

Numerical Approximation for the Multigroup Diffusion Equation and Acceleration Technique

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Abstract

The aim of this paper is to study and compare several numerical methods for the multigroup diffusion equations. We recall the definitions of standard nodal and mixed-hybrid elements. Convergence tests are computed to evaluate the different methods and numerical core calculations complete these results which allowed us to compare the numerical elements. To study all aspects of the multigroup diffusion we look more closely at the multigroup discretization problem. An acceleration technique to improve the thermal iteration convergence is exposed and tested on a thermal light-reactor.

Key-words: Neutronic diffusion, mixed-hybrid elements, nodal methods, acceleration technique.

1 Introduction

Much attention has been devoted for the neutronic diffusion equation to improve the quality of the numerical methods and the physical models.

One of the basic ideas to ensure the results accuracy is to introduce a fine discretization for the energy space. The diffusion calculations are usually computed with two neutronic groups : the thermal neutrons and the fast neutrons groups. The choice of a multigroup discretization (more than two groups) seems to be an improvement for the reactor calculations. We can indicate some applications for which this fine discretization will be of great interest :

- Spectrum effect evaluation,

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- Interface calculations,
- Reflector models ...

In this paper we will then consider the multigroup diffusion equations :

$$\begin{cases} -div(D_g \vec{grad} \phi_g) + (\Sigma_g^a + \sum_{g' \neq g} \Sigma_{gg'}^s) \phi_g = \frac{\chi_g}{\lambda} \sum_{g'=1}^n \nu \Sigma_{g'}^f \phi_{g'} + \sum_{g' \neq g} \Sigma_{g'g} \phi_{g'} \\ g = 1, n \end{cases} \quad (1)$$

where we use standart notations for neutronic coefficients.

To solve problem (1) we can define 3 stages :

- the inner stage which consists in inversing the numerical method matrix for each group,
- the scattering stage which consists in converging over the transfer term and usually concerns the thermal groups for which the up-scattering phenomenon exists,
- the outer stage which usually fits with an power-method iteration.

In Sec.2 we will look more closely at the internal stage by studying different mixed-hybrid and nodal elements. Sec.3 is devoted to the theoretical and numerical convergence orders evaluation for each element.

Numerical tests on reactor cores will be computed to compare the methods in real situations.

In Sec.4 we will be concerned with the thermal stage specific to the fine multigroup calculations. We will present an acceleration technique due to Adams and Morel [1] and adapted to the diffusion case. A numerical example will illustrate the interest of the method.

We will conclude in Sec.5 over the numerical methods to propose a global multigroup calculation scheme.

2 Numerical methods for the spatial discretization

We will consider the typical second order elliptic equation subject to homogeneous Dirichlet boundary conditions :

$$\begin{cases} -div(D \vec{grad} \phi) + \Sigma \phi = S \text{ in } \Omega \subset \mathbb{R}^2, \\ \phi = 0 \text{ on } \Gamma = \partial\Omega, \end{cases} \quad (2)$$

which defines the problem solved during the inner stage described above.

We will make the following assumptions :

$$\left. \begin{array}{l} D \geq \nu > 0 \\ \Sigma \geq 0 \\ S \in L^2(\Omega). \end{array} \right\} \text{ almost everywhere in } \Omega,$$

We shall recall the usual Fick law which defines a relation between the current and the flux :

$$\vec{J} = -D \text{grad} \phi \text{ in } \Omega. \quad (3)$$

In this paper, $(T_h)_h$ represents a regular family of triangulation of the domain Ω each being composed of rectangles :

$$\Omega = \bigcup_{K \in T_h} K.$$

We will denote the different polynomial spaces by :

$$\left\{ \begin{array}{l} Q_{kl} = \{x^\alpha y^\beta; \alpha \leq k, \beta \leq l\}, \\ \mathcal{P}_k = \{x^\alpha y^\beta; \alpha + \beta \leq k\}. \end{array} \right.$$

In the following, nodal methods are summarized briefly and the particular $\Sigma 4$ nodal method is presented. Next the mixed-hybrid formulation will be recalled and the elements detailed.

2.1 Σ nodal method

The basic principles of nodal methods consists in considering a decomposition of the core in relatively large homogeneous cells where the flux is treated in mean-value term. These methods are derived from physical considerations as they consider a physical integrated balance equation on each cell. A detailed review of the advances in nodal methods can be found in [7].

In the so-called sum or Σ nodal scheme of index k the equations are derived by imposing the conditions that the balance equation be satisfied on each node for all weighted polynomials of degree $\leq k - 2$ in x or y and that the mean values of the flux and the mean values of the normal current be continuous through the edges of the node [9].

