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Numerical analysis of the neutron multigroup SP_N equations

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Abstract

The multigroup neutron SP_N equations, which are an approximation of the neutron transport equation, are used to model nuclear reactor cores. In their steady state, these equations can be written as a source problem or an eigenvalue problem. We study the resolution of those two problems with an H^1 -conforming finite element method and a Discontinuous Galerkin method, namely the Symmetric Interior Penalty Galerkin method.

1 Introduction

The neutron transport equation describes the neutron flux density in a reactor core. It depends on 7 variables: 3 for the space, 2 for the motion direction, 1 for the energy (or the speed), and 1 for the time.

The energy variable is discretized using the multigroup theory [9]. In this method, the entire range of neutron energies is divided into G intervals, called energy groups. In each energy group, the neutron flux density is lumped and all parameters are averaged. We denote by $\mathcal{I}_G := \{1, \dots, G\}$, the set of energy group indices.

Concerning the motion direction, the P_N transport equations are obtained by developing the neutron flux on the spherical harmonics from order 0 to order

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N . This approach is very time-consuming. The simplified P_N (SP_N) transport theory [11] was developed to address this issue. The two fundamental hypotheses to obtain the SP_N equations are that locally, the angular flux has a planar symmetry; and that the axis system evolves slowly. The neutron flux and the scattering cross sections are then developed on the Legendre polynomials. From a mathematical point of view, SP_N equations correspond to tensorized $1D$ P_N transport equations, so that some couplings are missing. Consequently, the SP_N equations do not converge to transport equations. Nevertheless, they are commonly used by physicists since their resolution is cheap in terms of computational cost. The order N is odd, and the number of SP_N odd (resp. even) moments is $\hat{N} := \frac{N+1}{2}$. We will denote by $\mathcal{I}_e$ (resp. $\mathcal{I}_o$) the subset of even (resp. odd) integers of the integer set $\{0, \dots, N\}$.

Finally, the (motion direction and energy) discretization of the neutron flux is such that there are $\hat{N} \times G$ even and odd moments of the neutron flux.

We will denote by $\phi = ((\phi_m^g)_{m \in \mathcal{I}_e})_{g \in \mathcal{I}_G} \in \mathbb{R}^{\hat{N} \times G}$ the set of functions containing, for all energy group g , the even moments of the neutron flux.

Likewise, we will denote by $\mathbf{p} = ((p_{x,m}^g)_{m \in \mathcal{I}_o})_{g \in \mathcal{I}_G}^d \in \left(\mathbb{R}^{\hat{N} \times G}\right)^d$ the set of functions containing the odd moments of the neutron flux.

Note that while modelling the core of a pressurized water reactor, the number of groups is such that $2 \leq G \lesssim 30$, physicists usually choose $N = 1$ or 3 , more rarely $N = 5$.

2 Setting of the model

The reactor core is modelled by a bounded, connected and open subset $\mathcal{R}$ of $\mathbb{R}^d$, $d = 1, 2, 3$, having a Lipschitz boundary which is piecewise regular. The coefficients are piecewise regular, so that we split $\mathcal{R}$ into $\tilde{N}$ open disjoint parts $(\mathcal{R}_i)_{i=1}^{\tilde{N}}$ with Lipschitz, piecewise regular boundaries: $\overline{\mathcal{R}} = \cup_{i=1}^{\tilde{N}} \overline{\mathcal{R}_i}$. For this reason, we will use the following space of piecewise regular functions:

$$\mathcal{PW}^{1,\infty}(\mathcal{R}) = \left\{ D \in L^\infty(\mathcal{R}) \mid \vec{\nabla} D|_{\mathcal{R}_i} \in (L^\infty(\mathcal{R}_i))^d, i = 1, \dots, \tilde{N} \right\}.$$

For a set of functions $\psi = (\phi_m^g)_{m,g} \in \mathbb{R}^{\hat{N} \times G}$, we make the following abuse of notation: $\vec{\nabla} \psi = ((\partial_x \psi_m^g)_{m,g})_{x=1}^d \in \left(\mathbb{R}^{\hat{N} \times G}\right)^d$.

For a set of vector valued functions $\mathbf{q} = ((q_{x,m}^g)_{m,g})_{x=1}^d \in \left(\mathbb{R}^{\hat{N} \times G}\right)^d$, we make the following abuse of notation:

$$\operatorname{div} \mathbf{q} = (\operatorname{div} ((q_{x,m}^g)_{x=1}^d))_{m,g}, \quad \mathbf{q} \cdot \mathbf{p} = \left(\sum_{x=1}^d q_{x,m}^g p_{x,m}^g \right)_{m,g} \in \mathbb{R}^{\hat{N} \times G}.$$

Let us use these notations: for $E \subset \mathbb{R}^d$, $L(E) = L^2(E)$; $L := L^2(\mathcal{R})$; $V := H_0^1(\mathcal{R})$; $V' := H^{-1}(\mathcal{R})$ its dual and $Q := H(\operatorname{div}, \mathcal{R})$. For $W = L(E)$, L , V or

Q we define the product space $\underline{W} := W^{\hat{N} \times G}$ endowed with the following scalar product and associated norm:

$$(\mathbf{u}, \mathbf{v})_{\underline{W}} = \sum_{g \in \mathcal{I}_G} \sum_{m \in \mathcal{I}_{e,o}} (\mathbf{u}_m^g, \mathbf{v}_m^g)_W, \quad \|\mathbf{u}\|_{\underline{W}}^2 = \sum_{g \in \mathcal{I}_G} \sum_{m \in \mathcal{I}_{e,o}} \|\mathbf{u}_m^g\|_W^2. \quad (1)$$

We also set $\underline{V}' := (V')^{\hat{N} \times G}$, $\underline{\mathbf{L}}(E) = (\underline{L}(E))^d$ and $\underline{L}^p(\cdot) = (L^p(\cdot))^{\hat{N} \times G}$. Let $\mathbf{q} \in \left(\mathbb{R}^{\hat{N} \times G}\right)^d$ and $\mathbb{M} \in \left(\mathbb{R}^{\hat{N} \times \hat{N}}\right)^{G \times G}$. We set $\mathbf{q}_x = (q_{x,m}^g)_{m,g}$ and we use the notation $\mathbb{M}\mathbf{q} = (\mathbb{M}\mathbf{q}_x)_{x=1}^d$.

