M2AN - MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

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M2AN - Modélisation mathématique et analyse numérique, tome 30, n° 6 (1996), p. 743-762

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MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

(Vol. 30, n° 6, 1996, p. 743 à 762)

ERROR ANALYSIS FOR THE FINITE ELEMENT APPROXIMATION OF A RADIATIVE TRANSFER MODEL (*)

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Abstract. — *This note deals with the numerical solution of a weakly singular integral equation arising in radiative or neutron transfer physics. In contrast to the common discrete ordinates method, the approach considered here is designed for physical applications where the major interest is in computing the scalar flux or only a limited number of flow intensities in arbitrary directions rather than the whole radiative field. Apart from a global convergence result, we also derive interior* a priori *and* a posteriori *error estimates particularly tempting for astrophysical applications where the computational boundary is mostly artificial.*

Résumé. — *Cette note traite de la solution numérique d'une équation intégrale faiblement singulière qui joue un rôle important en astrophysique et en physique des neutrons. Contrairement à la méthode des « ordinations discrètes » conventionnelle, notre méthode est particulièrement intéressante pour des problèmes mettant en jeu une intensité moyenne ou un petit nombre d'intensités spécifiées. En plus d'un résultat global de convergence, nous présentons des estimations d'erreurs locales non seulement* a priori *mais aussi* a posteriori *particulièrement intéressantes pour des applications en astrophysique qui ont, pour la plupart, des frontières artificielles.*

INTRODUCTION

The radiative (or neutron) transfer equation is of key importance for understanding various transport phenomena in astronomy as well as in nuclear and environmental physics. A simplified n-dimensional ($n = 2, 3$) version with $(n-1)$-dimensional ordinate space of this integro-differential equation reads

$$n_\theta \cdot \nabla u(x,\theta) + \kappa(x)\, u(x,\theta) = \hat{\lambda}(x) \int_{S_n} R(\theta,\theta^*)\, u(x,\theta^*)\, d\theta^* + f(x)\,,$$

$$(x,\theta) \in \Omega \times S_n \qquad (0.1a)$$

(*) Manuscript received October 5, 1994.

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M² AN Modélisation mathématique et Analyse numérique 0764-583X/96/06/$ 7.00
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with inflow boundary conditions

$$u(x, \theta) = b(x, \theta), \quad x \in \Gamma_\theta^- . \tag{0.1b}$$

Here, Ω is a bounded subdomain of $\mathbf{R}^n$ with piecewise smooth boundary, $\lambda(x) > 0$, $\kappa(x) > 0$ and $f(x) \in L_2(\Omega)$, while S_n represents the unit sphere in $\mathbf{R}^n$ (ordinate space with parametrization θ) with n_θ being the unit vector associated to a point on S_n. Further, $\Gamma_\theta^- = \{x \in \partial\Omega ; n_\theta \cdot n(x) < 0\}$, where $n(x)$ denotes the outward normal in x with respect to $\partial\Omega$.

Problem (0.1) can be understood as describing the changes of a flow intensity u in a point x with flow direction θ if the particle flow is subject to losses due to scattering and absorption (represented by the term $(\kappa(x)\, u(x, \theta))$, retrieves some particles by means of recombination (the integral term) and is further stimulated by internal sources $f(x)$ (for a more detailed introduction, see [1], [2], [6] or [15]). The redistribution function $R(\theta, \theta^*)$ is a measure for the radiation retrieved by these recombinational processes and describes the number of particles which, due to scattering, change their flow direction from θ^* to θ. In this note, we focus on the special case that $R(\theta, \theta^*) = R(\theta^*)$, and, for simplicity, assume $R(\theta^*) \equiv 1$, i.e., isotropic scattering in Ω. Finally, $b(x, \theta)$ is considered to be a sufficiently smooth function describing radiation entering Ω from the outside.

A large part of numerical research for radiative transfer problems has been directed towards particle methods like the Monte-Carlo-method which avoids the straightforward solution of (0.1) by following the path of individual particles as they are exposed to the specific physical conditions created by κ, λ and f. Another family of numerical methods, the so-called discrete ordinates methods (DOM) (see [12] or [13]), replaces the integral on the right hand side by a finite quadrature sum, thus getting a highly-coupled system of partial differential equations which are then solved in an iterative process (see [12]) using a characteristic method (see [15]), a finite difference scheme (see [2]) or a finite element discretization (see [12]). Indeed, recent research (see [7] and [18]) shows that DOM schemes including finite element upwind strategies for handling the resulting transport equations are efficient tools for solving a large class of radiative transfer problems.

Nevertheless, the DOM is not entirely devoid of disadvantages. First of all, some practical applications require knowledge only of the mean value of the intensity u, i.e., the « scalar flux »,

$$U(x) := \int_{S_n} u(x, \theta^*)\, d\theta^* .$$

In these cases, of course, the DOM delivers much more numerical information than is actually needed. Further, the DOM inherently entails iterative processes

such as the so-called A-iteration still favoured by many authors (see [2] or [6]) because of its apparent simplicity, or more efficient techniques like the conjugate gradient-type methods recently proposed by Turek [18]. In addition, the ordinates have to be spread in a uniform manner on the unit circle in order to guarantee convergence of the DOM (see [6] or [12]), so that a user whose interest focuses only on very few directions and the respective flow intensities would be forced to include many unnecessary ordinates in the computational process to get satisfactory results. Also, due to the possibly reduced regularity of the scalar flux at the boundary (see [16] for a detailed discussion), most DOM schemes suffer, at least in theoretical considerations, from a distinct lack of precision, which seriously impairs all efforts to construct fully-discrete schemes of higher order for the scalar flux (see [6]). Finally, the mathematical theory developed for the DOM so far does not suggest how to efficiently include the idea of adaptivity (see, e.g., [4] and [5] for proto-type examples concerning both elliptic and parabolic problems) into these considerations.