We shall consider in this paper the particular case $k = 4$.

This method can be improved by proceeding to some transverse averaging of the given equations (partial integration in the transverse direction).

As said above, the equations are derived through physical arguments, namely :

- neutronic balance equation,

- current and flux continuity in mean value through cell interfaces.

Considering the $\Sigma 4$ method the approximation space for the restriction $\phi_{h|K}$ to the node K is $Q_{4,0} \times Q_{0,4}$. The flux expansion doesn't contain any crossed term. Figure 1 illustrate the 9 degrees of freedom from the method (5 cell values and 4 edge values).

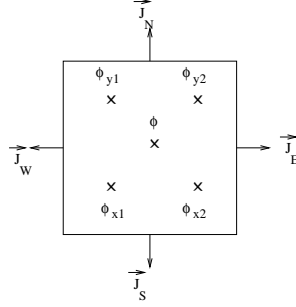


Figure 1: *Degrees of freedom for the $\Sigma 4$ nodal method.*

The equivalence between this nodal method and a non conforming element can be proved (see for instance [3], [8]).

The flux is approximated in each node K by a polynomial of degree 4 :

$$\begin{aligned} \phi(x, y) = & a_0 + a_1 f_1(x) + a_2 f_2(x) + a_3 f_3(x) + a_4 f_4(x) \\ & + b_1 f_1(x) + b_2 f_2(x) + b_3 f_3(x) + b_4 f_4(x) \end{aligned}$$

where we can express the a_i and b_i coefficients with the degrees of freedom and the basis functions f_i (see [9] for more details).

The transverse integration technique may be used to improve the accuracy of the method by evaluating the physical leakages ie neutrons leaving the cell through the transverse face [6].

The basic idea is to proceed to some transverse averaging of the given equation (2). The original equation is then integrated in the y -direction to obtain the x -transverse equation :

$$\frac{\partial J_x}{\partial x} + \Sigma \phi_x = S_x - \left(-\frac{D}{\Delta y} \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} \frac{\partial^2 \phi}{\partial y^2} dy \right),$$

where the cell is $K = [-\frac{\Delta x}{2}, \frac{\Delta x}{2}] \times [-\frac{\Delta y}{2}, \frac{\Delta y}{2}]$ with the notations :

$$\left\{ \begin{array}{l} \phi_x(x) = \frac{1}{\Delta y} \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} \phi(x, y) dy, \\ J_x(x) = -\frac{D}{\Delta y} \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} \frac{\partial \phi}{\partial x}(x, y) dy, \\ S_x(x) = \frac{1}{\Delta y} \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} S(x, y) dy. \end{array} \right.$$

We call transverse leakages in the x -direction :

$$F_x(x) = -\frac{D}{\Delta y} \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} \frac{\partial^2 \phi}{\partial y^2}(x, y) dy.$$

The result of the transverse averaging procedure is a set of 2 one-dimensional transverse equations :

$$\left\{ \begin{array}{l} -D \frac{\partial^2 \phi_x}{\partial x^2}(x) + \Sigma \phi_x(x) = S_x(x) - F_x(x), \\ -D \frac{\partial^2 \phi_y}{\partial y^2}(y) + \Sigma \phi_y(y) = S_y(y) - F_y(y). \end{array} \right.$$

An easy computation shows that :

$$\frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} F_x(x) dx = \frac{1}{\Delta y} (J_N - J_S).$$

The quadratic approximation for the transverse leakages satisfies :

$$F_x(x) = \bar{F}_x + F_1 f_1(x) + F_2 f_2(x).$$

Several choices are possible to evaluate the coefficients F_1 and F_2 [6].

The transverse averaging procedure doesn't modify the matrix of the nodal method since the transverse coefficients only appear in the second member of the system.

2.2 Mixed-hybrid variational formulation

We should first recall the mixed dual formulation. We consider (2) and (3) as a first-order coupled equations set :

$$\left\{ \begin{array}{l} \vec{J} + \overrightarrow{grad} \phi = 0 \text{ in } \Omega, \\ div \vec{J} + \Sigma \phi = S \text{ in } \Omega. \end{array} \right.$$