Given a source term $S_f \in \underline{L}$, the multigroup SP_N equations with zero-flux boundary conditions¹ read as coupled diffusion-like equations set in a mixed formulation:

$$\text{Solve in } (\phi, \mathbf{p}) \in \underline{V} \times \underline{Q} \mid \begin{cases} \mathbb{T}_o \mathbf{p} + \vec{\nabla}(\mathbb{H}\phi) &= 0, \\ {}^t\mathbb{H} \operatorname{div} \mathbf{p} + \mathbb{T}_e \phi &= S_f. \end{cases} \quad (2)$$

When S_f depends on ϕ , the steady state multigroup SP_N equations read as the following generalized eigenproblem:

$$\text{Solve in } (\lambda, \phi, \mathbf{p}) \in \mathbb{R}^* \times \underline{V} \times \underline{Q} \mid \begin{cases} \mathbb{T}_o \mathbf{p} + \vec{\nabla}(\mathbb{H}\phi) &= 0, \\ {}^t\mathbb{H} \operatorname{div} \mathbf{p} + \mathbb{T}_e \phi &= \lambda^{-1} \mathbb{M}_f \phi. \end{cases} \quad (3)$$

The physical solution to Problem (3) corresponds to the eigenfunction associated to the smallest eigenvalue, which in addition is simple [7]. In neutronics, the *multiplication factor* $k_{eff} = \max_{\lambda} \lambda$ characterizes the physical state of the core reactor: if $k_{eff} = 1$: the nuclear chain reaction is self-sustaining; if $k_{eff} > 1$: the chain reaction is diverging; if $k_{eff} < 1$: the chain reaction vanishes.

The matrices $\mathbb{H}$, $\mathbb{T}_e$, $\mathbb{T}_o$, $\mathbb{M}_f \in \left(\mathbb{R}^{\hat{N} \times \hat{N}}\right)^{G \times G}$ are such that $\forall (g, g') \in \mathcal{I}_G \times \mathcal{I}_G$ ($\delta_{\cdot, \cdot}$ is the Kronecker symbol):

- $(\mathbb{H})_{g,g'} = \delta_{g,g'} \hat{\mathbb{H}} \in \mathbb{R}^{\hat{N} \times \hat{N}}$, with $\forall (i, j) \in \{1, \dots, \hat{N}\}^2$, $\hat{\mathbb{H}}_{i,j} = \delta_{i,j} + \delta_{i,j-1}$.
- $(\mathbb{T}_e)_{g,g} := \mathbb{T}_e^g \in \mathbb{R}^{\hat{N} \times \hat{N}}$ denotes the even removal matrix, such that:

$$\mathbb{T}_e^g = \operatorname{diag} (t_0 \sigma_{r,0}^g, t_2 \sigma_{r,2}^g, \dots),$$

$(\mathbb{T}_o)_{g,g} := \mathbb{T}_o^g \in \mathbb{R}^{\hat{N} \times \hat{N}}$ denotes the odd removal matrix, such that:

$$\mathbb{T}_o^g = \operatorname{diag} (t_1 \sigma_{r,1}^g, t_3 \sigma_{r,3}^g, \dots),$$

where $\forall m \in \mathcal{I}_{e,o}$, $\sigma_{r,m}^g := \sigma_t^g - \sigma_{s,m}^{g \rightarrow g}$, and $\forall m > 0$, $t_m > 0$.

The coefficient σ_t^g is the macroscopic total cross section of energy group g , and the coefficients $\sigma_{s,m}^{g \rightarrow g}$ denote the P_N moments of the macroscopic self scattering cross sections from energy group g to itself.

¹ie: for $1 \leq g \leq G$, $m \in \mathcal{I}_e$, $(\phi_m^g)|_{\partial \mathcal{R}} = 0$.

- For $g' \neq g$:

$(\mathbb{T}_e)_{g,g'} := -\mathbb{S}_e^{g' \rightarrow g} \in \mathbb{R}^{\hat{N} \times \hat{N}}$ denotes the even scattering matrix, such that:

$$\mathbb{S}_e^{g' \rightarrow g} = \text{diag} \left(t_0 \sigma_{s,0}^{g' \rightarrow g}, t_2 \sigma_{s,2}^{g' \rightarrow g}, \dots \right),$$

$(\mathbb{T}_o)_{g,g'} := -\mathbb{S}_o^{g' \rightarrow g} \in \mathbb{R}^{\hat{N} \times \hat{N}}$ denotes the odd scattering matrix, such that:

$$\mathbb{S}_o^{g' \rightarrow g} = \text{diag} \left(t_1 \sigma_{s,1}^{g' \rightarrow g}, t_3 \sigma_{s,3}^{g' \rightarrow g}, \dots \right),$$

where $\sigma_{s,m}^{g' \rightarrow g}$ are the P_N moments of the macroscopic scattering cross sections from energy group g' to energy group g .

- $(\mathbb{M}_f)_{g,g'} := \chi^g \mathbb{M}_f^{g'} \in \mathbb{R}^{\hat{N} \times \hat{N}}$ is such that $\mathbb{M}_f^{g'} \phi^{g'} = {}^t(\nu \underline{\sigma}_f^{g'} \phi_0^{g'}, 0, \dots)$ where the coefficient $\nu \underline{\sigma}_f^{g'}$ is the product of the number of neutrons emitted per fission times the macroscopic fission cross section; and the coefficient χ_g is the fission spectrum of energy group g .

The coefficients of the matrices $\mathbb{T}_{e,o}$, $\mathbb{M}_f$ are supposed to be such that:

$$\left\{ \begin{array}{ll} (0) & \forall g, g' \in \mathcal{I}_G, \forall m \in \mathcal{I}_{e,o} : \\ & (\sigma_{r,m}^g, \sigma_{s,m}^{g' \rightarrow g}, \nu \underline{\sigma}_f^g) \in \mathcal{PW}^{1,\infty}(\mathcal{R}) \times L^\infty(\mathcal{R}) \times L^\infty(\mathcal{R}). \\ (i) & \exists (\sigma_{r,(e,o)})^*, (\sigma_{r,(e,o)})^* > 0 \mid \forall g \in \mathcal{I}_G, \forall m \in \mathcal{I}_{e,o} : \\ & (\sigma_{r,(e,o)})^* \leq t_m \sigma_{r,m}^g \leq (\sigma_{r,(e,o)})^* \text{ a.e. in } \mathcal{R}. \\ (ii) & \exists (\nu \underline{\sigma}_f)^* > 0 \mid \forall g \in \mathcal{I}_G, 0 \leq \nu \underline{\sigma}_f^g \leq (\nu \underline{\sigma}_f)^* \text{ a.e. in } \mathcal{R} \text{ and } \exists g' \mid \nu \underline{\sigma}_f^{g'} \neq 0. \\ (iii) & \exists 0 < \varepsilon < \frac{1}{G-1} \mid \forall m \in \mathcal{I}_{e,o}, \forall g, g' \in \mathcal{I}_G, g' \neq g, \\ & |\sigma_{s,m}^{g \rightarrow g'}| \leq \varepsilon \sigma_{r,m}^g \text{ a.e. in } \mathcal{R}. \end{array} \right. \quad (4)$$

It happens that the coefficient $\nu \underline{\sigma}_f^g$ vanishes in some regions.

