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# Free Boundary Problems with Nonlinear Source Terms*

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**Summary.** The method of lines is used to semi-discretize the non-linear Poisson equation over a domain with a free boundary. The resulting multipoint free boundary problem is solved with a line Gauss-Seidel method which is shown to converge monotonically. The method of lines solution is then shown to converge to the continuous solution of the variational inequality form of the obstacle problem. Some numerical results for the diffusion-reaction equation indicate that the method is applicable to more general free boundary problems for nonlinear elliptic equations.

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## I. Introduction

Front tracking for free and moving boundary problems refers to numerical methods for differential equations over unknown domains which explicitly use the geometry of the domain in the solution process. Such methods are applied routinely to one and multi-dimensional elliptic, parabolic and hyperbolic equations. They are often conceptually simple, numerically robust, and relatively independent of the structure and data of the problem provided that the free boundaries are indeed trackable. Surveys of numerical methods for free boundary problems in general and front tracking in particular may be found in [13, 17, 9], and [5].

Although front tracking is widely used in practice only few theoretical results exist which a priori assure its success. Moreover, most of the existing analytic work applies either to interval problems for ordinary differential equations (e.g. the minimum fuel problem of optimal control [15]), to one dimensional diffusion problems of Stefan type (see, e.g. [4]), or to one dimensional

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hyperbolic problems (see, e.g. [7]). An analysis of multi-dimensional front tracking is only now beginning.

In our own work we have used a fully implicit sequentially one dimensional front tracking method to solve multi-dimensional free boundary problems. As demonstrated in [11] a numerical algorithm results which is applicable to a variety of potential and diffusion problems. Moreover, for the Reynolds equation describing the hydrodynamic lubrication of a journal bearing it is possible to establish that the iteration required in the sequentially one dimensional algorithm is convergent, and that the discrete numerical solution converges to the continuous solution as mesh sizes go to zero [12].

It is the purpose of this paper to discuss again front tracking based on sequentially one dimensional methods. In overall outline our approach here is similar to that of [12]; however, by using monotonicity instead of fixed point arguments nonlinear field equations can be treated. Thus, our new analysis applies not only to the Reynolds equation but also to certain (time discretized) diffusion problems involving Michaelis-Menten or second order irreversible reactions. Finally, some numerical experiments with reaction diffusion equations are described which show that the numerical method is practically unaffected by the presence of nonlinear source terms in the field equations.

## 2. The Algorithm

We shall begin by considering front tracking for the following free boundary problem on the rectangle $R=(0,\bar{X})\times(0,\bar{Y})$.

$$\Delta u = f(x,y,u) \qquad (x,y)\in D, \tag{2.1 a}$$

$$u = g(x,y) \qquad (x,y)\in \partial D_1, \tag{2.1 b}$$

$$u = \frac{\partial u}{\partial n} = 0 \qquad (x,y)\in \partial D_2 \quad \text{if } x<\bar{X}, \tag{2.1 c}$$

$$u = g(x,y) \qquad (x,y)\in \partial D \quad \text{if } x=\bar{X}. \tag{2.1 d}$$

Here $D$ is a domain in $R$. Its boundary consists of two parts $\partial D_1$ and $\partial D_2$.

The given boundary $\partial D_1$ lies on the lines $x=0$, $y=0$ and $y=\bar{Y}$. $\partial D_2$ denotes the unknown free boundary which is assumed to be expressible as $x=s(y)$ and which bounds $D$ on the right. $s(y)$ is allowed to coincide in part or completely with the fixed boundary $x=\bar{X}$. When this occurs the free boundary condition (2.1c) is replaced by (2.1d). The geometry of the problem is apparent from Fig. 1. Problem (2.1) may be considered to be a typical obstacle problem (see, e.g. [8]).

We shall be interested in non-negative solutions of problem (2.1). To insure their existence and computability several hypotheses will be imposed on the data.

H1): $f$ and $g$ are continuously differentiable on $\bar{R}\times\{u: u\geqq 0\}$ and $\partial R$, respectively.

H2): $f(x,y,u)=f_1(x,y,u)+f_2(x,y,u)$ where

i) $\frac{\partial f_1}{\partial u} \geqq a_0 > -\lambda_0 = -\left\{\left(\frac{\pi}{\overline{X}}\right)^2 + \left(\frac{\pi}{\overline{Y}}\right)^2\right\}$, $u \geqq 0$,

ii) $\sup|f_2(x,y,u)| \equiv \|f_2\| < \infty$ where the supremum is taken over $R \times \{u: u \geqq 0\}$.

H3): $g(x,y) \geqq 0$ on $\partial R$.

H4): $\max\{g(0,y), -f(0,y,0)\} > 0$, $y \in (0,\overline{Y})$.

Hypothesis H1) can be relaxed somewhat, but minimal smoothness conditions are not central to our analysis. Hypothesis H2) allows an application of standard monotonicity arguments as, for example, in [1, p. 369]. We note that if in any given application a free boundary $x=s(y)$ has been computed, then one may set a posteriori $\overline{X} = \max_y s(y)$ and verify whether H2) holds for the calculation. H3) is consistent with the expressed aim to find non-negative solutions. The hypothesis H4) will be seen to assure that $D \neq \{\emptyset\}$.

Problem (2.1) will be discretized with the method of lines. We define a uniform partition $0=y_0<y_1<\ldots<y_{N+1}=\overline{Y}$ with mesh width $\Delta y$ and replace (2.1) by the system of nonlinear ordinary differential equations

$$u_i'' + \frac{u_{i+1}+u_{i-1}-2u_i}{\Delta y^2} = f(x, y_i, u_i), \tag{2.2a}$$

$$u_i(0) = g(0, y_i) \equiv g_i(0), \tag{2.2b}$$

$$u_i(s_i) = u_i'(s_i) = 0 \qquad \text{if } s_i < \overline{X}, \tag{2.2c}$$

$$u_i(s_i) = g(\overline{X}, y_i) \equiv g_i(\overline{X}) \qquad \text{if } s_i = \overline{X}. \tag{2.2d}$$

For $u_0$ and $u_{N+1}$ we choose $g_0(x)$ and $g_{N+1}(x)$, respectively. Thus along each line $y=y_i$ the solution $\{u_i, s_i\}$ of a multi-point free boundary problem must be found.

In order to define a numerical algorithm for (2.2) an a priori bound for the solution of (2.2) is needed. Such a bound can be computed with the following two lemmas which are also used in subsequent convergence proofs.

**Lemma 2.1.** *Let $\{\alpha_i\}_{i=0}^{N+1}$ be a set of real numbers with $\alpha_0=\alpha_{N+1}=0$. Then*

$$\sum_{i=1}^{N} \alpha_i^2 \leqq K(\Delta y) \sum_{i=1}^{N+1} \left(\frac{\alpha_i - \alpha_{i-1}}{\Delta y}\right)^2$$

*where* $\lim_{\Delta y \to 0} K(\Delta y) = \left(\frac{\overline{Y}}{\pi}\right)^2$.