The mixed dual variational formulation is then :

$$\left\{ \begin{array}{l} \text{Find } (\vec{J}, \phi) \in H(\text{div}, \Omega) \times L^2(\Omega) \text{ so that} \\ \int_{\Omega} \frac{\vec{J}}{D} \cdot \vec{q} \, d\Omega - \int_{\Omega} \phi \, \text{div} \vec{q} \, d\Omega = 0 \quad \forall \vec{q} \in H(\text{div}, \Omega), \\ - \int_{\Omega} v \, \text{div} \vec{J} \, d\Omega - \int_{\Omega} \Sigma v \phi \, d\Omega = - \int_{\Omega} S v \, d\Omega \quad \forall v \in L^2(\Omega). \end{array} \right. \quad (4)$$

As ϕ needs only to be in $L^2(\Omega)$, it can in particular be discontinuous at the interfaces but \vec{J} needs to be in $H(\text{div}, \Omega)$ which implies [10] that its normal component to any interface must be continuous. This conformity condition may be relaxed by hybridation leading to the mixed-hybrid formulation where \vec{J} is no longer in $H(\text{div}, \Omega)$. As a consequence boundary terms appear on each interface and a supplementary equation is needed :

$$\left\{ \begin{array}{l} \text{Find } (\vec{J}, \phi, \phi_F) \in W \times L^2(\Omega) \times L_0^2(\partial T_h) \text{ so that} \\ \int_{\Omega} \frac{\vec{J}}{D} \cdot \vec{q} \, d\Omega + \sum_{K \in T_h} \left(\int_K \phi \, \text{div} \vec{q} - \int_{\partial K} \phi_F \vec{q} \cdot \vec{n} \right) = 0 \quad \forall \vec{q} \in H(\text{div}, \Omega), \\ \sum_{K \in T_h} \int_K v \, \text{div} \vec{J} \, d\Omega + \int_{\Omega} \Sigma v \phi \, d\Omega = \int_{\Omega} S v \, d\Omega \quad \forall v \in L^2(\Omega), \\ \sum_{K \in T_h} \int_{\partial K} \mu \vec{J} \cdot \vec{n} = 0 \quad \forall \mu \in L_0^2(\partial T_h), \end{array} \right. \quad (5)$$

where $W = \left\{ \vec{J} \in (L^2(\Omega))^2, \vec{J}|_K \in H(\text{div}, K) \right\}$ and $\partial T_h = \bigcup_{K \in T_h} \partial K$.

2.2.1 RT $_k$ Finite Element

We will denote by P_n the normalized Legendre polynomial over $[-1, 1]$.

Over the reference cell, cell moments are defined as follows :

$$m^{ij}(u) = \frac{1}{N_i N_j} \int_{-1}^1 P_i(x) P_j(y) u(x, y) \, dx \, dy.$$

Over the West, East, South and North edges of the reference cell, the fol-

lowing moments are defined :

$$\left\{ \begin{array}{l} m_W^i(u) = \frac{1}{N_i} \int_{-1}^1 P_i(y) u(-1, y) dy, \\ m_E^i(u) = \frac{1}{N_i} \int_{-1}^1 P_i(y) u(1, y) dy, \\ m_S^i(u) = \frac{1}{N_i} \int_{-1}^1 P_i(x) u(x, -1) dx, \\ m_N^i(u) = \frac{1}{N_i} \int_{-1}^1 P_i(x) u(x, 1) dx, \end{array} \right.$$

with $N_i = \frac{2}{2i+1}$ the normalized factor.

The degrees of freedom and the polynomial spaces for the RTk element are given by [5] :

- scalar variable u

$$\mathcal{D}_k = \left\{ m_K^{ij}(u_h), i, j = 0, \dots, k \right\}$$

$$\mathcal{S}_k = Q_{kk}.$$

- vector variable $\vec{q} = (q_1, q_2)$

$$\mathcal{D}_k = \mathcal{D}_{k1} \cup \mathcal{D}_{k2},$$

$$\mathcal{S}_k = \mathcal{S}_{k1} \cup \mathcal{S}_{k2} = Q_{k+1,k} \times Q_{k,k+1},$$

$$\text{where } \left\{ \begin{array}{l} \mathcal{D}_{k1} = \left\{ m_{E/W}^i(q_{h1}), i = 0, \dots, k; m_K^{ij}(q_{h1}), \begin{array}{l} i = 0, \dots, k-1, \\ j = 0, \dots, k \end{array} \right\}, \\ \mathcal{D}_{k2} = \left\{ m_{N/S}^i(q_{h2}), i = 0, \dots, k; m_K^{ij}(q_{h2}), \begin{array}{l} i = 0, \dots, k, \\ j = 0, \dots, k-1 \end{array} \right\} \end{array} \right.$$

Figure 2 illustrate the degrees of freedom for the case $k = 0$ and $k = 1$. The basis functions can be found in [5].

