocation method.

features, which are clearly seen in Table 4 for a specific case:

1. For a given order of discretization, the variational and nodal collocation methods offer similar accuracy.
2. The reference solution, obtained through the analytic nodal method, is bounded by the variational and nodal collocation solutions, respectively. This bounding effect is observed for the eigenvalue and for most zonal powers.

It is worth mentioning that the band width of matrices $\mathbf{X}_{gg}$, $\mathbf{Y}_{gg}$, and $\mathbf{Z}_{gg}$ is equal to K + 1 with the variational collocation method, while it is equal to 2K with the nodal collocation method. This feature tends to penalize the nodal collocation method in terms of calculation efficiency and memory utilization.

It is not possible to conclude that one discretization method is numerically more stable than the other. The variational collocation method is more stable for solving the Tihange test problem while the nodal collocation method seems to be preferable for the IAEA benchmarks.

Figures 2 and 3 illustrate the thermal flux distributions obtained for the IAEA-2D benchmark when a third order discretization is used. The distribution corresponding to the variational collocation method

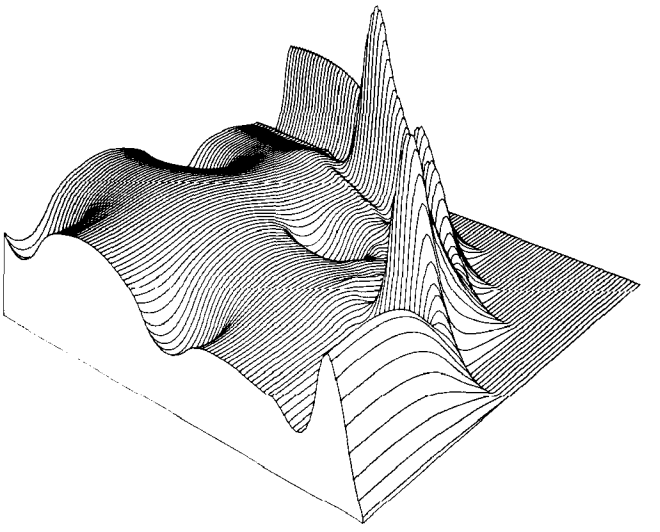

Figure 2: Distribution of thermal flux for a discretization of the IAEA-2D benchmark by the variational collocation method.

is formed from the assembly of bicubic polynomials and does not have any discontinuities at element boundaries. On the other hand, the distribution corresponding to the nodal collocation method consists of the assembly of piecewise continuous biparabolic polynomials. The discontinuities, located on element boundaries, are responsible for the incompatibility of a Legendre representation with the variational formalism presented in reference 1. While reconstructing the neutron flux obtained by the nodal collocation method, we have lost one order of representation on the trial functions. However, this causes no practical handicap during the later stages of calculation requiring such a reconstruction.

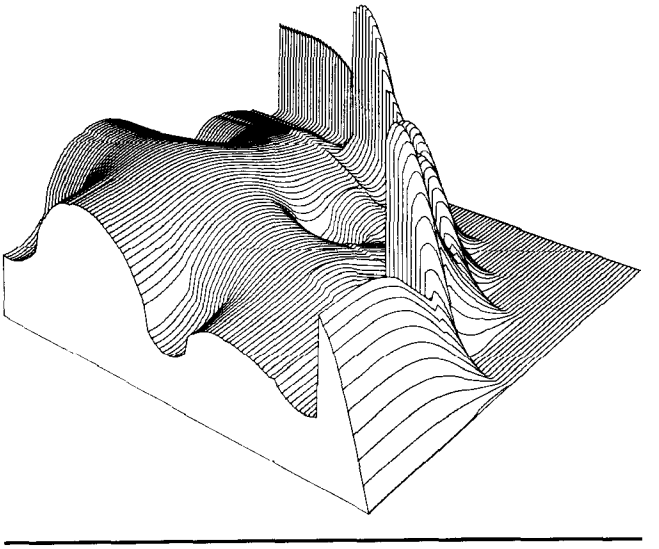

Figure 3: Distribution of thermal flux for a discretization of the IAEA-2D benchmark by the nodal collocation method.

Conclusions

We have described a new family of numerical techniques for discretizing the neutron diffusion equation. These collocation methods makes it possible to increase the order of discretization by varying the degree of polynomials used as trial functions. The minimum order, corresponding to a linear representation, is equivalent to the mesh-corner or mesh-centered finite difference method.

The variational and nodal collocation methods appear to be linked, in so far as they provide lower and upper limits for the exact solution of the diffusion equation. This property has not been proven analytically, but it has nevertheless been observed in the majority of numerical tests carried out so far.

The variational and nodal collocation methods also share a certain number of interesting properties for numerical applications: they are compatible with an ADI preconditioning and permit reconstruction of flux after convergence. They therefore share the main advantages of the finite element method, without being committed by its main drawback.

The main criticism that could be made of collocation methods is their reliance on tensorial expansions of trial polynomials. This means that when going from one to three dimensions, for a given order of discretization, the number of unknowns associated with each element is cubed. This approach, while mathematically coherent, requires more computer resources than methods based on the quadratic transverse leakage approximation [4].

Work is now underway to use this new diffusion module in fuel management and design applications, such as:

1. OPTEX-4 for the 3-D optimization of fuel enrichment, burnup, and adjuster grading in a CANDU reactor, using generalized perturbation theory [8, 9];
2. XSTATIC for the solution of the space-time kinetics equations using the generalized quasistatic algorithm;
3. a new diffusion module for the FMDP family of codes [13].

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