*Proof.* We apply the Rayleigh-Ritz inequality $\int_a^b f^2\,dx \leqq ((b-a)/\pi)^2 \int_a^b f'^2\,dx$ for $f \in H_0^1[a,b]$ to the function

$$f(y) = \sum_{i=0}^{N+1} \alpha_i \varphi_i(y)$$

where $\varphi_i(y)$ is the standard Chapeau function centered at $y_i$. Integration with respect to $y$ leads to

$$\sum_{i=1}^{N} (\tfrac{1}{3}\alpha_i\alpha_{i-1}+\tfrac{2}{3}\alpha_i^2) \leqq \left(\frac{\bar{Y}}{\pi}\right)^2 \sum_{i=1}^{N+1} \left(\frac{\alpha_i-\alpha_{i-1}}{\Delta y}\right)^2.$$

Writing $\alpha_i\alpha_{i-1}=\alpha_i^2+\alpha_i(\alpha_{i-1}-\alpha_i)$ and applying the algebraic geometric mean inequality to the term $\alpha_i(\alpha_{i-1}-\alpha_i)$ we obtain

$$\left(1-\frac{\Delta y}{6}\right) \sum_{i=1}^{N} \alpha_i^2 \leqq \left[\left(\frac{\bar{Y}}{\pi}\right)^2+\frac{\Delta y}{6}\right] \sum_{i=1}^{N+1} \left(\frac{\alpha_i-\alpha_{i-1}}{\Delta y}\right)^2.$$

Hence the lemma follows with $K(\Delta y)=\left[\left(\frac{\bar{Y}}{\pi}\right)^2+\frac{\Delta y}{6}\right] \Big/ \left[1-\frac{\Delta y}{6}\right]$.

Let $H=\prod_{i=1}^{N} H_0^1[0,\bar{X}]$ denote the Hilbert space of vectors $u=(u_1,\dots,u_N)$, $u_i\in H_0^1[0,\bar{X}]$, with inner product

$$\langle u,v\rangle = \sum_{i=1}^{N+1} \Delta y \int_0^{\bar{X}} \left\{u_i' v_i' + \left(\frac{u_i-u_{i-1}}{\Delta y}\right)\left(\frac{v_i-v_{i-1}}{\Delta y}\right)\right\} dx$$

and norm $\|u\|^2=\langle u,u\rangle$ where $u_0\equiv u_{N+1}\equiv 0$. Then one can use the Lax-Milgram lemma to prove the following result.

**Lemma 2.2.** *The fixed boundary value problem*

$$\psi_i''+\frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{\Delta y^2}-a_0\psi_i=\alpha_i(x), \qquad i=1,\dots,N, \tag{2.3}$$

$$\psi_i(0)=\psi_i(\bar{X})=0,$$

$$\psi_0(x)\equiv\psi_{N+1}(x)\equiv 0$$

*for $\alpha_i\in C^0(0,\bar{X}]$ has a unique solution for sufficiently small $\Delta y$. If $\alpha_i\leqq 0$ then this solution is non-negative.*

*Proof.* We remark that an analogous result for the continuous problem $\Delta\psi - a_0\psi\leqq 0$ is well-known because $a_0$ dominates the first eigenvalue of the Laplacian on $R$. For the above discrete problem the lemma can be eastablished by defining on $H$ the bilinear operator

$$B[u,v]=\langle u,v\rangle + a_0 \sum_{i=1}^{N} \Delta y \int_0^{\bar{X}} u_i v_i$$

and proving its continuity and coercivity on $H$. In fact, continuity in $u$ and $v$ follows by inspection because the Rayleigh-Ritz inequality applies to each component $u_i$ and $v_i$. To show that $B[u,u]\geqq\gamma\|u\|^2$ for $\gamma>0$ we apply Lemma 2.1 to obtain the inequality

$$\sum_{i=1}^{N} \Delta y \int_0^{\bar{X}} u_i u_i\, dx \leqq \sum_{i=1}^{N} \alpha\Delta y \left(\frac{\bar{X}}{\pi}\right)^2 \int_0^{\bar{X}} u_i'^2\, dx$$

$$+(1-\alpha)\sum_{i=1}^{N+1} \Delta y K(\Delta y) \int_0^{\bar{X}} \left(\frac{u_i-u_{i-1}}{\Delta y}\right)^2 dx$$

for any $\alpha\in[0,1]$. The coefficients of both integrals on the right are equal if $\alpha = K(\Delta y)/\left[\left(\frac{\bar{X}}{\pi}\right)^2 + K(\Delta y)\right]$. Thus

$$\left|a_0 \sum_{i=1}^{N} \Delta y \int_0^{\bar{X}} u_i^2\,dx\right| \leqq |a_0|\,K(\Delta y)\left(\frac{\bar{X}}{\pi}\right)^2 \Big/ \left[\left(\frac{\bar{X}}{\pi}\right)^2 + K(\Delta y)\right]\langle u,u\rangle.$$

But in view of H2) and Lemma 2.1.

$$\lim_{\Delta y+0} |a_0|\,K(\Delta y)\left(\frac{\bar{X}}{\pi}\right)^2 \Big/ \left[\left(\frac{\bar{X}}{\pi}\right)^2 + K(\Delta y)\right] < 1.$$

Hence for sufficiently small $\Delta y$ it follows that $B[u,u]\geqq\gamma\|u\|^2$ for some $\gamma>0$. By the Lax-Milgram lemma there exists a unique solution $\{\psi_i\}_{i=1}^N$ of (2.3). If $\alpha_i\leqq 0$ then let $\bar{\psi}_i=\min\{\psi_i,0\}$. A straightforward calculation shows that

$$B[\psi,\bar{\psi}] = -\sum_{i=1}^{N} \Delta y \int_0^{\bar{X}} \alpha_i \bar{\psi}_i\,dx \leqq 0$$

and

$$B[\psi,\bar{\psi}] \geqq B[\bar{\psi},\bar{\psi}] \geqq 0.$$

These inequalities can hold only if $\bar{\psi}\equiv 0$ for $i=1,\dots,N$. Hence each $\psi_i$ is non-negative.

**Corollary 2.1.** *If the bound on* $a_0$ *in* H2) *is strengthened to*

$$a_0 > -\frac{16}{\bar{X}^2-\bar{Y}^2}$$

*then each* $\psi_i$ *can be bounded above by* $\mu_i = M(x(\bar{X}-x)+y_i(\bar{Y}-y_i))$ *for sufficiently large* $M>0$.

*Proof.* We compute

$$\mu_i'' + \frac{\mu_{i+1}-\mu_{i-1}-2\mu_i}{\Delta y^2} - a_0\mu_i = -4M - a_0\mu_i$$

$$\leqq \left(-1+|a_0|\frac{(\bar{X}^2+\bar{Y}^2)}{16}\right)(4M) \leqq -\gamma M \quad \text{for some } \gamma>0.$$

Hence for sufficiently large $M$ we can assure $\gamma M \geqq \max_{i,j}|\alpha_0|$. The conclusion follows by applying Lemma 2.2 to $\mu_i-\psi_i$. Note that $M$ is independent of $\Delta y$.

In order to give an algorithm for (2.2) we shall denote by $\psi_i$ the solution of (2.3) when

$$\alpha_i = -\max_R |f_1(x,y,0)| - \|f_2\| + \min\{a_0,0\}\,\|g\|$$

and write $\Gamma_i = \psi_i + \|g\|$ where $\|g\| = \max_{\partial R} g(x,y)$ and $\psi_0=\psi_{N+1}\equiv 0$.

