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NUMERICAL SOLUTION OF SEMI-LINEAR  
ELLIPTIC PROBLEMS ON UNBOUNDED DOMAINS

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ABSTRACT

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~~We~~ present the derivation and implementation of asymptotic boundary conditions at "artificial" boundaries for semi-linear elliptic boundary value problems on semi-infinite cylindrical domains. A general theory developed by the authors in a previous work [11] is applied to establish the existence of exact boundary conditions and to obtain useful approximations to them. ~~They~~ are based on the Laplace transform solution of the linearized problem at infinity. ~~We~~ discuss the incorporation of these conditions in a finite difference scheme and present the results of a numerical experiment: the solution of the Bratu problem in a two dimensional stepped channel. ~~We~~ also examine certain problems concerning the existence of solutions on infinite domains.

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## SIGNIFICANCE AND EXPLANATION

Many computational problems arising in applied mathematics are posed in infinite pipes and channels. One of the most important examples of this is the problem of incompressible fluid flow in such a geometry. As computations are only possible on finite domains, "artificial" boundaries must be introduced and boundary conditions must be imposed there. For the fluids problem these are referred to as inflow and outflow boundary conditions.

In a previous work the authors developed a general theory of boundary conditions at artificial boundaries. In this work we show how to apply that theory to the numerical solution of semi-linear elliptic problems. Such problems are well-suited for numerical experimentation for a variety of reasons: first, the abstract theory can be directly applied to them; second, the derivation of boundary conditions for these problems is formally applicable to the equations of incompressible flow; third, the problems are physically and mathematically interesting in their own right.

We illustrate the large reduction in the error brought about by use of the asymptotic boundary conditions through presentation of the results of computations on the Bratu problem. This deals with the existence of stable solutions to the equation  $\nabla^2 u = -\lambda e^u$ , which is used as a model of thermal ignition. For  $\lambda$  sufficiently large and positive, solutions do not exist and, hence, ignition is said to have taken place. The problem is to determine the minimum value of  $\lambda$  for which this occurs. We present some results concerning the change in the critical value of  $\lambda$  due to finite perturbations of infinite domains.

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The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

NUMERICAL SOLUTION OF SEMI-LINEAR ELLIPTIC  
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Thomas M. Hagstrom\* and H. B. Keller\*\*

1. Introduction

We consider boundary value problems of the form:

$$(1.1) \quad \begin{aligned} a) \quad & Lu(x, y) = f(u, \chi), \quad (x, \chi) \in [0, \infty) \times \Omega, \quad \Omega \subset \mathbb{R}^{n-1}; \\ b) \quad & a_{\Omega}(\chi) \frac{\partial u}{\partial \nu} + b_{\Omega}(\chi)u = c_{\Omega}(\chi), \quad \chi \in \partial\Omega; \\ c) \quad & a_0(\chi) \frac{\partial u}{\partial x} + b_0(\chi)u = c_0(\chi), \quad x = 0; \\ d) \quad & \lim_{x \rightarrow \infty} u(x, \chi) = u_{\infty}(\chi), \quad \lim_{x \rightarrow \infty} \frac{\partial u}{\partial x}(x, \chi) = 0. \end{aligned}$$

Here,  $L$  is a linear uniformly elliptic second-order operator which is independent of  $x$ :

$$(1.2) \quad \begin{aligned} a) \quad & L \equiv \frac{\partial^2}{\partial x^2} + L_1 \cdot \frac{\partial}{\partial x} + L_2; \\ b) \quad & L_1 \equiv \sum_{i=1}^{n-1} a_{ni}(\chi) \frac{\partial}{\partial y_i} + a_n(\chi); \\ c) \quad & L_2 \equiv \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} a_{ij}(\chi) \frac{\partial^2}{\partial y_i \partial y_j} + \sum_{i=1}^{n-1} a_i(\chi) \frac{\partial}{\partial y_i} + a(\chi). \end{aligned}$$

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The expression  $\frac{\partial}{\partial \nu}$  denotes the conormal derivative associated with  $L$  and  $\Omega$ . The function  $u_\infty(\chi)$  must satisfy the limiting cross-sectional problem obtained by formally letting  $x \rightarrow \infty$  and setting  $u_x \equiv u_{xx} \equiv 0$  in (1.1a,b) to get:

$$(1.3) \quad \begin{aligned} \text{a) } & L_2 u_\infty = f(u_\infty, \chi), \quad \chi \in \Omega; \\ \text{b) } & a_\Omega(\chi) \frac{\partial u_\infty}{\partial \nu} + b_\Omega(\chi) u_\infty = c_\Omega(\chi), \quad \chi \in \partial\Omega. \end{aligned}$$

Equations such as (1.1a) arise, for example, in equilibrium problems in non-linear heat generation. (See, e.g., Aris [3].) Furthermore, the method we describe can be generalized to systems and to higher order equations [11]. As such it has potential for application to steady state problems of fluid flow in pipes and channels.

Our procedure is to introduce an artificial boundary at some point  $\tau > 0$ , impose boundary conditions there and solve the resulting finite problem on  $[0, \tau] \times \Omega$  by a standard numerical technique. A theory of boundary conditions at an artificial boundary has been developed by the authors in [11] and we use it here. Indeed, one of the purposes of this work is to illustrate the power of the general theory.

Other authors have discussed the problem of deriving boundary conditions at an artificial boundary for linear elliptic problems. Gustafsson and Kreiss [10] point out the possibility of deriving exact conditions by use of a Laplace transformation in  $x$ . Fix and Marin [7] and Goldstein [9] use a related approach to solve problems in underwater acoustics and wave propagation in cylindrical waveguides. The first approximation to the boundary condition given by our method coincides with that obtained by applying the Laplace transform method to the problem linearized about  $u_\infty(\chi)$ .

In section 2 of this work we state the basic results of [11] and show how they can be applied to (1.1). In particular, we present detailed asymptotic expansions of the exact boundary conditions and state sufficient conditions for their validity. Extensions to other problems are also discussed. In section 3 the inclusion of the expansions in a discrete approximation is described and their efficient use is considered.

A special case of (1.1a), the Bratu problem in a two-dimensional channel, is introduced in section 4. We discuss its physical interpretation and quote various existence results for finite domains. The results of some numerical experiments are presented assessing the effects of varying the location of the artificial boundary and the number of terms in the asymptotic expansion. Some questions concerning the existence of solutions in unbounded domains are also examined.

