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Properties of Solutions and Eigenfunctions of Multigroup Diffusion Problems

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"Properties of Solutions and Eigenfunctions of Multigroup Diffusion Problems"

by

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ABSTRACT

A variational formulation of the static multigroup diffusion equations for heterogeneous assemblies provides a rigorous mathematical foundation for the solution of the time eigenvalue and the time-dependent initial value problems. Theorems on existence, uniqueness, regularity, and positivity are stated, and a proof that the generalized eigenfunctions are complete in L^2 is indicated.

"Eigenschaften der Lösungen und der Eigenfunktionen der Mehrgruppen-Diffusions-Probleme"

KURZFASSUNG

Durch eine variationstheoretische Formulierung der statischen Mehrgruppen-Diffusionsgleichungen für heterogene Anordnungen wird die Lösung der Zeiteigenwert- und der zeitabhängigen Anfangswertaufgabe mathematisch begründet.
Sätze über Existenz, Eindeutigkeit, Regularität und Positivität werden mitgeteilt; es wird ein Beweis angedeutet, daß die verallgemeinerten Eigenfunktionen vollständig in L^2 sind.

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INTRODUCTION

A basic paper in the theory of the differential equations for multigroup neutron diffusion has for some time been that of Habetler and Martino [1]; these authors offered an approach to strict mathematical analysis of the time-dependent diffusion equations as well as of the effective multiplication rate eigenvalue problem. For example, Habetler and Martino showed the completeness of eigenfunctions (of the time rate eigenvalue problem) for one-dimensional problems and for homogeneous two- and three-dimensional problems. A main result of the present work is the completeness of eigenfunctions for general heterogeneous problems in the higher dimensions.

In addition to this extension of previous results, the present author has noticed important mathematical points in Habetler and Martino's work which at least need further clarification. For this reason, a somewhat different approach in this paper - the weak or variational formulation of the static problem - will be developed systematically from the beginning. This approach employs functional analysis and much of the recent theory of elliptic boundary value problems. We shall summarize rather completely the results of our analysis; full proofs will appear elsewhere [2]. We also choose to omit discussion of the multiplication rate eigenvalue problem, and concentrate on the time-dependent equations and the related time rate eigenvalue problem. Starting from the weak formulation, we establish the existence and uniqueness of solutions to the initial value problem, the completeness of generalized eigenfunctions, and positivity properties of solutions.

PROBLEM

The following assumptions suffice for all the results of this paper. The multigroup diffusion equations determine a neutron flux distribution $\phi(x) = (\phi_1(x), \phi_2(x), \ldots, \phi_G(x))$ in G energy groups within a space domain Ω. Here Ω will be a bounded connected open set in Euclidean n-space, $n = 1,2,3$, with boundary $\partial\Omega$ made up of a finite number of intersecting smooth $(n-1)$-dimensional surfaces. To specify smoothness we introduce the following definitions. A function f satisfies a <u>Hölder condition</u> with Hölder exponent $\mu > 0$ if $|f(x) - f(y)| \leq M|x-y|^{\mu}$. The class $C^{j,\mu}(F)$ consists of functions on a set F whose partial derivatives up to order j satisfy a Hölder condition uniformly in F. An $(n-1)$-dimensional surface will be called $C^{j,\mu}$ if it is represented by local coordinate functions which, together with their inverses, are in $C^{j,\mu}(B)$, where B is a unit ball in n-space, and the surface is locally the image of a plane in B. Using these terms, the surfaces making up $\partial\Omega$ must be $C^{2,\mu}$, and $\partial\Omega$ as a whole must be $C^{0,1}$. (The latter condition prevents the surfaces from joining in sharp cusps.) Ω may also be subdivided by further $C^{2,\mu}$ surfaces into open subsets Ω_r, $r = 1,2,\ldots R$. These usually correspond to different material regions. A point where two of the smooth surfaces intersect is called a corner. (See Figure.)