Let $\Gamma$ be a positive constant such that $\Gamma\geqq\max\Gamma_i$, $x\in[0,\bar{X}]$, $i=1,\dots,N$, and set

$$K=\max\left|\frac{\partial f}{\partial u}(x,y,u)\right| \tag{2.4}$$

where the maximum is taken over the compact set $\bar{R}\,x\,[0,\Gamma]$. Then in analogy to the usual monotone methods for nonlinear elliptic equations (see, e.g. [1]) we shall generate a solution $\{u_i^*, s_i^*\}_{i=1}^N$ with the Gauss-Seidel iteration

$$Lu_i^m \equiv u_i^{m\prime\prime} - \left[\frac{2}{\Delta y^2}+K\right] u_i^m = F_i^m(x) \tag{2.5}$$

$$u_i^m(0)=g_i(0)$$
$$u_i^m(s_i^m)=u_i^{m\prime}(s_i^m)=0 \quad \text{if } s_i^m<\bar{X}$$
$$u_i^m(x)=g_i(\bar{X}) \quad \text{if } s_i^m=\bar{X}.$$

where

$$F_i^m(x) = -\frac{u_{i-1}^m+u_{i+1}^{m-1}}{\Delta y^2}+f(x,y_i,u_i^{m-1})-K\,u_i^{m-1}, \tag{2.6}$$

and where $m$ denotes the iteration. The functions $\{u_i^0\}$ are suitable initial guesses to be discussed below, and $s_i^m$ is the computed free boundary on the line $y=y_i$ in iteration $m$.

The solution $\{u_i^m, s_i^m\}$ of each scalar problem (2.5) is found exactly as described in [11]. For ease of reference the basic steps are outlined below. We emphasize, however, that the question of convergence of $\{u_i^m, s_i^m\}$ to a solution of (2.5) as $m\to\infty$ and to a solution of (2.1) as $\Delta y\to 0$ is completely independent of the algorithm used to solve each scalar problem (2.5).

In order to compute $u_i^m$ and $s_i^m$ we employ the Riccati transformation

$$u_i^m(x)=R(x)\,v_i^m(x)+w_i^m(x) \tag{2.7}$$

where $v_i^m(x)=u_i^{m\prime}(x)$, and where $R$ and $w_i^m$ are the solutions of

$$R'=1-\left[\frac{2}{\Delta y^2}+K\right]R^2, \qquad R(0)=0, \tag{2.8}$$

$$w_i^{m\prime}=-\left[\frac{2}{\Delta y^2}+K\right]R\,w_i^m-R(x)\,F_i^m(x), \qquad w_i^m(x)=g_i(0). \tag{2.9}$$

The Riccati transformation and the boundary conditions $u_i^m(s_i^m)=v_i^m(s_i^m)=0$ imply that $s_i^m$ must be a root of the equation

$$w_i^m(x)=0. \tag{2.10}$$

Throughout this paper we shall agree to choose the smallest root of (2.10) on $(0,\bar{X})$. If no such root exists we shall set $s_i^m=\bar{X}$. Finally, $v_i^m$ is computed from

$$v_i^{m\prime}=\left[\frac{2}{\Delta y^2}+K\right][R(x)\,v_i^m+w_i^m(x)]+F_i^m(x) \tag{2.11}$$

$$v_i^m(s_i^m)=\begin{cases}0 & \text{if } s_i^m<\bar{X}\\ \dfrac{g_i(\bar{X})-w_i^m(\bar{X})}{R(\bar{X})} & \text{if } s_m^i=\bar{X}.\end{cases}$$

The existence of a positive solution $R$ of (2.8) on $(0,\bar{X}]$ follows by inspection. The other two equations are linear and have bounded solutions for bounded source terms. Finally, if $s_i^m<\bar{X}$ we shall set $u_i^m\equiv 0$ on $[s_i^m,\bar{X}]$ so that each $u_i^m\in C^1[0,\bar{X}]$.

It is straightforward to extend the results of [12] to characterize the iterates $\{u_i^m\}$. We shall summarize the necessary results and outline their proof.

**Lemma 2.3.** *Let* $u_i^0(0)\geqq 0$ *for* $i=1,\dots,N$. *Then* $s_i^m>0$ *and* $u_i^m>0$ *on* $(0,s_i^m)$ *for* $1\leqq i\leqq N$ *and* $m=1,2,\dots$.

*Proof.* Consider $u_i^m(x)$ for arbitrary $i$ and $m$. Either $w_i^m(0)=g_i(0)>0$ or $w_i^m(0)=w_i^{m\prime}(0)=0$ and $w_i^{m\prime\prime}(0)=-F_i^m(0)>0$ because of H4). In either case $w_i^m>0$ on some interval $(0,s_i^m)$. If $u_i^m$ has a relative minimum at $x^*\in(0,s_i^m)$ then $v_i^m(x^*)=0$ and $u_i^m(x^*)=w_i^m(x^*)>0$.

The next lemmas depend on the observation that if $u_j^k-u_j^{k-1}\geqq 0$ for all $j$ and $k$ preceding the calculation along the line $y=y_i$ in iteration $m$ then because of (2.4)

$$F_i^m(x)-F_i^{m-1}(x)\leqq 0. \tag{2.12}$$

**Lemma 2.4.** *Let* $u_i^0\equiv 0$, $s_i^0=0$ *for* $i=1,\dots,N$. *Then* $u_i^m\geqq u_i^{m-1}$ *and* $s_i^m\geqq s_i^{m-1}$.

*Proof.* The result is true for $m=1$ by Lemma 2.3. Suppose next that $s_i^k\geqq s_i^{k-1}$ and $u_i^k\geqq u_i^{k-1}$ for all $j$ and $k$ preceding the computation along the line $y=y_i$ in iteration $m$. Then

$$(w_i^m-w_i^{m-1})'=-\left[\frac{2}{\Delta y^2}+K\right]R(x)(w_i^m-w_i^{m-1})$$
$$-R(x)\left[F_i^m(x)-F_i^{m-1}(x)\right],\qquad (w_i^m-w_i^{m-1})(0)=0$$

and (2.12) imply that $w_i^m\geqq w_i^{m-1}$ and hence that $s_i^m\geqq s_i^{m-1}$. The maximum principle is then applied to $L(u_i^m-u_i^{m-1})\leqq 0$ on $(0,s_i^{m-1})$ to conclude that $u_i^m\geqq u_i^{m-1}$ on $(0,s_i^{m-1})$ and hence on $[0,\bar{X}]$.

The sequence $\{u_i^m,s_i^m\}$ provides monotonely increasing lower bounds for the solution of (2.2). We can also obtain monotonely decreasing upper bounds

**Lemma 2.5.** *Let* $U_i^0=\Gamma_i$, $S_i^0=\bar{X}$. *Then the Gauss-Seidel iterates* $\{U_i^m,S_i^m\}$ *satisfy* $U_i^m\leqq U_i^{m-1}$ *and* $S_i^m\leqq S_i^{m-1}$.

*Proof.* By hypothesis $S_i^1\leqq S_i^0$ and by direct calculation $L(U_1^1-\Gamma_1)\geqq 0$. The maximum principle can now be applied inductively.

**Lemma 2.6.** *For the sequences* $\{u_i^m\}$ *and* $\{U_i^m\}$ *of Lemma* 2.4 *and* 2.5 *we have* $0\leqq u_i^m\leqq U_i^m\leqq\Gamma_i$.

*Proof.* We observe that $s_i^0<S_i^0$ and $u_i^0\leqq U_i^0$. If we assume that $u_j^k\leqq U_j^k$ for all $j$ and $k$ prior to the calculation along line $y=y_i$ in iteration $m$ then as in Lemma 2.4 we find that $s_i^m\leqq S_i^m$ and $u_i^m\leqq U_i^m$ on $(0,s_i^m)$ and hence on $[0,\bar{X}]$.

Thus, the solution of (2.2), if it exists, is bracketed by monotone sequences of functions and boundary points.

**Theorem 2.1.** *The sequence* $\{u_i^m,s_i^m\}$ *converges to a solution* $\{u_i^*,s_i^*\}$ *of the discrete free boundary problem* (2.2).

