Singularities and Error Estimates in Non-Conforming Approximation of Two-Dimensional Diffusion Problem

P. Lesaint* V. Louvet†

Abstract

The solution of a two dimensional diffusion problem with discontinuous coefficients is analyzed on a particular two-regions domain. The solution is shown to contain a singular part, and the particular behavior is quantitatively evaluated. It is well known that the degree of regularity of the solution for such problem determines the accuracy of the numerical techniques used to approximate the solution. The presence of singular points will then affect the convergence orders for numerical solution of the problem. This consequences are analyzed by deriving some error estimates for a non-conforming approximation. The real effects of the singularity are then studied on numerical calculations for different non-conforming elements. We will conclude from these tests that the damages due to the singularity are not as many important as theory may proceed.

Rsum

On étudie dans ce travail un problème de diffusion à coefficients discontinus dans le cas particulier d’un domaine composé de deux régions distinctes. La solution contient alors une partie singulière que nous évaluons en étudiant la forme analytique du flux aux points singuliers. Sachant que le degré de régularité de la fonction joue un rôle primordial sur la précision des méthodes numéricques utilisées, nous étudions l’impact des singularités sur les majorations d’erreur d’une approximation non conforme. Les tests numériques complétent cette analyse par une étude des dégradations dues aux singularités et qui s’avèrent moindres que ce que la théorie laisse supposer.

Key-words: Neutronic diffusion, Singularities, error estimates, non-conforming approximation.

*Laboratoire de Calcul Scientifique - Université de Franche Comté, 16 route de Gray, 25000 Besançon, France.
†E.D.F./D.E.R./R.N.E./Ph.R., 1 avenue du Général de Gaulle, 92141 Clamart Cedex, France. Email: Violaine.Maugain@der.edfgdf.fr
1 Introduction

Much attentions has been devoted in the last two decade to improve the quality of the methods used in neutronic calculations. The Finite Element Method (FEM) has attracted much interest and the nodal methods introduced during the late 1970’s constitute accurate and fast methods which share may attractive features of the Finite Element Method as well as of the Finite Difference Method.

The relationship between nodal schemes and non-conforming formulations of the FEM are explicitely detailed in [5] and [6]. In this work, we should consider a non-conforming approximation for the error estimates.

The domaine defined by a nuclear reactor is hardly heterogeneous and each region has specific neutronic constants.

The two-dimensional monocinetic diffusion problem can be written as:

\[
\begin{cases}
-\text{div}(D \nabla u) + \sigma u = S & \text{on } \Omega, \\
u = 0 & \text{on } \partial \Omega.
\end{cases}
\] (1)

The neutronic coefficients \( D \) and \( \sigma \) are supposed to be piecewise constant on \( \Omega \). The continuous system (1) is equivalent to the transmission problem:

\[
\begin{cases}
-\text{div}(D_i \nabla u_i) + \sigma_i u_i = S_i & \text{on } \Omega_i, \\
u_i = 0 & \text{on } \partial \Omega_i \cap \partial \Omega, \\
u_i = u_j & \text{on } (\partial \Omega_i \cap \partial \Omega_j) \setminus \partial \Omega, \\
D_i \frac{\partial u_i}{\partial n_i} + D_j \frac{\partial u_j}{\partial n_j} = 0 & \text{on } (\partial \Omega_i \cap \partial \Omega_j) \setminus \partial \Omega,
\end{cases}
\] (2)

where \( i = 1 \) to \( n \) and \( n \) refer to the number of regions of the domain \( \Omega \).

When \( n = 1 \), ie \( \Omega \) is homogeneous, the regularity of \( u \) is in \( H^2(\Omega) \). If \( n > 1 \), ie \( \Omega \) is heterogeneous, the transmission condition of (2) damages the degree of regularity when the coefficients \( D_i \) are discontinuous across the interfaces.