## 2. Construction of the Boundary Conditions

In order to conform to the notation of [11], we write the problem as a first order ordinary differential equation in a Banach space. Letting  $v \equiv u - u_\infty$  we introduce:

$$(2.1) \quad w(x) \equiv \begin{pmatrix} \frac{\partial v}{\partial x}(x, \chi) \\ v(x, \chi) \end{pmatrix} \equiv \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}.$$

We seek a solution,  $v$ , which for each  $x$  is an element of the space  $W_2^0(\Omega)$  - that subspace of the Sobolev space  $W_2(\Omega)$  consisting of functions which satisfy the homogeneous version of (1.1b), i.e. with  $C_\Omega \equiv 0$ . Here for each  $x$  we require:

$$(2.2) \quad \begin{aligned} \text{a) } w(x) \in \mathcal{B} &\equiv \left\{ \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} : w_1 \in W_1(\Omega), w_2 \in W_2(\Omega), (2.2b) \text{ holds.} \right\} \\ \text{b) } a_\Omega \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} n_i a_{ij} \frac{\partial w_2}{\partial y_j} + a_\Omega \sum_{i=1}^{n-1} n_i a_{ni} w_1 + b_\Omega w_2 &= 0, \quad \chi \in \partial\Omega. \end{aligned}$$

Here  $n_i$  is the  $i^{\text{th}}$  component of the unit normal to  $\partial\Omega$ . Choosing  $\tau > 0$  as the location of the artificial boundary, we rewrite the equation in the tail in the abstract form:

$$(2.3) \quad \begin{aligned} \text{a) } \frac{dw}{dx} &= Aw + R(w), \quad x > \tau; \\ \text{b) } \lim_{x \rightarrow \infty} w(x) &= 0; \end{aligned}$$

where

$$(2.4) \quad \begin{aligned} \text{a) } A \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} &\equiv \begin{pmatrix} -L_1 w_1 - L_2 w_2 + f_u(u_\infty) w_2 \\ w_1 \end{pmatrix}; \\ \text{b) } R \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} &\equiv \begin{pmatrix} f(u_\infty + w_2) - f_u(u_\infty) w_2 - f(u_\infty) \\ 0 \end{pmatrix}. \end{aligned}$$

In [11] an explicit approximation to the solution of (2.3) is constructed in terms of the eigenfunctions of  $A$ . That is, we consider pairs

$(\lambda_\ell, w_\ell) \in \mathbb{C} \times \mathcal{B}$  such that:

$$(2.5) \quad Aw_\ell = \lambda_\ell w_\ell, \quad \ell = 1, 2, \dots; \quad \|w_\ell\| \neq 0.$$

We assume that:

- a) The eigenvalues,  $\lambda_\ell$ , are distinct and bounded away from the imaginary axis.
- (2.6) b) The eigenfunctions,  $w_\ell$ , form a Riesz basis of  $\mathcal{B}$ . (See, e.g., Gohberg and Krein [8] for a discussion of non-orthonormal bases.)

Note that (2.6a) ensures that the linearized problem has an exponential dichotomy. From (2.4a) we see that (2.5) is equivalent to the eigenvalue problem obtained by application of a Laplace transformation in  $x$  to the linearization of (1.1) about  $u_\infty$ :

$$(2.7) \quad \begin{aligned} & \text{a) } L_2 Y_\ell - f_u(u_\infty) Y_\ell + \lambda_\ell L_1 Y_\ell + \lambda_\ell^2 Y_\ell = 0, \quad Y_\ell \in \Omega; \\ & \text{b) } a_\Omega \sum_{i=1}^{n-1} n_i \left\{ \left( \sum_{j=1}^{n-1} a_{ij} \frac{\partial Y_\ell}{\partial y_j} \right) + \lambda_\ell a_{ni} Y_\ell \right\} + b_\Omega Y_\ell = 0, \quad Y_\ell \in \partial\Omega; \\ & \text{c) } w_\ell \equiv \begin{pmatrix} \lambda_\ell Y_\ell \\ Y_\ell \end{pmatrix}. \end{aligned}$$

Condition (2.6b) can be particularly difficult to check for nonselfadjoint problems. (See, e.g., Berezanskii [6] for a discussion of the selfadjoint case.) Agmon [1] treats the case  $L_1 \equiv 0$  while Agmon and Nirenberg [2] give sufficient conditions for completeness in the class of initial data leading to absolutely integrable solutions in the tail. Note

that the set of all decaying solutions of the linearized problem is generated by those  $w_\ell$  whose eigenvalues have negative real part. We denote this subspace of  $B$  by  $A$  :

$$(2.8) \quad A \equiv \text{span}\{w_\ell : \text{Re}\lambda_\ell < 0\}.$$

We now state our fundamental result concerning the existence of solutions of (2.3):

Theorem 2.9 Let  $\delta > 0$  satisfy

$$(2.9) \quad \delta < \frac{1}{2\gamma\alpha(K_1 + K_2 + K_3)\left(\frac{1}{\lambda_+} + \frac{1}{\lambda_-}\right)},$$

where

$$a) \quad \lambda_+ = \inf_{\text{Re}\lambda_\ell > 0} \text{Re}(\lambda_\ell), \quad \lambda_- = \inf_{\text{Re}\lambda_\ell < 0} (-\text{Re}(\lambda_\ell));$$

$$b) \quad K_1 \equiv \sup_{\substack{|\tilde{v}| < 2\gamma\delta \\ \chi \in \Omega}} |f_{uu}(u_\infty + \tilde{v}, \chi)|;$$

$$c) \quad K_2 \equiv \sum_{i=1}^{n-1} \sup_{\substack{|\tilde{v}| < 2\gamma\delta \\ \chi \in \Omega}} |f_{uuy_i}(u_\infty + \tilde{v}, \chi)|;$$

$$(2.10) \quad d) \quad K_3 \equiv \sum_{i=1}^{n-1} \sup_{\chi \in \Omega} |(u_\infty(\chi))_{y_i}| \sup_{\substack{|\tilde{v}| < 2\gamma\delta \\ \chi \in \Omega}} |f_{uuu}(u_\infty + \tilde{v}, \chi)|;$$

e)  $\gamma$  is a constant appearing in Sobolev's inequality (see Agmon [1]),

$$|u| \leq \gamma(\|u\|_{W_2(\Omega)} + \|u\|_{W_0(\Omega)});$$

f)  $\alpha_1, \alpha_2$  are constants such that if  $w = \sum_\ell c_\ell w_\ell$  then:

$$\alpha_1 \left( \sum_\ell |c_\ell|^2 \right)^{1/2} \leq \|w\| \leq \alpha_2 \left( \sum_\ell |c_\ell|^2 \right)^{1/2}, \quad \alpha \equiv \frac{\alpha_2}{\alpha_1}.$$

(Such a  $\delta$  clearly exists if the necessary derivatives of  $f$  are continuous near  $u_\infty$ .) Then, for any  $\xi \in A$  which also satisfies:

$$(2.11) \quad \|\xi\|_B < \frac{\delta}{2\alpha},$$

there exists a solution,  $w(x)$ , of (2.3) such that, if  $Q_\infty$  is the projection operator into  $A$  whose nullspace is the span of the  $w_\ell$  whose eigenvalues have positive real part, then:

$$(2.12) \quad Q_\infty w(\tau) = \xi.$$

Furthermore,  $w(x)$  is unique among small solutions satisfying (2.12). /

We note that Theorem 2.9 is the specialization of some results of [11] to the present case. The proof, as given there, follows this path: (i) a solution,  $w_0(x)$ , of the linearized problem satisfying  $w_0(\tau) = \xi$  is written down, (ii)  $w(x)$  is represented as  $w_0(x) + \tilde{w}(x)$ , (iii) an integral equation for  $\tilde{w}$  is derived from an integral representation (in this case a Green's function representation) of solutions of the linearized inhomogeneous equations, (iv) the existence of  $\tilde{w}$  is established by a contraction mapping argument. In order to carry out step (iv), it is necessary to prove certain estimates. This leads to the inequality (2.9). As their derivation is straightforward, we postpone its presentation to the appendix.

