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On the numerical solution of free boundary problems for reaction-diffusion systems

by

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1. Introduction

Sequentially one dimensional methods have been suggested repeatedly for the numerical solution of free boundary problems for an elliptic (or time discretized parabolic) equation in $\mathbf{R}_n$. If the elliptic equation is approximated with the method of lines, and a sweep method is used in a line SOR iteration, then a numerical method is obtained which is conceptually simple, easy to program and robust in its numerical performance. Moreover, for model problems with the right variational structure the algorithm is known to converge [5].

We now would like to consider nonlinearly coupled elliptic equations with multiple free boundaries. They may arise, for example, after reaction-diffusion equations are time discretized. While fixed boundary problems for such systems have received some attention in the numerical analysis literature [2], [3], their free boundary analogs are only now beginning to appear, primarily in connection with heat and mass transport [1].

It is the purpose of this contribution to indicate that with virtually no increase in conceptual or programming complexity the common line SOR-sweep method can be used to solve systems of elliptic free boundary problems. In this initial research only problems with a rigidly prescribed structure are considered for which the free boundary problem is well posed and for which the iteration required to solve the discretized problem will converge monotonically. The convergence of the solution of the discrete problem to that of the continuous problem is proved in [5] for a single nonlinear elliptic problem but unresolved for systems.

To give an idea of the numerical performance of this method two reaction-diffusion problems with multiple free boundaries are solved. The examples indicate that the numerical method will perform reliably well outside the conditions for which its validity can be proved at this time. This research was supported by NSF Grant MCS 8302548.

2. Statement of the Problem

We shall consider the computation of non-negative solutions u_i for the following nonlinear elliptic system

$$\begin{gathered} L_i u_i = f_i(\vec{u}, x, y),\ 0 < x < 1,\ 0 < y < s_i(x),\ i = 1, \ldots, m \\ u_i(x, 0) = g_i(x) \\ \frac{\partial u}{\partial n}(0, y) = \frac{\partial u}{\partial n}(1, y) = 0 \end{gathered} \tag{2.1}$$

where L_i is a linear elliptic operator on $(0, 1) \times (0, 1)$ and where $\vec{u}$ stands for the vector $(u_1, \ldots, u_m)$. In (2.1) $s_i(x)$ denotes the free boundary corresponding to the component u_i. It is to be determined from the Cauchy conditions

$$u_i(x, s_i(x)) = \frac{\partial u_i}{\partial n}(x, s_i(x)) = 0. \tag{2.2}$$

We shall assume that s_i is constrained to lie in the interval $(0, 1]$. If $s_i(x) = 1$ then the free boundary condition (2.2) is replaced by the Dirichlet condition

$$u_i(x, s_i(x)) = 0,\ s_i(x) = 1. \tag{2.3}$$

Thus our formulation includes nonlinear systems on the fixed domain $(0, 1) \times (0, 1)$.

While the algorithm proposed below applies to more general problems than (2.1, 2), its analysis is usually intractible unless the problem has a well defined structure. In particular, we shall assume that the question of existence of a solution $\vec{u}^* = (u_1^*, \ldots, u_m^*)$ for (2.1, 2) can be answered with the theory of variational inequalities. To discuss whether (2.1, 2) is well posed the following notation is employed.

$D = (0, 1) \times (0, 1) \subset \mathbf{R}_2$

$(f, g) = \int_D fg\, dx\, dy$, $\langle f, g \rangle$ and $\|f\|$ are the inner product and norm on $H^1(D)$.

H = closure in $H^1(D)$ of C^∞ functions with compact support on $[0, 1] \times [0, 1)$.

$\dot{H} = \{\vec{u} : \vec{u} = (u_1, \ldots, u_m), u_i \in H$ for each $i\}$.

$$\frac{\partial u_i}{\partial n}(0, y) = \frac{\partial u_i}{\partial n}(1, y) = 0$$
$$u_i(x, s_i(x)) = \frac{\partial u_i}{\partial n}(x, s_i(x)) = 0. \tag{3.2}$$

The reason for this change of (2.1) is to insure that the derivatives of the right hand side of (3.1) with respect to u_i, $i = 1, \ldots, m$ are non-positive which will allow the repeated application of the maximum principle.