The degree of regularity of the solution determines the accuracy of the numerical element used. To illustrate this behavior we consider a particular domain with two different regions (the generalization is straightforward). Sec.2 present an analyze of the analytical solution in a neighborhood of the singular point. Sec.3 derives some error estimates for a non-conforming approximation under the hypothesis that the solution has a singular part. The singularity will be shown to damage the estimation in theory. To verify this result, Sec.4 report some numerical studies in the same geometry. The regions are taken to be the most usual case in core reactor. We will conclude in Sec.5 on the theorical developments and on their applications on industrial calculations.
2 Analytical solution in neighbourhood of singular points

Let us consider the solution of problem (1) which is equivalent to the problem (2) on a domain \( \Omega = \Omega_1 \cup \Omega_2 \) defined on figure 1.

Figure 1: An internal singular point.

In the domain \( \Omega \) we consider the disk \( \Omega_0 = \{(r, \theta), 0 \leq r \leq r_0, 0 \leq \theta \leq 2\pi\} \) with \( \Omega_0 \subset \Omega \) centered at the typical interior corner \( P \).

We introduce the Sturm-Liouville problem:

\[
\begin{cases}
\frac{d}{d\theta} \left( D \frac{d\varphi}{d\theta} \right) + \alpha^2 \varphi = 0 \quad \text{on } \Omega, \\
\varphi, \quad D\varphi' \text{ continuous in } \theta, \text{ and } 0.
\end{cases}
\]

(3)

As a classical result [9] the problem (3) have a countable number of eigenvalues \( \alpha_k \) and the eigenfunctions \( \varphi_k \) are periodic and complete in \( L^2([0, 2\pi]) \). They satisfy two orthogonality relations:

\[
\begin{cases}
\int_0^{2\pi} D\varphi_i \varphi_j d\theta = \delta_{ij}, \\
\int_0^{2\pi} D\varphi_i' \varphi_j' d\theta = \delta_{ij} \alpha_j^2.
\end{cases}
\]

(4)

The set \( \{\varphi_k\}_k \) represent a orthonormal basis of \( L^2([0, 2\pi]) \). It is also possible to expand the flux \( u(r, \theta) \) in an infinite sum of the form:

\[
u(r, \theta) = \sum_{n=1}^{\infty} w_n(r) \varphi_n(\theta),
\]

(5)

The variational formulation of problem (1) can be written as:

\[
\int_{\Omega} (-\nabla(D\nabla u)v + \sigma uv) dxdy = \int_{\Omega} Svdxdy
\]

\[
\forall v \in V = \{v \in H^1(\Omega), v = 0 \text{ sur } \partial\Omega\}.
\]

Using polar coordinates, it gives:

\[
\int_0^{2\pi} \int_0^{r_0} (D \frac{\partial u}{\partial r} \frac{\partial v}{\partial r} + \frac{D}{r^2} \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} + \sigma uv) r dr d\theta = \int_0^{2\pi} \int_0^{r_0} Svr dr d\theta,
\]

(6)

if \( v \) is taken to cancel out of \( \Omega_0 \).
The particular choice of $v$ define by $v(r, \theta) = \psi(r) \varphi_n(\theta)$ where $\psi(r) = 0$ for $r \geq r_0$ and the orthogonality conditions (4) simplify the equation (6):

$$\int_0^{r_0} \left( \frac{\partial w_n}{\partial r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \alpha_n^2 w_n(r) \psi(r) \right) r dr = \int_0^{r_0} f_n(r) \psi(r) r dr.$$

by noting $\tilde{S}(r, \theta) = S(r, \theta) - \sigma u(r, \theta)$ and $f_n(r) = \int_0^{2\pi} \tilde{S}(r, \theta) \varphi_n(\theta) d\theta.$

By integrating by part, we arrive at a differential equation for the function $w_n$:

$$-\frac{1}{r} \frac{d}{dr} \left( r \frac{dw_n}{dr} \right) + \frac{\alpha_n^2}{r^2} w_n(r) = f_n(r). \quad (7)$$

Solving problems (3) and (7) will then give the analytical solution for the neutronic flux in $\Omega.$

