Mathematical Methods in Energy Research

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PREFACE

During the Academic Year 1982-83 the Mathematics Department at the University of Wyoming sponsored a special year devoted to the mathematics of energy. In light of the abundance of energy and mineral resources in Wyoming, and the resultant importance of the State in the nation's long-term energy outlook, it seems only natural that one should emphasize on campus the importance of mathematical modelling and analysis in energy exploration and production as well as in the associated environmental concerns. Indeed, besides serving as an introduction for both faculty and students to potential research areas in mathematics, the emphasis on physical applications and origins of problems provides an interdisciplinary forum for faculty and students from many other science and engineering departments.

As evidenced by the list of participants and the short-term visitors in the Special Lecture Series, the Energy Year program stressed the close cooperation between mathematicians in academia and those in industry, as well as interaction with mathematical researchers in other areas of science and engineering.

The major areas discussed in courses, seminars, and the visiting lecture series can be loosely grouped under the following five headings: (1) Mathematical modelling related to hydrocarbon recovery, flow in porous media, combustion and chemical reactors. (2) Mathematical analysis of coupled systems of nonlinear partial differential equations. (3) Numerical analysis of transport-dominated flow in two and three dimensions. (4) Computational algorithm development for large, sparse, nonlinear, nonsymmetric systems of equations. (5) Inverse problems, especially related to reflective seismology and geophysical prospecting.

The papers appearing in this Proceedings are quite varied in nature, some are expansions of topics presented in the Energy Year Lecture Series, and others represent recent research on a subject appropriate to these Proceedings. The reader interested in a more systematic expository development of the general subject matter is referred to the first three volumes of the new SIAM series Frontiers in Applied Mathematics. Volume 1, edited by Dr. Richard Ewing, deals with the mathematics of reservoir simulation; Volume 2, edited by Dr. John Buckmaster, concerns combustion and chemical stability; and Volume 3, edited by Dr. Robert Burridge, treats seismic exploration and inversion. It should be mentioned that these volumes are, in part, also an outgrowth of the Special Energy Year at Wyoming.

It is a pleasure to express our gratitude to all who made this special year possible and contributed to its success, including the participants and visitors from academia and industry who gave generously of their time and effort and to the authors who contributed to this volume. Special thanks are due to several individuals. Dr. Richard E. Ewing, the J. E. Warren Professor of Energy and Environment, organized the scientific program and served as a focus for the year's activities. My colleagues, Professors John George, Eli Isaacson, and Duane Porter provided invaluable help. Their efforts during the year were unflagging. I would like to express appreciation to SIAM for its encouragement and support of these Proceedings and to the Rocky Mountain Mathematics Consortium for sponsoring the two summer schools that inaugurated and capped the Energy Year, respectively. Funding for the Energy Year was generously provided by the Mobil Foundation, the National Science Foundation, and the University of Wyoming.

Finally, to close on a personal note, this Special Year in Mathematics Related to Energy launched a period of expansion and development at the University of Wyoming in applied mathematics and interdisciplinary mathematical research on energy and environment. Whatever success will be achieved is due in large part to Dr. L. Milton Woods, Executive Vice President of Mobil Oil Corporation, whose support has been crucial and inspirational. It is a pleasure to be able to record in a formal way our great appreciation to him.

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CONTENTS

PART I: NUMERICAL AND ANALYTICAL METHODS IN PARTIAL DIFFERENTIAL EQUATIONS

ON THE NUMERICAL SOLUTION OF CONVECTION DOMINATED CONVECTION-DIFFUSION PROBLEMS

O. AXELSSON*

Abstract.
A modified form using an embedding method simplifies the presentation of the streamlined diffusion finite element method of Hughes and Brooks for the numerical solution of convection dominated convection-diffusion flow problems. The modification also makes it more clear which types of boundary conditions to choose in connection with a method of separating the layer part calculation of the solution. We discuss also more classical methods, such as exponentially upwinded Galerkin methods and a new defect-correction method.

1. Introduction.

The numerical solution of convection dominated convection-diffusion problems is difficult because the solution has layers and a standard Galerkin method may result in severely oscillating approximate solutions, unless the finite element mesh is very fine. Furthermore, even if the exact solution is smooth (i.e. has no layers) such methods do not in general give optimal orders of accuracy in the discretization parameter (h).