For ease of exposition only we shall assume from now on that $L_i u_i \equiv \equiv D_i \Delta u_i$ where $D_i > 0$ for $i = 1, \ldots, m$. The system (3.1, 2) will be approximated with the method of lines by discretizing the x-variable. For given $N > 0$ let $x_j = j/N$, $j = 0, \ldots, N$ denote $N+1$ lines. Then (3.1, 2) is replaced along the line $x = x_j$ by

$$l_i u_{i,j} \equiv u''_{i,j} - \left[\frac{2}{\Delta x^2} + K\right] u_{i,j} = G_{i,j}(\vec{u}_j, x_j, y) \tag{3.3}$$

where $\Delta x = 1/N$ and

$$G_{i,j}(\vec{u}_j, x_j, y) = -\frac{1}{\Delta x^2}(u_{i,j+1} + u_{i,j-1}) + $$
$$+ f_i(u_{1,j}, \ldots, u_{m,j}, x_j, y) - K u_{i,j}.$$

The boundary conditions at $x = 0$ and $x = 1$ are accounted for by setting

$$u_{i,-1} = u_{i,1} \text{ and } u_{i,N+1} = u_{i,N-1}.$$

The function $u_{i,j}$ is subject to the boundary conditions

$$u_{i,j}(0) = g_i(x_j),\ u_{i,j}(s_{i,j}) = 0 \tag{3.4}$$

and

$$u'_{i,j}(s_{i,j}) = 0 \text{ when } s_{i,j} < 1.$$

(We remark that the subsequent analysis requires that a convection term in (3.1) involving $\partial u_i/\partial x$ be discretized with a one sided difference quotient which assures that $\partial G_{i,j}/\partial u_{i,j\pm 1} \leqslant 0$. However, in actual calculations a central difference quotient can usually be used. A convection term like $\partial u_i/\partial y$ enters the differential equation (3.3) as u'_i).

The multi-point problem (3.3, 4) is solved iteratively in line SOR fashion. We make an initial quess $\{s^0_{i,j}, u^0_{i,j}\}$ for $i = 1, \ldots, M$ and $j = 0, \ldots, N$. We then compute for $k = 1, 2, \ldots$ along successive lines the new boundaries $\{s^k_{i,j}\}$ and functions $\{u_{i,j}^k\}$ by solving for fixed j

$$l_i \tilde{u}_{i,j} = G_{i,j}^k(y) \qquad i = 1, \dots, M \tag{3.5}$$
$$\tilde{u}_{i,j}(0) = g_i(x_j)$$
$$\tilde{u}_{i,j}(s_{i,j}^k) = \tilde{u}'_{i,j}(s_{i,j}^k) = 0$$

and setting

$$u_{i,j}^k = u_{i,j}^{k-1} + \omega(\tilde{u}_{i,j} - u_{i,j}^{k-1}).$$

Here $\omega \in (0, 2)$ is a relaxation factor which is generally chosen on the basis of experience. For $\omega = 1$ the SOR iteration is called a line Gauss-Seidel method.

The source term $G_{i,j}^u(y)$ in (3.5) is given by

$$G_{i,j}^k(y) = -\frac{1}{\Delta x^2}(u_{i,j+1}^{k-1} + u_{i,j-1}^k) + \\ + f(u_{1,j}^k, \dots, u_{i,j}^{k-1}, \dots, u_{m,j}^{k-1}, x_j, y) - K u_{i,j}^{k-1}$$

and incorporates the newest available data. After $\{u_{i,j}^k\}$ is known we advance to the next line x_{j+1}. After running through the lines from $j = 0$ to $j = N$ we begin iteration $k+1$ on line $j = 0$.

(3.5) describes a scalar second order free boundary problem. Its solution $\{s_{i,j}^k \, \tilde{u}_{i,j}\}$ is found with the sweep method described in [5]. In summary, we use the Riccati transformation

$$\tilde{u}_{i,j} = R_i(y)\,\tilde{u}'_{i,j} + w_{i,j}^k(y) \tag{3.6}$$

where R_i and $w_{i,j}^k$ are solutions of

$$R'_i = 1 - \left[\frac{2}{\Delta x^2} + K\right] R_i, \; R_i(0) = 0 \tag{3.7}$$

$$w_{i,j}^{k\prime} = -\left[\frac{2}{\Delta x^2} + K\right] R_i(y)\, w_{i,j}^k - R_i(y)\, G_{i,j}^k(y), \; w_{i,j}^k(0) = g_i(x_j).$$