2.1 Evaluation of $w_n$

We consider the following second-order linear differential equation for the function $w$:

$$w'' = -\frac{w'}{r} + \frac{\alpha^2}{r^2} w - f. \quad (8)$$

The general solution of (8) contains a term in $r^\alpha$ which can be responsible of the singular behavior of the flux if $0 < \alpha < 1.$

We should now study the Sturm Liouville problem (3) to estimate the value of $\alpha.$

2.2 Solution of the Sturm Liouville problem

Two-region domains are frequently encountered in neutronics calculations of nuclear reactor cores. The most usual case for rectangular geometry is $\theta_s = \frac{\pi}{2}.$

Solving the Sturm Liouville (3) leads to general solution in each $\Omega_i$:

$$\varphi_i = \varphi_{\Omega_i} = A_i \cos(\alpha \theta) + B_i \sin(\alpha \theta).$$

Expressing the continuity conditions we obtain a system of homogeneous algebraic equations:

$$\begin{cases}
A_1 = A_2 \cos(2\pi \alpha) + B_2 \sin(2\pi \alpha), \\
A_1 \cos(\frac{\alpha \pi}{2}) + B_1 \sin(\frac{\alpha \pi}{2}) = A_2 \cos(\frac{\alpha \pi}{2}) + B_2 \sin(\frac{\alpha \pi}{2}), \\
D_1 B_1 \alpha = -D_2 A_2 \alpha \sin(2\pi \alpha) + D_2 B_2 \alpha \cos(2\pi \alpha), \\
-D_1 A_1 \alpha \sin(\frac{\alpha \pi}{2}) + D_1 B_1 \alpha \cos(\frac{\alpha \pi}{2}) = -D_2 A_2 \alpha \sin(\frac{\alpha \pi}{2}) + D_2 B_2 \alpha \cos(\frac{\alpha \pi}{2}).
\end{cases} \quad (9)$$
The compatibility condition requires the determinant of (9) to be equal to zero. Solving this problem leads to the equation:

\[-\sin^2 \gamma \left[ \cos(2\gamma)(2\Delta^2 + 4\Delta + 2) + \Delta^2 + 6\Delta + 1 \right] = 0 \tag{10}\]

with \( \Delta = \frac{D_2}{D_1} \) and \( \gamma = \frac{\alpha \pi}{2} \).

The solution of (10) gives two sequences of eigenvalues as follows:

\[
\begin{align*}
\alpha_n &= 2n \quad n \geq 1, \\
\cos(2\gamma) &= \frac{-\left(\Delta^2 + 6\Delta + 1\right)}{2\Delta^2 + 4\Delta + 2}.
\end{align*}
\tag{11}
\]

The first sequence of eigenvalues satisfies \( \alpha_n \geq 1 \). It doesn’t define any singularity.

The function \( f(x) = \frac{x^2 + 6x + 1}{2x^2 + 4x + 2} \) verifies the inequality:

\[\frac{1}{2} \leq f(x) \leq 1 \quad \forall x \in \mathbb{R}^+.\]

The second equation of (11) is then valid. Its solution gives \( \alpha \) as a function of \( \Delta \):

\[\alpha = \frac{1}{\pi} \arccos \left( \frac{-\left(\Delta^2 + 6\Delta + 1\right)}{2\Delta^2 + 4\Delta + 2} \right). \tag{12}\]

We can find a similar expression in [13] for continuous-media percolation.

All we have said above is valid for an interior point. On the external boundary \( \partial \Omega \) the continuity conditions should be replace by the appropriate boundary conditions [8].