The nonphysical oscillations may be damped out by introducing an artificial diffusion term in the discrete problem of O(h) (see for instance [15]). Alternatively, one may use upwinded basisfunctions such as in [17]. In the limit case, and for piecewise linear finite element basisfunctions, this latter method approaches an upwinded difference method. Besides the usual limitation in the order of accuracy, classical artificial diffusion or upwind finite elements have the

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undesirable property of smearing sharp fronts in the directions perpendicular to the streamlines. This is caused by the fact that the artificial diffusion term acts in all coordinate directions. In some problems, such as miscible displacements problems one encounters also an undesirable grid-orientation effect: the approximate solution may depend heavily on the orientation of the grid, see [8].

By use of an exponentially damped weightfunction used in the layer elements only (see for instance [1]), one may damp oscillations caused by a downstream layer (see below), but the oscillations due to characteristic layers remain. Use of an exponentially damped weightfunction all over the domain may cause numerical instabilities when evaluating the exponential functions. See however the discussion at the end of Section 3 about the use of such a method for the approximate symmetrization of the given problem.

To be more specific we shall consider the numerical solution of the convection-diffusion problem:

(1.1) $L_\varepsilon u = -\underline{\nabla}\cdot(\varepsilon\underline{\nabla}u) + \underline{v}\cdot\underline{\nabla}u + qu = f$ in $\Omega \subset \mathbb{R}^n$, $u = \alpha$ on Γ_-, $u = 0$ on $\Gamma_{D_0} \subset \Gamma_0$, $\underline{\nabla}u\cdot\underline{\hat{n}} = 0$ on $\Gamma_0 \setminus \Gamma_{D_0}$ and boundary conditions on Γ_+ to be specified later. Here some concentration u (of a chemical, of heat, etc) is driven by a velocity field $\underline{v}$ and

$$\Gamma_- = \{\underline{x} \in \partial\Omega;\ \underline{v}\cdot\underline{\hat{n}} < 0\}$$

$$\Gamma_0 = \Gamma_{0,1} \cup \Gamma_{0,2} = \{\underline{x} \in \partial\Omega;\ \underline{v}\cdot\underline{\hat{n}} = 0\}$$

$$\Gamma_+ = \{\underline{x} \in \partial\Omega;\ \underline{v}\cdot\underline{\hat{n}} > 0\}$$

are the inflow, the characteristic and outflow boundary parts, respectively, of $\partial\Omega$ (see figure 1 for an example). ε is a diffusion tensor the components of which are small for convection dominated flows. For most of the discussion there is no limitation in assuming that ε is a scalar parameter.

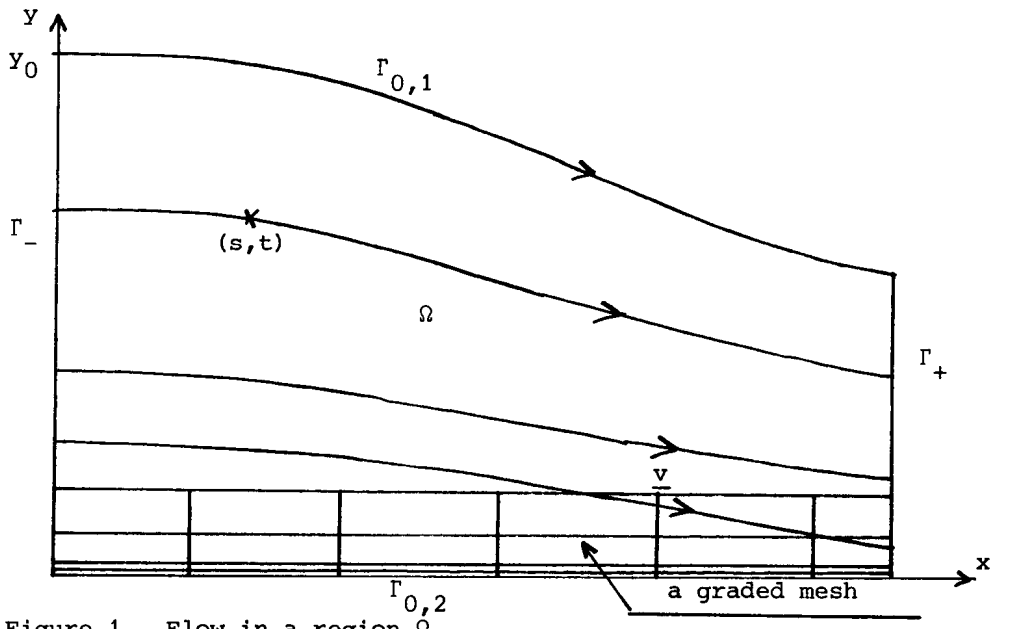

Figure 1. Flow in a region Ω.