2.2.2 BDM1 Finite Element

The general case BDMk has the following degrees of freedom and polynomial spaces :

- scalar variable u

$$\mathcal{D}_k = \left\{ m_K^{ij}(u_h), 0 \leq i + j \leq k-1 \right\}$$

$$\mathcal{S}_k = \mathcal{P}_{k-1}.$$

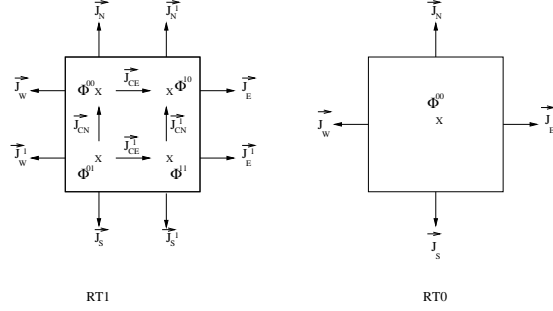


Figure 2: *Degrees of freedom for RTk element.*

- vector variable $\vec{q} = (q_1, q_2)$

$$\mathcal{D}_k = \left\{ \begin{array}{l} m_{E/W}^i(q_{h1}), i = 0, \dots, k; m_K^{ij}(q_{h1}), 0 \leq i + j \leq k - 2 \\ m_{N/S}^i(q_{h2}), i = 0, \dots, k; m_K^{ij}(q_{h2}), 0 \leq i + j \leq k - 2 \end{array} \right\}$$

$$\mathcal{S}_k = \{ \mathcal{P}_k \times \mathcal{P}_k \} \oplus \text{span} \left\{ \begin{pmatrix} P_{k+1,0} \\ -(2k+1)P_{k,1} \end{pmatrix}, \begin{pmatrix} -(2k+1)P_{1,k} \\ P_{0,k+1} \end{pmatrix} \right\}.$$

The degrees of freedom for the particular case BDM1 are indicated on figure 3.

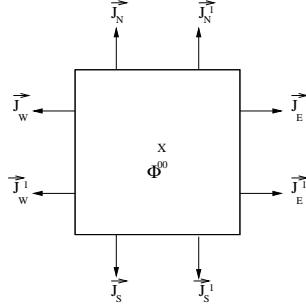


Figure 3: *Degrees of freedom for the BDM1 element.*

Rewriting the mixed-hybrid formulation using the basis function yields to the matrix of the method. In order to simplify the resolution we shall eliminate the cell-moments and we obtain a tridiagonal system for the current in each direction (see [8] for more details).

As a post-processing of the method the Lagrange multipliers can be used to improve the accuracy of the approximate solution [2].

Using this flux reconstruction yields to the equivalence between the mixed-hybrid element and some nodal schemes [5]. We can then consider a non-conforming approximation to evaluate the convergence orders of the different methods.

3 Convergence evaluation

We begin by recalling the main results about the convergence orders of the numerical methods presented above. We consider the non-conforming formulation :

$$\left\{ \begin{array}{l} \text{Find } \phi_h \in V_h \text{ so that} \\ a_h(\phi_h, v_h) = f(v_h) \quad \forall v_h \in V_h, \\ \text{with } \left\{ \begin{array}{l} a_h(\phi_h, v_h) = \sum_{K \in \mathcal{T}_h} \int_K (D \vec{\text{grad}} \phi_h \vec{\text{grad}} v_h + \Sigma \phi_h v_h) dx dy, \\ f(v_h) = \int_{\Omega} S v_h dx dy. \end{array} \right. \end{array} \right. \quad (6)$$

We define the usual norm on V_h : $\|v_h\|_h = \left(\sum_{K \in \mathcal{T}_h} |v_h|_{1,K}^2 \right)^{\frac{1}{2}}$.

As we said, each element can be rewrite as a non conforming formulation.

For the $\Sigma 2$ nodal method equivalent to the RT0 mixed-hybrid element the approximate space is :

$$V_h = \{v_h \in L^2(\Omega), v_h|_K \in \mathcal{Q}_{20} \times \mathcal{Q}_{02}, v_h = 0 \text{ sur } \partial\Omega\}.$$

For the $\Sigma 4$ nodal method :

$$V_h = \{v_h \in L^2(\Omega), v_h|_K \in \mathcal{Q}_{40} \times \mathcal{Q}_{04}, v_h = 0 \text{ sur } \partial\Omega\}.$$

We can formulate the classical result ([3], [8]) :