*Proof.* It follows from Lemma 2.6 that for each $i$ the sequence $\{u_i^m\}$ is uniformly bounded. Equation (2.5) then assures that $u_i^{m\prime\prime}$ is also uniformly bounded on $(0, s_i^m)$ and $(s_i^m, \bar{X})$. Thus, $\{u_i^m\}$ and $\{u_i^{m\prime}\}$ simultaneously are sequences of uniformly bounded equi-continuous functions so that $u_i^m$ converges monotonically to a continuously differentiable function $u_i^*$ as $m \to \infty$. At the same time the monotone sequence $\{s_i^m\}$ converges to a limit $s_i^*$ for each $i = 1, \ldots, N$. Moreover, let $[0, \tilde{x}] \in [0, s_i^*)$ then there exists an $m_0$ such that $\tilde{x} < s_i^{m_0}$ for all $m \geqq m_0$. On $(0, \tilde{x})$ the function $u_i^{m\prime\prime\prime}$ satisfies the equation $u_i^{m\prime\prime\prime} = \left[\frac{2}{\Delta y^2} + K\right] u_i^{m\prime} + F_i^{m\prime}(x)$.

Since $u_j^m \in C^1[0, \bar{X}]$ for all $j$ it follows that $u_i^{m\prime\prime}$ also is bounded and equicontinuous. Hence $u_i^m \to u_i^{*\prime\prime}$ as $m \to \infty$. Taking limits in Eq. (2.5) we see that $u_i^*$ is a solution of (2.6). Moreover because $u_i^m(x) \equiv 0$ on $[s_i^m, \bar{X}]$ we may conclude that $u_i^* = u_i^{*\prime} = 0$ at $x = s_i^*$. If $s_i^m = \bar{X}$ then $u_i^*(s_i^*) = g_i(\bar{X})$ by construction. Thus $\{u_i^*, s_i^*\}$ is a solution of the free boundary problem (2.2).

An analogous argument may be applied to show that the sequence $\{U_i^m, S_i^m\}$ converges to a solution $\{U_i^*, S_i^*\}$ of (2.2). However, the hypotheses imposed so far only guarantee existence of a solution, not its uniqueness. One can verify, for example, that if $f$ and $g$ are determined such that

$$u(x, y) = (S - x)^2 (s - x)^2, \quad 0 < s < S < \bar{X}$$

is a solution of $\Delta u = f$ then $f \equiv f(x)$ and $g \equiv g(x)$ satisfy the conditions H1–H4). But two distinct solutions of (2.1) result if we truncate $u$ after $s$ or $S$ and continue it as the zero function. In fact, one may observe that the increasing sequence $\{u_i^m\}$ converges to the minimal positive solution of (2.2). The monotone sequence $\{U_i^m\}$ will converge to the maximal solution whenever the corresponding Eq. (2.10) has a single root $S_i^m$ on $[0, X]$.

Uniqueness of the numerical solution can be guaranteed under the following additional hypotheses.

H5): $f_2(x, y, u) \equiv 0$

H6): $G_i(x) \equiv f(x, y_i, 0) - \dfrac{u_{i+1}^* + u_{i-1}^*}{\Delta y^2} \geqq 0$ on $[s_i^*, \bar{X}]$, $s_i^* < \bar{X}$,

where $\{u_i^*, s_i^*\}$ is the minimal solution obtained above. Hypothesis H5) is common to force uniqueness of the solution of the Dirichlet problem [1]. Hypothesis H6) is related to the condition $(\Delta u - f) u \leqq 0$ in the complementarity formulation of free boundary problems but shows the effect of the by-lines approximation. We note that $G_i(s_i^*) \geqq 0$ because otherwise $w_i^{*\prime}(s_i^*) > 0$ which contradicts that $s_i^*$ is the first zero of $w_i^*$ on $(0, s_i^*)$. We also note that since convergence of $\{u_i^m, s_i^m\}$ to $\{u_i^*, s_i^*\}$ is guaranteed the hypothesis H6 can be verified a posteriori.

**Theorem 2.2.** *Under the hypotheses* H5, 6) *the solution of* (2.2) *is unique for sufficiently small* $\Delta y$.

*Proof.* Let $\Delta_i = U_i^* - u_i^*$ on $[0, \bar{X}]$ where $\{U_i^*\}$ is any other non-negative solution. Then integration and summation by parts yield

$$\sum_{i=1}^{N} \Delta y \int_0^X \left[\Delta_i'' + \frac{\Delta_{i+1}+\Delta_{i-1}-2\Delta_i}{\Delta y^2}\right] \Delta_i \, dx$$
$$= -\sum_{i=1}^{N+1} \Delta y \int_0^X \left\{\Delta_i'^2 + \left(\frac{\Delta_i - \Delta_{i-1}}{\Delta y}\right)^2\right\} dx.$$

On the other hand, $U_i^*$ and $u_i^*$ satisfy (2.2) which leads to the identity

$$\sum_{i=1}^{N+1} \Delta y \int_0^X \left\{-\Delta_2'^2 - \left(\frac{\Delta_i - \Delta_{i-1}}{\Delta y}\right)^2 - [f(x, y_i, U_i^*) - f(x, y_i, u_i^*)]\, \Delta_i\right\} dx$$
$$= \sum_{i=1}^{N} \Delta y \int_{s_i^*}^{X} G_i(x)\, U_i^*(x)\, dx \geqq 0.$$

Since $[f(x, y, U_i^*) - f(x, y_i, u_i^*)]\, \Delta_i \geqq a_0 \Delta^2$ we see with the notation used in Lemma 2.2 that

$$-B[\Delta, \Delta] \geqq \sum_{i=1}^{N} \Delta y \int_{s_i^*}^{X} G_i(x)\, U_i^*(x)\, dx.$$

Hence $\Delta_i \equiv 0$ for $i = 1, \ldots, N$, and the solution is unique.

It is apparent that the above theory applies to more general problems than just Poisson's equation with Dirichlet boundary data. Since the key tool is the maximum principle one can treat equations like

$$L\tilde{u} \equiv \nabla \circ k \nabla u + a(x) \circ \nabla u = f(x, y, u)$$

provided the by-lines approximation also satisfies the maximum principle. Moreover, Neumann or reflection data can be given on $\partial D_1$. However, inhomogeneous data on the free boundary require careful estimation (see the method of lines for the dam problem described in [10]). The actual numerical performance of the above iterative method is not very sensitive to the boundary data on $x = s(y)$.

## 3. Convergence of the Method of Lines Approximation

The convergence of the discrete solution of (2.2) to the continuous solution of (2.1) as $\Delta y \to 0$ will be shown as in [12] by relating the computed solution $\{u_i\}$ to that of a variational inequality underlying (2.1). However, the nonlinearity of $f$ causes some technical complications.

We shall retain the hypotheses H 1,3,4,5). To simplify exposition only we shall replace H 2) by

H 2') $\dfrac{\partial f}{\partial u} \geqq 0, \quad u \geqq 0.$

In addition, our technique of proof requires that hypothesis H 6) be strengthened to

H 6') $G_i(x) \equiv f(x, y_i, 0) - \dfrac{u_{i+1}^* - u_{i-1}^*}{\Delta y^2} \geqq 0, \quad x \geqq s_i^*$

for any solution of (2.2).

In the proof of uniqueness of the numerical solution given above the hypothesis H6) could be verified a posteriori for a given $\Delta y$, whereas in H6′) the inequality $G_i \geqq 0$ has to hold a priori for all $\Delta y$. As we shall see below this condition can often be established with the maximum principle. In addition we shall assume that the boundary function $g$ is the restriction of a non-negative function $\tilde{g} \in C^0(R) \cap H^{2,s}(R)$ for some $s>2$. For example $\tilde{g}$ may be the classical solution of $\Delta \tilde{g}=0$, $\tilde{g}=g|_{\partial R}$. For ease of notation we shall identify $\tilde{g}$ with $g$.