The solution we have constructed,  $\bar{w}(x;\xi)$ , can now be used to write down an exact boundary condition at  $x = \tau$ . Written in abstract form it is (see [11]):

$$(2.13) \quad (I - Q_\infty)w(\tau) = -\int_\tau^\infty S(\tau,p)(I - Q_\infty)R(\bar{w}(p, Q_\infty w(\tau)))dp,$$

Here, the combination  $S(s,t)(I - Q_\infty)$  is the solution operator of the linearized problem restricted to the span of  $w_\ell$  whose eigenvalues have positive real part. Its existence is guaranteed only for  $s \leq t$ . Equation

(2.13) is an exact condition in that there exists a small solution,  $w$ , of (2.3) if and only if  $w(\tau)$  satisfies (2.13).

A useful approximation to (2.13) is obtained in terms of the eigenfunctions,  $w_\ell$ . The iterative process implicit in the contraction argument is truncated to give some approximation,  $\bar{w}^{(n)}(x;\xi)$ , to  $\bar{w}(x;\xi)$ . Furthermore, the nonlinearity  $R$  is replaced by a finite Taylor series. Then the integrals involved only contain exponential functions of the integration variable and can be evaluated explicitly. The result is an expression relating the expansion coefficients. (See [11], eq. (6.1) . . . rewrite the quadratic approximation below for an expansion in terms of  $Y_\ell(\chi)$ . This, in turn, makes use of solutions of the adjoint problem:

$$(2.14) \quad \begin{aligned} \text{a) } & L_2^* \bar{Y}_\ell - f_u(u_\infty) \bar{Y}_\ell + \lambda_\ell^* L_1^* \bar{Y}_\ell + \lambda_\ell^{*2} \bar{Y}_\ell = 0, \quad \chi \in \Omega; \\ \text{b) } & a_\Omega \frac{\partial \bar{Y}_\ell}{\partial v} + \left( b_\Omega + a_\Omega \sum_{i=1}^{n-1} n_i \left( \sum_{j=1}^{n-1} \frac{\partial a_{ij}}{\partial y_j} - a_i \right) \right) \bar{Y}_\ell = 0, \quad \chi \in \partial\Omega. \end{aligned}$$

Here,  $L_2^*$  and  $L_1^*$  are the formal adjoints of  $L_2$  and  $L_1$ . We choose our normalization so that:

$$(2.15) \quad \begin{aligned} \text{a) } & \int_\Omega d\chi \left[ (\lambda_\ell + \lambda_m + a_n) \bar{Y}_\ell^* - \sum_{i=1}^{n-1} \frac{\partial}{\partial y_i} (a_{ni} \bar{Y}_\ell^*) \right] Y_m = \delta_{\ell m}; \\ \text{b) } & \|Y_m\|_{W_2(\Omega)} = 1. \end{aligned}$$

Given the pair  $\begin{pmatrix} v_x(\tau, \chi) \\ v(\tau, \chi) \end{pmatrix}$  we define expansion coefficients in the following way:

$$(2.16) \quad \begin{aligned} C_\ell & \equiv \int_\Omega d\chi \left\{ \bar{Y}_\ell^*(\chi) v_x(\tau, \chi) \right. \\ & \left. + \left[ (\lambda_\ell + a_n(\chi)) \bar{Y}_\ell^*(\chi) - \sum_{i=1}^{n-1} \frac{\partial}{\partial y_i} (a_{ni}(\chi) \bar{Y}_\ell^*(\chi)) \right] v(\tau, \chi) \right\}. \end{aligned}$$

We further define matrix elements of the quadratic approximation to R:

$$(2.17) \quad \alpha_{mn}^{(\ell)} \equiv \frac{1}{2} \int_{\Omega} d\chi \bar{Y}_{\ell}^*(\chi) f_{uu}(u_{\infty}, \chi) Y_m(\chi) Y_n(\chi).$$

We then have as an  $O(\|v(\tau, \chi)\|^2)$  approximation to (2.13):

$$(2.18) \quad C_{\ell} = \sum_{\substack{m \\ \operatorname{Re} \lambda_m < 0}} \sum_{\substack{n \\ \operatorname{Re} \lambda_n < 0}} \alpha_{mn}^{(\ell)} \frac{C_m C_n}{\lambda_m + \lambda_n - \lambda_{\ell}}, \quad \forall \ell \text{ such that } \operatorname{Re} \lambda_{\ell} > 0.$$

Equations (2.16) and (2.18) take on a more familiar form when the eigenvalue problem, (2.7), is selfadjoint. In particular we consider the case when  $L$  is the laplacian and the boundary conditions are of Dirichlet type.

We then have:

$$(2.19) \quad \text{a) } \sum_{i=1}^{n-1} \frac{\partial^2 Y_{\ell}}{\partial y_i^2} - f_u(u_{\infty}) Y_{\ell} + \lambda_{\ell}^2 Y_{\ell} = 0, \quad \chi \in \Omega;$$

$$\text{b) } Y_{\ell}(\chi) = 0, \quad \chi \in \partial\Omega.$$

Define  $\phi_{\ell} \equiv Y_{\ell} Y_{\ell}$  to be normalized in  $L_2(\Omega)$ :

$$(2.20) \quad \int_{\Omega} d\chi \phi_{\ell}^2(\chi) = 1.$$

Then we have by (2.15a):

$$(2.21) \quad \bar{Y}_{\ell}(\chi) = \frac{Y_{\ell}}{2\lambda_{\ell}} \phi_{\ell}.$$

Note that each eigenfunction  $Y_{\ell}$  corresponds to two distinct eigenvalues,  $\pm \lambda_{\ell}$ . Consider the expansion of the pair  $\begin{pmatrix} v \\ x \end{pmatrix}$  in terms of the two bases:

$$(2.22) \quad \begin{pmatrix} v \\ x(x, \chi) \end{pmatrix} = \sum_{\ell} \left\{ C_{\ell}^+(x) \begin{pmatrix} \lambda_{\ell} Y_{\ell} \\ Y_{\ell} \end{pmatrix} + \bar{C}_{\ell}^-(x) \begin{pmatrix} -\lambda_{\ell} Y_{\ell} \\ Y_{\ell} \end{pmatrix} \right\} = \sum_{\ell} \begin{pmatrix} h_{\ell}^+(x) \\ h_{\ell}^-(x) \end{pmatrix} \phi_{\ell}.$$