Theorem 1 *Let ϕ be the exact solution of the neutronic diffusion problem. Write ϕ_h the approximate solution using the $\Sigma 2$ or $\Sigma 4$ nodal method. Then we have the error estimation :*

$$\|\phi - \phi_h\|_h \sim O(h).$$

For the nodal scheme equivalent to the RT1 mixed-hybrid element :

$$V_h = \{v_h \in L^2(\Omega), v_h|_K \in \mathcal{Q}_{31} \times \mathcal{Q}_{13}, v_h = 0 \text{ sur } \partial\Omega\}$$

which lead to the theorem ([4]) :

Theorem 2 *If ϕ_h is the approximate solution using the RT1 mixed-hybrid element then :*

$$\|\phi - \phi_h\|_h \sim O(h^2).$$

If we consider the non-conforming scheme (6) with

$$V_h = \{v_h \in L^2(\Omega), v_h|_K \in \mathcal{B}_1, v_h = 0 \text{ sur } \partial\Omega\},$$

where

$$\mathcal{B}_k = \mathcal{P}_{k+1} \oplus \mathcal{R}_k \oplus \text{span}\{P_{i,i}, P_{i+1,i}, P_{i,i+1}, P_{i+2,i} - P_{i,i+2} : \frac{(k+1)}{2} < i \leq k\}$$

and

$$\mathcal{R}_k = \text{span} \{P_{i+1,i}, P_{i,i+1}, P_{i+2,i} - P_{i,i+2}, i = k + 1/2\} \text{ } k \text{ impair,}$$

$$\{P_{i+2,i} - P_{i,i+2}, i = k/2\} \text{ } k \text{ pair.}$$

which is equivalent to the BDM1 mixed-hybrid element, then we have the result [5] :

Theorem 3 *Let ϕ_h be the mixed-hybrid BDM1 approximate solution. Then the error estimation is :*

$$\|\phi - \phi_h\|_h \sim O(h).$$

For more details, we refer the reader to [8].

The L^2 -estimation give a supplementary order using a Aubin-Nitsche characterization.

We will now check this theoretical result by performing numerical calculations. Let us define a homogeneous simple configuration illustrate by figure 4.

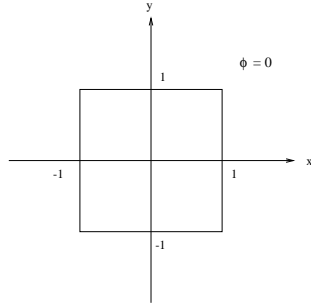


Figure 4: *Convergence test geometry.*

We consider the problem :

$$\begin{cases} -D\Delta\phi + \Sigma\phi = S & \text{dans } \Omega, \\ \phi = 0 & \text{sur } \partial\Omega, \end{cases}$$

with the exact solution $\phi(x, y) = (1 - x^4)(1 - y^4)$.

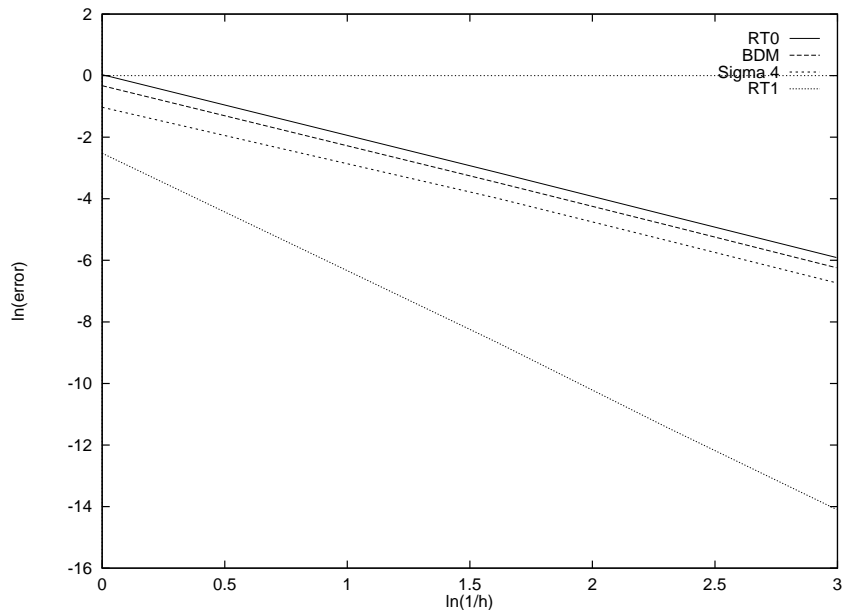


Figure 5: *Convergence curves.*

With the use of quadrature schemes we evaluate the exact L^2 -error between the solution ϕ and the approximate solution ϕ_h .