Let $K$ be the closed convex set in $H^1(R)$ defined by

$$K=\{v: v\in H^1(R), 0\leqq v \leqq \Gamma, v-g\in H_0^1(R)\},$$

where $\Gamma$ is independent of $\Delta y$ (see Corollary 2.1). Then we can consider the variational inequality

$$\langle Au, v-u\rangle \leqq 0, \qquad v\in K \tag{3.1}$$

where $A$ is the nonlinear mapping from $H^1(R)$ to $H^{-1}(R)$ defined by

$$\langle Au, \varphi\rangle = (-\Delta u + f(x,y,u), \varphi), \qquad \varphi \in H^1(R)$$

and where $(u,v)=\int_R uv\,dx\,dy$. Under the hypotheses H1–5) we can state

**Theorem 3.1.** *The variational inequality* (3.1) *has a unique solution* $u\in K$. *Moreover,* $u\in C^{1,\lambda}(\bar{R})\cap H^{2,s}(R)$ *for* $\lambda = 1-\frac{2}{s}$.

For a proof of the existence of a generalized solution for (3.1) and for its regularity we refer to [8].

It will be convenient to define

$$B(u,v)=\int_R \nabla u \circ \nabla v\,dx\,dy$$

and to rewrite (3.1) as

$$B(u,u-v)+(f,u-v)\leqq 0. \tag{3.2}$$

Let us define next the subspace $M_N \subset H^1(R)$ consisting of all functions of the type

$$v_N(x,y)=\sum_{i=0}^{N+1} \varphi_i(y)\,\psi_i(x)$$

where again each $\varphi_i$ is the one-dimensional Chapeau function centered at $y=y_i$, and where $\psi_i(x)\in H^1[0,x]$. We note for further reference that for any two sets $\{\alpha_i\}_{i=0}^{N+1}$, $\{\beta_j\}_{j=0}^{N+1}$ we obtain by integration and rearrangement

$$\begin{aligned}
&\int_0^Y \left(\sum_{i=0}^{N+1}\alpha_i\varphi_i(y)\right)\left(\sum_{j=0}^{N+1}\beta_j\varphi_j(y)\right)dy \\
&\quad=\sum_{i=0}^{N}\Delta y\left(\frac{\alpha_i\beta_i}{3}+\frac{\alpha_i\beta_{i+1}}{6}\right)+\sum_{i=1}^{N+1}\Delta y\left(\frac{\alpha_i\beta_i}{3}+\frac{\alpha_i\beta_{i-1}}{6}\right) \\
&\quad=\Delta y\sum_{i=0}^{N+1}\alpha_i\beta_i-\frac{\Delta y}{6}\sum_{i=1}^{N+1}(\alpha_i-\alpha_{i-1})(\beta_i-\beta_{i-1}) \\
&\qquad -\tfrac{1}{2}\Delta y(\alpha_0\beta_0+\alpha_{N+1}\beta_{N+1}).
\end{aligned} \tag{3.3}$$

It is straightforward to verify with this identity that $\{v_N^k\}$ is a Cauchy sequence in $M_N$ if and only if $\{\psi_i^k\}$ is a Cauchy sequence in $H^1[0,x]$. Hence $M_N$ is a closed subspace of $H^1(R)$.

If $\{u_i\}_{i=0}^{N+1}$ is the computed solution of (2.2) we can define a function $U_N \in M_N$ by

$$U_N(x,y)=\sum_{i=0}^{N+1}\varphi_i(y)\,u_i(x).$$

It follows immediately from Lemma 2.2 that $U_N \in K$. Let $\| \ \|_0$ and $\| \ \|_1$ denote the usual norms on $L_2(R)$ and $H^1(R)$. Then we can give

**Lemma 3.1.** *$\|U_N\|_1 \leqq k$ for some constant $k$ and all sufficiently small $\Delta y$.*

*Proof.* Let $W_N=U_N-G_N$ where $G_N=\sum\varphi_i(y)\,g(x,y_i)$. Then from (3.3)

$$\begin{aligned}
B(W_N,W_N) &\leqq \sum_{i=1}^{N+1}\Delta y\int_0^X\left\{w_i'^2+\left(\frac{w_i-w_{i-1}}{\Delta y}\right)^2\right\}dx\\
&=\sum_{i=1}^{N+1}\Delta y\int_0^X\left\{-w_i''-\frac{w_{i+1}+w_{i-1}-2w_i}{\Delta y^2}\right\}w_i\,dx\\
&\leqq \sum_{i=1}^{N+1}\Delta y\int_0^X\{-f(x,y_i,u_i)+\Delta g_i\}\,w_i\,dx.
\end{aligned}$$

Since $W_N \in H_0(R)$ it follows from the boundedness of the right hand side that $\|W_N\|_1 \leqq k$ and hence that $\|U_N\|_1 \leqq k$. For any $V_N \in M_N \cap K$ we compute with the aid of (3.3)

$$\begin{aligned}
B(U_N,U_N-V_N)=\sum_{i=1}^{N+1}\Delta y\int_0^X\Bigg\{&\left(\frac{u_i-u_{i-1}}{\Delta y}\right)\left(\frac{u_i-u_{i-1}}{\Delta y}-\frac{v_i-v_{i-1}}{\Delta y}\right)\\
&+u_i'(u_i'-v_i')-\tfrac{1}{6}(u_i'-u_{i-1}')(u_i'-u_{i-1}'-(v_i'-v_{i-1}'))\Bigg\}dx,
\end{aligned}$$

where we have taken into account that $u_0-v_0\equiv u_{N+1}-v_{N+1}=0$. Let us set

$$R_1=\sum_{i=1}^{N+1}\frac{\Delta y}{6}\int_0^X(u_i'-u_{i-1}')(u_i'-u_{i-1}'-(v_i'-v_{i-1}'))\,dx.$$

Summation and integration by parts yield

$$B(U_N,U_N-V_N)=-\sum_{i=1}^{N}\Delta y\int_0^X\left\{\frac{u_{i+1}-u_{i-1}-2u_i}{\Delta y^2}+u_i''\right\}(u_i-v_i)\,dx-R_1.$$

Since $\{u_i\}$ is a solution of (2.2) on $(0,s_i)$ we can write

$$\begin{aligned}
B(U_N,U_N-V_N)=-\sum_{i=1}^{N}\Delta y\Bigg\{&\int_0^X-f(x,y_i,u_i)(u_i-v_i)\\
&+\int_{s_i}^X G_i(x)(u_i-v_i)\,dx\Bigg\}-R_1. \qquad (3.4)
\end{aligned}$$

For any $U_N \in M_N$ let us define

$$f_N(x, y, U_N) = \sum_{i=0}^{N+1} \varphi_i(y) f(x, y_i, u_i) \tag{3.5}$$

then it follows from (3.3) that

$$(f_N, U_N - V_N) = \sum_{i=1}^{N} \Delta y \int_0^{\bar{X}} f(x, y_i, u_i)(u_i - v_i)\, dx - R_2$$

where

$$R_2 = -\sum_{i=1}^{N+1} \frac{\Delta y}{6} \int_0^{\bar{X}} [f(x, y_i, u_i) - f(x, y_{i-1}, u_{i-1})][u_i - v_i - (u_{i-1} - v_{i-1})]\, dx.$$

We can now rewrite (3.4) as

$$B(U_N, U_N - V_N) + (f_N, U_N - V_N) = \sum_{i=1}^{N} \Delta y \int_{s_i}^{\bar{X}} G_i(x)(u_i - v_i)\, dx - R_1 - R_2.$$

