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On discontinuous Galerkin and discrete ordinates approximations for neutron transport equation and the critical eigenvalue

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Summary. — The objective of this paper is to give a mathematical framework for a fully discrete numerical approach for the study of the neutron transport equation in a cylindrical domain (container model). More specifically, we consider the discontinuous Galerkin (DG) finite element method for spatial approximation of the mono-energetic, critical neutron transport equation in an infinite cylindrical domain $\widetilde{\Omega}$ in \mathbf{R}^3 with a polygonal convex cross-section Ω . The velocity discretization rely on a special quadrature rule developed to give optimal estimates in discrete ordinate parameters compatible with the quasiuniform spatial mesh. We use interpolation spaces and derive optimal error estimates, up to maximal available regularity, for the fully discrete scalar flux. Finally we employ a duality argument and prove superconvergence estimates for the critical eigenvalue.

PACS 28.20.Fc - Neutorn absorption.

PACS 28.20.Gd - Neutron diffusion.

PACS 28.20.Cz - Neutron scattering.

1. – Description

We start with an eigenvalue problem for the critical neutron transport equation:

(1)
$$\begin{cases} -v \cdot \nabla_x \varphi - \Sigma \varphi + \int_V \sigma_s \varphi(x, v') d\mu(v') + \frac{1}{\lambda} \int_V \sigma_f \varphi(x, v') d\mu(v') = 0, \\ \varphi = 0 \text{ on } \Gamma_v^- := \{(x, v) \in \partial\Omega \times V : v \cdot n(x) < 0\}, \end{cases}$$

where λ is a positive parameter and $\varphi = \varphi(x, v)$ is a non-negative function. The space variable x is in an open set $\widetilde{\Omega} \subset \mathbf{R}^d$, the domain of the core of the reactor, and the velocity

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variable v is in a closed subset $V \subset \mathbf{R}^d$, the admissible velocity domain. Further, Γ^- denotes the inflow boundary and n(x) is the outward unit normal at the point $x \in \partial \Omega$. The kernels $\sigma_s := \sigma_s(x, v, v')$ and $\sigma_f := \sigma_f(x, v, v')$ describe the pure scattering and fission, respectively, while $\Sigma := \Sigma(x, v)$ represents the total cross-section.

In this note we study the numerical solution of the *mono-energetic* critical equation in a cylindrical domain $\widetilde{\Omega}$ in \mathbf{R}^3 with a polygonal convex cross-section Ω . Thus the velocity domain is the unit sphere $S^2 \subset \mathbf{R}^3$. All involved functions are assumed to be constant in the direction of the symmetry axis of the cylinder. This allows us to reduce the problem to \mathbf{R}^2 by projection along the symmetry axis of the cylinder. Therefore we study the *mono-energetic* version of the (1) in a bounded convex polygonal domain $\Omega \subset \mathbf{R}^2$, where due to the projection the integration over velocity domain $\mathbf{D} \subset \mathbf{R}^2$ is now associated by the measure $w(\eta) := (1 - |\eta|^2)^{-1/2}$. Furthermore, we assume that the kernels satisfy

$$\Sigma(x,v) = \Sigma(|v|), \quad \sigma_s(x,v,v') = \sigma_s(v,v') \quad \text{and} \quad \sigma_f(x,v,v') = \sigma_f(|v|,|v'|).$$

Since Σ and σ_f depend only on |v|, thus for the mono-energetic model they are constant. We may normalize σ_f to 1 and use the same notation for λ and the stretched $\lambda \to \lambda |\sigma_f|$.

