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OFFICE OF CONTRACT ADMINISTRATION
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Date: 13 September 1979

Project Title: Locally One Dimensional Numerical Methods for Multidimensional Free Surface Problems

Project No: G-37-618

Project Director: Dr. Gunter H. Meyer

Sponsor: U. S. Army Research Office; Research Triangle Park, North Carolina 27709

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Research Triangle Park, N.C. 27709

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Closeout:

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Defense Priority Rating: None

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SPONSORED PROJECT TERMINATION/CLOSEOUT SHEETDate 4/11/84Project No. G-37-618School/~~Lab~~ MathematicsIncludes Subproject No.(s) N/AProject Director(s) Dr. Gunter H. MeyerGTRI / ~~GRI~~Sponsor U.S.Army Research Office; Research Triangle Park, NC 27709Title Locally One Dimensional Numerical Methods for Multidimensional Free
Surface ProblemsEffective Completion Date: 12/31/82 (Performance) 2/28/83 (Reports)and Contract Closeout Actions Remaining:

- ☐ None
- ☐ Final Invoice or Final Fiscal Report
- ☐ Closing Documents
- ☒ Final Report of Inventions Patent Questionnaire attached for Project Director
- ☒ Govt. Property Inventory & Related Certificate
- ☐ Classified Material Certificate
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PROGRESS REPORT

(TWENTY COPIES REQUIRED)

1. ARO PROPOSAL NUMBER: P-16373-M
2. PERIOD COVERED BY REPORT: August-December 1979
3. TITLE OF PROPOSAL: Locally one dimensional numerical methods for multidimensional free surface problems.
4. CONTRACT OR GRANT NUMBER: DAAG29-79-C-0145
5. NAME OF INSTITUTION: Georgia Institute of Technology
6. AUTHOR(S) OF REPORT: Gunter H. Meyer
7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

On the computational solution of elliptic and parabolic free boundary problems, to appear in the Proceedings of the Bimestre on Free Boundary Problems, Pavia 1979.
8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

Robert Boisvert, graduate student, summer 1979

16373-M

GUNTER H. MEYER
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BRIEF OUTLINE OF RESEARCH FINDINGS

Work has been completed on the convergence of the line SOR iteration for the method of lines approximation to the dam problem. In this porous medium flow problem the free boundary is a streamline which results in a coupling of the differential equations along the lines not only through the discretized Laplacian but also through the conditions on the free boundary. Under the hypothesis common in the variational treatment of the problem it can be shown that an iterative solution of the discrete free multipoint problem does indeed converge. The convergence of the discrete solution to the continuous solution, however, has not yet been established. In addition, numerical experiments have been carried out on the dam problem. They show that the method is readily applicable to problems with variable permeabilities without the need for Baiocchi type transformations. Our result will be included in the proceedings of the "Bimestre on Free Boundary Problems" held in Paria, Italy last September-October.

On the Computational Solution of Elliptic and Parabolic Free Boundary Problems

Gunter H. Meyer

Georgia Institute of Technology

The dominant difficulty in solving free boundary and interface problems numerically is introduced by the nonlinearity due to the unknown free surface. For the analytical and numerical solution of such problems a variety of approaches have been proposed which differ greatly in their applicability and effectiveness. It is the purpose of this paper to give an updated survey over some commonly used numerical methods for free surface problems, and then to describe in more detail the method of lines approach for the problem of percolation through a porous dam. An analysis of the iterative solution of the method of lines equations is presented in the second part of the paper.

1. Some Methods for Free Boundary Problems. Numerical methods for free surface problems can conveniently be grouped into "fixed domain methods" and "front tracking methods". A critical discussion of individual methods in each group may be found in [6], [7], and [12]. In this paper we shall attempt to update the earlier discussions for some selected methods.

Fixed domain methods require the solution of the free surface problem on an a priori given domain by absorbing the phenomena on the free boundary into the differential or integral field equations. Thus, the discretization required for

This research was supported in part by the U. S. Army Research Office under Grant DA AG29-76-G-0261 and carried out while the author was a Senior Visiting Fellow at the Institute of Computational Mathematics of Brunel University under Science Research Council Grant GR/A49256.