Inspired by these deficiencies of the DOM, this note tries to explore a different approach for solving (0.1), which appears quite justified in the case of isotropic scattering. It explicitly uses the fact that the scalar flux obeys the following Fredholm integral equation :

$$(I - T_\lambda)\, U(x) = Tf(x) + B(x) \quad \text{in } \Omega\,, \tag{0.2}$$

where T and T_λ are certain weakly singular integral operators, $B(x)$ represents inflowing radiation, while I denotes the identity. Integral equations like (0.2) feature in quite a lot of physical problems ; however, in many applications, the operator T in (0.2) is mostly replaced by the identity, making it a little easier to evaluate the right hand side. As soon as a reliable, stable and precise numerical solution technique for (0.2) is available, equation (0.1) boils down to a simple set of linear transport equations which may then be solved by a standard integration process. We emphasize that (0.2) differs from the problems usually associated with the boundary element method where a differential equation in Ω becomes an integral equation on the closed manifold $\partial\Omega$.

The following discussion is primarily devoted to the cause of investigating the theoretical properties of a finite element approach for solving (0.2). A central objective is to couple the concepts of adaptivity and of interior error estimates (in the spirit of Nitsche and Schatz [14]) so as to gain an interior *a posteriori* error estimate that ensures a sufficient degree of grid refinement away from the boundary while not overly refining the mesh close to it. One of the big problems surrounding the actual use of conventional *a posteriori* error estimates for adaptive mesh control is the global character of the estimates in contrast to the local, i.e. element-wise, character of the mesh-refinement necessary to guarantee efficiency. Eriksson and Johnson make up for this deficiency by simply equilibrating the error over all elements which, at least for the model problems presented in [4] and [5], provides satisfactory

results. A general abstract analysis of global *a posteriori* error estimates for the boundary integral method has been provided in [3]. So far, it seems that local *a posteriori* error estimates have only been reported for certain pseudodifferential equations in [19].

The outline of this paper is as follows. Section 1 gives a more detailed summary of the theoretical properties of (0.1), derives equation (0.2) and briefly illuminates its specific analytical behaviour. In Section 2, we introduce a class of finite element methods for solving (0.2), discuss its main advantages and disadvantages and prove, largely using techniques borrowed from L_2-projection theory, global *a priori* H^{-1}- and L_2-error estimates. Also, this section strives to critically review techniques designed to boost the L_2-convergence rate without excessive additional computational effort. An *a priori* and an *a posteriori* localization result for the L_2-error away from the critical boundary layer of the exact solution will be unveiled in Section 3, opening up the way for locally adaptive finite element techniques in numerical radiative transfer. Combining the finite element approach for the mean intensity U with a simple characteristic method gives us the solution of (0.1) for an arbitrary ordinate θ with increased accuracy. Numerical tests concerning the reliability and efficiency of adaptive grid refinement for radiative transfer problems will be presented in a forthcoming work [8].

Let us finally introduce some notation to be used throughout this paper. $\|\cdot\|_{0;\Omega}$ denotes the L_2-norm on Ω, whereas $(\cdot,\cdot)$ indicates the corresponding L_2-scalar product and $H^m(\Omega)$ (m being a positive integer) the usual Sobolev-space with norm $\|\cdot\|_{m;\Omega}$. $H^m(\Omega)$ with m a noninteger is to be understood as a suitable interpolation space as in [12]. Departing from the usual notation we let $\|\cdot\|_{-m;\Omega}$ be the norm of the dual of $H^m(\Omega)'$ defined by (see [10])

$$\|f\|_{-m} := \sup_{\chi \in H^m(\Omega)} \frac{(f,\chi)}{\|\chi\|_{m;\Omega}}. \tag{0.3}$$

For a fixed domain Ω, we may omit the Ω-index. If not otherwise indicated, C will be used as some generic constant and h will serve as a parameter characterizing the mesh-size of the finite element meshes.

1. THE CONTINUOUS PROBLEM

Let us first outline some basic analytical properties of the radiative transfer model equation (0.1) with $R(\theta,\theta^*) \equiv 1$ and the corresponding integral equation (0.2) for the scalar flux. Abbreviating the right side of (0.1) as $g(x)$, we get

$$n_\theta \cdot \nabla u(x,\theta) + \kappa(x)\, u(x,\theta) = g(x), \quad (x,\theta) \in \Omega \times S_n \tag{1.1a}$$

and

$$u(x, \theta) = b(x, \theta), \quad x \in \Gamma_\theta^- . \tag{1.1b}$$

Since (1.1) can also be interpreted as an ordinary differential equation along the straight characteristics (i.e., in n_θ-direction), we can explicitly define a solution operator T_θ for (1.1) by

$$u(x, \theta) = T_\theta g(x) := \int_0^{d(x,\theta)} \times \exp\left(- \int_0^s \kappa(x - tn_\theta)\, dt \right) g(x - sn_\theta)\, ds$$

$$+ \exp(-d(x, \theta))\, b(x - d(x, \theta)\, n_\theta), \tag{1.2}$$

where $d(x, \theta)$ denotes the distance of x from the inflow boundary Γ_θ^- in negative n_θ-direction. After an integration over the unit sphere, (1.2) results in

$$U(x) := \int_{S_n} u(x, \theta)\, d\theta$$

$$= \int_{S_n} \int_0^{d(x,\theta)} \times \exp\left(- \int_0^s \kappa(x - tn_\theta)\, dt \right) (\lambda U + f)(x - sn_\theta)\, ds\, d\theta + B(x),$$

with

$$B(x) := \int_{S_n} \exp(-d(x, \theta))\, b(x - d(x, \theta)\, n_\theta)\, d\theta .$$

Substituting $y := x - sn_\theta$ and $n_\theta = \dfrac{x - y}{s} = \dfrac{x - y}{|x - y|}$ furnishes

$$U(x) = \int_\Omega \exp\left(- \int_0^{|x-y|} \kappa\left(x - t \frac{x - y}{|x - y|} \right) dt \right) \times$$

$$\times (\lambda(y)\, U(y) + f(y)) \frac{1}{|x - y|^{n-1}}\, dy + B(x) . \tag{1.3}$$

Utilizing the weakly singular integral operators T_λ and T defined by

$$T_\lambda g(x) := \int_\Omega \exp\left(- \int_0^{|x-y|} \kappa\left(x - t \frac{x - y}{|x - y|} \right) dt \right) \frac{g(y)}{|x - y|^{n-1}}\, \lambda(y)\, dy ,$$

and

$$Tg(x) := T_1 g(x)$$

(1.3) may be written as

$$(I - T_\lambda) U(x) = Tf(x) + B(x) . \tag{1.4}$$

For the numerical analysis to come we need some basic stability properties of the operator T. Mikhlin has shown in [12] that T maps $L_2(\Omega)$ into $H^1(\Omega)$ and satisfies

$$\| Tg \|_1 \leq C \| g \|_0 , \tag{1.5}$$

so that U, for λ sufficiently small and H sufficiently smooth, fulfils

$$\| U \|_1 \leq C \| f \|_0 \tag{1.6}$$

with a positive constant $C = C(\lambda, T, \Omega)$.