For a general PDE, for a solution in the Sobolev space $H^k(\Omega)$ the optimal finite element convergence rate for elliptic and parabolic problems is of $\mathcal{O}(h^k)$ whereas the corresponding optimal error estimate for hyperbolic problems is $\mathcal{O}(h^{k-1})$, where h is the mesh size. From the convergence point of view, discontinuous Galerkin is designed to regain an $\mathcal{O}(h^{1/2})$ of this loss. The equation (1) is an integro-differential equation with a hyperbolic differential operator and the scalar flux in $H^{3/2-\varepsilon}(\Omega)$. This is maximal available regularity (no matter the shape of the convex domain Ω) therefore our finite element rate $\mathcal{O}(h^{1-\varepsilon})$ is optimal. Our velocity discretization relies on an N-points radial Gauss rule combined with an M-points angular trapezoidal rule. The former leads to singular integrals for the 5th derivative of the scalar flux and therefore is at best of order $\mathcal{O}(N^{-4})$, the latter (trapezoidal rule) is of order $\mathcal{O}(M^{-2})$. The paper is touching these limits. We also use a duality argument and derive eigenvalues estimates of order $\mathcal{O}(h^{3-\varepsilon})$. This study follows a pattern developed by Pitkäranta and Scott in in [10], Johnson and Pitkäranta in [6] and also by the first author in [1]- [4]. Other finite element and related studies of this type considered by, e.g. [5], [7], [8] yield suboptimal convergence.

2. – The continuous problem

The projection of mono-energetic version of (1) onto the cross-section Ω of $\widetilde{\Omega}$ is ([1]):

(2)
$$\left\{ \begin{array}{l} -\mu \cdot \nabla_x \varphi - \Sigma \varphi + \int_{\mathbf{D}} \sigma_s(\mu, \eta) \varphi(x, \eta) w(\eta) \, d\eta + \frac{1}{\lambda} \int_{\mathbf{D}} \varphi(x, \eta) w(\eta) \, d\eta = 0 \\ \varphi = 0 \text{ on } \Gamma_{\mu}^- := \left\{ (x, \mu) \in \partial \Omega \times \mathbf{D} : \ \mu \cdot n(x) < 0 \right\}, \qquad w(\eta) := (1 - |\eta|^2)^{-1/2} \end{array} \right.$$

In contrary to the mono-energetic version of (1), where $\mu \in S^2 \Rightarrow |\mu| = 1$, the projected equation (2) allows small velocities as well and we have $|\mu| \leq 1$. We shall use the spaces

$$(3a) \quad L_w^p(\Omega \times \mathbf{D}) = L^p(\Omega \times \mathbf{D}, w \, dx d\mu), \qquad 1 \le p < \infty, \qquad w(\mu) := (1 - |\mu|^2)^{-1/2}$$

$$(3b) \quad W^p_w(\Omega \times \mathbf{D}) = \Big\{ \varphi \in L^p_w(\Omega \times \mathbf{D}), \ \mu \cdot \nabla_x \varphi \in L^p_w(\Omega \times \mathbf{D}) \Big\}.$$

The total cross-section Σ is split into the scattering (Σ_s) and fission (Σ_f) cross-sections: $\Sigma = \Sigma_s + \Sigma_f$, with $\Sigma_s > 0$ and $\Sigma_f > 0$ where Σ_s is defined as

(4)
$$\Sigma_s := \int_{\mathbf{D}} \sigma_s(\eta, \mu) w(\eta) \, d\eta.$$

To proceed we let $L_w^p := L_w^p(\Omega \times \mathbf{D})$, and define the operators S, A, K_s and K_f by

$$S\varphi = -\mu \cdot \nabla_x \varphi - \Sigma \varphi, \qquad A\varphi = S\varphi + K_s \varphi, \qquad \mathcal{D}(A) = \mathcal{D}(S), \text{ with } K_s \varphi(x, \mu) = \int_{\mathbf{D}} \sigma_s(\mu, \eta) \varphi(x, \eta) w(\eta) \, d\eta, \qquad \text{and} \quad K_f \varphi(x, \mu) = \int_{\mathbf{D}} \varphi(x, \eta) w(\eta) \, d\eta,$$

Note that the operators K_s and K_f are bounded on L_w^p . We also recall that the operators S and A generate strongly continuous semigroups on L_w^p denoted by $\{e^{tS}, t \geq 0\}$ and $\{e^{tA}, t \geq 0\}$, respectively. In the sequel, we may replace the conservative assumption (4) by a somewhat stronger one, viz $\exists \delta > 0$ such that