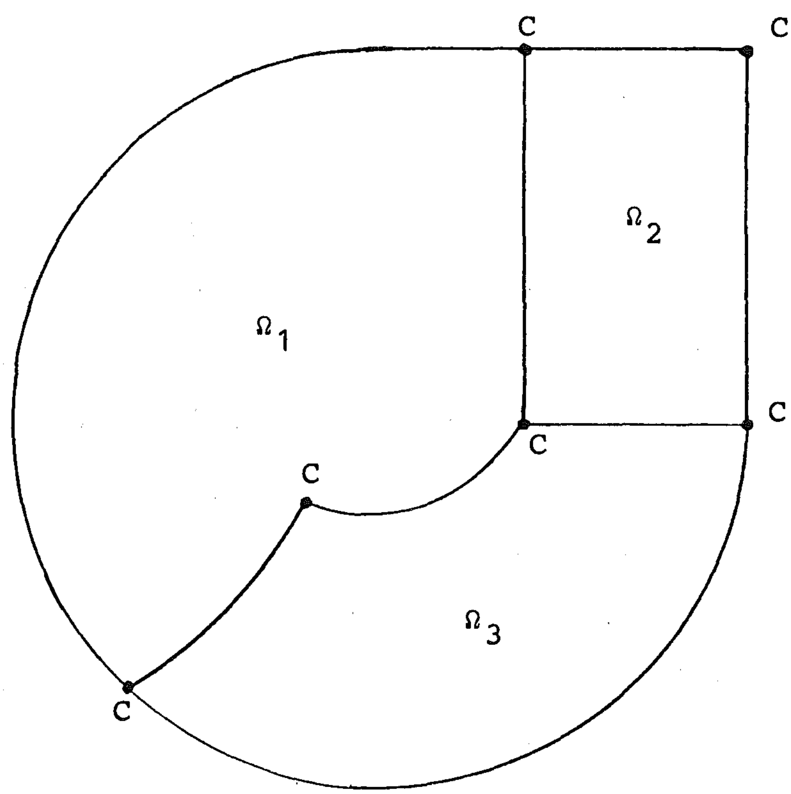

Figure: A possible plane region Ω showing corners indicated by C.

On Ω we have group diffusion coefficients $d_g(x)$, $g = 1,2,\ldots,G$, and group transfer cross sections $\sigma_{gh}(x)$, $g,h = 1,2,\ldots,G$. The latter include absorption and scattering processes, and all fission processes as well. The time-dependent differential equations for multi-group diffusion would be

$$v_g^{-1}\,\partial\phi_g/\partial t - \nabla\cdot d_g\nabla\,\phi_g + \sum_{h=1}^{G}\sigma_{gh}\,\phi_h = s_g\,, \tag{1}$$

where s_g are inhomogeneous neutron sources; or,

$$V^{-1}\,\partial\phi/\partial t - D\phi + S\phi = s. \tag{2}$$

The d_g must be in $C^{1,\mu}(\Omega_r)$ for each subregion Ω_r, real, positive, and everywhere greater than some positive minimum value δ. The neutron group velocities v_g shall be in $C^{0,\mu}(\Omega_r)$ for each r, and also positive with positive minimum. The σ_{gh} must be $C^{0,\mu}(\Omega_r)$, real, and non-positive for $g \neq h$. Note that we allow arbitrary up- and down-scattering and an unrestricted form of the fission matrix. The only additional restriction, for positivity theorems only, will be transitivity of the σ_{gh}.

With equation (1) come certain boundary conditions and continuity conditions. At present, only the Dirichlet boundary condition

$$\phi = 0 \quad \text{on} \quad \partial\Omega \tag{3}$$

will be considered. Continuity conditions arise at surfaces $\partial\Omega_r \cap \partial\Omega_s$ across which the coefficients have jump discontinuities. At points where $\partial\Omega_r$ is smooth, and hence has a well-defined normal vector, one requires

ϕ_g and the normal component of $d_g \nabla \phi_g$ continuous across each interface. (4)

Points where $\partial\Omega_r$ is not smooth are the corners.

The time-dependent equation (2) is closely related to the time rate eigenvalue equation

$$-D\phi + S\phi \equiv -L\phi = \lambda\phi. \tag{5}$$

The same conditions (3) and (4) go with this equation as well. Neutron velocities may be included by replacing L with VL - this remark applies throughout the sequel. A study of (5) yields valuable information about (2).

WEAK SOLUTIONS

Let $L^2(\Omega)$ be the space of complex measurable vector functions ϕ on Ω whose norms

$$\|\phi\| = \int_\Omega |\phi(x)|^2 \, dx$$

are finite; $L^2(\Omega)$ is a Hilbert space with inner product $(\phi,\psi) = \int_\Omega \phi\overline{\psi}\, dx$. Weak solutions will be functions in the Hilbert space $H_0^1(\Omega)$: from the set of functions having bounded continuous first partial derivatives and satisfying the boundary condition (3), one takes the completion in the norm

$$\|\phi\|_1 = \|\phi\| + \int_\Omega |\nabla\phi(x)|^2\, dx ,$$

that is, all possible limits of sequences converging in $\|\cdot\|_1$, to obtain $H_0^1(\Omega)$. Functions in $H_0^1(\Omega)$ have first partial derivatives, belonging to $L^2(\Omega)$, in a generalized sense; they need not be continuously differentiable in the usual sense [(3)]. Such functions also satisfy the zero Dirichlet boundary condition in a generalized sense.