Hypothesis 4—(iii) is valid while modelling the core of a pressurized water reactor: the scattering cross-sections are weaker than the removal cross-sections of an order $0 < \varepsilon \ll 1$. Thus, the matrices ${}^t\mathbb{T}_{e,o}$ are strictly diagonally dominant matrices: they are invertible.

Let us set $\mathbb{D} = {}^t\mathbb{H} \mathbb{T}_o^{-1} \mathbb{H}$.

Problem 2 can be written as a set of coupled primal diffusion-like equations with single unknown $\phi \in \underline{V}$:

$$\text{Solve in } \phi \in \underline{V} \mid -\text{div} \left(\mathbb{D} \vec{\nabla} \phi \right) + \mathbb{T}_e \phi = S_f. \quad (5)$$

The variational formulation of (5) writes:

$$\text{Solve in } \phi \in \underline{V} \mid \forall \psi \in \underline{V} : c(\phi, \psi) = \ell(\psi), \quad (6)$$

$$\text{where: } \left\{ \begin{array}{ll} c : \underline{V} \times \underline{V} & \rightarrow \mathbb{R} \\ c(\phi, \psi) & = (\mathbb{D} \vec{\nabla} \phi, \vec{\nabla} \psi)_{\underline{L}} + (\mathbb{T}_e \phi, \psi)_{\underline{L}} \end{array} \right., \text{ and } \left\{ \begin{array}{ll} \ell : \underline{V} & \rightarrow \mathbb{R} \\ \ell(\psi) & = (S_f, \psi)_{\underline{L}} \end{array} \right. .$$

Theorem 1 *Suppose that $\mathbb{D}$ is positive definite. For a given source term $S_f \in \underline{L}$, it exists a unique $\phi \in \underline{V}$ that solves Problem 6. In addition, it holds: $\|\phi\|_{\underline{V}} \lesssim \|S_f\|_{\underline{L}}$.*

Proof: The bilinear form c and the linear form ℓ are continuous and under the hypothesis on $\mathbb{D}$, the bilinear form c is coercive: we can apply Lax-Milgram theorem to conclude. $\square$

In the same way, Problem 3 can be written as:

$$\text{Solve in } (\lambda, \phi) \in \mathbb{R}^* \times \underline{V} \setminus \{0\} \mid -\operatorname{div} \left(\mathbb{D} \vec{\nabla} \phi \right) + \mathbb{T}_e \phi = \lambda^{-1} \mathbb{M}_f \phi. \quad (7)$$

The variational formulation of (7) writes:

$$\text{Solve in } (\lambda, \phi) \in \mathbb{R}^* \times \underline{V} \setminus \{0\} \mid \forall \psi \in \underline{V}: c(\phi, \psi) = \lambda^{-1} \ell_f(\phi, \psi), \quad (8)$$

$$\text{where: } \begin{cases} \ell_f : \underline{L} \times \underline{L} & \rightarrow \mathbb{R} \\ \ell_f(\phi, \psi) & = (\mathbb{M}_f \phi, \psi)_{\underline{L}} \end{cases}.$$

Theorem 2 *Suppose that $\mathbb{D}$ is positive definite. There exists a unique compact operator $T_f : \underline{L} \rightarrow \underline{L}$ such that $\forall (\phi, \psi) \in \underline{L} \times \underline{V}: c(T_f \phi, \psi) = \ell_f(\phi, \psi)$.*

Proof: The bilinear form c is a continuous and under the hypothesis on $\mathbb{D}$, it is coercive onto $\underline{V} \times \underline{V}$. The bilinear form ℓ_f is a continuous onto $\underline{L} \times \underline{V}$. Finally, $\underline{V}$ is a subset of $\underline{L}$ with a compact embedding. We can then apply the work of Babuška and Osborn in [2]. $\square$

Thus, the couple (ϕ, λ^{-1}) is a solution to Problem 8 iff the couple (ϕ, λ) is an eigenpair of operator T_f . Moreover, Problem 8 admits a countable number of eigenvalues.

We propose first to derive conditions on the macroscopic cross sections so that Problems 5 and 7 are well-posed. Then we obtain a priori error estimates for a discretization performed with some H^1 -conforming FEM and a Discontinuous Galerkin method, namely the Symmetric Interior Penalty Galerkin method (SIPG) [8, Chapter 4]. The outline is as follows: in Section 3, we exhibit some conditions so that the matrix $\mathbb{T}_o^{-1}$ and $\mathbb{T}_e$ are positive definite. Then we study the discretization of the source problem (5) in Section 5, and the discretization of the eigenproblem in Section 6. Finally, we perform in Section 7 a numerical study of convergence on a benchmark representative of a nuclear core.

3 Properties of $\mathbb{T}_e$ and $\mathbb{T}_o^{-1}$

Consider the diagonal matrix containing the even (resp. odd) removal macroscopic cross sections: $\mathbb{T}_{r,(e,o)} = \operatorname{diag}(\mathbb{T}_{e,o}^1, \dots, \mathbb{T}_{e,o}^G)$. We split $\mathbb{T}_{e,o}$ so that: $\mathbb{T}_{e,o} = \mathbb{T}_{r,(e,o)}(\mathbb{I} - \varepsilon \mathbb{U}_{e,o})$, where $\mathbb{I} \in \left(\mathbb{R}^{\hat{N} \times \hat{N}} \right)^{G \times G}$ is the identity matrix, and:

$$\begin{aligned} \forall g, g' \in \mathcal{I}_G, g' \neq g, \quad (\mathbb{U}_{e,o})_{g,g'} &= \operatorname{diag} \left(\left(\frac{\sigma_{s,m}^{g' \rightarrow g}}{\varepsilon \sigma_{r,m}^g} \right)_{m \in \mathcal{I}_{e,o}} \right) \in \mathbb{R}^{\hat{N} \times \hat{N}}; \\ \forall g \in \mathcal{I}_G, \quad (\mathbb{U}_{e,o})_{g,g} &= 0 \in \mathbb{R}^{\hat{N} \times \hat{N}}. \end{aligned}$$

We have then: $\|\mathbb{U}_{e,o}\|_2 \lesssim \frac{\alpha_{s,(e,o)}}{\varepsilon}$ where: $\alpha_{s,(e,o)} := (G-1) \max_{m \in \mathcal{I}_{e,o}} \max_{g \neq g' \in \mathcal{I}_G} \sup_{\vec{x} \in \mathcal{R}} \frac{|\sigma_{s,m}^{g' \rightarrow g}(\vec{x})|}{\sigma_{r,m}^g(\vec{x})}$.