(5)
$$\Sigma_s \ge \int_{\mathbf{D}} \sigma_s(\eta, \mu) w(\eta) d\eta + \delta.$$

3. – The semi-discrete problem - Quadrature rule

Let $\Delta_n = \{\mu_i\}_{i=1}^n \subset \mathbf{D}$ be a discrete set of quadrature points associated with the, positive, quadrature weights w_{μ_i} (note that w_{μ_i} approximates $w(\mu_i)$) and introduce the discrete operators K_s^n and K_f^n , approximating the operators K_s and K_f , respectively

(6a)
$$K_s^n \varphi(x,\mu) := \sum_{\eta \in \Delta_n} \sigma_s(\mu,\eta) \varphi(x,\eta) w_{\eta} \approx \int_{\mathbf{D}} \sigma_s(\mu,\eta) \varphi(x,\eta) w(\eta) d\eta,$$

(6b)
$$K_f^n \varphi(x, \mu) := \sum_{\eta \in \Delta_n} \varphi(x, \eta) w_{\eta} \approx \int_{\mathbf{D}} \varphi(x, \eta) w(\eta) d\eta.$$

We also introduce the semi-discrete $l_w^2(\Delta_n; L^2(\Omega))$ space associated with the norm

$$\left(\sum_{\mu \in \Delta_n} w_\mu \int_{\Omega} |\varphi(x,\mu)|^2 dx\right)^{1/2}.$$

Note that the operators K_s^n and K_f^n are bounded on $l_w^2(\Delta_n; L^2(\Omega))$ and we have

$$||K_s^n|| \le \sup_{(\mu,\eta)\in\mathbf{D}^2} \left(\sigma_s(\mu,\eta)\right) \left(\sum_{\eta\in\Delta_n} w_\eta\right), \qquad ||K_f^n|| \le \left(\sum_{\eta\in\Delta_n} w_\eta\right).$$

More specifically writing $\eta \in \Delta_n$ in polar coordinates as $\eta = r(\cos \theta, \sin \theta)$, $r = |\eta|$ we may choose a uniform quadrature rule on θ with a uniform weight of $2\pi/M$, where M is the number of quadrature points in θ (unit circle). As for the radial quadrature, we choose a particular Gauss rule on (0,1) with the quadrature points and weights given by $(r_k, A_k), k = 1, \ldots, N$, where N is the number of quadrature points in (0, 1), see [10]. We let n = MN be the total number of quadrature points on **D**, then we can prove that Lemma 3.1. Let $f \in C_{2,\theta}^{4,r}(\mathbf{D}, L_1(\Omega))$, then there exist constants C > 0 and small $\varepsilon_1 > 0$,

$$\left| \int_{\mathbf{D}} f(x, \mu, \eta) \frac{d\eta}{\sqrt{1 - |\eta|^2}} - \sum_{i=1}^n f(x, \mu, \eta_i) w_{\eta_i} \right| \le C \left(\frac{1}{N^4} + \frac{1}{M^{2 - \varepsilon_1}} \right) ||f||_{L_1(\Omega)},$$

where $C_{2,\theta}^{4,r}(\mathbf{D}, L_1(\Omega))$ denotes the space functions, defined in $\mathbf{D} \times \Omega$ that are in $L_1(\Omega)$ and are continuously differentiable 4 times in r and twice in θ .