The expansion coefficients are related by:

$$c_{\ell}^{+} = \frac{\gamma_{\ell}}{2} \left( h_{\ell} + \frac{h'_{\ell}}{\lambda_{\ell}} \right), \quad (2.23)$$

$$c_{\ell}^{-} = \frac{\gamma_{\ell}}{2} \left( h_{\ell} - \frac{h'_{\ell}}{\lambda_{\ell}} \right).$$

Define matrix elements in the new basis by:

$$\bar{\alpha}_{mn}^{(\ell)} = \frac{1}{2} \int_{\Omega} d\mathcal{Y} f_{uu}(u_{\infty}, \mathcal{Y}) \phi_{\ell}(\mathcal{Y}) \phi_m(\mathcal{Y}) \phi_n(\mathcal{Y}). \quad (2.24)$$

They are related to the old matrix elements through:

$$\alpha_{mn}^{(\ell)} = \frac{\gamma_{\ell}}{2\lambda_{\ell}\gamma_m\gamma_n} \bar{\alpha}_{mn}^{(\ell)}. \quad (2.25)$$

Using (2.23) and (2.25) the boundary condition (2.18) becomes:

$$h'_{\ell} + \lambda_{\ell} h_{\ell} = - \sum_m \sum_n \frac{\bar{\alpha}_{mn}^{(\ell)}}{\lambda_m + \lambda_n + \lambda_{\ell}} \frac{1}{4} \left( h_m - \frac{h'_m}{\lambda_m} \right) \left( h_n - \frac{h'_n}{\lambda_n} \right), \quad (2.26)$$

which can be replaced, to the same quadratic order of approximation, by:

$$h'_{\ell} = -\lambda_{\ell} h_{\ell} - \sum_m \sum_n \frac{\bar{\alpha}_{mn}^{(\ell)}}{\lambda_m + \lambda_n + \lambda_{\ell}} h_m h_n. \quad (2.27)$$

Condition (2.27) is used in the calculations presented in section 4.

In closing this section we note that the analysis given above can easily be extended to a variety of different situations. The assumption concerning the lack of dependence of the domain and coefficients on  $x$  is necessary only in the tail, i.e. for  $x$  sufficiently large. In fact, the asymptotic expansions given in [11] allow for a dependence of the coefficients on  $x$  so long as they approach their limiting values sufficiently fast. Also, the restriction to scalar equations is not needed.

### 3. Discrete Approximations

We show how to implement the boundary conditions discussed above in a numerical computation. For simplicity we assume a one dimensional cross-section,  $\Omega$ , with Dirichlet boundary conditions. We also consider centered finite difference approximations to the derivatives with a uniform mesh width. Let  $p$  denote the number of gridpoints in a cross-section,  $h$  be the mesh width and  $i$ ,  $1 \leq i \leq p$ , parametrize the points in a cross-section. Then, if  $j$  parametrizes the  $x$  coordinate, the index,  $k$ , of a mesh point is given by  $k = p(j-1) + i$ . At an interior point a finite difference approximation to (1.1a) is given by:

$$\begin{aligned}
 & \frac{1}{h^2}(u(k+p) - 2u(k) + u(k-p)) + \frac{a_2(y_i)}{2h}(u(k+p) - u(k-p)) \\
 & + \frac{a_{11}(y_i)}{h^2}(u(k+1) - 2u(k) + u(k-1)) \\
 (3.1) \quad & + \frac{a_{21}(y_i)}{h^2}(u(k+p+1) + u(k-p-1) - u(k-p+1) - u(k-p-1)) \\
 & + \frac{a_1(y_i)}{2h}(u(k+1) - u(k-1)) + a(y_i)u(k) - f(u(k), y_i) = 0 .
 \end{aligned}$$

In order to implement (2.18), it is necessary to solve the eigenvalue problems (2.7) and (2.14). We approximate these on the same cross-sectional mesh as the full equation. We must therefore assume that the eigenvalues and eigenfunctions which are approximated well on this mesh are enough to resolve the solution. (See Kreiss [13] for a discussion of the approximate solution of nonselfadjoint eigenvalue problems.) We denote our approximate solutions to (2.7) and (2.14) by the pairs  $(\hat{\lambda}_\ell, \hat{Y}_\ell(y_i))$ ,  $(\hat{\lambda}_\ell^*, \hat{\bar{Y}}_\ell(y_i))$ . Approximate expansion coefficients  $\hat{C}_\ell$  are given by:

$$\begin{aligned}
 \hat{C}_\ell &= \frac{1}{p} \sum_{i=1}^p \{ \hat{Y}_\ell^*(y_i) v_x(\tau, y_i) + [(\hat{\lambda}_\ell + a_2(y_i)) \hat{Y}_\ell^*(y_i) \\
 (3.2) \quad &- \frac{1}{2h} (a_{21}(y_{i+1}) \hat{Y}_\ell^*(y_{i+1}) - a_{21}(y_{i-1}) \hat{Y}_\ell^*(y_{i-1})) \} v(\tau, y_i) \},
 \end{aligned}$$

and, if approximations,  $\hat{\alpha}_{mn}^{(\ell)}$ , to the matrix elements  $\alpha_{mn}^{(\ell)}$  are calculated in a similar fashion, (2.18) can be replaced by:

$$(3.3) \quad \hat{C}_\ell = \sum_{\substack{m \\ \text{Re} \lambda_m < 0}} \sum_{\substack{n \\ \text{Re} \lambda_n < 0}} \hat{\alpha}_{mn}^{(\ell)} \frac{\hat{C}_m \hat{C}_n}{\hat{\lambda}_m + \hat{\lambda}_n - \hat{\lambda}_\ell}, \quad \forall \ell \text{ such that } \text{Re} \hat{\lambda}_0 > 0.$$

We note that  $v(\tau, y_i) \equiv u(\tau, y_i) - u_\infty(y_i)$  and that  $v_x(\tau, y_i)$  must be replaced by a difference approximation. A simple approach is to take  $\tau$  half way between vertical grid lines and to calculate  $v(\tau, y_i)$  by averaging. In general, there will be  $2p$  eigenvalues,  $\hat{\lambda}_\ell$ , of the discrete problem. Equation (3.3) represents as many equations as there are eigenvalues with positive real part. If this is not equal to  $p$ , then we cannot expect the discrete equations to be well-posed. (One reason for this might be that the original problem is ill-posed.)