Let us set $\alpha_{r,(e,o)} = \frac{(\sigma_{r,(e,o)})^*}{(\sigma_{r,(e,o)})_*} > 1$. We have the following properties.

Property 3 Suppose that $\alpha_{s,e} < \frac{1}{\alpha_{r,e}}$. The matrix $\mathbb{T}_e$ is such that:

$$\forall X \in \mathbb{R}^{\hat{N} \times G} \quad (\mathbb{T}_e X | X) \geq \tau_e \|X\|_2^2 \text{ where } \tau_e = (\sigma_{r,e})_* (1 - \alpha_{r,e} \alpha_{s,e}). \quad (9)$$

Proof: We have: $\forall X \in \mathbb{R}^{\hat{N} \times G}$, $(\mathbb{T}_e X | X) = (\mathbb{T}_{r,e} X | X) - \varepsilon (\mathbb{U}_e X | \mathbb{T}_{r,e} X)$, so that: $(\mathbb{T}_e X | X) \geq (\sigma_{r,e})_* - \varepsilon \|\mathbb{U}_e\|_2 \|\mathbb{T}_{r,e}\|_2 \|X\|_2$, where $\|\mathbb{T}_{r,e}\|_2 \leq (\sigma_{r,e})^*$. $\square$

Property 4 Suppose that $\alpha_{s,o} < \frac{1}{\alpha_{r,o} + 1}$, the matrix $\mathbb{T}_o^{-1}$ is such that:

$$\forall X \in \mathbb{R}^{\hat{N} \times G} \quad (\mathbb{T}_o^{-1} X | X) \geq \tau_o \|X\|_2^2 \text{ where } \tau_o = \frac{1}{(\sigma_{r,o})^*} \left(1 - \frac{\alpha_{r,o} \alpha_{s,o}}{1 - \alpha_{s,o}} \right). \quad (10)$$

Proof: The Taylor expansion of $\mathbb{T}_o^{-1}$ writes: $\mathbb{T}_o^{-1} = \left(\mathbb{I} + \sum_{l>0} \varepsilon^l \mathbb{U}_o^l \right) \mathbb{T}_{r,o}^{-1}$.

We get that $\forall X \in \mathbb{R}^{\hat{N} \times G}$:

$$\begin{aligned} (\mathbb{T}_o^{-1} X | X) &= (\mathbb{T}_{r,o}^{-1} X | X) + \sum_{l>0} \varepsilon^l (\mathbb{U}_o^l \mathbb{T}_{r,o}^{-1} X | X) \\ &\geq \frac{1}{(\sigma_{r,o})^*} \left(1 - \alpha_{r,o} \sum_{l>0} \varepsilon^l \|\mathbb{U}_o\|_2^l \right) \|X\|_2^2, \\ &\geq \frac{1}{(\sigma_{r,o})^*} \left(1 - \alpha_{r,o} \frac{\varepsilon \|\mathbb{U}_o\|_2}{1 - \varepsilon \|\mathbb{U}_o\|_2} \right) \|X\|_2^2, \\ &\geq \frac{1}{(\sigma_{r,o})^*} \left(1 - \frac{\alpha_{r,o} \alpha_{s,o}}{1 - \alpha_{s,o}} \right) \|X\|_2^2. \end{aligned}$$

$\square$

Under assumptions of Properties 3 and 4 the matrices $\mathbb{T}_e$ and $\mathbb{T}_o^{-1}$ are positive definite. Moreover, one can show that $\|\mathbb{H} \vec{\nabla} \phi\|_{\underline{\mathbf{L}}} \gtrsim \|\vec{\nabla} \phi\|_{\underline{\mathbf{L}}}$ [12]. We infer that the matrix $\mathbb{D}$ is positive definite and that there exists a constant $C_{\mathbb{D}} > 0$ such that for all $\xi \in \mathbb{R}^{\hat{N} \times G}$,

$$(\mathbb{D} \xi | \mathbb{D} \xi) \leq C_{\mathbb{D}} \|\xi\|_2^2. \quad (11)$$

From now on, we suppose that this property holds.

4 Discretizations

Let $\mathcal{T}_h$ be a shape-regular mesh of $\mathcal{R}$, with mesh size h . We denote by K its elements and F its facets. To simplify the presentation, we assume that the meshes are such that in every element, the cross-sections are regular. We define by $\mathcal{F}_h^i$ the set of interior faces of $\mathcal{T}_h$, $\mathcal{F}_h^b$ the set of boundary facets and $\mathcal{F}_h = \mathcal{F}_h^i \cup \mathcal{F}_h^b$. We denote by N_∂ the maximum number of mesh faces composing the boundary of mesh elements

$$N_\partial := \max_{K \in \mathcal{T}_h} \text{Card}\{F \in \mathcal{F}_h, F \subset \partial K\}.$$

We will first consider an H^1 -conforming finite element method (FEM). For $k \in \mathbb{N}^*$, $V_h^k \subset V$ and $\underline{V}_h^k \subset \underline{V}$ are the finite dimension spaces defined by:

$$V_h^k = \{v_h \in V, \forall K \in \mathcal{T}_h, v_h|_K \in \mathbb{P}_k\}, \quad \underline{V}_h^k := (V_h^k)^{\hat{N} \times G}.$$

The discrete variational formulation associated to Problem (6) writes:

$$\text{Solve in } \phi_h \in \underline{V}_h^k \mid \forall \psi_h \in \underline{V}_h^k : c(\phi_h, \psi_h) = \ell(\psi_h), \quad (12)$$

Similarly, the discrete variational formulation associated to Problem (7) writes:

$$\text{Solve in } (\lambda_h, \phi_h) \in \mathbb{R}^* \times \underline{V}_h^k \setminus \{0\} \mid \forall \psi \in \underline{V}_h^k : c(\phi_h, \psi_h) = \lambda_h^{-1} \ell_f(\phi_h, \psi_h). \quad (13)$$

Then, we will consider a non-conforming FEM. We define the broken spaces:

$$V_{\text{NC}} = \{v \in L^2(\mathcal{R}) \mid \forall K \in \mathcal{T}_h, v \in H^1(K)\}, \quad \underline{V}_{\text{NC}} = (V_{\text{NC}})^{\hat{N} \times G}.$$