Since both T and T_λ are compact as mappings in $L_2(\Omega)$, (1.4) is a weakly singular Fredholm equation of the second kind. Assuming from now on $1 \notin \sigma(T_\lambda)$, where $\sigma(T_\lambda)$ denotes the spectrum of T_λ, we obtain that $(I - T_\lambda)^{-1}$ exists on $L_2(\Omega)$, i.e., for a given $f \in L_2(\Omega)$, there exists a unique solution $U(x) = (I - T_\lambda)^{-1} Tf(x)$ of (1.4). This solution can then be inserted into (0.1) to get the unique solution of our radiative transfer model equation for any ordinate θ desired.

For reasons of simplicity, let us for now consider κ to be equal to one, $\lambda > 0$ to be a constant parameter, and set $b(x, \theta) \equiv 0$ on $\partial\Omega$ so that (1.4) becomes

$$(I - \lambda T) U(x) = Tf(x) \tag{1.7}$$

with

$$Tg(x) := \int_\Omega \exp(- |x - y|) \frac{g(y)}{|x - y|^{n-1}} dy ,$$

which means that existence and uniqueness of a solution to both (1.7) and (0.1) can be guaranteed for $\lambda^{-1} \notin \sigma(T)$. Let us also note that T is self-adjoint as shown in [1].

For numerical purposes, we would like to have some information about the smoothness of the solution U of (1.7). However, the smoothing property of T is, because of its weakly singular character, limited. In fact, various authors have shown (see, for example, [16]) that the generic regularity of U is

$U \in H^{3/2-\varepsilon}(\Omega)$, $\varepsilon > 0$. Note that even for an ideally smooth f with $f \neq 0$ near the boundary $\partial\Omega$, this singularity (which manifests itself mainly in areas close to the boundary, see [16]) cannot be outweighed.

2. A FINITE ELEMENT APPROACH

This section aims to establish some basic properties of the finite element method as applied to equation (1.7). We may formulate the following variational analogue of (1.7) :

Given $f \in L_2(\Omega)$, find $U \in L_2(\Omega)$ such that

$$((I - \lambda T)\, U, \varphi) = (Tf, \varphi) \quad \forall \varphi \in L_2(\Omega)\,. \tag{2.1}$$

In order to derive a corresponding finite element form of (2.1), we now take $V_h \subset L_2(\Omega)$ to be a finite-dimensional subspace characterized by the local approximation properties

$$\inf_{v_h \in V_h} \|v - v_h\|_{0;\Omega_1} \leq Ch^{2-k} \|v\|_{k;\Omega_1}\,, \quad k = 1, 2\,,$$

for all $v \in H^k(\Omega_1)$ and appropriate subdomains $\Omega_1 \subset \Omega$, where h is a mesh-width parameter. A typical example of this situation is furnished by the space of piecewise linear, continuous (or discontinuous) elements on a regular decomposition K_h of the domain Ω into triangles or tetrahedra K. Using this definition, the corresponding discrete analogue of (2.1) then reads : Find $U_h \in V_h$, such that

$$((I - \lambda T)\, U_h, \varphi_h) = (Tf, \varphi_h) \quad \forall \varphi_h \in V_h\,. \tag{2.2}$$

For λ sufficiently small, there holds for all $v \in L_2(\Omega)$:

$$((I - \lambda T)\, v, v) \geq (1 - \lambda \|T\|_0)\, \|v\|_0^2 = \gamma \|v\|_0^2 \quad \text{with } \gamma > 0\,, \tag{2.3}$$

which indicates an easy way to establish both existence and uniqueness of a solution $U_h \in V_h$ of (2.2), using the finite-dimensional character of V_h. In order to get an impression of the size of the scattering parameters λ allowed for the ensuing estimates, we must find an upper bound for the L_2-operator norm of T. First of all, the definitions of T and T_θ (see (1.2)) yield

$$\|T\|_0 = \left\| \int_{S_n} T_\theta \, d\theta \right\|_0 \leq \mu(S_n) \sup_\theta \|T_\theta\|_0\,,$$

where $\mu(S_n) := 2\,\Gamma(1/2)^n\, \Gamma(n/2)^{-1}$ is the measure of the n-dimensional unit-sphere with Γ denoting the Gamma-function. The size of $\|T_\theta\|_0$ follows

from a close look at the actual size of the stability constant featuring in the standard L_2-stability estimate of (1.1) as can be seen in [6]. We obtain $\|T_0\|_0 \leq 1$ and thus $\|T\|_0 \leq \mu(S_n)$, so that λ should comply by $\lambda \leq \lambda_0 < \mu(S_n)^{-1}$.

Remark : In a general physical setting, the function $\kappa(\,.\,)$ in (0.1) and (1.3) would have to be replaced by $\kappa(\,.\,) + \lambda(\,.\,)$, thus creating an additional dependence of the operator T_λ on λ. Setting both κ and λ constant, a stability analysis of the corresponding transport problem

$$n_0 \cdot \nabla u(x, 0) + (\kappa + \lambda)\, u(x, 0) = g(x)$$

quickly reveals that the critical scattering parameter λ_0 must obey $\lambda_0 < \kappa/(\mu(S_n) - 1)$.