By hypothesis $G_i(x) \geqq 0$ and $u_i \equiv 0$, $v_i \geqq 0$ on $[s_i, \bar{X}]$. Hence the computed solution $U_N \subset H^1(R)$ satisfies

$$B(U_N, U_N - V_N) + (f_N, U_N - V_N) \leqq R_N \tag{3.6}$$

where

$$R_N = -R_1 - R_2.$$

In order to prove convergence of $U_N$ to $u$ as $\Delta y \to 0$ we adapt the calculation of [3]. It follows from

$$B(U_N, U_N - V_N) + (f_N, U_N - V_N) \leqq R_N, \qquad V_N \in M_N \cap K_N,$$
$$B(u, u - v) + (f, u - v) \leqq 0, \qquad v \in K$$

that

$$\begin{aligned} B(u - U_N, u - U_N) \leqq & B(U_N - u, V_N - u) + B(u, v - U_N) + B(u, V_N - u) \\ & + (f, v - U_N) + (f, V_N - u) + (f - f_N, U_N - V_N) + R_N \\ = & B(U_n - u, V_N - u) + (f - \Delta u, v - U_N + V_N - u) \\ & + (f - f_N, U_N - u_N + u - V_N) + R_N. \end{aligned} \tag{3.7}$$

If we write

$$\hat{f}(x, y, U_N) = f(x, y, \sum \varphi_i(y) u_i)$$

then

$$(f - f_N, U_N - u) = (f - \hat{f}, U_N - u) + (\hat{f} - f_N, U_N - u)$$

so that $\frac{\partial f}{\partial u} \geqq 0$ implies that

$$(f - f_N, U_N - u) \leqq (\hat{f} - f_N, U_N - u).$$

We now can estimate

$$
\begin{aligned}
B(u-U_N, u-U_N) \leqq & \|f-\Delta u\|_0 \{\|V_N - v\|_0 + \|v-U_N\|_0\} \\
& + \|\hat{f}-f_N\|_0 \|U_N - u\|_0 + \|f-f_N\|_0 \|u-V_N\|_0 \\
& + \|\nabla(u-U_N)\|_0 \|\nabla(V_N-u)\|_0 + R_N
\end{aligned}
\tag{3.8}
$$

where so far $v$ and $V_N$ are arbitrary in $K$ and $M_N \cap K$.

Since $u-U_N \equiv 0$ for $y=0$ and $y=\bar{Y}$ it follows that there is a constant $\gamma>0$ such that

$$\gamma \|u-U_N\|_1^2 \leqq B(u-U_N, u-U_N).$$

Let us now choose

$$
\begin{aligned}
v(x,y) &= u(x,y), \\
V_N(x,y) &= \sum_{i=0}^{N+1} \varphi_i(y)\, u(x, y_i)
\end{aligned}
$$

where $u$ is the solution guaranteed by Theorem 3.1. Since $f$ is smooth, $u \in C^{1,\lambda} \cap H^{2,s}$, $s>2$ and $\|U_N\|_1 \leqq k$ for some generic constant $k$ which is independent of $\Delta y$, it follows from approximation theory (see, e.g. [16]) that

$$
\begin{aligned}
\|V_N - u\|_0 &\leqq k\,\Delta y^2 \\
\|\nabla(V_N - u)\|_0 &\leqq k\,\Delta y, \\
\|\hat{f} - f_N\|_0 &\leqq k\,\Delta y.
\end{aligned}
$$

If we now use the algebraic geometric mean inequality $ab \leqq \frac{a^2}{2\varepsilon} + \frac{\varepsilon b^2}{2}$ then (3.8) leads to the following estimate

$$\|u-U_N\|_1^2 \leqq k\,\Delta y^2 + R_N \tag{3.9}$$

for some constant $k>0$. Hence convergence is assured if $\lim_{\Delta y \to 0} R_N \to 0$. We observe from the definition of $R_N$ and the assumption $\frac{\partial f}{\partial u} \geqq 0$ that

$$
\begin{aligned}
R_N \leqq & \sum_{i=1}^{N+1} \frac{\Delta y}{6} \int_0^X (u_i' - u_{i-1}')(v_i' - v_{i-1}')\,dx \\
& + \sum_{i=1}^{N+1} \frac{\Delta y}{6} \int_0^X (f(x, y_i, u_i) - f(x, y_{i-1}, u_{i-1}))(v_i - v_{i-1})\,dx \\
& - \sum_{i=1}^{N+1} \frac{\Delta y}{6} \int_0^X [f(x, y_i, u_{i-1}) - f(x, y_{i-1}, u_{i-1})](u_i - u_{i-1})\,dx.
\end{aligned}
$$

Since $u(x,y) \in C^{1,\lambda}(R)$ it follows that $|v_i' - v_{i-1}'| \leqq k\,\Delta y^\lambda$ and $|v_i - v_{i-1}| \leqq k\,\Delta y$. Since also $\|U_N\|_1 \leqq k$ we see immediately that

$$\lim_{\Delta y \to 0} R_N \leqq 0.$$

Thus we have proven

**Theorem 3.2.** *The method of lines solution $U_N$ obtained by linearily interpolating the computed solution $\{u_i\}_{N+1}^N$ between lines converges in $H^1(R)$ to the unique solution $u$ of* (3.1) *as $\Delta y \to 0$.*

We note that the above estimates guarantee a convergence rate of $\Delta y^{\lambda/2}$. An improvement of this rate would require an a priori estimate for $|u_i' - u_{i-1}'|$. Also, if hypothesis H2) applies rather than $\frac{\partial f}{\partial u} \geqq 0$ then the above estimates must be handled with greater care. In particular, the coercivity of the variational inequality on $M_N$ must be maintained which requires that $U_N$ and $u$ satisfy the same boundary conditions on $\partial R$. Thus, one should prove first convergence of $U_N$ to $\tilde{u}$ and then convergence of $\tilde{u}$ to $u$ where $\tilde{u}$ satisfies piecewise linear boundary data on $x=0$ and $x=\bar{X}$.

The final point to consider is whether condition H6′) can reasonably be verified a priori. A useful tool in this connection is a simple one-dimensional version of the "moving parallel plane" version of the maximum principle [6]. For definiteness we shall introduce it as follows. Let $x_c$ be arbitrary in $\left[\frac{\bar{X}}{2}, \bar{X}\right]$ and let $x_L$ and $x_R$ denote points in $[0, \bar{X}]$ which are an equal distance to the left and right of $x_c$. Assume that the following additional hypotheses are satisfied

H7 a) $g(\bar{X}, y) = 0$ for $y \in (0, \bar{Y})$,

b) $g(x_L, y) \geqq g(x_R, y)$ for any $x_L, x_R \in (0, \bar{X})$ and $y = 0, \bar{Y}$.

c) $f(x_L, y, u) \leqq f(x_R, y, u)$ for any $x_L, x_R \in (0, \bar{X})$, $y \in (0, \bar{Y})$, $u \geqq 0$.

We note that b) and c) imply that $g$ and $-f$ are decreasing on $\left[\frac{\bar{X}}{2}, \bar{X}\right]$ and that $g(x,y)$ and $-f(x,y,u)$ for $x < \frac{\bar{X}}{2}$ lie above the left reflection of $g$ and $-f$ about $x = \frac{\bar{X}}{2}$.