The variational formulation of the static problem (5) amounts to replacing the differential equation (and continuity conditions) for ϕ by a condition on ϕ expressed with a bilinear form. For motivation, we recall that the static diffusion equation (for one group) can be derived from the condition

$$\int_{\partial V} j \cdot \nu\, dS = \int_V (-\sigma\phi - s)\, dx$$

for all volumes $V \subset \Omega$, together with the diffusion law $j = d\nabla\phi$. Now if χ_V is a function which equals 1 inside V and zero outside, then $\nabla\chi_V$ is a Dirac distribution for line integration along an outward normal across ∂V, so the left side above can be re-written

$$-\int_\Omega d\nabla\phi \cdot \nabla\chi_V \, dx = \int_\Omega (-\sigma\phi - s)\, \chi_V \, dx ,$$

a condition which we still require for all χ_V with $V \subset \Omega$. The variational formulation we are about to introduce is the same condition, but instead of all step functions χ_V we use all $\psi \in H_o^1(\Omega)$.

To be precise, $\phi \in H_o^1(\Omega)$ will be a <u>weak</u> <u>solution</u> of the equations

$$-\nabla\cdot d_g \nabla\phi_g + \sum_h \sigma_{gh}\phi_h = s_g \tag{6}$$

if

$$\begin{aligned} B(\phi,\psi) &\equiv \int_\Omega \Big(\sum_g d_g \nabla\phi_g \cdot \nabla\overline{\psi}_g + \sum_{g,h} \sigma_{gh}\phi_h\overline{\psi}_g\Big)\, dx \\ &= \int_\Omega \sum_g s_g \overline{\psi}_g \, dx = (s,\psi) \end{aligned} \tag{7}$$

holds for all $\psi \in H_o^1(\Omega)$.

This weak formulation has become well known in the mathematical theory of elliptic partial differential equations, and a number of results can be borrowed from the established theory [3],[4],[5]. For a given bilinear form B, consider all pairs $\{\phi, s\}$ such that $B(\phi,\psi) = (s,\psi)$ for all $\psi \in H_o^1(\Omega)$. Let the set of all ϕ's from such pairs be Ⓓ, which is a subset of $H_o^1(\Omega)$. It is not hard to show that any $\phi \in$ Ⓓ corresponds to exactly one $s \in L^2(\Omega)$, which makes possible the

<u>Definition</u>: The mapping $\phi \to s$ is denoted by $\underline{\underline{L}}$, so that a weak solution ϕ of (6) is a solution of the operator equation $\underline{\underline{L}}\phi = s$.

In fact, $\underline{\underline{L}}$ is a closed linear operator in $L^2(\Omega)$, and one establishes the following a priori estimate:

$$\delta \| \phi \|_1 \leq \| (\underline{\underline{L}} + \lambda_o)\phi \| \leq \| \underline{\underline{L}}\phi \| + \lambda_o \| \phi \| \tag{8}$$

for some $\lambda_o > 0$ and all $\phi \in$ Ⓓ. One also discovers, using the Lax-Milgram theorem [3], that every $s \in L^2(\Omega)$ has a solution of $(\underline{\underline{L}} + \lambda_o)\phi = s$; by (8) this solution ϕ is unique, so $\underline{\underline{L}} + \lambda_o$ has an inverse, which maps $L^2(\Omega)$ back onto Ⓓ $\subset H_o^1(\Omega)$. Rellich's theorem [3] states that $H_o^1(\Omega)$ is a compact subspace of $L^2(\Omega)$, so $(\underline{\underline{L}} + \lambda_o)^{-1}$ is a compact operator. Applying the Riesz-Schauder spectral theory of compact operators [6], one can reach

<u>Theorem 1</u>: The spectrum of $\underline{\underline{L}}$ consists of a countable sequence of isolated eigenvalues of finite multiplicity which tend to infinity.

Presently we will locate the eigenvalues more precisely.

REGULARITY

The operator $\underline{\underline{L}}$ has been defined from the weak formulation (7), but it is perhaps still unclear why we say that a solution of $\underline{\underline{L}}\phi = s$ is called a weak solution of the differential equations (6). Weak solutions need only have partial derivatives of first order, and these in a generalized sense. We would like to know that weak solutions are more regular: that they actually have continuous partial derivatives of second order inside Ω_r which satisfy (6).