Let us now prove two simple L_2- and H^{-1}-error estimates taking explicitly into account the reduced regularity of U in (1.7).

LEMMA 2.1 : *For* $0 < \lambda \leq \lambda_0$, *there holds*

$$\|U - U_h\|_{-1} + h\|U - U_h\|_0 \leq Ch^2\|f\|_0$$

with a positive constant $C = C(\lambda, \Omega)$ *and the norm* $\|\,.\,\|_{-1}$ *being defined in* (0.3).

Proof: Making use of Galerkin orthogonality, we have, setting $e := U - U_h$,

$$((I - \lambda T)\, e, e) = ((I - \lambda T)\, e, U - P_h U)\,,$$

where P_h represents the L_2-projection into V_h. Furthermore, standard L_2-estimates give

$$\begin{aligned}((I - \lambda T)\, e, U - P_h U) &\leq \|I - \lambda T\|_0\, \|e\|_0\, \|U - P_h U\|_0 \\ &\leq Ch\|I - \lambda T\|_0\, \|e\|_0\, \|U\|_1 \\ &\leq Ch\|e\|_0\, \|f\|_0\,,\end{aligned}$$

where stability estimate (1.6) has been used. The desired L_2-error estimate follows now from (2.3).

In order to prove a global H^{-1}-error estimate, we consider an auxiliary dual problem

$$(I - \lambda T)\, \varphi = g \quad \text{in } \Omega$$

with $g(x)$ being an arbitrary function in $H^1(\Omega)$. Observing that T is self-adjoint and employing once more the Galerkin orthogonality, we get

$$(e, g) = (e, (I - \lambda T)\varphi) = ((I - \lambda T)e, \varphi - P_h\varphi)$$

$$\leq C\|e\|_0 \|I - \lambda T\|_0 \|\varphi - P_h\varphi\|_0 \leq Ch\|e\|_0 \|\varphi\|_1 .$$

In view of the *a priori* bound (1.6), this estimate may also be written as

$$\|e\|_{-1} \leq Ch\|e\|_0 \leq Ch^2\|f\|_0 ,$$

thus finishing the proof. □

Remark: Making use of the maximal regularity available for U and employing a suitable interpolation argument, the results of Lemma 2.1 can theoretically be sharpened to

$$\|U - U_h\|_{-1} + h\|U - U_h\|_0 \leq C_\varepsilon h^{5/2-\varepsilon}\|f\|_0 .$$

The global *a priori* results above are only sub-optimal as both lag at least about half a power of h behind the interpolation error due to the pollution effect of the boundary. Therefore, several authors have explored different strategies to make up for this distinct lack of accuracy. One popular way to do so has been considered by Graham [9] who has, for the one-dimensional analogue of (1.7), developed a specific mesh refinement technique designed to at least partly suppress the effect of the loss of regularity close the boundary. Of course, it is quite possible to apply Graham's idea also to the n-dimensional equation discussed above, but since the boundary in our case is a manifold in $\mathbf{R}^n$ rather than merely two points, the additional computational cost would render this technique rather useless. In addition, as already mentioned before, the boundary $\partial\Omega$ may be a purely mathematical one of only limited physical importance.

Another perhaps for higher-dimensional problems more feasible way to boost the accuracy of our finite element method is to post-process the discrete solution U_h in the framework of a smoothing operation. Sloan and Thomée [17] have proposed such a technique based on the simple post-processing step

$$\tilde{U}_h(x) := \lambda T U_h(x) + Tf(x) ,$$

and have demonstrated that $\tilde{U}_h$ satisfies

$$\|\tilde{U}_h - U\|_0 \leq C\|U_h - U\|_{-1} ,$$

provided that T fulfils

$$\| Tg \|_0 \leq C \| g \|_{-1} .$$

The latter follows immediately from the fact that T is self-adjoint as well as from (1.5). Notice that the computation of TU_h is, at least in principle, inherent in the process of calculating the finite element solution U_h, so that computing $\tilde{U}_h$ should theoretically not increase the computational cost.

However, as already mentioned, numerous publications concerning the singularity of U Imply that the non-smooth character of U is confined to areas close to the boundary (see [16]), while there is apparently no reason to boost accuracy in the interior of Ω. Therefore, it would indeed be very desirable to have some kind of interior error estimate valid only in areas of higher regularity.

3. INTERIOR ERROR ANALYSIS

This section is devoted to presenting an *a priori* interior L_2-error estimate and a corresponding *a posteriori* analogue designed for use in adaptive finite element codes. Let U and U_h be the solutions of (2.1) and (2.2), respectively. The following theorem gives a simple proof for an *a priori* interior error estimate for the finite element approach outlined in the previous section.

THEOREM 3.1 : *For any fixed subdomains* Ω_1 *and* $\tilde{\Omega}_1$, $\Omega_1 \subset\subset \tilde{\Omega}_1 \subset\subset \Omega$, *such that* $U \in H^2(\tilde{\Omega}_1)$, *there holds*

$$\| U - U_h \|_{0;\Omega_1} \leq C \{ h^2 \| U \|_{2;\tilde{\Omega}_1} + \| U - U_h \|_{-1;\Omega} \} , \tag{3.1}$$

where $C > 0$ *depends on* Ω_1, $\tilde{\Omega}_1$, Ω *as well as on* $\operatorname{dist}(\partial\tilde{\Omega}_1, \partial\Omega)$ *and* $\operatorname{dist}(\partial\Omega_1, \partial\tilde{\Omega}_1)$.