For $(\phi, \psi) \in \underline{V}_{\text{NC}} \times \underline{V}_{\text{NC}}$, and $\mathbb{T} \in \mathbb{R}^{\hat{N} \times G}$, we set:

$$\left(\mathbb{D} \vec{\nabla}_h \phi, \vec{\nabla}_h \psi \right)_{\mathcal{T}_h} = \sum_{K \in \mathcal{T}_h} \left(\mathbb{D} \vec{\nabla} \phi, \vec{\nabla} \psi \right)_{\underline{\mathbf{L}}(K)}, \quad \text{and} \quad \left\| \vec{\nabla}_h \psi \right\|_{\mathcal{T}_h} = \left(\vec{\nabla}_h \psi, \vec{\nabla}_h \psi \right)_{\mathcal{T}_h}^{1/2}.$$

For $F \in \mathcal{F}_h^i$ such that $F = \partial K_1 \cap \partial K_2$, we define the average $\{\mathbb{D} \vec{\nabla}_h \psi\}$ and the jump $[\![\psi]\!]$ as:

$$\begin{aligned} \{\mathbb{D} \vec{\nabla}_h \psi\}|_F &= \frac{1}{2} \left((\mathbb{D}_1 \vec{\nabla} \psi_1)|_F + (\mathbb{D}_2 \vec{\nabla} \psi_2)|_F \right) \in \left(\mathbb{R}^{\hat{N} \times G} \right)^d, \\ [\![\psi]\!]|_F &= \psi_1|_F \mathbf{n}_1 + \psi_2|_F \mathbf{n}_2 \in \left(\mathbb{R}^{\hat{N} \times G} \right)^d. \end{aligned}$$

where $\mathbf{n}_i$ is the unit outward normal to K_i at face F and $\mathbb{D}_i = \mathbb{D}|_{K_i}$, $\psi_i = \psi|_{K_i}$.

For $F \in \mathcal{F}_h^b$ such that $F \in K$, we set $\{\mathbb{D} \vec{\nabla}_h \psi\}|_F = \mathbb{D}|_K \vec{\nabla} \psi|_K$ and $[\![\psi]\!]|_F = (\psi_K)|_F \mathbf{n}$, where $\psi_K = \psi|_K$ and $\mathbf{n}$ is the unit outward normal to K at face F .

For $k \in \mathbb{N}^*$, $V_{h,\text{NC}}^k \subset H^1(\mathcal{T}_h)$ and $\underline{V}_{h,\text{NC}}^k$ are the finite dimension spaces defined by:

$$V_{h,\text{NC}}^k = \{v_h \in L^1(\mathcal{R}); \forall K \in \mathcal{T}_h, v_h|_K \in \mathbb{P}_k\}, \quad \underline{V}_{h,\text{NC}}^k := (V_{h,\text{NC}}^k)^{\hat{N} \times G}.$$

For $\phi_h, \psi_h \in \underline{V}_{h,\text{NC}}^k$, we set: $\left(\{\mathbb{D} \vec{\nabla}_h \phi_h\}, \llbracket \psi_h \rrbracket\right)_{\mathcal{F}_h^i} = \sum_{F \in \mathcal{F}_h^i} \left(\{\mathbb{D} \vec{\nabla}_h \phi_h\}, \llbracket \psi_h \rrbracket\right)_{\underline{\mathbf{L}}(F)}.$

Let us set

$$c_h(\phi_h, \psi_h) = c_{\mathcal{T}_h}(\phi_h, \psi_h) + c_{\mathcal{F}_h}(\phi_h, \psi_h), \quad (14)$$

with

$$\begin{aligned} c_{\mathcal{T}_h}(\phi_h, \psi_h) &= \left(\mathbb{D} \vec{\nabla}_h \phi_h, \vec{\nabla}_h \psi_h\right)_{\mathcal{T}_h} + (\mathbb{T}_e \phi_h, \psi_h)_{\underline{\mathbf{L}}}, \\ c_{\mathcal{F}_h}(\phi_h, \psi_h) &= \sum_{F \in \mathcal{F}_h} \frac{\alpha}{h_F} (\llbracket \phi_h \rrbracket, \llbracket \psi_h \rrbracket)_{\underline{\mathbf{L}}(F)} - \left(\{\mathbb{D} \vec{\nabla}_h \psi_h\}, \llbracket \phi_h \rrbracket\right)_{\mathcal{F}_h^i} - \left(\{\mathbb{D} \vec{\nabla}_h \phi_h\}, \llbracket \psi_h \rrbracket\right)_{\mathcal{F}_h^i}, \end{aligned}$$

where α is a stabilization parameter.

The Symmetric Interior Penalty Galerkin method (SIPG) associated to Problem (6) writes:

$$\text{Solve in } \phi_h \in \underline{V}_{h,\text{NC}}^k \mid \forall \psi_h \in \underline{V}_{h,\text{NC}}^k : c_h(\phi_h, \psi_h) = \ell(\psi_h). \quad (15)$$

Similarly, the SIPG method associated to Problem (8) writes:

$$\begin{aligned} \text{Solve in } (\lambda_h, \phi_h) \in \mathbb{R}^* \times \underline{V}_{h,\text{NC}}^k \setminus \{0\} \mid \forall \psi_h \in \underline{V}_{h,\text{NC}}^k : \\ c_h(\phi_h, \psi_h) = \lambda_h^{-1} \ell_f(\phi_h, \psi_h). \end{aligned} \quad (16)$$

5 The source problem

5.1 Conforming discretization

Theorem 5 *Suppose that there exists $r_{\max}$ in $[0, 1]$ such that $\forall r \in [0, r_{\max}[$, $\phi \in (H^{1+r}(\mathcal{R}))^{\hat{N} \times G}$ ([6], Proposition 1). Let us set $\mu = \min(r_{\max}, k)$. The solution of (12), ϕ_h is such that: $\|\phi - \phi_h\|_{\underline{V}} \lesssim h^\mu \|S_f\|_{\underline{\mathbf{L}}}$ and $\|\phi - \phi_h\|_{\underline{\mathbf{L}}} \lesssim h^{2\mu} \|S_f\|_{\underline{\mathbf{L}}}$.*

Proof: From Céa's lemma and Aubin-Nitsche lemma as detailed in ([10], §2.3). $\square$

5.2 SIPG discretization

Assumption 5.1 (Regularity of exact solution and space V^*) *Let us denote by $W^{2,p}(\mathcal{T}_h)$ the broken Sobolev space spanned by those functions v such that for all $K \in \mathcal{T}_h$, $v|_K \in W^{2,p}(K)$. We set $\underline{W}^{2,p}(\mathcal{T}_h) = (W^{2,p}(\mathcal{T}_h))^{\hat{N} \times G}$. We assume that $d \geq 2$ and that there is $2d/(d+2) < p \leq 2$ such that, for the exact solution $\phi \in \underline{V}^* := \underline{V} \cap \underline{W}^{2,p}(\mathcal{T}_h)$. This holds for our assumptions on the coefficients, which are piecewise constant with respect to the triangulation [15].*

This assumption requires $p > 1$ for $d = 2$ and $p > 6/5$ for $d = 3$. In particular, we observe that, in two space dimensions, $\phi \in \underline{W}^{2,p}(\mathcal{T}_h)$ in polygonal domains. Moreover, using Sobolev embeddings [4, Sect. IX.3], this implies

$$\phi \in (H^{1+\alpha_p}(\mathcal{R}))^{\hat{N} \times G}, \quad \alpha_p = \frac{d+2}{2} - \frac{d}{p} > 0.$$

We state the following lemma [8, Lemma 1.46, p.27].