In practice, the characteristic boundaries are often physical, like a wall. We shall assume that the vector function $\underline{v}$ is $[C^1(\Omega)]^n$, that $q \in C^1(\bar{\Omega})$ and that $f \in L^2(\Omega)$. We also make the standard assumption that $q - \frac{1}{2}\nabla\cdot\underline{v} \geq q_0 \geq 0 \ \forall \underline{x} \in \Omega$. In general $q_0 = 0$ but in some cases we shall assume that $q_0 > 0$. For part of the theoretical analysis we may introduce a new coordinate system (s,t) where t is the parametric representation of Γ_- ($t=y/y_0$ in Fig. 1) and $s = s(t)$ the parametric representation of the vector field line beginning at t on Γ_-. We let $\frac{d\underline{x}(s,t)}{ds} = \underline{v}(\underline{x}(s,t))$, $0 < s < s^*(t)$, $\underline{x}(0) = \begin{bmatrix} 0 \\ ty_0 \end{bmatrix}$ (in Fig. 1). The solution of the reduced equation $L_0 u = f$ (which is a scalar first order hyperbolic equation) satisfies then $\frac{du(s,t)}{ds} + qu(s,t) = f(s,t)$, $0 < s < s^*(t)$, $u(0,t) = \alpha(0,ty_0)$, i.e. for each t, an ordinary differential equation along the characteristic lines. Clearly when ε is small, the solution of (1.1) is essentially governed by the reduced solution and in general the boundary conditions on $\Gamma_0 \cup \Gamma_+$ are not satisfied. Hence there arises layers

along $\Gamma_0 \cup \Gamma_+$.
Along and close to $\Gamma_{0,2}$ (similar considerations are valid for $\Gamma_{0,1}$), the differential equation is essentially governed by

$$L_\varepsilon u \simeq -\varepsilon u_{yy} + v_1 u_x + qu = f,$$

i.e. a parabolic equation. For this one finds a layer in the solution of width $O(\sqrt{\varepsilon})$. At Γ_+ there arises an exponential layer of width $O(\varepsilon)$ if u is imposed there (i.e. if a Dirichlet condition is valid at Γ_+), otherwise, depending on the boundary condition, there arises a layer in some derivative of u (but not in u itself).

In many problems one is mainly interested in the behaviour of the layer along $\Gamma_0 = \Gamma_{0,1} \cup \Gamma_{0,2}$ but not in the one at Γ_+. In such cases we may select a boundary condition at Γ_+ for convenience of smoothness and ease of programming of the numerical method to be used, because the exact boundary condition at Γ_+ has negligible influence on the solution in the interior of Ω away from Γ_+.
Our aim is to calculate the solution of (1.1) numerically with error estimates of high order and valid uniformly in ε. Two difficulties arise then. The first is associated with the lack of regularity of the solution valid uniformly in ε. Typically when there is a layer at Γ_+, the solution $u = u_\varepsilon$ satisfies
$\varepsilon^{3/2}\| u_\varepsilon \|_2 + \varepsilon^{1/2}\| u_\varepsilon \|_1 + \| u_\varepsilon \|_0 \le C[\| f \|_0 + |\alpha|_{\Gamma_-}]$ where $\| \cdot \|_s$ is the Sobolev norm of s'th order and $|\cdot|_{\Gamma_-}$ is the L_2 norm on Γ_-. By considering a one-dimensional problem it follows that this inequality is sharp in the sence that $\| u_\varepsilon \|_2$ diverges as $\varepsilon^{-3/2}$ as $\varepsilon \to 0$. For problems without an outflow layer a somewhat better regularity result may be derived, see e.g. [4].

The second difficulty is due to the lack of coercivity valid uniformly in ε. If $q - \frac{1}{2}\underline{\nabla}\cdot\underline{v} \ge q_0 > 0 \ \forall \underline{x} \in \Omega$, we have only $\int_\Omega (L_\varepsilon u) u d\Omega \ge c[\varepsilon \| u \|_1^2 + \| u \|_0^2]$ and this is the cause of a degraded order of accuracy of the classical Galerkin method (see Section 3) for small values of ε.