Proof : We choose a cut-off function $\omega \in C_0^\infty(\Omega)$ obeying $\omega \equiv 1$ in Ω_1 and $\omega \equiv 0$ in $\Omega \backslash \tilde{\Omega}_1$, thus getting for $\lambda \leq \lambda_0$

$$\gamma \| e \|^2_{0;\Omega_1} \leq \gamma \| \omega e \|^2_{0;\Omega} \leq ((I - \lambda T) \omega e, \omega e) , \tag{3.2}$$

with γ as in (2.3). The commutator property, or even simpler, the smoothing property of T (see (1.5) or [12]) then induces

$$\begin{aligned} ((I - \lambda T) \omega e, \omega e) &= ((I - \lambda T) e, \omega^2 e) + \lambda ((\omega T - T\omega) e, \omega e) \\ &\leq ((I - \lambda T) e, \omega^2 e) + C \| e \|_{-1;\Omega} \| \omega e \|_{0;\Omega} . \end{aligned}$$

Using Galerkin-orthogonality leads us to

$$\gamma \| \omega e \|_{0;\Omega}^2 \leq ((I - \lambda T) e, \omega^2 e - P_h(\omega^2 e)) + C \| e \|_{-1;\Omega} \| \omega e \|_{0;\Omega}$$

$$\leq (e, \omega^2 e - P_h(\omega^2 e)) + |\lambda(\omega T e, we)| + C \| e \|_{-1;\Omega} \| \omega e \|_{0;\Omega}$$

$$\leq (U - P_h U, \omega^2 e - P_h(\omega^2 e)) + C \| e \|_{-1;\Omega} \| \omega e \|_{0;\Omega}$$

$$\leq (\omega(U - P_h U), \omega e) + C \| e \|_{-1;\Omega} \| \omega e \|_{0;\Omega},$$

where again, P_h denotes the L_2-projection into V_h. Then, using the approximation properties of P_h as well as (3.2) above, we obtain the desired result. □

In conjunction with the global negative Sobolov-norm estimate of Lemma 2.1, Theorem 3.1 guarantees an optimal interior L_2-error estimate away from the boundary of Ω. In order to prove an *a posteriori* result as sharp as possible, we must first derive an interior analogue of (1.6) with enhanced regularity properties.

LEMMA 3.2: *For domains* $\Omega_1 \subset\subset \tilde{\Omega}_1 \subset\subset \Omega$ $\delta := \text{dist}(\partial\Omega_1, \partial\tilde{\Omega}_1) > 0$, *and for any* $v \in L_2(\Omega)$ *there holds*

$$\| Tv \|_{0;\Omega_1} \leq C \| v \|_{-1;\tilde{\Omega}_1} + C_\varepsilon(\delta) \| v \|_{-3/2+\varepsilon;\Omega\setminus\tilde{\Omega}_1}, \tag{3.3}$$

where $C_\varepsilon(\delta) = O(\delta^{-n-1/2})$ *and* $\varepsilon > 0$ *is arbitrarily small, but fixed.*

Proof: The proof relies strongly on the fact that the domains Ω_1 and $\Omega\setminus\tilde{\Omega}_1$ are disjoint. There holds

$$\| Tv \|_{0;\Omega_1}^2 = \int_{\Omega_1} \left| \int_{\Omega} \exp(-|x-y|) \frac{v(y)}{|x-y|^{n-1}} dy \right|^2 dx$$

$$\leq 2 \int_{\Omega_1} \left| \int_{\Omega\setminus\tilde{\Omega}_1} \exp(-|x-y|) \frac{v(y)}{|x-y|^{n-1}} dy \right|^2 dx$$

$$+ 2 \int_{\Omega_1} \left| \int_{\tilde{\Omega}_1} \exp(-|x-y|) \frac{v(y)}{|x-y|^{n-1}} dy \right|^2 dx.$$

The second term on the right side can, in view of the smoothing property of T, be majorized by $C\|v\|^2_{-1;\tilde{\Omega}_1}$, giving us the first term for (3.3). In order to cope with the second term, we use

$$\int_{\Omega_1}\left|\int_{\Omega\setminus\tilde{\Omega}_1}\exp(-|x-y|)\,\frac{v(y)}{|x-y|^{n-1}}\,dy\right|^2 dx =$$

$$= \int_{\Omega_1}\left|\int_{\Omega\setminus\tilde{\Omega}_1}\exp(-|x-y|)\,\frac{\chi(y)\,v(y)}{|x-y|^{n-1}}\,dy\right|^2 dx,$$

where $\chi \in C^\infty(\Omega)$ with $\chi \equiv 1$ in $\Omega\setminus\tilde{\Omega}_1$ and $\chi \equiv 0$ in

$$U_{\delta/2}(\Omega_1) := \{x \in \Omega : \operatorname{dist}(x, \Omega_1) \leq \delta/2\}.$$

It follows that

$$\exp(-|x-y|)\,\frac{\chi(y)}{|x-y|^{n-1}} \in C^\infty(\Omega_1 \times \Omega\setminus\tilde{\Omega}_1),$$

thus inducing

$$\int_{\Omega_1}\left|\int_{\Omega\setminus\tilde{\Omega}_1}\exp(-|x-y|)\,\frac{v(y)}{|x-y|^{n-1}}\,dy\right|^2 dx$$

$$\leq C\|v\|^2_{-3/2+\varepsilon;\,\Omega\setminus\tilde{\Omega}_1}\int_{\Omega_1}\left\|\frac{\exp(-|x-\cdot|)}{|x-\cdot|^{n-1}}\right\|^2_{3/2-\varepsilon;\,\Omega\setminus\tilde{\Omega}_1} dx$$

$$\leq C_\varepsilon(\delta)\,\|v\|^2_{-3/2+\varepsilon;\,\Omega\setminus\tilde{\Omega}_1}. \tag{3.4}$$

□

Let us now derive an interior *a posteriori* error estimate for (1.7). The proof of such a local estimate for our integral equation is easier than for most PDE's as the relation between the error e and the residual $R(U_h) := Tf - (I-\lambda T)\,U_h = (I-\lambda T)\,e$ is rather weak. From now on we assume, as usual, $h = h(x)$ to be a piecewise constant function of x.