Lemma 6 Suppose that $(\mathcal{T}_h)_h$ is a shape- and contact-regular mesh sequence. Then, we have for all $h > 0$:

$$\forall \psi_h \in \underline{V}_{h,\text{NC}}^k, \forall K \in \mathcal{T}_h, \forall F \in \partial K, \quad h_K^{1/2} \|\psi_h\|_{\underline{L}^2(F)} \leq C_{tr} \|\psi_h\|_{\underline{L}^2(K)}, \quad (17)$$

where h_K is the diameter of element K .

We aim at asserting the discrete coercivity using the following norm:

$$\forall \psi_h \in \underline{V}_{h,\text{NC}}^k, \quad \|\psi_h\|_{sip}^2 := c_{\mathcal{T}_h}(\psi_h, \psi_h) + \|\psi_h\|_J^2$$

with the jump semi-norm

$$\|\psi_h\|_J^2 := \sum_{F \in \mathcal{F}_h} \frac{1}{h_F} \|\llbracket \psi_h \rrbracket\|_{\underline{L}(F)}^2.$$

Under assumption (4), there exists $\beta > 0$ we have for all $\psi_h \in \underline{V}_{h,\text{NC}}^k$

$$c_{\mathcal{T}_h}(\psi_h, \psi_h) \geq \beta \left(\left\| \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h}^2 + \|\psi_h\|_{\underline{L}}^2 \right), \quad (18)$$

so that

$$\|\psi_h\|_{sip}^2 \geq \beta \left(\left\| \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h}^2 + \|\psi_h\|_{\underline{L}}^2 + \|\psi_h\|_J^2 \right).$$

Lemma 7 (Discrete coercivity) Let $\underline{\alpha} := C_{tr}^2 N_{\partial} \frac{C_{\mathbb{D}}}{\beta}$ where

- C_{tr} results from the discrete trace inequality (17),
- N_{∂} is defined in Section 4,
- $C_{\mathbb{D}}$ is defined in (11).

For all $\alpha \geq \underline{\alpha}$, the SIP bilinear form defined by (14) is coercive on $\underline{V}_{h,\text{NC}}^k$ with respect to the $\|\cdot\|_{sip}$ -norm, i.e.,

$$c_h(\psi_h, \psi_h) \geq C_{\alpha} \|\psi_h\|_{sip}^2,$$

$$\text{with } C_{\alpha} := \left(\alpha - C_{tr}^2 N_{\partial} \frac{C_{\mathbb{D}}}{\beta} \right) \min \left\{ \frac{1}{2}, \beta \left(\alpha + C_{tr}^2 N_{\partial} \frac{C_{\mathbb{D}}}{\beta} \right)^{-1} \right\}.$$

Proof: We follow the proof of [8, Lemma 4.12]. For all $\psi_h \in \underline{V}_{h,\text{NC}}^k$,

$$\begin{aligned} & c_h(\psi_h, \psi_h) \\ &= c_{\mathcal{T}_h}(\psi_h, \psi_h) + c_{\mathcal{F}_h}(\psi_h, \psi_h) \\ &= c_{\mathcal{T}_h}(\psi_h, \psi_h) + \sum_{F \in \mathcal{F}_h} \frac{\alpha}{h_F} \|\llbracket \psi_h \rrbracket\|_{\underline{L}(F)}^2 - 2 \left(\{\mathbb{D} \vec{\nabla}_h \psi_h\}, \llbracket \psi_h \rrbracket \right)_{\mathcal{F}_h^i} \\ &\geq c_{\mathcal{T}_h}(\psi_h, \psi_h) + \alpha \|\psi_h\|_J^2 - 2C_{tr}(N_{\partial})^{1/2} \left\| \mathbb{D} \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h} \|\psi_h\|_J \end{aligned}$$

where we used Cauchy-Schwarz and Lemma 6 in the last line. Using the inequality $2ab \leq \varepsilon a + \varepsilon^{-1}b$ for any $\varepsilon > 0$, we obtain

$$\begin{aligned} 2C_{tr}(N_\partial)^{1/2} \left\| \mathbb{D} \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h} \|\psi_h\|_J &\leq \varepsilon C_{tr}^2 N_\partial \left\| \mathbb{D} \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h}^2 + \varepsilon^{-1} \|\psi_h\|_J^2 \\ &\leq \varepsilon C_{tr}^2 N_\partial C_{\mathbb{D}} \left\| \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h}^2 + \varepsilon^{-1} \|\psi_h\|_J^2. \end{aligned}$$

Using (18), we obtain that there exists a constant $\beta > 0$ such that

$$\begin{aligned} c_h(\psi_h, \psi_h) &\geq \beta(1 - \varepsilon \underline{\alpha}) \left\| \vec{\nabla}_h \psi_h \right\|_{\mathcal{T}_h}^2 + \beta \|\psi_h\|_{\underline{L}}^2 + (\alpha - \varepsilon^{-1}) \|\psi_h\|_J^2. \end{aligned}$$

Choosing $\varepsilon = 2(\alpha + \underline{\alpha})^{-1}$ yields the assertion. $\square$

Thus, it only remains to prove boundedness. To this purpose, we need to define $\underline{V}^{\star, h} = \underline{V}^\star + \underline{V}_{h, \text{NC}}^k$ and the following norm

$$\|\psi\|_{sip, \star} := \left(\|\psi\|_{sip}^p + \sum_{K \in \mathcal{T}_h} h_K^{1+\gamma_p} \left\| \vec{\nabla} \psi|_K \cdot \mathbf{n}_K \right\|_{\underline{L}^p(\partial K)} \right)^{1/p},$$

where $\gamma_p = \frac{d(p-2)}{2}$ and $\mathbf{n}_K$ is the unit outward normal to K . Following [8, Section 4.2], we obtain the following results.