**Lemma 3.2.** *Let $\{u_i, s_i\}$ be the computed minimal solution of* (2.2). *Assume also that $s_i^1 \geqq \frac{\bar{X}}{2}$. Then $u_i(x_L) \geqq u_i(x_R)$.*

*Proof.* Since $u_i^0 \equiv 0$ the result is true for $m=0$ and $i=1, \ldots, N$. Suppose the lemma is true for all $u_j^k$ prior to the calculation along line $y = y_i$ in iteration $m$. Because of monotonicity $s_i^m \geqq s_i^1 \geqq \frac{\bar{X}}{2}$. Now let $x_c$ be arbitrary in $\left[\frac{\bar{X}}{2}, \bar{X}\right)$. If $x_c > s_i^m$ then the conclusion follows because $u_i^m > 0$ on $[0, s_i^m)$ and $u_i^m \equiv 0$ on $[s_i^m, \bar{X}]$. If $x_c < s_i^m$ we set $x_E = x_c - (s_i^m - x_c)$ and define $v(x_L)$ by $v(x_L) = u_i^m(x_R)$ where $x_R = x_c + (x_c - x_L)$ for $x_L \in [x_E, x_c]$. Thus $v(x_L)$ is the left reflection of $u_i^m$ about $x_c$. In particular $v(x_E) = u_i^m(s_i^m) = 0$ where H7a) is used if $s_i^m = \bar{X}$. On $(x_E, x_c)$ we see that $v''(x_L) = u_i^m(x_R)''$ so that

$$L(u_i^m - v) = F_i^m(x_L) - F_i^m(x_R),$$
$$(u_i^m - v)(x_E) = u_i^m(x_E) > 0,$$
$$(u_i^m - v)(x_c) = 0.$$

But $F_i^m(x_L)-F_i^m(x_R)\leqq 0$ by the induction hypothesis and H7c) and by H7b) for $i=1$ and $N$. By the maximum principle $u_i^m(x_L)\geqq u_i^m(x_R)$. Since the lemma is true for all $i$ and $m$ it remains valid in the limit as $m\to\infty$.

Since Lemma 3.2 implies $u_i'\leqq 0$ on $\left[\frac{\bar{X}}{2}, \bar{X}\right]$ and since $G_i(s_i)\geqq 0$ it follows immediately that $G_i(x)\geqq 0$ on $[s_i, \bar{X}]$ so that H6) can be verified a priori. We also note that $s_i^1\geqq\frac{\bar{X}}{2}$ is assured, for example, if $f(x,y,u)\leqq 0$ for $x\in\left[0,\frac{\bar{X}}{2}\right]$, $y\in(0,\bar{Y})$, $u\geqq 0$ because (2.10) cannot have a root unless $f(x,y,u)$ is positive.

Finally, we remark that on occasion the boundary data and source term allow an application of the standard maximum principle to $u_i'$. For example, if $Lu_i'\geqq 0$ on $(0,s_i^m)$ then $u_i'$ cannot have an interior positive maximum. If, in addition $(u_i'^m)'(0)>0$ then $u_i'^m$ cannot have a positive maximum on $[0,x]$. We note that $(u_i^{m\prime})'(0)>0$ is induced if in the continuous problem

$$\lim_{x\to 0} u_{xx}=f(x,y,u)-g_{yy}(0,y)>0.$$

As we noted above, $\frac{\partial f}{\partial x}(x,y,u)\geqq 0$ and $u_i'\leqq 0$ imply $G_i'(x)\geqq 0$ and hence H6).

## 4. Applications

Numerical results referred to in this section were obtained with the research code described in [11]. In this program the Eq. (2.8) is solved in closed form while the linear Eqs. (2.9) and (2.11) are solved with the trapezoidal rule. The root of (2.10) is found by linear interpolation. Throughout, the iteration is terminated when the maximum absolute change in $u_i^m$ and $s_i^m$ from one iteration to the next falls below $10^{-8}$. However, the monotone convergence guaranteed by the above theory for the line Gauss-Seidel iteration was generally sacrificed to the improved convergence rates of the line SOR method.

### *a) The Reynolds Equation*

In [12] a convergence proof of front tracking for the linear Reynolds equation was given which applied to the hydrodynamic lubrication of a finite journal bearing. If the above theory is applied to this problem one can verify that fewer restrictions on the bearing geometry and inlet pressures need to be imposed. Moreover, the monotone convergence of the upper and lower bounding solutions to a common limit which was observed from the numerical results in [12] now follows directly from Theorem 2.2 above. And finally, hypothesis H6′) which was verified through the use of an ad-hoc bounding function, now follows from the generalized maximum principle Lemma 3.2. In fact, hypothesis H2) in [12] is essentially hypothesis H7c) above.

*b) The Obstacle Problem*

It is well known that the formulation (2.1) arises in the description of the general obstacle problem which usually is analyzed as a variational inequality. Thus the above theory is applicable to those obstacle problems whose free boundaries are single valued "trackable" functions.

A model obstacle problem is given in [2] for the Poisson equation

$$\Delta u = 1$$

where the boundary data are determined from the analytic solution

$$u = \frac{(x+1)^2 + y^2}{4} - \frac{1}{2} - \frac{1}{2} \ln \frac{(x+1)^2 + y^2}{2}$$

and where the free boundary is given by

$$(x+1)^2 + y^2 = 2.$$

It is easy to verify by induction that $u_i^{m\prime} \leqq 0$ for $i = 0, \ldots, N+1$ and all $m$. Hence the method of lines provides a convergent numerical algorithm for this problem. The program of [11] was used to solve this free boundary problem on the domain $[0, 0.5] \times [0, 1]$ chosen in [2] for a finite element calculation. Equiva-

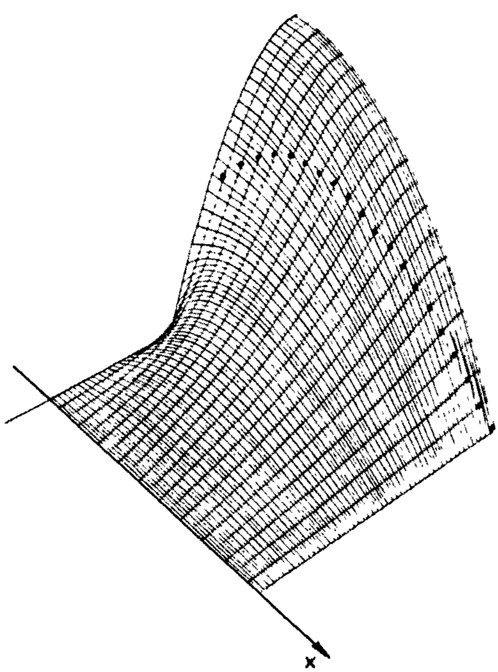


**Fig. 1.** Plot of membrane and obstacle for problem (4.1). $\Delta x = 1/20$, $\Delta y = 1/100$, $w = 1.6$; 51 iterations for convergence. Computing time on the Cyber 730 was 60 s

Please note: In this and subsequent figures $x$ is discretized and $y$ is retained as the continuous variable for the method of lines approximations.

lent results were obtained. With $\Delta y = 0.05$ the absolute error $s_i - s(y_i)$ increased from $2.10^{-5}$ for $i=1$ to $3.5 \cdot 10^{-3}$ for $i=N$. Reduced accuracy near $y=1$ is to be expected because the free boundary becomes less orthogonal to the mesh lines as $y \to 1$.

The above obstacle problem is benign because the obstacle has vanishing slope on $y=1$ so that $u \in C^{1,\lambda}(\bar{R})$. In contrast, consider the obstacle problem where an elastic membrane $w$ over the unit square is displaced by a parabolic punch $v = 1 - x^2 - 4(y-1)^2$. Then the difference $u = w - v$ satisfies

$$\begin{aligned} \Delta u &= 10 \qquad & (x,y) \in D \\ u &= \max(-v, 0) \qquad & (x,y) \in \partial D \end{aligned} \tag{4.1}$$

and

$$u = \frac{\partial u}{\partial n} = 0 \qquad x = s(y).$$

In this case $s_0 = 0.5$ and $s_i \geqq s_0$. Theorems 2.1 and 2.2 remain valid because Lemma 3.2 may be applied. On the other hand, the proof of Theorem 3.2 does not hold because $u \notin C^{1,\lambda}(\bar{R})$. Numerical results do show convergence as $\Delta y \to 0$. A plot of the membrane is given in Fig. 1.