Lemma 3.2. Assume (5) then for sufficiently large n and all $\mu \in \mathbf{D}$ we have that

(7)
$$\Sigma_s \ge \max \left(\sum_{\eta \in \Delta_n} (\sigma_s(\eta, \mu) w_{\eta}, \sum_{\eta \in \Delta_n} \sigma_s(\mu, \eta) w_{\eta} \right).$$

Remark 3.1. The proof of Lemma 3.1 (rather lengthy and technical) is a consequence of the stated regularity assumptions on f and interpolation theory results. These details are beyond the scope of this note, however, can be derived from the results in [3]. The proof of Lemma 3.2 is based on (5) and Lemma 3.1 which for sufficiently large n, yields

$$\sum_{\eta \in \Delta_n} \sigma_s(\eta, \mu) w_{\eta} \leq \left| \sum_{\eta \in \Delta_n} \sigma_s(\eta, \mu) w_{\eta} - \int_{\mathbf{D}} \sigma_s(\eta, \mu) w(\eta) d\eta \right| + \int_{\mathbf{D}} \sigma_s(\eta, \mu) w(\eta) d\eta$$
$$\leq C(N^{-4} + M^{-2+\varepsilon_1}) - \delta + \Sigma_s \leq \Sigma_s.$$

4. - The Fully-Discrete Problem - Discontinuous Galerkin method

Let $\{C_h\}$ be a family of quasiuniform triangulations $C_h = \{K\}$ of Ω indexed by the parameter h, the maximum diameter of triangles $K \in C_h$ and introduce the finite element space V_h of functions which are allowed to be discontinuous over enter-element boundaries:

$$V_h = \left\{ v \in L^2(\Omega) : v \Big|_K \text{ is linear, } \forall K \in \mathcal{C}_h \right\}.$$

For $\mu \in D$ and $g \in L_2(\Omega)$, let $T^h_{\mu}g \in V_h$ be the solution $u(.,\mu) \in V_h$ such that $\forall v \in V_h$

$$(8) \ \sum_{K \in \mathcal{C}_h} \left[\left(\mu. \nabla u + \Sigma u, v \right)_K + \int_{\partial K_-} [u] v_+ |\mu \cdot n| d\sigma \right] = \int_{\Omega} gv dx, \qquad u = 0, \quad \text{ on } \Gamma_\mu^-.$$

where

$$\begin{split} & \left(u,v\right)_K = \int_K uv dx, \qquad \partial K_- = \big\{x \in \partial K: \ \mu \cdot n(x) < 0\big\}, \\ & \left[v\right] = v_+ - v_-, \ v_\pm(x) = \lim_{s \to 0_+} v(x+s\mu) \text{ for } x \in \partial K, \end{split}$$

n = n(x) is the outward unit normal to ∂K at $x \in \partial K$, $d\sigma$ is the surface measure on ∂K . To continue we need to introduce the adjoint operator $(T_{\mu}^{h})^{\star}$ of T_{μ}^{h} . For a given $\mu \in D$ and $f \in L^{2}(\Omega)$, we define $(T_{\mu}^{h})^{\star} f \in V_{h}$ as the solution $u(\cdot, \mu) \in V_{h}$ of the dual problem

$$\begin{cases} \sum_{K \in \mathcal{C}_h} \left[\left(-\mu \cdot \nabla u + \Sigma u, v \right)_K - \int_{\partial K_-} [u] v_- |\mu \cdot n| d\sigma \right] = 0, & \forall v \in V_h \\ u = \tilde{g}, & \text{on} \quad \Gamma_{\mu}^+ := \left\{ x \in \partial \Omega : \ \mu \cdot n(x) > 0 \right\}, & (\tilde{g} \text{ is given}), \end{cases}$$

 $(T_{\mu}^{h})^{\star}$ is well defined adjoint of the operator T_{μ}^{h} in $L^{2}(\Omega)$. We simplify the notation by introducing $T = (-S)^{-1}$ on L_{w}^{p} . Then the critical eigenvalue problem is formulated as

$$\lambda (Id - TK_s)\varphi = TK_f\varphi,$$

where, in each occasion, Id appears as the identity operator in the relevant space.