Theorem 2 : Let $\underline{\underline{L}}\phi = s$, where $s \in C^{0,\mu}$ in each Ω_r. Then for some $\mu' > 0$, $\phi \in C^{0,\mu'}(\bar{\Omega})$ and takes the value zero continuously at $\partial\Omega$. Any point inside Ω_r has a neighborhood in which $\phi \in C^{2,\mu'}$ and satisfies the differential equations (6). At any point in $\partial\Omega_r$ where the interface is $C^{2,\mu}$, $\phi \in C^{2,\mu'}$ up to the interface from inside Ω_r and from inside the neighboring Ω_s, and satisfies the continuity conditions (4).

Remarks: The proof draws on results well known in the theory of elliptic boundary value problems. The hard part is proving the regularity (i.e. differentiability) of ϕ; once that is known, the differential equations and the continuity conditions can be derived by integrating the bilinear form by parts and using the arbitrary nature of ψ.

We emphasize that Theorem 2 does not claim the second derivatives of ϕ are bounded up to a corner point. In fact, recent work [7],[8] has shown examples where this is false. This raises substantial objection to the analysis of Habetler and Martino, who seem to claim that second derivatives are bounded at corners. For example, one may only integrate by parts over a region away from corner singularities. The weak formulation has the advantage of defining a uniquely solvable problem and avoids many difficulties related to corner singularities. Also, as we tried to show in motivating (7), the weak formulation has some physical sense.

TIME-DEPENDENT EQUATION

A basic tool for mathematical analysis of the time-dependent diffusion equations (1) is an estimate for the resolvent of $-\underline{\underline{L}}$, $R(z;-\underline{\underline{L}}) = (-\underline{\underline{L}}-z)^{-1}$. In Hilbert space this estimate follows without great difficulty if the spectrum of $-\underline{\underline{L}}$ be shown to lie near the negative real axis in the complex plane. Our multigroup diffusion operator $-\underline{\underline{L}}$ consists of a self-adjoint operator $-\underline{\underline{D}}$ with spectrum on the negative real axis, perturbed by a bounded operator $\underline{\underline{S}}$. One finds that the spectrum of $-\underline{\underline{L}}$ (which by Theorem 1 consists only of eigenvalues) thus falls within a semi-infinite band of fixed width about the negative real axis.

Theorem 3: For any $\varepsilon > 0$ there are constants $\lambda, C > 0$ such that

$$\| (\underline{\underline{L}} + z)^{-1} \| \leq C/|z| \tag{9}$$

for all complex z with $|z| \geq \lambda$ and $|\arg z| \leq \pi - \varepsilon$.

This estimate represents the main condition under which $-\underline{\underline{L}}$ generates an analytic semigroup (9) of operators $U(t)$ for $t \geq 0$. Recall that this semigroup, also written $\exp(-t\underline{\underline{L}})$, has the properties $\exp(-(t+s)\underline{\underline{L}}) = \exp(-t\underline{\underline{L}}) \cdot \exp(-s\underline{\underline{L}})$ and $(d/dt) \exp(-t\underline{\underline{L}}) = -\underline{\underline{L}} \exp(-t\underline{\underline{L}})$. According to the Hille-Yosida semigroup theory, Theorem 3 further implies $U(t)$ is analytic in t for complex t with $\mathrm{Re}\, t > 0$, and tends strongly in $L^2(\Omega)$ to the identity operator as $t \to 0$. One can construct $U(t)$ from $\underline{\underline{L}}$ by a modified inverse Laplace transform of $\underline{\underline{L}}$; the transformation integral converges due to (9).

The semigroup $U(t)$ gives solutions to an abstract initial value problem. Let $\phi_0 \in L^2(\Omega)$, and define

$$\phi(t) = U(t)\, \phi_0.$$

Then $\phi(t)$ is a function of t with values in $L^2(\Omega)$. By the properties above, $\phi(t)$ is a solution of the abstract Cauchy problem

$$d\phi/dt + \underline{\underline{L}}\phi = 0$$
$$\phi(t) \to \phi_o \text{ in } L^2(\Omega) \text{ as } t \to 0.$$

Here the derivative is taken abstractly, in the sense of functions with values in a Banach space; it does not mean a partial derivative of $\phi(x,t)$ with respect to t. However, using a more refined analysis of our particular $\underline{\underline{L}}$, and estimates in the supremum norm on Ω, the existence of the partial derivative in t can be established.