As expected, all of this is simplified in the selfadjoint case. Then, (3.3) can be replaced by a discrete analogue of (2.27) where

$$\begin{aligned}
 \hat{h}_\ell^i &= \frac{1}{p} \sum_{i=1}^p \phi_\ell(y_i) v_x(\tau, y_i); \\
 (3.4) \quad \hat{h}_\ell &= \frac{1}{p} \sum_{i=1}^p \phi_\ell(y_i) v(\tau, y_i).
 \end{aligned}$$

Since the  $p$ -vectors  $\phi_\ell(y_i)$  are orthogonal, our approximation to (2.27) can be rewritten in the convenient form:

$$\begin{aligned}
 v_x(\tau, y_i) &= - \sum_{\ell=1}^P \sum_{j=1}^P \phi_{\ell}(y_i) \hat{\lambda}_{\ell} \phi_{\ell}(y_j) v(\tau, y_j) \\
 (3.5) \quad & - \frac{1}{P} \sum_{\ell=1}^P \sum_{m=1}^P \sum_{n=1}^P \phi_{\ell}(y_i) \frac{\alpha_{mn}}{\lambda_m + \lambda_n + \lambda_{\ell}} \left( \sum_{j=1}^P \phi_m(y_j) v(\tau, y_j) \right) \left( \sum_{j=1}^P \phi_n(y_j) v(\tau, y_j) \right).
 \end{aligned}$$

We now consider the solution of the system of nonlinear equations by Newton's method. From (3.1) we see that the interior of the Jacobian will be banded with band width at most  $p + 1$ . Assuming we use (3.3) to relate two vertical grid lines, the last  $p$  rows will have nonzero elements in the last  $2p$  columns, increasing the band width by as much as  $p$ . If, however, (3.5) can be used, it is possible to write the condition in such a way that the band width is not increased. Therefore, in the latter case, no extra work is needed to solve the system by banded Gaussian elimination. In the former, a bordering technique is necessary to avoid significant additional calculation. The effect of the nonlocal boundary conditions on the performance of iterative techniques has not been examined in general. Bayliss, Goldstein and Turkel [5] have found that the use of the linear version of (3.5) has essentially no effect on the convergence of their preconditioned conjugate gradient algorithm for the Helmholtz equation in three dimensions.

A significant number of new calculations are, however, required to evaluate the Jacobian. From (3.5) we see that, for the quadratic approximation, this involves an evaluation of

$$\begin{aligned}
 Q_{ij} &\equiv \sum_{\ell=1}^P A_{ij\ell} v(\tau, y_{\ell}), \\
 (3.6) \quad A_{ij\ell} &\equiv \sum_{m=1}^P \sum_{n=1}^P \sum_{K=1}^P \phi_m(y_i) \frac{\hat{\alpha}_{nK}^{(m)}}{\lambda_m + \lambda_n + \lambda_K} \phi_n(y_{\ell}) \phi_K(y_j).
 \end{aligned}$$

Since  $A_{ijl}$  can be evaluated beforehand, this entails  $O(p^3)$  new multiplications at each iteration. The direct solve itself requires  $O(p^3q)$  operations where  $q$  is the number of gridpoints in the  $x$  direction. There are two ways to reduce the error due to the introduction of the artificial boundary: first, to take more terms in the expansion of the boundary condition; second, to move the boundary further out. The latter requires  $O(p^3\Delta q)$  additional multiplications. The increased cost of evaluating the Jacobian in the former approach is  $O(p^{s+1})$  where  $s$  is the number of terms taken in the expansion. This suggests that the quadratic approximation is an efficient choice. These considerations might change, of course, if a different solver was used or if the dimension of the cross-section were higher.

#### 4. The Bratu Problem

We consider the following special case of (1.1a):

$$(4.1) \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\lambda e^u.$$

Equation (4.1), which is also associated with the names of Gelfand and Frank-Kamenetskii, arises in the theory of thermal ignition of gases. (See, e.g., Aris [3].) The problem of existence of positive solutions has been considered by various authors. We state below two theorems from the literature for the Dirichlet problem on a finite domain - that is (4.1) holds on some finite domain,  $D$ , and:

$$(4.2) \quad u = 0, \quad (x,y) \in \partial D.$$

Theorem 4.3 (Keller and Cohen [12]) Let  $\lambda > 0$  be such that (4.1, 4.2) has a positive solution. (We say that  $\lambda$  is in the spectrum.) Then, if  $0 < \lambda^* < \lambda$ ,  $\lambda^*$  is in the spectrum. Furthermore, for all  $\lambda$  in the spectrum, there exists a minimal positive solution,  $u_0(x,y; \lambda)$ , such that, if  $U(x,y; \lambda)$  is any other positive solution, then

$$(4.3) \quad u_0(x,y; \lambda) \leq U(x,y; \lambda) \quad \forall (x,y) \in D.$$

The minimal positive solution is stable in that the linearized eigenvalue problem

$$(4.4) \quad \begin{aligned} \text{a) } & \nabla^2 \phi + \lambda e^u \phi = \alpha \phi \quad \text{in } D; \\ \text{b) } & \phi = 0 \quad \text{on } \partial D; \end{aligned}$$

has only negative eigenvalues.

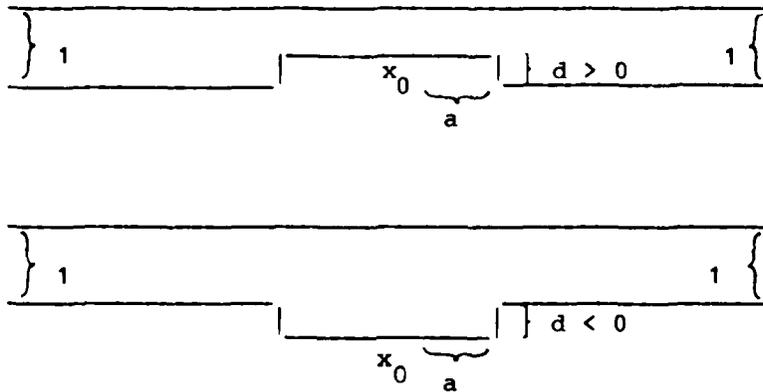
Theorem 4.5 (Bandle (4)) Let  $D' \subset D$ . Then, if  $\lambda$  is in the spectrum for  $D$ , it is in the spectrum for  $D'$ . Furthermore, the minimal positive solutions satisfy:

$$(4.5) \quad u_0(x,y; \lambda, D') \leq u_0(x,y; \lambda, D) \quad \forall (x,y) \in D'.$$

That is, the minimal equilibrium temperature increases with the size of the domain.