The fully discrete scheme: Find the parameter $\lambda_n^h > 0$ and a non-negative function $\varphi_n^h \in l_w^2(\Delta_n; L^2(\Omega))$ such that for $T_n^h \varphi(x, \mu) = T_\mu^h \varphi(\cdot, \mu) \in V_h$,

(9)
$$\lambda_n^h(Id - T_n^h K_s^n)\varphi_n^h = T_n^h K_f^n \varphi_n^h, \qquad \forall \mu \in \Delta_n, \quad \forall \varphi \in l_w^2(\Delta_n; L^2(\Omega)).$$

According to [1]-[3], the discrete operator T_n^h is bounded on $l_w^2(\Delta_n; L^2(\Omega))$, i.e. λ_n^h and $\varphi_n^h(.,\mu) \in V_h$, are solution of the fully discrete critical eigenvalue equation given by

$$\begin{cases} \sum_{K \in \mathcal{C}_h} \left[\left(\mu. \nabla \varphi_n^h + \Sigma \varphi_n^h, v \right)_K + \int_{\partial K_-} [\varphi_n^h] v_+ | \mu \cdot n | d\sigma \right] - \int_{\Omega} v(x) \sum_{\eta \in \Delta_n} \sigma_s(\mu, \eta) \varphi_n^h(x, \eta) w_\eta \\ - \frac{1}{\lambda_n^h} \int_{\Omega} v(x) \sum_{\eta \in \Delta_n} \varphi_n^h(x, \eta) w_\eta \ dx = 0; \qquad u = 0 \quad \text{on } \Gamma_\mu^-; \qquad \forall \mu \in \Delta_n, \quad \forall v \in V_h. \end{cases}$$

Lemma 4.1. For sufficiently large n, the operators $T_n^h K_f^n$ and $T_n^h K_s^n$ are uniformly bounded on $l_w^2(\Delta_n; L^2(\Omega))$. Moreover, there exists a constant $0 < \alpha < 1$ such that $||T_n^h K_s^n|| < \alpha$. Consequently the operator $(Id - T_n^h K_s^n)$ is invertible on $l_w^2(\Delta_n; L^2(\Omega))$ and the inverse operator $(Id - T_n^h K_s^n)^{-1}$ is uniformly bounded.

Proof. Let $\tau \in l_w^2(\Delta_n; L^2(\Omega))$ and $u = T_n^h K_s^n \tau$. For a given $\mu \in \Delta_n$ it follows from the definition of T_n^h , with the choice of u as a test function in (8), that

(10)
$$\int_{\Omega} u K_s^n \tau dx = \sum_{K \in \mathcal{C}_h} \left[\left(\mu \cdot \nabla u + \Sigma u, u \right)_K + \int_{\partial K_-} [u] u_+ |\mu \cdot n| d\sigma \right].$$

Let $\mathcal{E} = \bigcup \partial K$, $\partial K \subset \Omega \setminus \partial \Omega$, i.e. \mathcal{E} is the set of all the sides of the triangles $K \in \mathcal{C}_h$ which are not included in $\partial\Omega$. By using Green's formula we have that

$$\begin{split} &\sum_{K\in\mathcal{C}_h} \left[\left(\mu \cdot \nabla u, u \right)_K + \int_{\partial K_-} [u] u_+ |\mu \cdot n| d\Gamma \right] \\ &= \frac{1}{2} \sum_{K\in\mathcal{C}_h} \left[\int_{\partial K_+} |\mu \cdot n| |u_-|^2 d\Gamma - \int_{\partial K_-} |\mu \cdot n| |u_+|^2 d\Gamma + \int_{\partial K_-} [u] u_+ |\mu \cdot n| d\Gamma \right] \\ &= \sum_{\partial K_- \in \mathcal{E}} \left[\frac{1}{2} \int_{\partial K_-} |\mu \cdot n| |u_-|^2 d\Gamma + \frac{1}{2} \int_{\partial K_-} |\mu \cdot n| |u_+|^2 d\Gamma - \int_{\partial K_-} |\mu \cdot n| u_- u_+ d\Gamma \right] \\ &+ \frac{1}{2} \int_{\Gamma_\mu^+} |\mu \cdot n| |u_-|^2 d\Gamma = \sum_{\partial K_- \in \mathcal{E}} \left[\frac{1}{2} \int_{\partial K_-} |\mu \cdot n| \left[u \right]^2 d\Gamma \right] + \frac{1}{2} \int_{\Gamma_\mu^+} |\mu \cdot n| |u_-|^2 d\Gamma \geq 0. \end{split}$$