The integration of (3.7) is called the forward sweep. The free boundary $s_{i,j}^k$ is the smallest root on (0, 1) of

$$\tilde{u}'_{i,j} = 0. \tag{3.8}$$

If there is no such root we set $s_{i,j}^k = 1$. The solution $\tilde{u}_{i,j}$ is completed by solving the initial value problem

$$\tilde{u}''_{i,j} = \left[\frac{1}{\Delta x^2} + K\right] [R_i(y)\, \tilde{u}'_{i,j} + w^k_{i,j}] + G^k_{i,j}(y)$$
$$\tilde{u}_{i,j}(s^k_{i,j}) = -\frac{w^k_{i,j}(s^k_{i,j})}{R_i(s^k_{i,j})} \tag{3.9}$$

and substituting $\tilde{u}_{i,j}$ into (3.6). The solution of (3.9) is the reverse sweep.

We remark that this particular sweep method for the solution of (3.5) has proven to be convenient for both the analysis and numerical solution of (3.5), but other one-dimensional free boundary solvers might equally well be used. In particular, if the two point free boundary problem (3.5) exhibits boundary or internal transition layers then such high order sweep methods as continuous orthonormalization may be necessary. (For an application of this method to an obstacle problem for a highly loaded beam see [6]).

It is our goal to establish that this sequentially one dimensional method will converge as $k \to \infty$. We shall assume that $\omega = 1$ so that $\tilde{u}_{i,j} = u^k_{i,j}$.

Lemma 3.1. *If* $u^0_{i,j} \equiv 0$ *and* $s^0_{i,j} = 0$ *for* $i = 1, \ldots, m$ *and* $j = 0, \ldots, N$ *then* $0 \leqslant u^{k-1}_{i,j} \leqslant u^k_{i,j} \leqslant G$ *and* $0 < s^{k-1}_{i,j} \leqslant s^k_{i,j} \leqslant 1$.

Proof. We shall use induction. By hypothesis $w^1_{1,0}(0) > 0$ so that $s^1_{1,0} > 0$. Assume now that $u^1_{1,0}$ has a negative minimum at $y^* \in (0, s^1_{1,0})$ then $u^{1\prime}_{1,0}(y^*) = 0$ and $w^1_{1,0}(y^*) < 0$ by (3.6) which contradicts that $s^1_{1,0}$ is the smallest root of $w^1_{1,0}(y) = 0$ on $(0, 1]$. Hence $u^1_{1,0} \geqslant 0$ on $(0, s^1_{1,0})$. Finally, we observe that $l_1\, u^1_{1,0} = f_1(0, \ldots, 0, 0, y) \geqslant 0$ rules out an interior maximum for $u^1_{1,0}$ so that $u^1_{1,0}(y) \leqslant G$. Let us assume next that Lemma 3.1 holds for all u and s prior to the calculation of $u^k_{i,j}$ and $s^k_{i,j}$. The mean value theorem and the hypothesis *vi*) show that

$$G^k_{i,j}(y) - G^{k-1}_{i,j}(y) \leqslant 0$$

which implies that $w^k_{i,j}(y) \geqslant w^{k-1}_{i,j}(y)$ and hence that $s^k_{i,j} \geqslant s^{k-1}_{i,j}$. The positivity of $u^k_{i,j}$ follows as above and $u^{k-1}_{i,j} \leqslant u^k_{i,j}$ is guaranteed by the maximum principle for

$$l_i\,(u^k_{i,j} - u^{k-1}_{i,j}) \leqslant 0 \text{ on } (0, s^{k-1}_{i,j}).$$

Finally, we observe that

$$l_i\,(G - u^k_{i,j}) \leqslant 0$$

so that also $G \geqslant u^k_{i,j}$. ∎

We can now argue as in [5] to establish

Theorem 3.1. *The sequence* $\{u^k_{i,j}, s^k_{i,j}\}$ *converges monotonely to a solution* $\{u^*_{i,j}, s^*_{i,j}\}$ *of the multi-point free boundary problem* (3.1, 2).

For details of the proof we refer to the discussion in [5] for $m = 1$ which carries over without change since only the number but not the type of equations has changed.

It may be noted that we can equally well begin our iteration from an initial guess of $s_{i,j}^0 = 1$ and $u_{i,j}^0 \equiv G$. In this case a monotone decreasing sequence is obtained which converges to a solution $\{U_{i,j}^*, S_{i,j}^*\}$ of the discrete free boundary problem (3.1, 2). However, without further assumptions one cannot generally conclude that the solution of (3.1, 2) is unique (see [5]).