We consider the problem (4.1) on domains with infinite boundaries of the following types:

$$(4.6) \quad y \in [0,1], |x - x_0| > a; \quad y \in [d,1], |x - x_0| < a;$$



where  $d$  can be positive or negative. On the top and bottom of the channel and on the step at  $x = x_0 + a$  we require  $u = 0$ . As  $|x| \rightarrow \infty$  we require:

$$(4.7) \quad \lim_{|x| \rightarrow \infty} u(x,y) = u_\infty(y) .$$

Here,  $u_\infty(y)$  is a solution of the limiting cross-sectional problem:

$$(4.8) \quad \begin{aligned} \text{a) } u_\infty'' &= -\lambda e^{u_\infty}, \quad y \in (0,1); \\ \text{b) } u_\infty(0) &= u_\infty(1) = 0. \end{aligned}$$

We are now assuming that  $\lambda$  is in the spectrum of the cross-sectional problem at infinity. Furthermore, in order to ensure that condition (2.6a) is met, we must take  $u_\infty$  to be the minimal positive solution. It is possible to solve (4.8) analytically. The spectrum is found to range between 0 and  $\lambda_C$  where

$$(4.9) \quad \lambda_C = 3.51 \dots .$$

Finally, we seek solutions which are symmetric with respect to  $x_0$ . This allows us to consider solutions on the semi-infinite domain created by the restriction of the original domain to  $x > x_0$ . At  $x_0$  we impose the boundary condition:

$$(4.10) \quad \frac{\partial u}{\partial x}(x_0, y) = 0.$$

For the numerical solution of the problem an artificial boundary is introduced at the point  $x = \tau$ . Three different boundary conditions are imposed there:

- (i) the quadratic condition, (2.26);
- (ii) the linear approximation,  $h_\ell^i + \lambda_\ell h_\ell = 0$ ;
- (iii) the "naive" zero-order condition,  $\frac{\partial u}{\partial x} = 0$ .

Before discretization, the stepped channel was mapped to a straight channel using the conformal mapping, with  $d > 0$ :

$$(4.11) \quad \begin{aligned} \text{a) } & s + it = w = F^{-1}(z), \quad z = x + iy; \\ \text{b) } & F(w) = \frac{2}{\pi} \left\{ \ln \left[ (e^{\pi w} - 1)^{1/2} + (e^{\pi w} - (1-\alpha))^{1/2} \right] - \right. \\ & (1-\alpha)^{1/2} \ln \left[ (e^{\pi w} - (1-\alpha))^{1/2} + (1-\alpha)^{1/2} (e^{\pi w} - 1)^{1/2} \right] \left. \right\} + (1-\alpha)^{1/2} w; \\ \text{c) } & \alpha = 2d - d^2. \end{aligned}$$

For  $d < 0$ , set  $d^* = \frac{-d}{1-d}$  and replace  $F$  by  $\frac{-1}{1-d^*} F^{\text{conjg}}(-w^{\text{conjg}}; d^*) + d$ . The straight boundaries at  $x = x_0, \tau$  are mapped into slightly curved boundaries. The resulting perturbation of the boundary conditions are calculated using linear interpolation. The equations are discretized and solved (Newton's method and Gaussian elimination) as described in section 3. For all cases shown the uniform mesh width is  $h = .05$ . Due to the curvature of the boundary, it is necessary to implement the condition at  $x = \tau$  in such a way that the band width is increased. To avoid additional computation, a

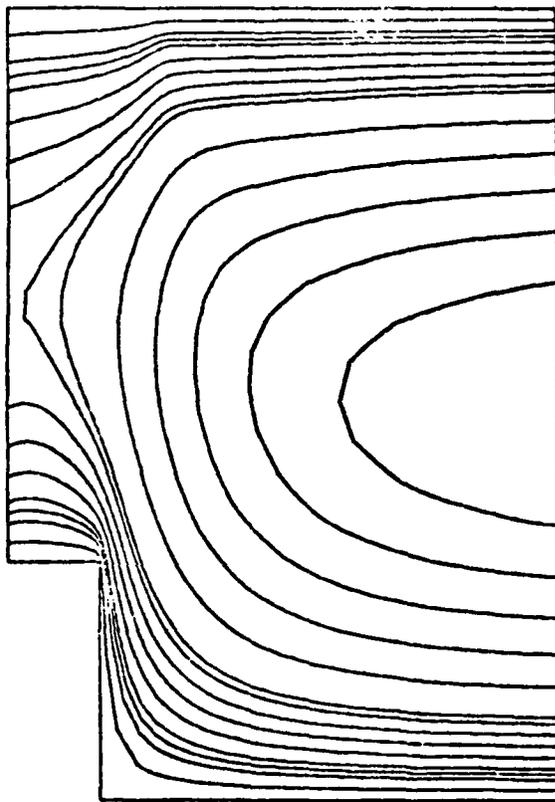
bordering technique is used to solve the Newton iterates. All calculations were performed on VAX 11/780 computers at the California Institute of Technology and the Mathematics Research Center.

If the step parameter,  $d$ , is taken to be zero a trivial solution exists - namely  $u = u_{\infty}(y)$ . Theorem 4.5 (which has not been established for an unbounded domain) suggests that solutions exist if  $0 < d < 1$ . We always found this to be the case. Presented below are results  $d = .4$  and  $\lambda = 3.51$ , very close to the critical value for the cross-section. The minimum eigenvalue of the cross-sectional problem is .66825, so the decay to  $u_{\infty}$  is relatively slow. In Table I we list the maximum error as a function of  $\tau$  and the order of the asymptotic boundary condition. (The exact solution is taken to be a finite difference solution on a large domain,  $\tau = 2.262$ , using the quadratic approximation to the boundary condition.)

$\tau$	# vertical gridlines to the right of step	B.C. approximation order	$\max_{x=\tau}  u^h - u_{\infty} $	$\ u^h - u_{\text{approx}}^h\ _{\infty}$
1.262	20	0: $u_x = 0$	.076	.0743
		1: linear		.0030
		2: quadratic		.0015
.764	10	0	.177	.1472
		1		.0082
		2		.0018
.520	5	0	.269	.1936
		1		.0154
		2		.0051
.381	2	0	.341	.2131
		1		.0213
		2		.0105

TABLE I

We see that the quadratic condition is consistently the best and that the naive condition is consistently the worst. The success of the quadratic condition is graphically displayed in Figures 1-4. Figure 1 shows the solution using the quadratic condition on a large domain,  $\tau = 1.262$ . (The step is located at  $x = -.057$ .) Plotted are level curves of  $u$ . In Figure 2 the same level curves are plotted for a solution on a small domain,  $\tau = .381$ . Figure 3 shows the superposition of the two solutions. As predicted by the linear error analysis (Hagstrom and Keller [11]), the error decays as we move into the interior. Figure 4 shows the superposition of the large domain solution and a solution on the small domain found using  $u_x(\tau, y) = 0$ . The level curves are seen to be greatly distorted.



$x = 0.057$

$x = 1.262$

FIGURE 1.



$x = 0.057$      $x = .381$

FIGURE 2.