Consequently, summing (10) over Δ_n , it follows that

(11)
$$\sum_{\mu \in \Delta_n} \left(\int_{\Omega} u(x,\mu) K_s^n \tau(x,\mu) dx \right) w_{\mu} \ge \sum_{\mu \in \Delta_n} \int_{\Omega} |u(x,\mu)|^2 dx \ w_{\mu}.$$

On the other hand by the repeated use of Cauchy-Schwarz inequality, and Lemma 3.2,

$$\begin{split} &\sum_{\mu \in \Delta_n} \left(\int_{\Omega} u(x,\mu) K_s^n \tau(x,\mu) dx \right) w_{\mu} = \sum_{\mu \in \Delta_n} \int_{\Omega} u(x,\mu) \sum_{\eta \in \Delta_n} \sigma_s(\mu,\eta) \tau(x,\eta) w_{\eta} w_{\mu} dx \\ &\leq \int_{\Omega} \sum_{\mu \in \Delta_n} |u(x,\mu)| \left(\sum_{\eta \in \Delta_n} \sigma(\mu,\eta) w_{\eta} \right)^{1/2} \times \left(\sum_{\eta \in \Delta_n} \sigma_s(\mu,\eta) |\tau(x,\eta)|^2 w_{\eta} \right)^{1/2} w_{\mu} dx \\ &\leq \left(\int_{\Omega} \sum_{\mu \in \Delta_n} \sum_{\eta \in \Delta_n} |u(x,\mu)|^2 \sigma_s w_{\mu} w_{\eta} dx \right)^{1/2} \times \left(\int_{\Omega} \sum_{\mu \in \Delta_n} \sum_{\eta \in \Delta_n} \sigma_s |\tau(x,\eta)|^2 w_{\mu} w_{\eta} dx \right)^{1/2} \\ &\leq \Sigma_s \left(\int_{\Omega} \sum_{\mu \in \Delta_n} |u(x,\mu)|^2 w_{\mu} dx \right)^{1/2} \times \left(\int_{\Omega} \sum_{\eta \in \Delta_n} |\tau(x,\eta)|^2 w_{\eta} dx \right)^{1/2}. \end{split}$$

Hence from the inequality (11) we deduce that

$$\left(\int_{\Omega} \sum_{\mu \in \Delta_n} |u(x,\mu)|^2 w_{\mu}\right)^{1/2} \leq \frac{\sum_s}{\sum} \left(\int_{\Omega} \sum_{\eta \in \Delta_n} |\tau(x,\eta)|^2 w_{\eta}\right)^{1/2}.$$

Therefore the operator norm of $T_n^h K_s^n$ is strictly smaller than $\Sigma_s \Sigma^{-1} < 1$. A similar, but simpler, calculus yields $||T_n^h K_f^n|| < \Sigma^{-1}$.

Lemma 4.2. Given μ in D, the operator T^h_{μ} is positive on $L^2(\Omega)$.

Proof. For $\mu \in \mathcal{D}$, let $u = T^h_{\mu}g$, where $g \in L^2(\Omega)$ is non-negative. We write $u = u^+ - u^-$ with $u^- = \max(0, -u)$ and $u^+ = \max(0, u)$. Choosing u^- as a test function in (8), and using the fact that the supports of u^+ and u^- are disconnected, we may write

(12)
$$\int_{\Omega} u^- g dx = -\sum_{K \in \mathcal{C}_b} \left[\left(\mu \cdot \nabla u^- + \Sigma u^-, u^- \right)_K + \int_{\partial K_-} [u^-] u_+^- |\mu \cdot n| d\sigma \right].$$

Now we assume that u^- has a non-empty support. Proceeding as in the proof of Lemma 4.1 we can prove, using the Green's formula, that

$$-\sum_{K\in\mathcal{C}_b} \left[\left(\mu \cdot \nabla u^- + \Sigma u^- , u^- \right)_K + \int_{\partial K_-} [u^-] u_+^- |\mu \cdot n| d\Gamma < 0. \right]$$

But $\int_{\Omega} u^{-}gdx \geq 0$, therefore, equation (12) implies that $u^{-} \equiv 0$.