THEOREM 3.3 : *For subdomains $\Omega_1 \subset\subset \tilde{\Omega}_1 \subset\subset \Omega$ as above, there holds*

$$\|U-U_h\|_{0;\,\Omega_1} \leq \|R(U_h)\|_{0;\,\Omega_1} + C_I\,\lambda\{C_1\|hR(U_h)\|_{0;\,\tilde{\Omega}_1} +$$

$$+ C_2\|h^{3/2-\varepsilon}R(U_h)\|_{0;\,\Omega\setminus\tilde{\Omega}_1}\}, \tag{3.5}$$

where

$$C_1 := \frac{C}{(1-\lambda\|T\|_{0;\tilde{\Omega}_1})^2}, \quad C_2 := \frac{C_\varepsilon(\delta)}{(1-\lambda\|T\|_{0;\Omega\setminus\tilde{\Omega}_1})^2},$$

while C_I denotes an interpolation constant depending only on the shape of the elements considered, C results from the application of (1.6), *$\delta := \mathrm{dist}(\partial\Omega_1, \partial\tilde{\Omega}_1) > 0$, and again, $\varepsilon > 0$ is arbitrarily small, but fixed.*

Remark : Note that using the results of Theorem 3.1 above, the residual obeys

$$\|R(U_h)\|_{0;\Omega_1} \equiv \|(I-\lambda T)\, e\|_{0;\Omega_1} \leq Ch^2$$

for U sufficiently smooth in Ω_1, i.e., the residual $R(U_h) = (I-\lambda T)(U-U_h)$ and the actual error $U-U_h$ correspond directly to each other.

Remark : Before we embark on the proof of Theorem 3.3, it is important to define the norm of T on an arbitrary subdomain $\tilde{\Omega}$ of Ω and to get an impression of its actual size. We set for $g \in L_2(\tilde{\Omega})$

$$Tg(x) := T\tilde{g}\,(x),$$

where

$$\tilde{g}\,(x) := \begin{cases} g(x) & \text{for } x \in \tilde{\Omega} \\ 0 & \textbf{else}. \end{cases}$$

Using this definition (Only points $y \in \tilde{\Omega}$ contribute to the computation of $(Tg(x)\,!)$, we can conclude

$$\|T\|_{0;\tilde{\Omega}} := \sup_{0\neq g\in L_2(\tilde{\Omega})} \frac{\|Tg\|_{0;\tilde{\Omega}}}{\|g\|_{0;\tilde{\Omega}}} = \sup_{0\neq g\in L_2(\tilde{\Omega})} \frac{\|T\tilde{g}\|_{0;\tilde{\Omega}}}{\|g\|_{0;\tilde{\Omega}}}$$

$$\leq \sup_{0\neq g\in L_2(\tilde{\Omega})} \frac{\|T\tilde{g}\|_{0;\Omega}}{\|g\|_{0;\tilde{\Omega}}} = \sup_{0\neq g\in L_2(\tilde{\Omega})} \frac{\|T\tilde{g}\|_{0;\Omega}}{\|\tilde{g}\|_{0;\Omega}} \leq \|T\|_{0;\Omega}.$$

Further, the stability constant corresponding to $\tilde{\Omega}$ can be majorized as

$$C_{s,\tilde{\Omega}} := \|(I-\lambda T)^{-1}\|_{0;\tilde{\Omega}} \leq \frac{1}{1-\lambda\|T\|_{0;\tilde{\Omega}}}.$$

Proof: The fairly simple relation between the error e and the residual $R(U_h)$ leads to

$$\|e\|_{0;\Omega_1} \leq \|R(U_h)\|_{0;\Omega_1} + \lambda \|Te\|_{0;\Omega_1}, \tag{3.6}$$

so that, making use of the local smoothing property of T as described in Lemma 3.2, there follows

$$\|e\|_{0;\Omega_1} \leq \|R(U_h)\|_{0;\Omega_1} + C\lambda\{\|e\|_{-1;\tilde{\Omega}_1} + \|e\|_{-3/2+\varepsilon;\Omega\setminus\tilde{\Omega}_1}\}.$$

Now we must employ a local duality argument to get a sharp upper bound for the term $\|e\|_{-1;\tilde{\Omega}_1}$. Set $\varphi \in L_2(\Omega) \cap H^1(\tilde{\Omega}_1)$ equal to zero in $\Omega\setminus\tilde{\Omega}_1$ and let φ in $\tilde{\Omega}_1$ be determined by

$$(I - \lambda T)\varphi = g \in H^1(\tilde{\Omega}_1),$$

which entails

$$\|\varphi\|_{1;\tilde{\Omega}_1} \leq C_{s,\tilde{\Omega}_1} \|g\|_{1;\tilde{\Omega}_1}.$$

Following the path leading to the global H^{-1}-estimate in Section 2, we arrive at

$$(e, g) \leq C_I C_{s,\tilde{\Omega}_1} \|he\|_{0;\tilde{\Omega}_1} \|g\|_{1;\tilde{\Omega}_1},$$

or

$$\|e\|_{-1;\tilde{\Omega}_1} \leq C_I C_{s,\tilde{\Omega}_1} \|he\|_{0;\tilde{\Omega}_1}.$$

A similar (global) estimate for $\|e\|_{-3/2+\varepsilon;\Omega\setminus\tilde{\Omega}_1}$ finally delivers

$$\|e\|_{0;\Omega_1} \leq \|R(U_h)\|_{0;\Omega_1} +$$

$$+ C_I \lambda\{CC_{s,\tilde{\Omega}_1} \|he\|_{0;\tilde{\Omega}_1} + C_\varepsilon(\delta) C_{s,\Omega\setminus\tilde{\Omega}_1} \|h^{3/2-\varepsilon} e\|_{0;\Omega\setminus\tilde{\Omega}_1}\}.$$