Finally, we remark that the above sequentially one-dimensional algorithm may describe an excessive decoupling of the components of $\vec{u}_j^*$ along each line. An alternative but more complicated method may treat (3.5) as a system in which case the scalar Riccati transformation (3.6) will be replaced by the affine transformation

$$\vec{u}_j^k = R(y)\,\vec{u}_j^{k\prime} + \vec{w}_j^{k\prime}(y)$$

where R is an $m \times m$ matrix. This approach may be particularly useful if $L_i u_i$ is replaced by a linear operator $L_i(\vec{u})$ involving several components of $\vec{u}$.

4. Numerical Examples

The research code used for the numerical examples of [5] was modified to solve the system (3.1, 2). Schematically, we can illustrate the program with the simple DO LOOPS

```
   10 CONTINUE
      K = K+1
      DO 20 J = 0, N
      DO 20 I = 1, M
      CALL THE FORWARD SWEEP (3.7)
      CALL THE FREE BOUNDARY PLACEMENT (3.8)
   20 CALL THE REVERSE SWEEP (3.9)
      IF NO CONVERGENCE GO TO 10.
```

The forward and backward sweep are carried out with the trapezoidal rule. The free boundary is found by linear interpolation between mesh points where $w_{i,j}^k$ changes sign. The iteration is terminated when maximum absolute changes in $\{u_{i,j}^k\}$ and $\{s_{i,j}^k\}$ fall below 10^{-6} from one iteration to the next. As usual, the monotone convergence guaranteed by Theorem 3.1 is sacrificed to the improved convergence rate achieved with overrelaxation. Unless indicated otherwise the results shown are no longer sensitive to changes in the mesh sizes.

Proof. By hypothesis iii) $f_i \in H \subset L_q$ for $2 \leqslant q < \infty$. Since u_i^* satisfies the variational inequality

$$(-L_i u_i, v_i - u_i) + (f_i(u^*, x, y), v_i - u_i) \geqslant 0$$

for all $v_i \geqslant 0$ the regularity theorem of [4, p. 108] may be used to conclude that $u_i \in C^{1,\lambda}(\bar{D})$ for $\lambda = 1 - \frac{2}{q}$. ∎

The regularity of $s_i(x)$ remains an open question. However, if the boundary of $\{x : u_i(x), y > 0\}$ is smooth then the free boundary condition (2.2) applies in the classical sense because u_i is continuously differentiable on $\bar{D}$.

3. The Algorithm

A natural extension of the method given in [5] will be applied to the system (2.1, 2). Three steps are involved. First, the partial differential equations are approximated by a system of ordinary differential equations (method of lines approximation). Then an iteration is defined which solves the system as a sequence of free boundary problems for a single second order ordinary differential equation (continuous line SOR method). Finally, the solution of the scalar free boundary problem is carried out with a sweep method.

The hypotheses of the preceding section guarantee the existence of a solution $\vec{u}^*$. We shall compute its approximation as a limit of monotone sequences for which we need to impose an additional condition on the data.

Hypothesis vi) $\frac{\partial f_i}{\partial u_j} \leqslant 0$, $i \neq j$, $\vec{u} \in \mathbf{K}$ and $(x, y) \in D$. This requirement is quite restrictive in applications and will receive attention in future research (see also Example 4.2). Next, let the constant G be defined by

$$G = \max_{1 \leqslant i \leqslant m} \max_{0 \leqslant x \leqslant 1} g_i(x)$$

and let $\mathbf{K}'$ denote the closed bounded set $\{\vec{u} : 0 \leqslant u_i \leqslant G\} \subset \mathbf{R}_m$. Then choose a constant K such that

$$K \geqslant \max_{1 \leqslant i \leqslant m} \max_{\vec{u} \in K'} \frac{\partial f_i}{\partial u_i}(\vec{u}, x, y), \text{ uniformly in } D.$$

Since $\frac{\partial f_i}{\partial u_i} \geqslant 0$ by hypothesis v) we see that K is non-negative. The numerical method will now be applied to the following modification of (2.1, 2).

$$\begin{aligned} L_i u_i - K u_i &= f_i(\vec{u}, x, y) - K u_i \\ u_i(x, 0) &= g_i(x) \end{aligned} \tag{3.1}$$

$$((\vec{u},\vec{v})) = \sum_{i=1}^{m} (u_i, v_i), \langle\langle \vec{u},\vec{v}\rangle\rangle = \sum_{i=1}^{m} \langle u_i, v_i\rangle.$$

$\mathbf{K} = \{\vec{u} \in H : u_i \geqslant 0$ a.e. for $i = 1, ..., m\}$.