Theorem 4: Let $\phi_o(x) \in L^2(\Omega)$. There exists a unique function $\phi(x,t)$ continuous in x and analytic in t on $\bar{\Omega} \times (0,T]$ and zero on $\partial\Omega \times (0,T]$, twice continuously differentiable in x in each $\Omega_r \times (0,T]$ and satisfying the time-dependent diffusion equation

$$v_g^{-1}\, \partial\phi_g/\partial t - \nabla\cdot d_g\nabla\phi_g + \sum_h \sigma_{gh}\phi_h = 0 \qquad (10)$$

there, and satisfying the continuity condition (4) on smooth parts of $\partial\Omega_r \cap \partial\Omega_s$ for $t > 0$, and $\phi(x,t) \to \phi_o(x)$ in $L^2(\Omega)$ as $t \to 0$.

Duhamel's principle yields solutions of the inhomogeneous equations (1) as well [9].

The resolvent estimate of Theorem 3 above can also be used in proving that the generalized eigenfunctions of $\underline{\underline{L}}$ are complete in $L^2(\Omega)$. We say a non-zero function ϕ

is a <u>generalized eigenfunction</u> of $\underline{\underline{L}}$ corresponding to the eigenvalue λ_j if for some positive integer k, $(\underline{\underline{L}} - \lambda_j)^k \phi = 0$. Using (9) and arguments adapted from Agmon (10) and Dunford and Schwartz (11), we get:

<u>Theorem 5</u>: The generalized eigenfunctions of $\underline{\underline{L}}$ are complete in $L^2(\Omega)$. Every $\phi_o \in L^2(\Omega)$ has a biorthogonal expansion in these generalized eigenfunctions converging in $L^2(\Omega)$, and the corresponding expansion for $\phi(x,t)$ converges in $L^2(\Omega)$ uniformly on $[0,T]$.

<u>Remarks:</u> By a biorthogonal expansion we mean an expansion in eigenfunctions of $\underline{\underline{L}}$, the coefficients of the expansion being found by inner products with corresponding eigen-functions of the adjoint of $\underline{\underline{L}}$ (which is an adjoint in the strict mathematical as well as the formal sense). Formulas may be found for example in Habetler and Martino (1). The convergence of the expansion for $\phi(x,t)$ depends on the fact that $-\underline{\underline{L}}$ generates a semigroup of bounded operators in $L^2(\Omega)$. Other partial results about completeness and convergence in supremum norm and in $\|\cdot\|_1$ are possible.

We repeat that neutron group velocities may always be included (occasionally with extra effort) by replacing $\underline{\underline{L}}$ with $\underline{\underline{V}}\,\underline{\underline{L}}$.

POSITIVITY

For physical reasons one expects that a positive initial neutron distribution will result in a flux which is positive for all later time. This expectation is confirmed mathematically for the time-dependent diffusion equations (10). For the next two theorems we need to assume the <u>transitivity</u> of the σ_{gh} , i.e. for any two groups g_1 and g_m there is a transitive chain of groups $g_1, g_2, \ldots g_m$ such that $\sigma_{g_i, g_{i+1}}$ is not everywhere zero.

<u>Theorem 6</u>: If ϕ_o is non-negative and not identically zero, then $\phi(x,t)$ of Theorem 4 is non-negative, and strictly positive except on $\partial\Omega$ and possibly at corners.

The proof that $\phi(x,t)$ is non-negative seems surprisingly difficult; but once ϕ is known to be non-negative, the strict positivity follows using classical maximum principles applied in each subregion Ω_r.

Aside from its intrinsic interest, the positivity of solutions of (10) also helps prove the existence of a dominant mode.

<u>Theorem 7</u>: There is a dominant mode for the time-dependent equations (10) which is positive and unique up to a constant factor, corresponding to a simple real eigenvalue of $\underline{\underline{L}}$ larger than the real part of any other eigenvalue.

One proves this theorem by applying results of Krein and Rutman[(12)] to the operator $U(t)$, which is a positive compact operator in $L^2(\Omega)$ for any particular $t > 0$.

CONCLUSIONS

The weak or variational formulation offers a useful starting point for rigorous mathematical analysis, especially as it allows one to bypass difficulties caused by singular solutions at corner points. From this basis, the existence and uniqueness of generalized solutions to the time-dependent initial value problem for multigroup diffusion can be established under very few restrictions. These generalized solutions are almost solutions in a classical sense; it remains only to show that initial values are taken on continuously. (We showed they are taken on in the square integral sense.) Solutions of the time-dependent problem are positive for positive time if the initial values are non-negative, and there is a positive dominant mode. The generalized eigenfunctions are complete in L^2, permitting biorthogonal expansions of arbitrary initial values and of the corresponding solutions for later time.

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