Now we are prepared to study the spectral problem (9).

Theorem 4.1. There exists a real and positive eigenvalue λ_n^h associated with a unique normalized non-negative eigenfunction $\varphi_n^h \in l_w^2(\Delta_n; L^2(\Omega))$ such that

$$\lambda_n^h (Id - T_n^h K_s^n) \varphi_n^h = T_n^h K_f^n \varphi_n^h.$$

Proof. To simplify the notation let $B := (Id - T_n^h K_s^n)^{-1} T_n^h K_f^n$. By Lemma 4.1 we have

$$B = (Id - T_n^h K_s^n)^{-1} T_n^h K_f^n = \sum_{m>0} (T_n^h K_s^n)^m T_n^h K_f^n.$$

By Lemma 4.2 the operator B is positive. Since T_{μ}^{h} and $(T_{\mu}^{h})^{\star}$ have finite dimensional ranges, and $(Id - T_n^h K_s^n)^{-1}$ is bounded, we deduce that B, its adjoint B^* and consequently, $(\ker B)^{\perp} = R(B^{\star})$ all have finite dimensional ranges, and the operator B acting from $(\ker B)^{\perp}$ into R(B) is a bijective positive matrix. Then the spectral radius of B is a positive eigenvalue, not necessary simple, associated with a unique normalized non-negative eigenfunction, i.e. $\varphi_n^h \in l_w^2(\Delta_n; L^2(\Omega))$, (see also the reasoning in [9]-[12]).

Theorem 4.2. Let u and u_h be the solutions of (2) and (8), respectively. Then we have

(13)
$$||u - u^h|| \le Ch^{1-\varepsilon} ||u||_{H^{3/2-\varepsilon}(\Omega)}, \quad \forall \text{ small } \varepsilon > 0.$$

Proof [sketchy]. For a convex domain Ω we have, cf [1]-[3] and the references therein, $u \in H^{3/2-\varepsilon}(\Omega)$. A weaker argument for a convex polygonal Ω is that the solution u has its first partial derivatives depending on the outward unit normal n to $\partial\Omega$, i.e. a linear combination of Heaviside functions. Thus, by a trace estimate, the maximal available regularity of u is just $u \in H^{3/2-\varepsilon}(\Omega)$ and hence the optimal convergence order for DG in this case is $\mathcal{O}(h^{1-\varepsilon})$. To deal with such fractional derivatives, we need embedding theorems between Sobolev and Besov spaces, which is beyond the scope of this paper. Therefore we skip these details and refer the reader to the procedure developed in [3].

5. – Eigenvalue estimates

Below we show that the largest eigenvalue λ^{-1} of the transport operator T, (which makes $(I - \lambda T)^{-1}$ singular), can be found more accurately than the pointwise scalar flux. Observe that, cf [2] the kernel of the integral operator T is symmetric and positive. Hence T is self-adjoint (on $L_2(\Omega)$), and thus has only real eigenvalues. Furthermore, by the Krien-Rutman theory, its largest eigenvalue is positive and simple. We prove that

Lemma 5.1. Let κ , κ_n and κ_n^h be the largest eigenvalues of the operators T, T_n and T_n^h , respectively. Then for any $\varepsilon > 0$ and $\varepsilon_1 > 0$, and any arbitrary quadrature set Q, there are constants $C = C(\varepsilon_1, \kappa)$ and $C(Q) = C(\varepsilon, \kappa, Q)$ such that for sufficiently large N and M (even) and sufficiently small h,