We note that H is a Hilbert space with inner product $\langle\langle , \rangle\rangle$ and that $\mathbf{K}$ is a closed convex subset of H.

In order to associate (2.1, 2) with a variational inequality we shall impose the following hypotheses

i) $(L_i u_i, u_i) \geqslant c \|u_i\|, c > 0, u_i \in H$

ii) g_i is continuous and positive on $[0, 1]$ for $i = 1, ..., m$

iii) $f_i : \mathbf{K} \to H$

iv) $f_i \geqslant 0$ for $\vec{u} \in \mathbf{K}$

v) If $F = (f_1, ..., f_m)$ then the derivative F' with respect to $\vec{u}$ exists for $\vec{u} \in \mathbf{K}$ and

$$\big((F'(\vec{u}, x, y)\vec{v}, \vec{v})\big) \geqq 0 \text{ for all } \vec{u} \in \mathbf{K} \text{ and } \vec{v} \in H.$$

Under these assumptions the above problem is well posed in the following sense. If u_i is a solution of (2.1, 2) which is extended as the zero function beyond the free boundary then (2.1, 2) can be written in complementarity form

$$\begin{aligned} -L_i u_i + f_i(\vec{u}, x, y) &\geqslant 0 \text{ on } D \\ (-L_i u_i + f_i(\vec{u}, x, y))\, u_i &= 0. \end{aligned} \tag{2.4}$$

As is well known (2.4) is formally equivalent to the variational inequality

$$(-L_i u_i, v_i - u_i) + (f_i(\vec{u}, x, y), v_i - u_i) \geqslant 0, \; i = 1, ..., m. \tag{2.5}$$

The solvability of these inequalities follows from an application of the results of [4].

THEOREM 2.1. *There exists a unique function $\vec{u}^* \in H$ whose components satisfy* (2.5).

Proof. Let $L\vec{u} = (L_1 u_1, ..., L_m u_m)$ then (2.5) can be written as the inequality

$$((-L\vec{u}, \vec{v} - \vec{u})) + \big((F(\vec{u}, x, y), \vec{v} - \vec{u})\big) \geqslant 0 \tag{2.6}$$

for $\vec{u}, \vec{v} \in \mathbf{K}$. The operator $Au \equiv -L\vec{u} + F(\vec{u}, x, y)$ maps $\mathbf{K}$ into H and satisfies $((A\vec{u} - A\vec{v}, \vec{u} - \vec{v})) \geqslant c\,\langle\langle \vec{u} - \vec{v}, \vec{u} - \vec{v}\rangle\rangle + \big((F'(\vec{w})(\vec{u} - \vec{v}), \vec{u} - \vec{v})\big)$ for some $\vec{w} \in \mathbf{K}$ between $\vec{u}$ and $\vec{v}$. The hypothesis v) assures that A is strongly monotone so that (2.6) has a unique solution $u^* \in \mathbf{K}$ by [4, p. 94]. ∎

THEOREM 2.2. $u_i \in H^2(D) \cap C^{1,\lambda}(\bar{D})$ *for any* $\lambda \in (0, 1)$.

EXAMPLE 4.1. *Michaelis-Menten reaction.* Consider the reaction problem for two components $u_1 \equiv u$ and $u_2 \equiv v$

$$\Delta u = f_1(u, v, x, y) \equiv \frac{u}{1+u+v} + \hat{f}_1(x, y)$$
$$\Delta v = f_2(u, v, x, y) \equiv \frac{v}{1+u+v} + \hat{f}_2(x, y), \tag{4.1}$$

where $\hat{f}_1, \hat{f}_2 \geqslant 0$. These equations model a "symbiotic interaction" between two species with population densities u and v [7, p. 221]. If $\hat{f}_1$ and $\hat{f}_2$ are differentiable then $f_1: \mathbf{K} \to H$ and $f_2: \mathbf{K} \to H$. We also verify that $\partial f_1/\partial u \geqslant 0$, $\partial f_1/\partial v$, $\partial f_2/\partial u \leqslant 0$ and $\partial f_2/\partial v \geqslant 0$. Moreover, if $0 \leqslant g_i(x) \leqslant 1$ then it is straightforward to verify that the matrix $(\partial f_i/\partial u_j)$ is positive definite (although not symmetric). Hence the system (4.1) satisfies all the conditions of Theorem 3.1 and can be solved monotonically with a line Gauss-Seidel method.