Repeating now the error-splitting procedure (3.6) on both $\tilde{\Omega}_1$ and $\Omega\setminus\tilde{\Omega}_1$, we get

$$\|he\|_{0;\tilde{\Omega}_1} \leq \|hR(U_h)\|_{0;\tilde{\Omega}_1} + \lambda \|hTe\|_{0;\tilde{\Omega}_1}$$

and

$$\|h^{3/2-\varepsilon} e\|_{0;\Omega\setminus\tilde{\Omega}_1} \leq \|h^{3/2-\varepsilon} R(U_h)\|_{0;\Omega\setminus\tilde{\Omega}_1} + \lambda \|h^{3/2-\varepsilon} Te\|_{0;\Omega\setminus\tilde{\Omega}_1},$$

thus yielding for λ sufficiently small (see above)

$$(1 - \lambda \| T \|_{0;\tilde{\Omega}_1}) \| he \|_{0;\tilde{\Omega}_1} \leq \| hR(U_h) \|_{0;\tilde{\Omega}_1}$$

and

$$(1 - \lambda \| T \|_{0;\Omega\setminus\tilde{\Omega}_1}) \| h^{3/2-\varepsilon} e \|_{0;\Omega\setminus\tilde{\Omega}_1} \leq \| h^{3/2-\varepsilon} R(U_h) \|_{0;\Omega\setminus\tilde{\Omega}_1}$$

which finishes our proof. □

Let us now analyze the local *a posteriori* error estimate (3.5) in a little more detail, particularly the size of the constants on the right hand side and their dependence on the parameter δ. Assuming optimal local behavior in the L_∞-norm and taking $\tilde{\Omega}_1$ as some sort of a cluster of elements containing Ω_1 (perhaps even ranging up close to the boundary) somewhere inside of Ω, the terms on the right hand side of (3.5) show the following asymptotic behavior for $U \in H^{3/2-\varepsilon}(\Omega) \cap H^2(\tilde{\Omega}_1)$:

$$\| R(U_h) \|_{0;\Omega_1} \leq Ch^2 \mu(\Omega_1)^{1/2},$$

$$\| hR(U_h) \|_{0;\tilde{\Omega}_1} \leq Ch^3 \mu(\tilde{\Omega}_1)^{1/2},$$

$$\| h^{3/2-\varepsilon} R(U_h) \|_{0;\Omega\setminus\tilde{\Omega}_1} \leq C_\varepsilon(\delta) h^{3-2\varepsilon}. \tag{3.7}$$

Due to the constant $C_\varepsilon(\delta)$ the global term in (3.7) behaves like $O(h^{3-2\varepsilon}\delta^{-n-1/2})$, forcing us to choose $\delta \approx O(1)$, i.e., $\tilde{\Omega}_1$ should be a sufficiently large domain around Ω_1 and may even comprise almost the whole of Ω with the exception of the boundary layer ; otherwise our interior error estimator would possible over-estimate the error on Ω_1. The practical value of (3.5) is mainly based on the fact that it strives to separate potential global pollution effects caused by the lack of regularity from phenomena which may result from a locally non-smooth character of the right hand side function f in the interior of Ω. A suitable mesh-refinement strategy may now be constructed by comparing the size of the local terms in (3.5) to that of the boundary term which is possibly responsible for introducing a global pollution effect. In case of dominating local terms, one would have to refine the mesh locally applying, for example, the error-equilibrating technique put forth in [4] and [5]. As a result of such a process, the local error may be majorized by an expression mainly dominated by the « global » boundary term, thus giving us a prescription for effective local error control.

Another notable aspect of (3.5) is the local character of the stability constants $C_{s,\tilde{\Omega}}$ and their specific dependence on λ, especially in the case of a non-constant scattering parameter. Replacing T by T_λ while omitting the constant λ-factor yields

$$C_{s,\tilde{\Omega}} = \|(I - T_\lambda)^{-1}\|_{0;\tilde{\Omega}} \leq (1 - \|T_\lambda\|_{0;\tilde{\Omega}})^{-1}.$$

In addition, there holds (for $\kappa \equiv 1$)

$$\|T_\lambda\|_{0;\tilde{\Omega}} = \sup_{0 \neq g \in L_2(\tilde{\Omega})} \frac{\|T_\lambda g\|_{0;\tilde{\Omega}}}{\|g\|_{0;\tilde{\Omega}}}$$

$$= \sup_{0 \neq g \in L_2(\tilde{\Omega})} \frac{\|T(\lambda g)\|_{0;\tilde{\Omega}}}{\|\lambda g\|_{0;\tilde{\Omega}}} \frac{\|\lambda g\|_{0;\tilde{\Omega}}}{\|g\|_{0;\tilde{\Omega}}} \leq |\lambda|_{\tilde{\Omega}} \|T\|_{0;\tilde{\Omega}},$$

and thus

$$C_{s,\tilde{\Omega}} \leq (1 - \|T_\lambda\|_{0;\tilde{\Omega}})^{-1} \leq (1 - |\lambda|_{\tilde{\Omega}} \|T\|_{0;\tilde{\Omega}})^{-1},$$

where $|\lambda|_{\tilde{\Omega}} := \max_{x \in \tilde{\Omega}} |\lambda|$. It follows that a locally large value of λ will automatically cause a locally large stability constant $C_{s,\tilde{\Omega}}$ for this subdomain, always provided that an erratic behavior of λ does not destroy the overall solvability of (1.4). As a result, our *a posteriori* error estimate is also able to differentiate between areas of negligible scattering and those with considerable scattering activity, i.e., it opens the way for the development of a λ-adaptive finite element technique.

Applying an L_2-duality argument, we can derive yet another possibly sharper local *a posteriori* error estimate for (2.2). Let $\varphi \in L_2(\Omega)$ be the solution of

$$(I - \lambda T)\varphi = \omega e \quad \text{in} \quad \Omega,$$

where $\omega \in C_0^\infty(\Omega)$, $\Omega_1 \subset\subset \tilde{\Omega}_1 \subset\subset \Omega$, is a cut-off function with $\omega \equiv 1$ in Ω_1 and $\omega \equiv 0$ in $\Omega \backslash \tilde{\Omega}_1$. There follows

$$\|e\|_{0;\Omega_1}^2 \leq \|\omega e\|_{0;\Omega}^2 = ((I - \lambda T)\varphi, \omega e)$$

$$= ((I - \lambda T) e, \omega\varphi - P_h(\omega\varphi)) + \lambda((\omega T - T\omega) e, \varphi) = I + II.$$