To overcome the problem associated with the lack of regularity

due to the layers we split the solution in three terms, a smooth one corresponding to Neuman boundary conditions or boundary conditions defined by the reduced equation at $\Gamma_0 \cup \Gamma_+$, a term in the form of a smooth function multiplying an exponential layer function at Γ_+ and a term taking care of a possible layer along Γ_0. In calculating the last term, we think of using a refined (graded) mesh along Γ_0 to resolve this layer (see Fig. 1.). This is not unreasonable, in as much the width of the layer is $O(\sqrt{\varepsilon})$ there. The smooth term may be calculated numerically by any of the methods discussed in Sections 3 and 4. This method of splitting the solution does however not handle possible interior layers. Methods of calculating the layers separately has been considered for one-dimensional problems in [5] and [6].

In order to reduce the non-physical smearing of sharp fronts (such as in an interior layer) in directions perpendicular to the convective field force, Raithby proposed in [19] an upwinded finite difference scheme which however was still only first order accurate but having an artificial diffusion term acting only in the direction of the streamlines. The idea was extended to finite elements by Hughes and Brooks in [11], and was further developed by Hughes and Brooks in a series of papers. The extra diffusion introduced by these so called streamline diffusion methods may be compensated for by a proper use of a Petrov-Galerkin formulation. The mathematical analysis of this method was done by Johnson and Nävert [13] for a problem with constant coefficients. Nävert extended the method in [18] to cover more general stationary and time-dependent problems. In particular he proved discretization error estimates valid in the interior of $\overline{\Omega}$.

In the present paper, we consider only global error estimates and valid uniformly with respect to ε. In section 3 we discuss the classical Galerkin method and in the last section we discuss a modified form of the streamline diffusion method. The modification is done by embedding the solution of the given problem in the solution space of a modified problem of a higher order with an artificial diffusion term acting along the streamlines. Then a classical Galerkin method may be applied on the new equation. For this we prove readily

almost optimal orders of convergence of the H^1- and L^2-discretization errors. The advantage of the modified form is that the analysis is somewhat simplified and we see easily which boundary conditions to use in order not to introduce extra layer effects, when we use the method of splitting the layer parts from the solution.

2. Method of separating the layer parts of the solution.

We shall use a modification of a method by Levinson (see e.g. [16]) to split off the layer parts of the solution. We shall assume that $\underline{\nabla}\cdot\underline{v} \le 0$, that ε is constant and that there exists a function g, such that $g = 0$ on Γ_+, $\underline{\nabla}g\cdot\hat{\underline{n}} = -\underline{v}\cdot\hat{\underline{n}}$ on $\Gamma\setminus\Gamma_+$ and that, at least approximately, $\underline{\nabla}g = -\underline{v}$ (see [1], p. 337, for a method to transform the problem to a form where this is satisfied). For ease of exposition, we assume in fact that this is satisfied exactly, i.e. $\underline{v}$ is a potential vector field. Then $\underline{\nabla}^2 g = -\underline{\nabla}\cdot\underline{v} \ge 0$ in Ω and because $\underline{\nabla}g\cdot\hat{\underline{n}} \le 0$ on Γ_+, it follows that $g > 0$ in Ω. Let at first $u = u_\varepsilon^{(0)} + u_\varepsilon^{(1)}$, where

$$L_\varepsilon u_\varepsilon^{(1)} = f,\ u_\varepsilon^{(1)} = \alpha \text{ on } \Gamma_-,\ \underline{\nabla}u_\varepsilon^{(1)}\cdot\hat{\underline{n}} = 0 \text{ on } \Gamma_0$$

and $u_\varepsilon^{(1)}$ satisfies the prescribed boundary conditions for u_ε at Γ_+. Assume in this section that these are also of Dirichlet type, i.e. $u_\varepsilon^{(1)} = \beta$ at Γ_+. For $u_\varepsilon^{(0)}$ we have then

$$L_\varepsilon u_\varepsilon^{(0)} = 0,\ u_\varepsilon^{(0)} = 0 \text{ on } \Gamma_- \cup \Gamma_+,\ \underline{\nabla}u_\varepsilon^{(0)}\cdot\hat{\underline{n}} = 0$$

on $\Gamma_0 \setminus \Gamma_{D_0}$ and $u_\varepsilon^{(0)} = u_\varepsilon - u_\varepsilon^{(1)}$ on Γ_{D_0}. Hence $u_\varepsilon^{(0)}$ contains the layer along the characteristic lines and $u_\varepsilon^{(1)}$ is free of such a layer. We now separate the downstream layer from $u_\varepsilon^{(1)}$,

$$u_\varepsilon^{(1)} = \tilde{u}_\varepsilon + z e^{-g/\varepsilon} \tag{2.1}$$

where g is defined above and where $\tilde{u}_\varepsilon, z$ will be defined below. Then

$$L_\varepsilon u_\varepsilon^{(1)} = L_\varepsilon \tilde{u}_\varepsilon + e^{-g/\varepsilon}\{[-\underline{\nabla}(\varepsilon\underline{\nabla}z) + (2\underline{\nabla}g+\underline{v})\cdot\underline{\nabla}z + (q+\nabla^2 g)z] - \tag{2.2}$$

$$- \frac{1}{\varepsilon}[\underline{v}\cdot\underline{\nabla}g + |\underline{\nabla}g|^2]z\} = f.$$