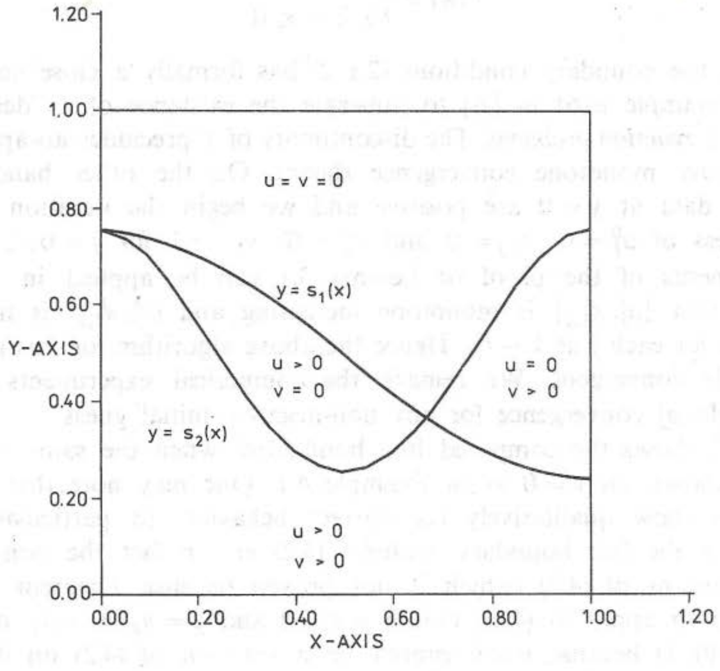

Fig. 4.1. Free boundaries for the Michaelis-Menten reaction system (4.1). $\Delta x = 1/20$, $\Delta y = 1/100$, $\omega = 1.7$. Convergence to 10^{-6} in 45 iterations. Maximum absolute error in the position of the free boundary is 0.0032 for $s_1(x)$ and 0.014 for $s_2(x)$. Cyber 855 execution time 160 sec.

Fig. 4.1 shows the computed solution which is obtained when $\hat{f}_1$ and $\hat{f}_2$ and g_1 and g_2 are determined such that

$$u(x, y) = \left(y - \frac{2+\cos(\pi x)}{4}\right)^2$$

and

$$v(x, y) = \left(y - \frac{2+\cos(2\pi x)}{4}\right)^2$$

are the analytic solutions. As already observed in [5], Michaelis-Menten reaction problems with or without free boundaries appear bengin for numerical methods.

EXAMPLE 4.2. The nonlinear system

$$\begin{aligned} \Delta u &= f(v) \\ \Delta v &= f(u) \end{aligned} \tag{4.2}$$

where

$$f(w) = \begin{cases} 1 & \text{if } w > 0 \\ 0 & \text{if } w \leqslant 0 \end{cases}$$

subject to the boundary conditions (2.1, 2) has formally a close connection with the example used in [8] to illustrate the existence of a "dead core" in *nonlinear reaction problems*. The discontinuity of f precludes an application of the above monotone convergence theory. On the other hand, if the boundary data at $y=0$ are positive and we begin the iteration with an initial guess of $u_j^0 = 0$, $s_{1,j} = 0$ and $v_j^0 = G$, $s_{2,j} = 1$ for $j = 0, \ldots, N$ then the arguments of the proof of Lemma 3.1 can be applied in order to conclude that $\{u_j^k, s_{1,j}^k\}$ is monotone increasing and $(v_j^k, s_{2,j}^k\}$ is monotone decreasing for each j as $k \to \infty$. Hence the above algorithm for this nonlinear problem is convergent. We remark that numerical experiments actually indicate global convergence for any non-negative initial guess.

Fig. 4.2 shows the computed free boundaries when the same boundary data are chosen on $y=0$ as in Example 4.1. One may note that the free boundaries show qualitatively the correct behavior. In particular, if the solutions of the free boundary problem (4.2) are in fact the non-negative $H^1(D)$ solutions of (4.2) (which is not proven because Theorem 2.2 does not appear to apply to (4.2)) then $y = s_1(x)$ and $y = s_2(x)$ may not cross in $(0, 1) \times (0, 1)$ because $u \equiv 0$ cannot be a solution of (4.2) on $0 < x < 1$ and $s_1(x) < y < 1$. The numerical free boundaries indeed do not cross.