Figure 5 indicate the numerical convergence curves.

An easy computation give the different numerical convergence orders :

- RT0 : 1.98,
- BDM1 : 1.97,
- Σ 4 : 1.89,
- RT1 : 3.86.

This numerical results confirm the theoretical estimations for the 3 first elements. For RT1 we establish a super-convergence of order ~ 4 .

For the Σ 4 nodal method with quadratical transverse leakages, we have to consider a heterogeneous domain otherwise the leakages cancel. On the configuration illustrated by figure 4, we consider different material by each quarter. The results are reported in figure 6.

We can evaluate the numerical convergence orders :

- classical Σ 4 method : 1.73 with a constant $C = 0.304$,
- Σ 4 method with quadratic leakages : 1.52 with $C = 0.121$.

The fall in convergence order can be explained by the presence of singularities due to the heterogeneity of the domain [8].

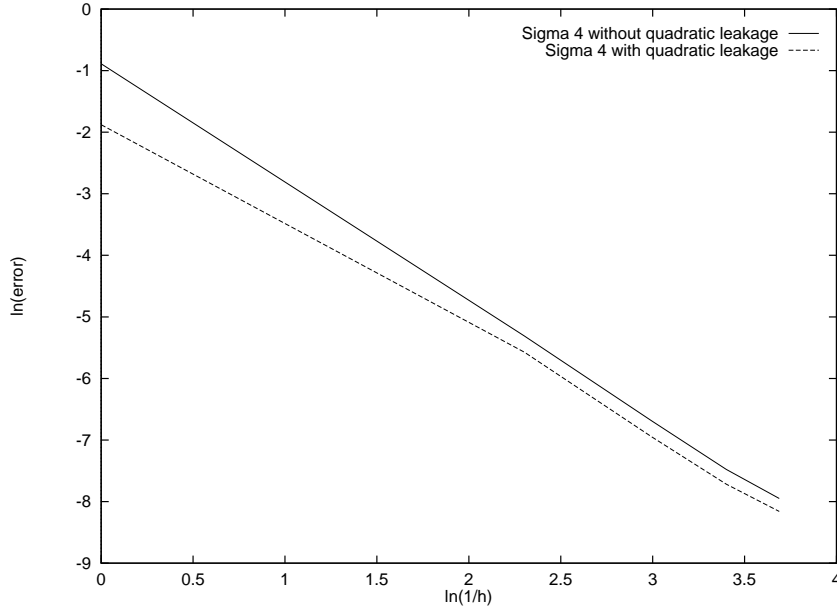


Figure 6: *Convergence curves for the $\Sigma 4$ nodal method with and without quadratic leakages.*

The convergence order seems to decrease with the quadratic leakages but the error constant is smaller which can explain that this approximation can be better in coarse-meshes.

To conclude with the numerical methods, we will now consider some real core calculations on two different reactors : a typical thermal light-water reactor (2 groups) and a fast breeder reactor due to Takeda (4 groups) [8].

The calculations results are summarized in table 1 for the PWR and in table 2 for the FBR.

We can conclude that the $\Sigma 4$ nodal method with quadratic leakages give quickly a good estimation. The RT0 and BDM1 elements are not so performant. The RT1 mixed-hybrid element is a good solution for each type of reactor.

The energy discretization used contains only one thermal neutronic group which eliminates the up-scattering problem. When more than one thermal group are considered, the supplementary iterations presented above can be very time-expensive. We will now propose an acceleration technique to reduce this iterations. The method, primary devoted to transport calculation acceleration, is due to Adams and Morel [1] and is adapted to the diffusion model.