In the case of zero flux boundary conditions as illustrate by figure 2 the solution of (3) is:

\[\varphi(\theta) = A \cos(\alpha \theta) + B \sin(\alpha \theta)\]

with the boundary conditions:

\[
\begin{align*}
A \cos(\alpha \theta_1) + B \sin(\alpha \theta_1) &= 0, \\
A \cos(\alpha \theta_2) + B \sin(\alpha \theta_2) &= 0.
\end{align*}
\]

\( \theta_1 = 0 \) which is always possible by rotation leads to the solution:

\[\alpha = \frac{\theta_2}{\pi}.\]

Figure 2: An external singular point.
2.3 \( \alpha \)-value according to \( \Delta \) and \( \theta_2 \)

From above developments the existence of singularity is effective:

- for an interior point:

\[
\alpha = \frac{1}{\pi} \arccos \frac{-(\Delta^2 + 6\Delta + 1)}{2\Delta^2 + 4\Delta + 2}
\]

for which we have the inequalities:

\[
\frac{2}{3} \leq \alpha \leq 1.
\]

- for an external point:

\[
\alpha = \frac{\theta_2}{\pi}
\]

which will give a singularity if \( \theta_2 > \pi \) that means for reentrant corner in the case of rectangular geometry.

The treatment of the multigroup diffusion equations is described in [2]. Cacuci presents in this reference the exact analytical solution in the general case.

All we have said above gives a particular form for the flux in the neighbourhood of the singular point:

\[
u(r, \theta) = r^\alpha \varphi(\theta) + u_r(r, \theta)
\]

with \( u_r \in H^2(\Omega) \) and \( \alpha \leq 1 \).

The consequences of this expression on error estimates for a non-conforming approximation is now studied.

3 Error estimates in a transmission problem

Some of the methods used in neutronic to solve the diffusion equations can be proved to be equivalent to non-conforming variational elements ([6], [5], [12]). It’s effectively the case for the elements presented in Sec.4.

In non conforming approximation the discrete solution \( u_h \in V_h \) is looked such that:

\[
a_h(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h \tag{13}
\]

where \( a_h(\cdot, \cdot) \) and \( f(\cdot) \) are the usual bilinear and linear forms:

\[
\begin{cases}
 a_h(u_h, v_h) = \sum_K \int_K (D \nabla u_h \cdot \nabla v_h + \sigma u_h v_h) dx dy, \\
 f(v_h) = \int_\Omega S v_h dx dy.
\end{cases}
\]
The domain $\Omega$ is supposed to be discretized by a triangulation $\tau_h$ using a coarse rectangular mesh : $\Omega = \bigcup_{K \in \tau_h} K$. We consider the assumption on the exact solution:

$$u = u_r + u_s$$

with $u_r \in H^2(\Omega)$ and $u_s = r^\alpha \varphi(\theta)$ with $0 < \alpha < 1$.

We will use the usual norm on $V_h$:

$$\| v_h \|_{h} = \left( \sum_{K} \frac{1}{|T|} | \nabla v_h |_{1,K}^2 \right)^{1/2}.$$ 

For an at least non-conforming $P_1$ approximation we have the following result:

**Theorem 1** Let $u$ be the exact solution and $u_h$ the approximate solution then:

$$\| u - u_h \|_{h} \sim O(h^\alpha) + O(h).$$

**Proof.** We give the proof only for the $\Sigma 4$ nodal method case. The other elements can be treated in the same way.

The triangular inequality gives:

$$\| u - u_h \|_{h} \leq \| u - r_h u \|_{h} + \| w_h - r_h u \|_{h}.$$

Estimation of $\| u - r_h u \|_{h}$

The regular part of $u$ is evaluated by the interpolation theorem:

$$\| u_r - r_h u_r \|_{h} \leq C h \| u_r \|_{2\Omega}.$$

We consider the configuration defined on figure 3 to estimates the term

$$\left( \sum_{K} \int_{K} (\nabla (u_s - r_h u_s))^2 dxdy \right)^{1/2}.$$

**Figure 3:** Domain decomposition.

$\Omega_j$ refer to the set of all black rectangles along the line $x + y = jh$. The decomposition of $\Omega$ yields

$$\sum_{K} \int_{K} (\frac{\partial}{\partial x} (u_s - r_h u_s))^2 dxdy = \int_{K_1} (\frac{\partial}{\partial x} (u_s - r_h u_s))^2 dxdy$$

$$ + \sum_{j=1}^{2(I-1)} \sum_{K \in \Omega_j} \int_{K} (\frac{\partial}{\partial x} (u_s - r_h u_s))^2 dxdy$$
with $Ih = 1$.