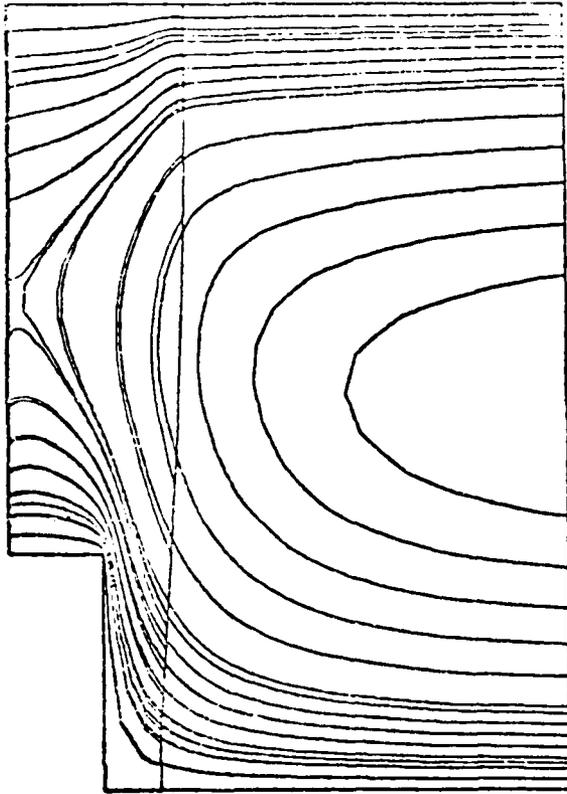


FIGURE 3.

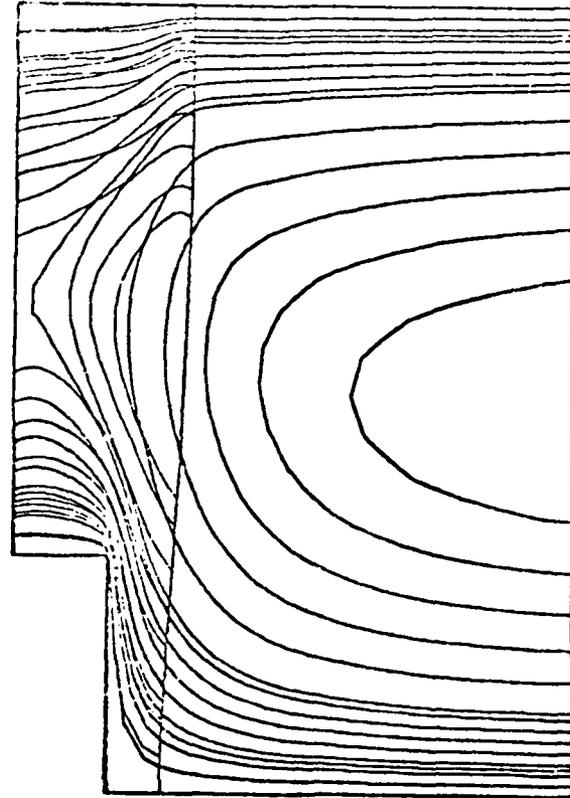


FIGURE 4.

A more interesting case, from the point of view of existence theory, occurs when  $d < 0$ . Then we may expect that the presence of the finite thick region will preclude the existence of steady solutions, even though the infinite part is thin enough for a one dimensional solution to exist ( $\lambda < \lambda_c$ ). In terms of the physical problem this says that a finite area of excess thickness can cause spontaneous ignition in a slab whose infinite part is stable.

In order to find critical values of  $\lambda$ , we used regular continuation in that parameter to generate initial guesses for Newton's method. The minimum

step size used was  $\Delta\lambda = .001$ . Tabulated in Table II are the critical values of  $\lambda$  thus found as functions of  $a = x_{\text{step}} - x_0$ , the half-width of the thick part. Here,  $d = .4$ . As expected, they vary between the one dimensional critical values of the thick region and the infinite region. Plotted in Figure 5 are the level curves of the solution for  $\lambda = 1.857$ ,  $a = 2.013$ , just before the steady solution ceases to exist. Here, the maximum of  $u$  at the left boundary is 1.27 while at infinity it is 0.3.

d	half-width: a	$\lambda_{\text{crit.}}$
-.4	$\infty$	1.791
-.4	2.994	1.821
-.4	2.013	1.858
-.4	1.028	1.978
-.4	.7415	2.049

TABLE II

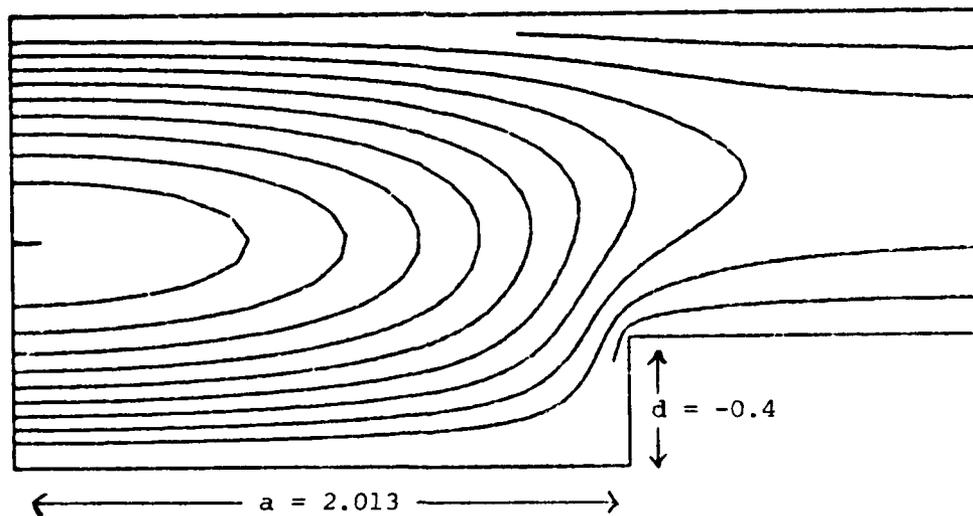


FIGURE 5.

In summary, the calculations we have presented confirm the usefulness of the asymptotic boundary conditions described in [11] and provide a practical example of their implementation.

Appendix: Proof of Theorem 2.9

We need to establish the conditions of [11], assumption 6.6. (here, we take  $\delta_1 = \frac{\delta}{2\alpha}$ .) Note that the combinations  $S(x, p; F_u(u_\infty))Q_\infty$ ,  $S(x, p; F_u(u_\infty))(I - Q_\infty)$  are easily represented in terms of the eigenfunction expansion - namely, if  $\phi = \sum_{\ell} c_{\ell} w_{\ell}$ ,

$$(A.1) \quad \begin{aligned} \text{a) } S(x, p; F_u(u_\infty))Q_\infty \phi &= \sum_{\substack{\ell \\ \operatorname{Re} \lambda_{\ell} < 0}} e^{\lambda_{\ell}(x-p)} c_{\ell} w_{\ell}, \quad x > p; \\ \text{b) } S(x, p; F_u(u_\infty))(I - Q_\infty) \phi &= \sum_{\substack{\ell \\ \operatorname{Re} \lambda_{\ell} > 0}} e^{\lambda_{\ell}(x-p)} c_{\ell} w_{\ell}, \quad x < p. \end{aligned}$$

From (2.10f) we then have:

$$(A.2) \quad \begin{aligned} \text{a) } \|S(x, p; F_u(u_\infty))Q_\infty\| &< a e^{-\lambda_-(x-p)}, \quad x > p; \\ \text{b) } \|S(x, p; F_u(u_\infty))(I - Q_\infty)\| &< a e^{\lambda_+(x-p)}, \quad x < p. \end{aligned}$$