Finally, we remark that the discontinuity of f at 0 may cause difficulties when the sweep equations are solved with the trapezoidal rule on a fixed mesh. Ideally the points $s_{i,j}^k$ should be added to the mesh when computing

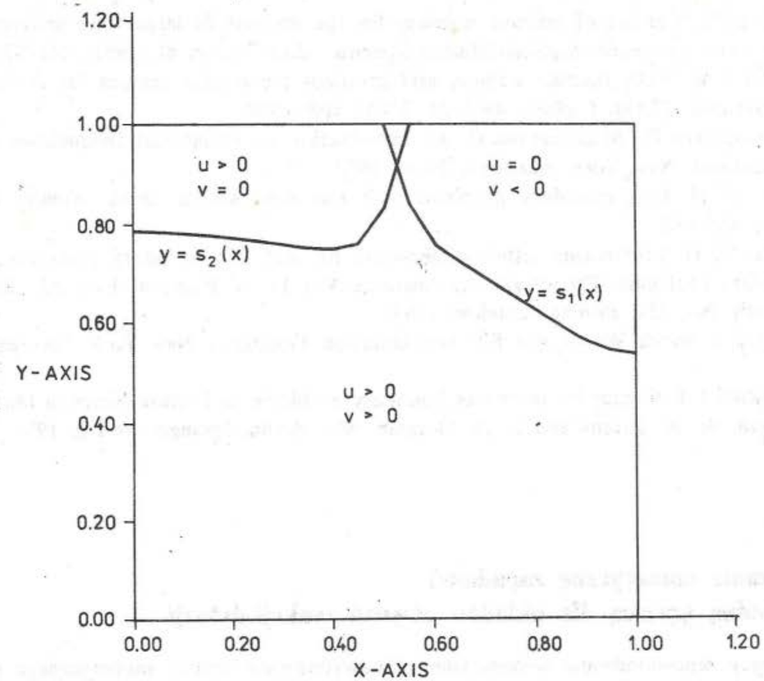

Fig. 4.2. Free boundaries for the reaction-diffusion system (4.2). $\Delta x = 1/20$, $\Delta y = 1/100$, $\omega = 1.7$. The computation was terminated after 200 iterations when the results oscillated slightly about a common value. The numerical free boundaries cross because of linear interpolation between computed points. Cyber 855 execution time 400 sec.

the next iterate. In the research code used here this modification was not incorporated. For monotone convergence no difficulties were observed, but arbitrary initial conditions and overrelaxation on occasion produced a cycling of the computed results from one iteration to the next. However, the change in the location of the free boundary always was too small to be noted in the computer plot. An additional complication arises in this example because the numerical results indicate that the free boundaries become tangent to the lines of computation where the free boundaries depart from $y = 1$. This behavior is reflected in changes of the free boundary on the line next to the contact point on $y = 1$ when the mesh width is changed. The remaining free boundary points do not move perceptibly.

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Rozwiązanie numeryczne zagadnień ze swobodną granicą dla układów równań reakcji-dyfuzji

W pracy zaproponowano sekwencyjnie jednowymiarowe metody numerycznego rozwiązywania zagadnień ze swobodną granicą dla równań eliptycznych (lub parabolicznych — zdyskretyzowanych w czasie) w R_n. Rozważa się nieliniowe sprężone układy równań eliptycznych z wieloma swobodnymi granicami. Układy takie odpowiadają zdyskretyzowanym w czasie równaniom reakcji — dyfuzji. Celem pracy jest pokazanie przydatności metody SOR do rozwiązywania takich problemów. Praca zawiera również wyniki odpowiednich eksperymentów numerycznych.

Численное решение проблем со свободной границей для систем уравнений реакции-диффузии

В работе представлены секвенциально одномерные методы численного решения проблем со свободной границей для эллиптических (или параболических дискретизированных по времени) уравнений в R_n. Рассуждены нелинейные сопряженные системы эллиптических уравнений с многими свободными границами. Такие системы соответствуют дискретизированным по времени уравнениям реакции-диффузии. Цель работы состоит в показании применяемости метода SOR для численного решения таких проблем. В работе представлены тоже результаты численных экспериментов.