### c) *Michaelis-Menten Reaction*

As a first example of a free boundary problem with a nonlinear source term we shall consider an extension of the oxygen diffusion-consumption model which is representative for a number of biological diffusion processes (see, e.g. [2]). Here an agent at concentration $u(x,y,t)$ is diffusing into the medium $D$. As it diffuses it is consumed at a rate determined by a Michaelis-Menten reaction. The concentration may be described by the free boundary problem

$$\Delta u - c u_t = f(x,y,u) \tag{4.2}$$

with

$$f(x,y,u) = \frac{\alpha u}{1+u} + \varepsilon(x,y)$$

where $\varepsilon(x,y)$ is a local threshold consumption rate. At the free boundary the concentration and its gradient vanish.

It is immediately verified that H2) holds for this choice of $f$ so that under suitable conditions on the boundary and initial data the time discretized diffusion equation can be solved with a convergent algorithm at each time level. Convergence as $\Delta t \to 0$ remains an open question.

For a numerical example we shall consider the steady-state case $c=0$ with the following additional data on the unit square $R$.

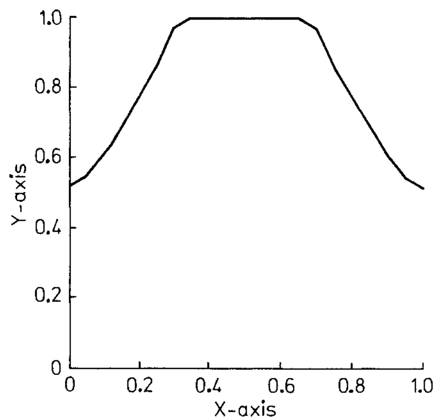


**Fig. 2.** Plot of the steady state free boundary for the Michaelis-Menten reaction problem (4.2). $\Delta x = 1/20$, $\Delta y = 1/100$, $w = 1.6$. 49 iterations for convergence. The same number of iterations was required for $K = \alpha = 1$ as for $K = \alpha = 0$

$$\varepsilon(x, y) = 8(y - 0.5)^2,$$

$$\frac{\partial u}{\partial n} = 0 \text{ when } y = 0 \text{ and } y = 1 \text{ and } s(y) = 1.$$

$$u(0, y) = y(1 - y).$$

Figure 2 shows $D$ and the free boundary. From the data symmetry about $y = 0.5$ is expected, although it is not specifically used in the program. We remark that the nonlinear source term had no discernible influence on the convergence of the line SOR iteration.

### *d) Second Order Reaction*

As a last example let us consider a two-component reaction problem where a substance at concentration $u$ diffuses into an immobile substance at concentration $v$ while undergoing a second order irreversivle reaction with it. The model equations and an application to the diffusion of oxygen in nickel are discussed in [14] where an asymptotic formula for the diffusion front is developed in one space dimension (which, however, does not correspond to a free boundary). Here we shall treat a two-dimensional problem in which movement into unreacted zones can occur only if the gradient on the diffusion front reaches a given threshold value. This problem goes considerably beyond the theory outlined above; however, the numerical method remains routinely applicable.

Specifically, for the same geometry as in examples b) and c) we shall consider the time dependent system

$$u_t = \Delta u - \text{kuv} \qquad 0 < x < s(y,t), \qquad y \in (0,1),$$
$$v_t = -\text{kuv}$$
$$u(x,y,0) = 0,$$
$$v(x,y,0) = v_0(x,y),$$
$$\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \qquad \text{on } y=0 \text{ and } y=1 \text{ and } x=1,\ t>0$$

and the free boundary condition

$$u=0, \qquad \frac{\partial u}{\partial n} = -\varepsilon \qquad \text{for } \varepsilon > 0 \text{ on } x = s(y,t).$$

This system is readily converted to a scalar problem for $u$ because

$$v(x,y,t) = v_0(x,y) \exp\left(-k \int_0^t u(x,y,r)\,dr\right).$$

Hence the scalar equation is

$$\Delta u - u_t = \text{kuv}_0 \exp\left(-k \int_0^t \text{udr}\right),$$

subject to the appropriate boundary conditions. We note in particular that the free boundary conditions must be rewritten as

$$u=0 \quad \text{and} \quad \left(1 + \left(\frac{\partial s}{\partial y}\right)^2\right) \frac{\partial u}{\partial x} = -\varepsilon$$

in order to compute along the lines $y = y_i$.

A fully time implicit approximation based on a backward difference quotient for $u_t$ and the trapezoid rule for the integral then leads to the following sequence of elliptic problems for $u \equiv u_n$ at time $t_n$

$$\Delta u = f(x,y,t,u)$$

where

$$f(x,y,t,u) = \frac{u - u_{n-1}}{\Delta t} + \text{kuv}\,\varphi(x,y,t_{n-1}) \exp\left(-k\,\Delta t\,\frac{u - u_{n-1}}{2}\right)$$
$$\varphi(x,y,t_n) = \varphi(x,y,t_{n-1}) \exp\left(-k\,\Delta t\,\frac{u - u_{n-1}}{2}\right)$$
$$\varphi(x,y,0) = 1.$$

For a boundary concentration of

$$u(x,y,t) = \frac{t}{1-t}(0,1 + 16\,y^2(1-y)^2), \qquad v_0(x,y) = 1$$

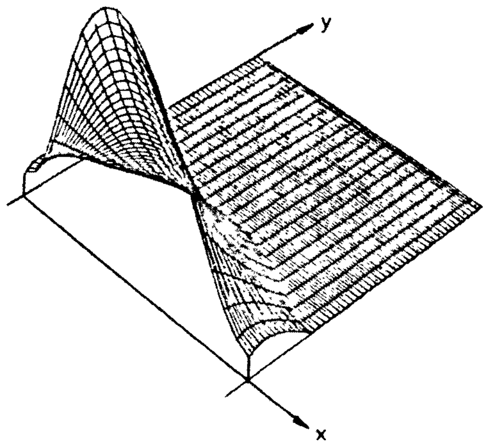


**Fig. 3.** Plot of $u(x, y, t)$ at $t=0.1$; $\Delta x=1/20$, $\Delta y=1/100$, $\Delta t=0.1/20$, $w=1.6$. About 34 iterations per time steps were required for convergence. Total computing time for 20 time steps was 240 sec on the Cyber 730

it follows immediately from the maximum principle that

$$0 \leqq u \leqq 1.1.$$

Since also $\varphi(x, y, t_n) \leqq 1$ it is simple to check that

$$\left|\frac{\partial f}{\partial u}\right| \leqq \frac{1}{\Delta t} + k$$

for sufficiently small $\Delta t$. Hence for the constant in (2.4) we shall use

$$K = \frac{1}{\Delta t} + k.$$

The algorithm outlined above is immediately applicable except that Eq. (2.10) is now replaced by

$$\tilde{w}_i(x) \equiv -R(x) \frac{\varepsilon}{1 + \left(\frac{s_{i+1}^{m-1} - s_{i-1}^{m}}{\Delta y}\right)^2} + w_i^m(x) = 0. \qquad (2.10')$$

Figure 3 shows a typical numerical solution for the reaction problem.

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