Since $u_s \in H^2(K)$ for $K \neq K_1$, \( \int_K \left( \frac{\partial}{\partial x} (u_s - r_h u_s) \right)^2 dx dy \leq C h^2 |u_s|^2_{2,K} \).

Evaluation in polar coordinates gives \( \left( \frac{\partial^2 u_s}{\partial x^2} \right)^2 \sim r^{2\alpha - 1} \).

As on $\Omega_j$, $r > \frac{jh\sqrt{2}}{2}$ we obtain:

\[
|u_s|^2_{2,\Omega_j} \leq C \sum_{j=1}^{2(I-1)} j^{2\alpha-1}(j + 1) h^{2\alpha-2}.
\]

But \( \sum_{j=1}^{2(I-1)} j^{2\alpha-3} \) converge since $0 < \alpha < 1$ therefore

\[
\int_K \left( \frac{\partial}{\partial x} (u_s - r_h u_s) \right)^2 dx dy \leq C h^{2\alpha} \quad \forall K \neq K_1
\]

and so $\| u_s - r_h u_s \|_{h,\Omega_j} \sim O(h^\alpha)$.

To estimate the norm on $K_1$, we note that

\[
r_h u_s = \sum_{i=1}^{4} \psi_i(x,y) \pi_i u_s + \sum_{i=5}^{9} \psi_i(x,y) \pi_i u_s
\]

where $\pi u_s$ denotes the degrees of freedom for $u_s$.

By the definition of the basis functions, $\frac{\partial \psi_i}{\partial x} \sim O(h^{-1})$ on $K_1$. An easy computation shows that

\[
\pi_i u_s \leq O(h^\alpha) \max_\theta |\varphi(\theta)|
\]

and consequently

\[
| \frac{\partial}{\partial x} (r_h u_s) | \leq C h^{\alpha-1} \max_\theta |\varphi(\theta)|
\]

Integrating on $K_1$ we obtain

\[
\int_{K_1} \left( \frac{\partial}{\partial x} (r_h u_s) \right)^2 dx dy \sim O(h^{2\alpha}).
\]

Since $u_s = r^\alpha \varphi(\theta)$ it follows that

\[
| \frac{\partial u_s}{\partial x} | \leq C r^{\alpha-1} \max_\theta (|\varphi(\theta)| + |\varphi'(\theta)|).
\]
Integrating on $K_1$ yields
\[
\int_{K_1} \left( \frac{\partial}{\partial x}(u_s) \right)^2 dxdy \sim O(h^{2\alpha})
\]
which gives the estimation
\[
\left[ \int_{K_1} \left( \frac{\partial}{\partial x}(u_s - r_h u_s) \right)^2 dxdy \right]^\frac{1}{2} \sim O(h^\alpha)
\]
It follows that $\| u - r_h u \|_h \sim O(h^\alpha) + O(h)$.

Estimation of $\| u_h - r_h u \|_h$

From the $V_h$-ellipticity of $a_h$ we have
\[
\| u_h - r_h u \|^2_h \leq C((S, w_h) - a_h(u, w_h) + a_h(u - r_h u, w_h))
\]
with $w_h = u_h - r_h u$.

By the definition of $a_h$ we can write
\[
(S, w_h) - a_h(u, w_h) = \sum_K \int_K (Sw_h - D\nabla u \nabla w_h - \sigma w_h) dxdy \tag{14}
\]
Suppose $u \in W^{2,q}(\Omega)$ with $1 < q < 2$. Let $q = \frac{2}{2 - \alpha} - \epsilon$. We introduce the notion of Green formula in $W^{p,q}$-Sobolev spaces following [1]. Replacing in (14) yields
\[
(S, w_h) - a_h(u, w_h) = \sum_K \int_{\partial K} D\frac{\partial u}{\partial n}(w_h - \pi w_h) ds
\]
with $\pi w_h$ the edge mean value of $w_h$.