We now estimate  $\max_x \|R(w^1) - R(w^2)\|$  where  $\max_x \|w^i\| < \delta$ ,  $w^i = \begin{pmatrix} w_1^i \\ w_2^i \end{pmatrix}$ . By (2.4b) and the definition of the norm we have:

$$(A.3) \quad \begin{aligned} &\|R(w^1) - R(w^2)\| \\ &= \|f(u_\infty + w_2^1, \chi) - f_u(u_\infty, \chi)w_2^1 - f(u_\infty + w_2^2, \chi) + f_u(u_\infty, \chi)w_2^2\|_{W_1(\Omega)}. \end{aligned}$$

We note that Sobolev's inequality (Agmon [1]) implies that:

$$(A.4) \quad |w_2^i| < 2\gamma \|w_2^i\|_{W_2(\Omega)} < 2\gamma \delta.$$

We have (suppressing the  $\chi$  in the argument of  $f$ ):

$$f(u_\infty + w_2^1) - f(u_\infty + w_2^2) - f_u(u_\infty)(w_2^1 - w_2^2) = \\ \int_0^1 dt \int_0^1 ds f_{uu}(u_\infty + s(w_2^2 + t(w_2^1 - w_2^2)))(w_2^1 - w_2^2)(w_2^2 + t(w_2^1 - w_2^2)).$$

Taking absolute values and integrating yields:

$$\|f(u_\infty + w_2^1) - f(u_\infty + w_2^2) - f_u(u_\infty)(w_2^1 - w_2^2)\|_{L_2(\Omega)} \\ \leq \frac{K_1}{2} \frac{1}{2} \|w_2^1 + w_2^2\| \|w_2^1 - w_2^2\|_{L_2(\Omega)} \\ \leq \frac{K_1}{2} \cdot \partial\gamma\delta \|w_2^1 - w_2^2\|_{L_2(\Omega)}.$$

Similarly we have:

$$\frac{\partial}{\partial y_i} (f(u_\infty + w_2^1) - f(u_\infty + w_2^2) - f_u(u_\infty)(w_2^1 - w_2^2)) \\ = (f_{y_i}(u_\infty + w_2^1) - f_{y_i}(u_\infty + w_2^2) - f_{uy_i}(u_\infty)(w_2^1 - w_2^2)) \\ + (f_u(u_\infty + w_2^1)(w_2^1)_{y_i} - f_u(u_\infty + w_2^2)(w_2^2)_{y_i} - f_u(u_\infty)(w_2^1 - w_2^2)_{y_i}) \\ + (u_\infty)_{y_i} (f_u(u_\infty + w_2^1) - f_u(u_\infty + w_2^2) - f_{uu}(u_\infty)(w_2^1 - w_2^2)).$$

The first and third terms of the right-hand side of the expression above are easily estimated in precisely the same fashion as used to produce (A.5). It is only necessary to replace  $|f_{uu}|$  by  $|f_{uuy_i}|$  for the first term and by  $|(u_\infty)_{y_i}| |f_{uuu}|$  for the third. For the second we have:

$$f_u(u_\infty + w_2^1)(w_2^1)_{y_i} - f_u(u_\infty + w_2^2)(w_2^2)_{y_i} - f_u(u_\infty)(w_2^1 - w_2^2)_{y_i} \\ = \int_0^1 dt f_{uu}(u_\infty + w_2^2 + t(w_2^1 - w_2^2))(w_2^1 - w_2^2)(w_2^2 + t(w_2^1 - w_2^2))_{y_i} \\ + \int_0^1 dt \int_0^1 ds f_{uu}(u_\infty + s(w_2^2 + t(w_2^1 - w_2^2)))(w_2^1 - w_2^2)_{y_i} (w_2^2 + t(w_2^1 - w_2^2)).$$

Taking absolute values and integrating the expression above yields, in combination with estimates of the other terms:

$$\begin{aligned}
 (A.6) \quad & \sum_i \left\| \frac{\partial}{\partial y_i} (f(u_\infty + w_2^1) - f(u_\infty + w_2^2) - f_u(u_\infty)(w_2^1 - w_2^2)) \right\|_{L_2(\Omega)} \\
 & < K_2 \cdot 2\gamma\delta \|w_2^1 - w_2^2\|_{L_2(\Omega)} + K_3 \cdot 2\gamma\delta \|w_2^1 - w_2^2\|_{L_2(\Omega)} \\
 & + \frac{K_1}{2} \cdot 2\gamma\delta \|w_2^1 - w_2^2\|_{W_2(\Omega)} + \frac{K_1}{2} \cdot 2\gamma\delta \sum_i \|(w_2^1 - w_2^2)_{y_i}\|_{L_2(\Omega)}.
 \end{aligned}$$

From (A.3), (A.5) and (A.6) we conclude:

$$(A.7) \quad \|R(w^1) - R(w^2)\| < 2\gamma\delta(K_1 + K_2 + K_3) \|w^1 - w^2\|,$$

which implies:

$$\begin{aligned}
 (A.8) \quad & \max_x \left\| \int_y^x dp S(x,p) Q_\infty (R(w^1) - R(w^2)) - \int_x^\infty dp S(x,p) (I - Q_\infty) (R(w^1) - R(w^2)) \right\| \\
 & < 2\gamma\delta\alpha(K_1 + K_2 + K_3) \left( \frac{1}{\lambda_-} + \frac{1}{\lambda_+} \right) \max_x \|w^1 - w^2\| \\
 & < \max_x \|w^1 - w^2\|.
 \end{aligned}$$

Similarly we have:

$$(A.9) \quad \|R(w^1)\| = \|f(u_\infty + w_2^1) - f_u(u_\infty)w_2^1 - f(u_\infty)\|_{W_1(\Omega)}.$$

Using the previous estimates (with  $w^2 \equiv 0$ ) we find:

$$(A.10) \quad \|R(w^1)\| < \gamma\delta^2(K_1 + K_2 + K_3),$$

which implies:

$$(A.11) \quad \max_x \left\| \int_\tau^x dp \int_\tau^x dp S(x,p) Q_\infty R(w^1) - \int_x^\infty dp S(x,p) (I - Q_\infty) R(w^1) \right\| < \frac{\delta}{2}.$$

Finally, we require  $\xi \in A$  such that  $\max_x \|S(x, \tau)\xi\| < \frac{\delta}{2}$ . From (A.2a) this becomes:

$$(A.12) \quad \|\xi\| < \frac{\delta}{2\alpha}.$$

All of the requirements for [11], assumption 6.6, have now been met, so the proof of Theorem 2.9 is complete. /

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20. ABSTRACT (cont.)

exact boundary conditions and to obtain useful approximations to them. They are based on the Laplace transform solution of the linearized problem at infinity. We discuss the incorporation of these conditions in a finite difference scheme and present the results of a numerical experiment: the solution of the Bratu problem in a two dimensional stepped channel. We also examine certain problems concerning the existence of solutions on infinite domains.

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