As in Theorem 3.1, term II allows the estimate

$$II \leq C(\omega, T)\lambda \|e\|_{-1;\Omega} \|\varphi\|_{0;\Omega} \leq C_s C(\omega, T)\lambda \|e\|_{-1;\Omega} \|\omega e\|_{0;\Omega},$$

e.g., produces a negligible term of higher order in h. Assuming $\bar{R} \in V_h$ to be some local approximation of R, the first term yields

$$I = ((I - \lambda T)\, e, \omega\varphi - P_h(\omega\varphi)) = (R(U_h) - \bar{R}(U_h), \omega\varphi - P_h(\omega\varphi))$$

$$\leq \sigma(\omega) \| R(U_h) - \bar{R}(U_h) \|_{0;\tilde{\Omega}_1} \| \omega e \|_{0;\Omega},$$

with $\sigma(\omega) := \dfrac{\| \omega\varphi \|_{0;\Omega}}{\| \omega e \|_{0;\Omega}}$ thus resulting in

$$\| e \|_{0;\Omega_1} \leq \sigma(\omega) \| R(U_h) - \bar{R}(U_h) \|_{0;\tilde{\Omega}_1} + \text{« global higher order term »} \tag{3.8}$$

The introduction of a suitable $\bar{R}$ is likely to reduce the size of the right hand side of (3.8), even for non-smooth R. Note that, given an approximation $\tilde{e}$ of e (take, for example, $\tilde{e} := U_h - U_{h/2}$), it is in principle possible to calculate the quantity $\sigma(\omega)$, thereby vindicating (3.8) as a real *a posteriori* error estimate.

Finally, let us now address the question of how to actually compute the radiative intensity $u(x, \theta)$ for an arbitrary ordinate θ. Setting κ for simplicity constant and inserting the discrete solution U_h of (2.2) into the transport equation (1.1) yields (note that the intensity now depends on the mesh-size h of the mesh used for the computation of U_h):

$$n_\theta \cdot \nabla u_h(x, \theta) + \kappa u_h(x, \theta) = \lambda U_h(x) + f(x). \tag{3.9}$$

As outlined in Section 1, the solution of (3.9) along one of the straight characteristics can be written as

$$u_h(x, \theta) = \int_0^{d(x,\theta)} \exp(-\kappa s)\, (\lambda U_h + f)\, (x - s n_\theta)\, ds, \tag{3.10}$$

thus giving us a simple prescription for actually computing $u_h(x, .)$, i.e., replacing the integral in (3.10) by a cubature formula (see also [15] for an application of the characteristic method to a real-world radiative transfer problem). This characteristic technique even allows us (for a sufficiently exact cubature rule) to derive an *a priori* interior error estimate for the radiative intensity without any further assumptions on the regularity of $u(x, .)$. Note that the evaluation of the integral in (3.10) is greatly facilitated by the fact that U_h is a piecewise linear function.

LEMMA 3.4 : *For any domain* $\Omega_1 \subset\subset \Omega$ *with* $\delta := \operatorname{dist}(\partial\Omega, \partial\Omega_1) > 0$ *and a sufficiently exact cubature rule for the characteristic method, the* L_2*-error for the radiative intensity obeys*

$$\|(u-u_h)(\,.\,,\theta)\|_{0;\Omega_1} \leq C\{\|U-U_h\|_{0;\Omega_1} + \\ + \exp(-\kappa\delta)\,\|U-U_h\|_{0;\Omega}\}\,, \quad (3.11)$$

so that for $\kappa\delta$ *sufficiently large, we can expect optimal interior accuracy for* $u_h(x,\,.\,)$.

Proof : Again, the idea is to split up the right hand side of (3.10) into a purely interior part and boundary contributions. There holds (neglecting the cubature error)

$$\|(u-u_h)(\,.\,,)\|^2_{0;\Omega_1} = \left\| \lambda \int_0^{d(\,.\,,\theta)} \exp(-\kappa s)\,(U-U_h)(\,.\,-sn_\theta)\,ds \right\|^2_{0;\Omega_1}$$

$$\leq \left\| \lambda \int_0^{d(\,.\,,)-\delta} \exp(-\kappa s)\,(U-U_h)(\,.\,-sn_\theta)\,ds \right\|^2_{0;\Omega_1} \cdot$$

$$+ \left\| \int_{d(\,.\,,\theta)-\delta}^{d(\,.\,,\theta)} \exp(-\kappa s)\,(U-U_h)(\,.\,-sn_\theta)\,ds \right\|^2_{0;\Omega_1}$$

Clearly, the first integral now includes only points x in the interior domain Ω_1 and can thus be majorized by $C\|U-U_h\|^2_{0;\Omega_1}$, producing the first term on the right hand side in (3.10). The second integral extends over the boundary region and therefore only permits the usual global estimate for the mean intensity U including, however, the multiplicative factor $\exp(-\kappa\delta)$. □

We may control the global term on the right hand side of (3.11) by assuming $\kappa\delta$ to be sufficiently large, i.e., by choosing

$$\exp(-\kappa\delta) \leq h^{1/2-\varepsilon} \approx h^{1/2}$$

which entails

$$\|(u-u_h)(\,.\,,\theta)\|_{0;\Omega_1} \leq Ch^2\,.$$

As a result, δ must obey $\delta \leq (2\kappa)^{-1} \ln(1/h)$, so that Ω_1 must lie sufficiently far away from $\partial\Omega$. We emphasize that for a negligible absorption

factor κ, this prescription may be impossible to fulfil so that (3.10) would guarantee only sub-optimal accuracy for u (always provided that an adequate numerical integration formula is used for solving the transport problem).

Remark : Of course, if a user is interested in getting precise information about the behavior of u in a fixed interior domain Ω_1, the distance δ has to grow like $\ln(1/h)$ to ensure optimal order convergence of the method, i.e., the domain Ω (the « observers's frame ») may have to be enlarged artificially. Consequently, several of the « constants » C, $C_\varepsilon(\delta)$, C_1, C_2, etc. used in various lemmata and theorems above also grow and could render our estimate useless if this growth with Ω turned out to be exponential. However, a thorough study of the dependence of these constants on Ω reveals only linear growth with increasing $\mu(\Omega)$ (see also [1], [6] and [12]), thus preserving the overall structure of (3.11).

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