Consider the application $\psi : u \mapsto \psi(u, w_h) = \int_{\partial K} \frac{\partial u}{\partial n}(w_h - \pi w_h) ds$.

By the Bramble Hilbert lemma and since $\psi$ is $P_1$-invariant we have on the reference cell $\tilde{K}$
\[
|\psi(\tilde{u})| \leq C|\tilde{u}|_{2,q,\tilde{K}}|\tilde{w}_h|_{1,\tilde{K}}.
\]

This gives
\[
|\int_{\partial K} D\frac{\partial u}{\partial n}(w_h - \pi w_h)| \leq h^{\frac{2q - 2}{q}} |u|_{2,q,K}|w_h|_{1,K}.
\]

Applying Hölder inequality yields
\[
|\sum_K \int_{\partial K} D\frac{\partial u}{\partial n}(w_h - \pi w_h)| \leq h^{\frac{2q - 2}{q}} \left( \sum_K \left| u_{2,q,K}^q \right|^{\frac{1}{q}} \left( \sum_K \left| w_h |_{1,K}^d \right|^{\frac{1}{d'}} \right) \right) = |u|_{2,q,\Omega}.
\]
Since norms are equivalent in finite dimension, we may evaluate the constant between \((\sum_K |w_h|_{1,K}^{d'})^{1/d'} \) and \(\|w_h\|_h\). By trace theorem we have on \(\hat{K}\)

\[
\int_K \left( \frac{\partial w_h}{\partial x} \right)^d \, dx \, dy \leq h^{2-d'} |\tilde{\phi}_h|_{1,\hat{K}}^{d'}.
\]

After summation we get

\[
(\sum_K |\tilde{\phi}_h|_{1,\hat{K}}^{d'})^{1/d'} \leq \left( \sum_K |\tilde{\phi}_h|_{1,\hat{K}}^{d' r} \right)^{1/d'} \left( \sum_K 1^{r'} \right)^{1/r'}.
\]

By choosing \(d' r = 2\) we obtain

\[
\left| \sum_K \int_{\partial K} D \frac{\partial u}{\partial n} (w_h - \pi w_h) \right| \leq h^{3-d/2} |u|_{2,q,\Omega} \|w_h\|_h
\]

which will be in \(O(h^\alpha)\) when \(\varepsilon \to 0\).

The proof will be complete by evaluating \(a_h(u-r_h u, w_h)\). We successively consider the applications

\[
u - r_h u \quad \mapsto \quad \int_K (\nabla (u - r_h u) \nabla w_h) \, dx \, dy
\]

\[
u - r_h u \quad \mapsto \quad \int_K \sigma(u - r_h u) w_h \, dx \, dy
\]

By the Bramble-Hilbert lemma it follows

\[
a_h(u - r_h u, w_h) \leq C h |u|_{2,q,\Omega} \|w_h\|_h
\]

which completes the proof.

We can applied the Aubin-Nitsche characterization to obtain the following \(L^2\)-estimation:

**Theorem 2** Let \(u\) be the exact solution and \(u_h\) the approximate solution of the non-conforming method (13) equivalent to the \(\Sigma_4\) nodal method then:

\[
|u - u_h|_0 \sim O(h^2 + h^{2\alpha} + h^{\alpha+1})
\]

*Proof.* See [12] for the complete proof.

The above result present a damaging theoretical effect on error estimates when the domain contain a singular point.

The following numerical calculations will illustrate the limitation on the convergence orders due to the presence of singular points.
4 Numerical tests on singular points domain

We have studied the same configuration as describe in Sec.2. \( \Omega \) is the \([-1,1] \times [-1,1] \) square filled with two regions as shown in figure 4.

The values of neutronic coefficients \( D_1, D_2, \sigma_1 \) and \( \sigma_2 \) are intended to represent one of the harder case find in thermal light-reactor: region 1 contains \( UO_2 \) and region 2 contains \( B_4C \) (a neutronic absorber).