Lemma 8 (Boundedness) *There is C_{bnd} , independent of h , such that for all $(\phi, \psi_h) \in \underline{V}^{\star, h} \times \underline{V}_h$*

$$c_h(\phi, \psi_h) \leq C_{bnd} \|\phi\|_{sip, \star} \|\psi_h\|_{sip}$$

Theorem 9 (Convergence) *Suppose that there exists $r_{\max}$ in $(0, 1]$ such that $\forall r \in [0, r_{\max}]$, $\phi \in (H^{1+r}(\mathcal{R}))^{\hat{N} \times G}$ ([6], Proposition 1). Then the solution of (15), ϕ_h is such that:*

$$\|\phi - \phi_h\|_{sip} \lesssim C \inf_{\psi_h \in \underline{V}_{h, \text{NC}}} \|\phi - \psi_h\|_{sip, \star},$$

where C is a constant independent of h . Moreover, under Assumption 5.1, there holds

$$\|\phi - \phi_h\|_{sip} \leq C |\phi|_{W^{2,p}(\mathcal{T}_h)} h^\mu,$$

where $\mu = r_{\max}$, C is a constant independent of h and p is such that $\mu = \frac{d+2}{2} - \frac{d}{p}$.

Theorem 10 (L^2 -norm estimate) *Suppose that there exists $r_{\max}$ in $(0, 1]$ such that $\forall r \in [0, r_{\max}]$, $\phi_m^g \in H^{1+r}(\mathcal{R})$ ([6], Proposition 1). Under Assumption 5.1, the solution of (15), ϕ_h is such that: $\|\phi - \phi_h\|_{\underline{L}} \lesssim h^{2\mu} \|S_f\|_{\underline{L}}$, where $\mu = r_{\max}$.*

Proof: We apply the Aubin-Nitsche similarly as in [8, Theorem 4.25]. $\square$

6 The eigenproblem

6.1 Conforming discretization

Theorem 11 *Let μ be the regularity of the eigenfunction φ associated to λ , and $\omega = \min(\mu, k)$. Let λ_h be the discrete eigenvalue associated to Problem (13). The following a priori error estimate holds: $|\lambda - \lambda_h| \lesssim h^{2\omega}$.*

Proof: As in the continuous case (Theorem 2), since the discretization is conforming, there exists a unique compact operator $T_h : \underline{V}_h^k \rightarrow \underline{V}_h^k$ such that $\forall(\phi_h, \psi_h) \in \underline{V}_h^k \times \underline{V}_h^k$: $c(T_h \phi_h, \psi_h) = \ell_f(\phi_h, \psi_h)$. According to Thm. 5, the sequence of the operators $(T_h)_h$ is pointwise converging towards T . As T_h and T are compact operators, the sequence of the operators $(T_h)_h$ is then converging in $\mathcal{L}(\underline{V})$ towards T : $\|T_h - T\|_{\mathcal{L}(\underline{V})} \rightarrow 0$. The norm convergence guarantees that there is no spectral pollution (see [17]). Moreover, we can apply Theorem 8.3 in [2] to state the error estimate on the eigenvalue. We remark that $(\mathbb{M}_f \phi, \phi)_{\underline{L}}$ is a norm over $\underline{V}_\lambda := \{\phi \in \underline{V} \mid \forall \psi \in \underline{V}, c(\phi, \psi) = \lambda \ell_f(\phi, \psi)\}$ [12, Section 5.2.2 p. 78]. $\square$

6.2 SIPG discretization

We recall that, in this section, we work under the assumption 5.1.

Theorem 12 *Let μ be the regularity of the eigenfunction φ associated to λ , and $\omega = \min(\mu, k)$. Let λ_h be the discrete eigenvalue associated to Problem (16). The following a priori error estimate holds: $|\lambda - \lambda_h| \lesssim h^{2\omega}$.*

Proof: We apply the theory developed in [1]. The proof is decomposed as follows. We first show that there is no spectral pollution. Then, we derive the error estimate.

Let $E : \underline{V} + \underline{V}_{h,\text{NC}}^k \rightarrow \underline{V} + \underline{V}_{h,\text{NC}}^k$ be the continuous spectral projector relative to λ defined by

$$E = \frac{1}{2\pi i} \int_{\Gamma} \left(z - T|_{\underline{V} + \underline{V}_{h,\text{NC}}^k} \right)^{-1} dz,$$

where Γ is a circle in the complex plane centred at λ which lies in $\rho(T|_{\underline{V} + \underline{V}_{h,\text{NC}}^k})$ and encloses no other points of $\sigma(T|_{\underline{V} + \underline{V}_{h,\text{NC}}^k})$. The absence of spectral pollution relies on two properties. First, using interpolation results [8, Assumption 4.31] we have for all $\phi \in E(\underline{V} + \underline{V}_{h,\text{NC}}^k)$,

$$\inf_{\psi_h \in \underline{V}_{h,\text{NC}}^k} \|\phi - \psi_h\|_{\text{sip}} \leq Ch^\mu,$$

where C is a constant independent of h . Second, we have for all $\phi_h \in \underline{V}_{h,\text{NC}}^k$,

$$\begin{aligned} \|(T - T_h)\phi_h\|_{\text{sip}} &\leq Ch^\mu |T\phi_h|_{W^{2,p}(\mathcal{T}_h)} \\ &\leq Ch^\mu \|T\phi_h\|_{(H^{1+\alpha_P}(\mathcal{R}))^{\bar{N} \times G}} \\ &\leq Ch^\mu \|\phi_h\|_{\underline{L}} \\ &\leq Ch^\mu \|\phi_h\|_{\text{sip}}, \end{aligned}$$

where we used Theorem 9 in the second line and regularity results [15] in the third line. Applying [1, Theorem 3.7], we obtain that there is no spectral pollution.

Moreover, we apply [1, Theorem 3.14] to state the error estimate on the eigenvalue,

$$|\lambda - \lambda_h| \leq C\delta_h\delta_{*,h},$$

where

$$\begin{aligned} \delta_h &= \gamma_h + \left\| (T - T_h)|_{E(\underline{V} + \underline{V}_{h,\text{NC}}^k)} \right\|_{\text{sip}} \\ \delta_{*,h} &= \gamma_{*,h} + \left\| (T_* - T_{*,h})|_{E(\underline{V} + \underline{V}_{h,\text{NC}}^k)} \right\|_{\text{sip}}, \end{aligned}$$

with

$$\begin{aligned} \gamma_h &= \delta(E(\underline{V} + \underline{V}_{h,\text{NC}}^k), \underline{V}_{h,\text{NC}}^k), \\ \gamma_{*,h} &= \delta(E_*(\underline{V} + \underline{V}_{h,\text{NC}}^k), \underline{V}_{h,\text{NC}}^k), \end{aligned}$$

where

$$\delta(Y, Z) = \sup_{y \in Y, \|y\|_{\text{sip}}=1} \left(\inf_{z \in Z} \|y - z\|_{\text{sip}} \right),$$

and $E_* : \underline{V} + \underline{V}_{h,\text{NC}}^k \rightarrow \underline{V} + \underline{V}_{h,\text{NC}}^k$ is the continuous spectral projector of the adjoint operator $T_*|_{\underline{V} + \underline{V}_{h,\text{NC}}^k}$ relative to $\bar{\lambda}$.