(14a)
$$\|\kappa - \kappa_n\| \le C \left(\frac{1}{N^4} + \frac{1}{M^{2-\varepsilon_1}}\right),$$

(14b)
$$\|\kappa - \kappa_n^h\| \le C \left(\frac{1}{N^4} + \frac{1}{M^{2-\varepsilon_1}}\right) + C(Q)h^{3-\varepsilon}.$$

Proof [sketchy]. To prove (14a) we recall the following classical result: for normalized \tilde{f} ,

$$(15) ||T - T_n|| \to 0 \implies d\mathcal{N}(\kappa - T) = d\mathcal{N}(\kappa_n - T_n) \implies ||\kappa - \kappa_n|| \le ||(T - T_n)\tilde{f}||,$$

where $d\mathcal{N}(\kappa - T)$ is the dimension of the null space of $(\kappa - T)$. But $||T - T_n|| \to 0$ is not necessarily true in our case and we can only show that $||T^3 - T_n^3||_p \to 0, \ 1 \le p \le \infty$, as $n \to \infty$ (see [2]). To circumvent this we use the splitting

(16)
$$T^3 - \Lambda = (T - \kappa)(T - \kappa e^{2\pi i/3})(T - \kappa e^{4\pi i/3}), \quad \text{with} \quad \Lambda := \kappa^3,$$

and the fact that T and T_n , being self-adjoint, have only real eigenvalues and since the critical (largest) eigenvalue is simple thus $d\mathcal{N}(\Lambda - T^3) = d\mathcal{N}(\kappa - T) = 1$. Now (14a) follows from Lemma 3.1 combined with compactness of the operator T and the identity

(17)
$$T^{3} - T_{n}^{3} = T^{2}(T - T_{n}) + T(T - T_{n})T_{n} + (T - T_{n})T_{n}^{2}.$$

To prove (14b) we define $U_n := \sum_{\mu \in \Delta_n} w_{\mu} u^{\mu}(x)$ and write a dual problem for (8) as

(18)
$$-\mu \cdot \nabla u^{\mu}(x) + u^{\mu}(x) = \lambda U_n(x) + \hat{g}(x), \quad \text{in } \Omega \times \mathbf{D}; \quad u^{\mu} = 0, \quad \text{on} \quad \Gamma_{\mu}^+.$$

By Galerkin orthogonality and using the bilinear operator $\mathcal{B}_{\mu}(u_n^{\mu}, v)$ associated to (8)

(19)
$$(U_n - U_n^h) = \sum_{\mu \in \Delta_n} w_{\mu} \Big[\mathcal{B}_{\mu} (u_n - u_n^{\mu}, v^{\mu} - \tilde{v}^{\mu}) - \lambda (U_n - U_n^h, v^{\mu} - \tilde{v}^{\mu}) \Big],$$

where \tilde{v}^{μ} is an interpolant of v^{μ} . Now using Theorem 4.2 and interpolation error estimates

$$(U_n - U_n^h, \hat{g}) \le C(Q)[h^{1-\varepsilon}h^2 - \lambda h^{1-\varepsilon}h^2] \le C(Q)h^{3-\varepsilon} \Longrightarrow ||U_n - U_n^h||_{L_1(\Omega)} \le C(Q)h^{3-\varepsilon}.$$

Thus, for κ_n and κ_n^h being the eigenvalues corresponding to T_n and T_n^h , respectively

(20)
$$\|\kappa_n - \kappa_n^h\| \le C(Q)h^{3-\varepsilon}.$$

Now (14b) is a consequence of combining (14a) and (20), and the proof is complete.

Concluding remarks. We present a numerical a fully discrete scheme that yields an optimal convergence for the discrete ordinates and the DG methods for the neutron transport equation in cylindrical media. The geometry is adequate in, e.g. reactor calculations and some kinetic models. In real applications all involved parameters should appear in their relevant physical ranges. Some future developments are, e.g. extension of the analysis to multi-energy group, and adaptive mesh refinement strategies.

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