We consider the following source for the problem (1):

\[
S(x,y) = (1 - x^4)(1 - y^4).
\]

We evaluate the \( L^2 \)-error between approximate solutions calculated by different elements:

- \( RTk \) mixed-hybrid element, for \( k = 0 \) and \( k = 1 \),
- \( \Sigma 4 \) nodal method,
- \( BDM1 \) mixed-hybrid element.

For a general description of this methods we refer the reader to [7] and [12].

If \( \beta \) is the searched convergence order, it can be estimated as [12]:

\[
\ln \left( \frac{\| \phi_h - \phi_{h/2} \|_2}{\| \phi_{h/2} - \phi_{h/4} \|_2} \right) \leq \beta \ln 2.
\]

Table 1 shows the calculated convergence orders.

<table>
<thead>
<tr>
<th>( h )</th>
<th>( RT0 )</th>
<th>( BDM1 )</th>
<th>( \Sigma 4 )</th>
<th>( RT1 )</th>
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<td>2.54</td>
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<td>2.03</td>
<td>1.92</td>
<td>3.15</td>
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</table>

Table 1: Convergence orders for the colorset \( UO_2-B_4C \).

The above results give an estimation for the singularity value. As \( \frac{D_1}{D_2} = 164.8 \) then \( \alpha = 0.67 \), which is closed to the limit.
The theoretical convergence orders on a homogeneous domain when the solution is sufficiently regular are 2 for RT0, BDM1 and Σ 4, and 3 for RT1. The values are reported in table 2. Numerical tests on homogeneous domain give a convergence order closed to 4 for the RT1 element which define a super-convergence phenomenon.

<table>
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<th>BDM1</th>
<th>Σ 4</th>
<th>RT1</th>
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<td>1/6</td>
<td>1.98</td>
<td>1.97</td>
<td>1.98</td>
<td>3.97</td>
</tr>
</tbody>
</table>

Table 2: Convergence orders for the homogeneous domain.

Table 1 shows that the presence of singularity doesn’t affect the convergence behavior of numerical methods of order 2, but for RT1 we only have 3,2. We can then presume that the regular term of the error estimate (15) \( O(h^2) \) (for the Σ 4 nodal method and the RT0 and BDM1 mixed-hybrid element) prevails over the other singular terms.

Some explanations can be found to understand the results:

- Numerical methods with high convergence order as RT1 need more regularity for the solution. They can be penalized by other terms of the flux expansion, which affect the regularity. This phenomenon can explain why RT1 suffer more than the other methods [8].

- The BDM1 mixed-hybrid element is less affected than the others (complementary calculations confirm this behavior). The presence of two degrees of freedom for each face allowed a best evaluation of interface problem and then a better result.

- The neutronic coefficient \( \sigma \) seems to have an effect on the calculation. Other results [12] shows that it compensates the singular behavior of the diffusion coefficients. If \( \sigma \) is taken constant, the degradation on the convergence order is more important.

Note that the colorset \( UO_2/B_4C \) is one of the most penalized case we can find in core reactor. The \( \alpha \)-value is closed to the limit \( \frac{2}{3} \).

5 Conclusions

The physic flux doesn’t have any particular behavior in the neighbourhhood of the interfaces of the domain. The diffusion model is in the beginning of
all singular problem. Unlike other physical phenomenon (see for instance [14]) the neutronic flux singularities are due to the mathematical form of the diffusion equation.

This elliptic equation has been analyzed to define an analytical form for the solution at singular points. We found a singular part in $r^\alpha \varphi(\theta)$ with $\frac{2}{3} < \alpha \leq 1$ for the particular case of two-regions domain.

This result allowed us to deriving error estimates for non-conforming approximation usually used in neutronic calculations.

Singularities seem to affect the theoretical convergence order. Calculations have been run to illustrate the limitation on the convergence. The numerical convergence orders are closed to the regular case for the second order elements, and decrease for the RT1 element.

Introduction of singular basis functions seems to be not necessary. This technique requires a detailed knowledge of the singular behavior of the flux and complicates the numerical method matrix. For an application to fast-breeder reactors in hexagonal geometry we refer the reader to the work of Cacuci ([3], [4]).

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References