Using again elliptic regularity results [15] and Theorem 9, we obtain

$$\begin{aligned} \left\| (T - T_h)|_{E(\underline{V} + \underline{V}_{h,\text{NC}}^k)} \right\|_{\text{sip}} &\leq Ch^\mu \\ \left\| (T_* - T_{*,h})|_{E(\underline{V} + \underline{V}_{h,\text{NC}}^k)} \right\|_{\text{sip}} &\leq Ch^\mu. \end{aligned}$$

Using elliptic regularity results, we get

$$\|\varphi\|_{(H^{1+\alpha_P}(\mathcal{R}))^{\bar{N} \times G}} \leq C\|\varphi\|_{\underline{L}} \leq C\|\varphi\|_{\underline{V}}.$$

Applying Theorem 9, we infer that

$$\begin{aligned}\gamma_h &\leq Ch^\mu \\ \gamma_{*,h} &\leq Ch^\mu.\end{aligned}$$

This concludes the proof. $\square$

7 Numerical Results

We consider the test case Model 2, case 1 from the benchmark of Takeda and Ikeda [19]. The geometry of the core is three-dimensional and the domain is $\{(x, y, z) \in \mathbb{R}^3, 0 \leq x \leq 140 \text{ cm}; 0 \leq y \leq 140 \text{ cm}; 0 \leq z \leq 150 \text{ cm}\}$. This test is defined with 4 energy groups, isotropic scattering and vacuum boundary conditions. Figure 1 represents the cross-sectional geometry on the plane $z = 75 \text{ cm}$.

Since the scattering is isotropic, the SP_3 formulation can easily be reformulated as a multigroup diffusion problem with 8 energy groups and an isotropic albedo boundary condition [3]. We then made the computations with the PRIAM solver from the code CRONOS2 [14] for the conforming case and with the MINARET solver [13] from the APOLLO3[®] code [18] for the SIPG discretization.

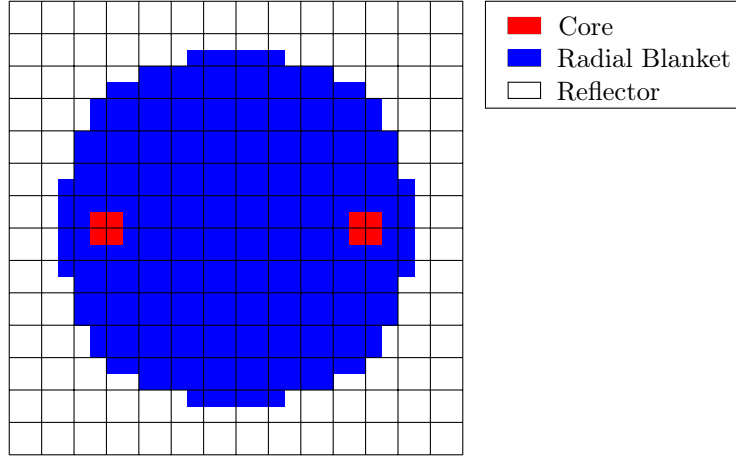


Figure 1: Cross-sectional view of the core ($z = 75 \text{ cm}$).

In Figure 2, we consider the convergence of the fundamental mode where we used the SP_3 formulation with Q^1 finite elements and a regular cartesian mesh of size h . The approximated order of convergence is 2.22.

In Figure 3, we consider the convergence of the fundamental mode for different the SP_N formulations with discontinuous P^1 finite elements and a prismatic mesh of size h . The approximated orders of convergence are given in Table 1.

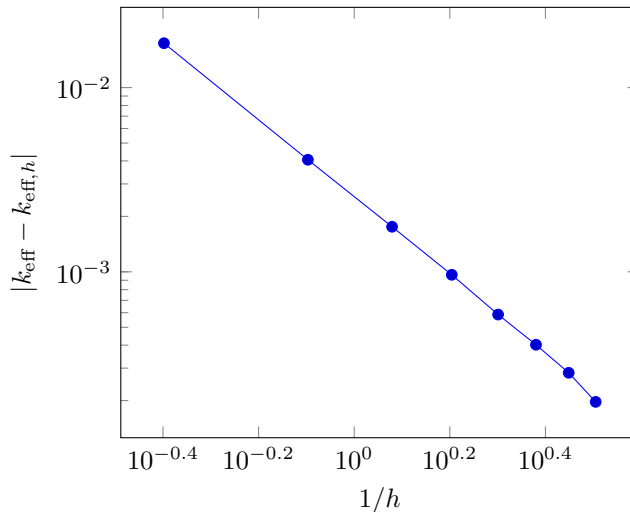


Figure 2: Error on the discrete eigenvalue for the SP_3 formulation with Q^1 finite elements

SP_3	SP_5	SP_7
1.88	1.96	1.92

Table 1: Approximated order of convergence associated to Figure 3

8 Conclusion

We did the numerical analysis of the approximation with an H^1 -conforming finite element method of the neutron multigroup SP_N equations. We also studied the numerical analysis of the approximation with the Symmetric Interior Penalty Galerkin method of the neutron multigroup SP_N equations. We then illustrated numerically the convergence results on a benchmark representative of a nuclear core. Those results can be extended to a mixed finite element method, see [5] for the diffusion case with an H^1 -conforming finite element method.

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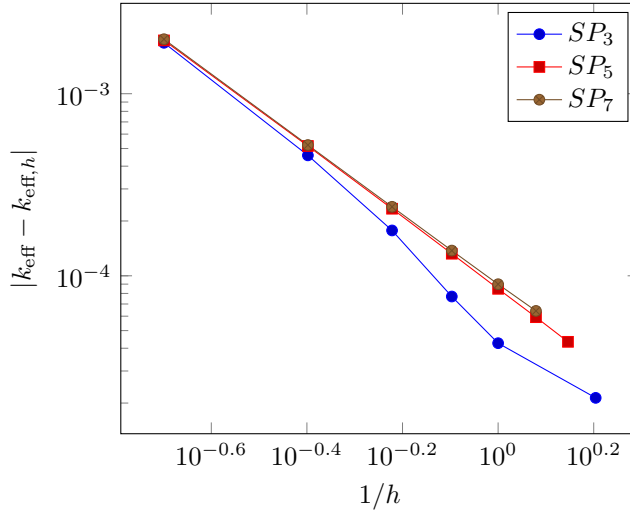


Figure 3: Error on the discrete eigenvalue for the SP_3 formulation with discontinuous linear finite elements

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