Method	Mesh	k_{eff}	Δk_{eff} in pcm	maximum error (%) mean error (%) on the power distribution
RT0	1 × 1	0.99440	-106.	-25.34 3.48
	2 × 2	0.99392	-58.	-9.18 1.61
	4 × 4	0.99353	-19.	-3.01 0.55
	8 × 8	0.99340	-6.	-0.87 0.16
	16 × 16	0.99336	-2.	-0.23 4.3E-02
	24 × 24	0.99335	-1.	-0.1 1.9E-02
BDM1	1 × 1	0.99420	-86.	-18.93 2.92
	2 × 2	0.99367	-33.	-7.27 1.21
	4 × 4	0.99346	-12.	-2.48 0.43
	8 × 8	0.99338	-4.	-0.73 0.13
	16 × 16	0.99335	-2.	-0.19 3.44E-02
	24 × 24	0.99335	-1.	-8.58E-02 1.55E-02
Σ_4	1 × 1	0.99378	-44.	-5.61 0.84
	2 × 2	0.99361	-27.	-2.55 0.41
	4 × 4	0.99342	-8.	-0.73 0.12
	8 × 8	0.99336	-2.	-0.20 3.75E-02
	16 × 16	0.99335	-1.	-4.84E-02 9.31E-03
	24 × 24	0.99334	0.	-2.42E-02 4.04E-03
Σ_4 with leakages	1 × 1	0.99344	-10.	-2.86 0.36
	2 × 2	0.99337	-3.	-0.27 3.99E-02
	4 × 4	0.99334	0.	-3.37E-02 4.40E-03
	8 × 8	0.99334	0.	-1.11E-02 1.29E-03
	16 × 16	0.99334	0.	4.31E-03 4.01E-04
	24 × 24	0.99334	0.	3.72E-03 1.06E-04
RT1	1 × 1	0.99380	-46.	-6.11 1.20
	2 × 2	0.99342	-8.	-1.20 0.25
	4 × 4	0.99335	-1.	-0.19 3.91E-02
	8 × 8	0.99334	0.	-2.23E-02 3.46E-03
	16 × 16	0.99334	0.	5.5E-03 3.08E-04
	24 × 24	0.99334	0.	5.5E-03 2.29E-04

Table 1: Results for the PWR.

Method	Mesh	k_{eff}	Δk_{eff} in pcm	maximum error (%)	mean error (%)
				on the power distribution	
RT0	1 × 1	0.91557	451.	38.17	8.21
	2 × 2	0.91888	120.	8.68	2.07
	4 × 4	0.91978	30.	2.18	0.52
	8 × 8	0.92000	8.	0.55	0.13
	16 × 16	0.92006	2.	0.13	3.18E-02
BDM1	1 × 1	0.91046	962.	41.84	9.22
	2 × 2	0.91756	252.	10.71	2.22
	4 × 4	0.91944	64.	2.69	0.55
	8 × 8	0.91992	16.	0.66	0.13
	16 × 16	0.92004	4.	0.16	3.34E-02
$\Sigma 4$	1 × 1	0.92524	-516.	-18.15	4.4
	2 × 2	0.92142	-134.	-4.3	1.09
	4 × 4	0.92042	-34.	1.07	0.27
	8 × 8	0.92017	-9.	-0.27	7.04E-02
	16 × 16	0.92011	-3.	-7.62E-02	1.85E-02
$\Sigma 4$ with leakages	1 × 1	0.92032	-24.	3.00	0.64
	2 × 2	0.92010	-2.	-0.27	6.72E-02
	4 × 4	0.92008	0.	5.03E-02	1.01E-02
	8 × 8	0.92008	0.	1.62E-02	2.85E-03
	16 × 16	0.92008	0.	-9.91E-03	1.88E-03
RT1	1 × 1	0.92000	8.	1.34	0.35
	2 × 2	0.92007	1.	0.12	2.53E-02
	4 × 4	0.92008	0.	1.61E-02	3.70E-03
	8 × 8	0.92008	0.	-1.0E-02	2.40E-03
	16 × 16	0.92008	0.	-1.12E-02	2.59E-03

Table 2: Results for the FBR

4 Thermal iterations acceleration

The usual method use to inverse the matricial system is the Gauss-Seidel method. Without up-scattering phenomenon, it converges in one iteration over the groups. With up-scattering phenomenon, convergence can be very slow.

The Gauss-Seidel iterative method can be described as follows :

$$-div D_g \overrightarrow{grad} \phi_g^{(n)} + (\Sigma_g^a + \sum_{g' \neq g} \Sigma_{gg'}^s) \phi_g^{(n)} = F_g + \sum_{g' < g} \Sigma_{g'g}^s \phi_{g'}^{(n)} + \sum_{g' > g} \Sigma_{g'g}^s \phi_{g'}^{(n-1)}.$$

Define $\Sigma_g^d = \Sigma_g^a + \sum_{g' \neq g} \Sigma_{gg'}^s$ and $\phi_g^{(n+\frac{1}{2})}$ the non-accelerated solution. We rewrite the standart Gauss-Seidel method :

$$-div D_g \overrightarrow{grad} \phi_g^{(n+\frac{1}{2})} + \Sigma_g^d \phi_g^{(n+\frac{1}{2})} = F_g + \sum_{g' < g} \Sigma_{g'g}^s \phi_{g'}^{(n+\frac{1}{2})} + \sum_{g' > g} \Sigma_{g'g}^s \phi_{g'}^{(n)}. \quad (7)$$