We shall let

(2.3) $L_\varepsilon \tilde{u}_\varepsilon = f$ in Ω, $\tilde{u}_\varepsilon = \alpha$ on Γ_- and $\underline{\nabla}\tilde{u}_\varepsilon \cdot \hat{\underline{n}} = 0$ on Γ_0 (i.e. the boundary conditions at $\Gamma_- \cup \Gamma_0$ as for $u_\varepsilon^{(1)}$). At Γ_+ we may choose proper boundary conditions in order to get a smooth solution $\tilde{u}_\varepsilon$ without layers. For simplicity, we take $\underline{\nabla}\tilde{u}_\varepsilon \cdot \hat{\underline{n}} = 0$. Since $\underline{\nabla}^2 g = -\underline{\nabla}\cdot\underline{v}$ it follows from (2.2) that z must satisfy $\underline{\nabla}\cdot(-\varepsilon\underline{\nabla}z) + (2\underline{\nabla}g+\underline{v})\cdot\underline{\nabla}z + (q+\underline{\nabla}^2 g)z = 0$ or

(2.4) $L_\varepsilon^* z = \underline{\nabla}\cdot(-\varepsilon\underline{\nabla}z) - \underline{\nabla}\cdot(\underline{v}z) + qz = 0$ in Ω.

The boundary conditions are

$$z = u_\varepsilon^{(1)} - \tilde{u}_\varepsilon \text{ on } \Gamma_+, \quad z = 0 \text{ on } \Gamma_-.$$

Further $\underline{\nabla}z\cdot\hat{\underline{n}} = 0$ on Γ_0 because

$$0 = \underline{\nabla}(u_\varepsilon^{(1)} - \tilde{u}_\varepsilon)\cdot\hat{\underline{n}} = [\underline{\nabla}z\cdot\hat{\underline{n}} - \frac{1}{\varepsilon}\underline{\nabla}g\cdot\hat{\underline{n}}]e^{-g/\varepsilon} = [\underline{\nabla}z\cdot\hat{\underline{n}} + \frac{1}{\varepsilon}\underline{v}\cdot\hat{\underline{n}}]e^{-g/\varepsilon}$$

and, by definition, $\underline{v}\cdot\hat{\underline{n}} = 0$ on Γ_0.

Hence z is the solution of the adjoint operator equation. For this the flow goes in the opposite direction and an exponential layer may now occur at Γ_-.

In the same way as above in (2.1), we may split off the layer part of z, i.e. $z = z^{(0)} = \tilde{z}_\varepsilon + z^{(1)}e^{-g^{(1)}/\varepsilon}$, where $g^{(1)}$ satisfies $\underline{\nabla}^2 g^{(1)} = \underline{\nabla}\cdot\underline{v}$ in Ω, $g^{(1)} = 0$ on Γ_- and $\underline{\nabla}g^{(1)}\cdot\hat{\underline{n}} = \underline{v}\cdot\hat{\underline{n}}$ on $\Gamma\backslash\Gamma_-$. $\tilde{z}_\varepsilon$ satisfies $L_\varepsilon^*\tilde{z}_\varepsilon = 0$ and $z^{(1)}$ satisfies $L_\varepsilon z^{(1)} = 0$. The process may be repeated until the corrections (the layer terms) are small enough. Note that, because $g > 0$ in the interior of Ω, the correction terms, $ze^{-g/\varepsilon}$ etc. are indeed small in the interior, when ε is small. This implies that we only have to calculate g numerically in the vicinity of Γ_+.

In the above fashion, our problem (1.1) is reduced to solving problems $L_\varepsilon\tilde{u}_\varepsilon = f$, $L_\varepsilon^*\tilde{z}_\varepsilon = 0$ etc., where the solution is smooth (has no layers).

Remark 2.1. Above we have assumed that $\alpha \in C^0(\Gamma_-)$. If α is discontinuous at some point on Γ_-, there arises an interior layer, of the same type as the characteristic boundary layers. Interior layers can't so easily be treated in the above way.