Consider that the accelerated solution $\phi_g^{(n+1)}$ must verify the diffusion equation :

$$-div D_g \overrightarrow{grad} \phi_g^{(n+1)} + \Sigma_g^d \phi_g^{(n+1)} = F_g + \sum_{g' \neq g} \Sigma_{g'g}^s \phi_{g'}^{(n+1)}. \quad (8)$$

By substrating equation (7) from equation (8), an equation for the error in the Gauss-Seidel iterate is obtained :

$$-div D_g \overrightarrow{grad} \varepsilon_g^{(n+\frac{1}{2})} + \Sigma_g^d \varepsilon_g^{(n+\frac{1}{2})} = \sum_{g' < g} \Sigma_{g'g}^s \varepsilon_{g'}^{(n+\frac{1}{2})} + \sum_{g' > g} \Sigma_{g'g}^s (\phi_{g'}^{(n+1)} - \phi_{g'}^{(n)}) \quad (9)$$

with $\varepsilon_g^{(n+\frac{1}{2})} = \phi_g^{(n+1)} - \phi_g^{(n+\frac{1}{2})}$.

Define the residual $R_g^{(n+\frac{1}{2})} = \sum_{g' > g} \Sigma_{g'g}^s (\phi_{g'}^{(n+1)} - \phi_{g'}^{(n)})$.

We next assume that the solution of this error equation is given by the product of a space-dependant function $E(x, y)$ and a spectral shape function ξ_g :

$$\varepsilon_g^{(n+\frac{1}{2})}(x, y) = E(x, y) \xi_g$$

where $\sum_g \xi_g = 1$.

Substituting into (9) and summing over all energy groups, we obtain :

$$-div \left[\langle D \rangle \overrightarrow{grad} E(x, y) + \langle \bar{D} \rangle E(x, y) \right] + \langle \Sigma \rangle E(x, y) = \langle R \rangle \quad (10)$$

where

$$\left\{ \begin{array}{l} \langle D \rangle = \sum_g \xi_g D_g, \\ \langle \bar{D} \rangle = \sum_g D_g \nabla \xi_g, \\ \langle \Sigma \rangle = \sum_g (\Sigma_g^d \xi_g - \sum_{g' \neq g} \Sigma_{g'g}^s \xi_{g'}), \\ \langle R \rangle = \sum_g R_g. \end{array} \right.$$

Note that equation (10) is not a standart diffusion equation because of the term containing the gradient of the shape function. In each homogeneous region, this gradient cancels and we obtain a classical monocinetic diffusion equation :

$$-div \langle D \rangle \overrightarrow{grad} E(x, y) + \langle \Sigma \rangle E(x, y) = \langle R \rangle .$$

The accelerated procedure will be then :

1. Gauss-Seidel iteration, evaluation of $\phi_g^{(n+\frac{1}{2})}$,
2. Calculation of the residual R and of $\langle R \rangle$ by summation,
3. Solving the monocinetic diffusion equation to evaluate $E(x, y)$,
4. Calculations of $\varepsilon_g^{(n+\frac{1}{2})}$,
5. Correction of the flux :

$$\phi_g^{(n+1)} = \phi_g^{(n+\frac{1}{2})} + \varepsilon_g^{(n+\frac{1}{2})}.$$

The known of the shape function ξ_g will complete the procedure. This is done by a Fourier analysis. For a detailed description we refer the reader to [1].

To evaluate the performance of the method we present the result of a calculation which compare the accelerated scheme to the standart Gauss-Seidel iterative procedure over a simple typical PWR constituted with a homogeneous combustible zone and a reflector.

The energy space is discretized in 6 groups with 3 thermal groups. The results are report in table 3. We indicate the number of thermal iterations for the first external iteration and the total number of thermal iteration. We evaluate the saving of time on the same computer configuration.

The benefit of the method on this simplified core are important. The supplementary development needed are then justified.

Method	1st external iteration	Total number of thermal iterations	Saving of Time %
non-acc.	69	624	/
Adams-Morel	4	84	75 %

Table 3: *Performance of the acceleration technique on a typical PWR*

5 Conclusions

We have presented a global study about the solution of the multigroup diffusion equation. Different numerical elements for the spatial discretization have been described. We can conclude on the good complementarity of the Σ_4 nodal method with quadratic leakages and the more accurate RT1 mixed-hybrid element which can be superior in interface evaluations.

The multigroup problem has been defined and a performant acceleration technique has been tested.

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