6-37-68

PROGRESS REPORT

(TWENTY COPIES REQUIRED)

1. ARO PROPOSAL NUMBER: P-16373-M
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3. TITLE OF PROPOSAL: Locally one dimensional numerical methods for
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4. CONTRACT OR GRANT NUMBER: DAAG29-79-C-0145
5. NAME OF INSTITUTION: Georgia Institute of Technology
6. AUTHOR(S) OF REPORT: Gunter H. Meyer
7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP
DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

A numerical method for the solidification of a binary alloy,
submitted to Int. J. Heat Mass Transfer
8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED
DURING THIS REPORTING PERIOD:

None

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BRIEF OUTLINE OF RESEARCH FINDINGS

Two particular objectives were pursued during the past six months. The first of these is the numerical solution of the binary alloy solidification problem in one space dimension. This process is characterized by simultaneous heat and mass transfer, both of which determine the evolution of the phase front. In earlier work we had shown that our sweep method in principle applies to this problem; however, thermal and mass diffusivities for a realistic problem differ by several orders of magnitude which complicates the numerical solution of the resulting stiff equations. We show that a Crank-Nicolson time discretization and a combination of the implicit Euler and trapezoidal rule can solve practical problems in binary alloy solidification. A report on this work has been submitted for publication (see below).

The main effort has been spent on examining the method of lines approach for non-standard two dimensional problems. As a model problem we have chosen Hele-Shaw flow with suction where the free boundary speeds up in time and eventually cusps. For particular initial conditions a closed form solution can be obtained with conformal methods. We are now checking how well our method can reproduce this solution. Finer grids appear necessary than for the usual Stefan problems, which, however, require long run times. To speed up our runs we are experimenting with a multi-grid algorithm for the method of lines. Preliminary results point to some time savings for this nonlinear problem.

A Numerical Method for the Solidification of a Binary Alloy

Gunter H. Meyer

School of Mathematics

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Atlanta, Georgia 30332, U.S.A.

Nomenclature

c , normalized concentration

\hat{c} , heat capacity, $J^{\circ}Ckg^{-1}$

D , mass diffusivity, m^2sec^{-1}

k , thermal conductivity, $J^{\circ}Cm^{-1}sec^{-1}$

L , length of slab, m

R , defined by equation (11)

r , mass flux, Dc'

1. Introduction. It is the purpose of this note to introduce a numerical method for the solidification of a one dimensional binary alloy. The method is a straightforward extension of the technique described in [3] for the two phase Stefan problem. It is applied to the heat and mass balance equations and specifically tracks the phase front. The method has several useful features. 1) It applies to the primary variables of temperature and solute concentration. 2) It permits solute diffusion both in the liquid and solid phase. 3) General phase diagrams are acceptable for the liquid-solid phase change. 4) The method is applicable to systems with heat and concentration dependent diffusion parameters. 5) The method is time implicit and can cope with discontinuous

PROGRESS REPORT
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3. TITLE OF PROPOSAL: Locally one dimensional numerical methods for multi-dimensional free surface problems
4. CONTRACT OR GRANT NUMBER: DAAG29-79-C-0145
5. NAME OF INSTITUTION: Georgia Institute of Technology
6. AUTHOR(S) OF REPORT: Gunter H. Meyer
7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:
 - 1) Hele-Shaw Flow with a Cusping Free Boundary, submitted to J. of Comp. Phys.
 - 2) Test Solutions for a One-Phase Problem Through Conformal Transformations, to appear in the Proceedings of the 1980 Oberwolfach Conference on Free Boundary Problems.
8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

none

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BRIEF OUTLINE OF RESEARCH FINDINGS

The examination of the method of lines for Hele-Shaw flow in the plane was continued. The problem looks like a one-phase Stefan problem but is ill-posed with regard to the initial domain. For example, a circular initial free boundary around a producing well at the center will move inward until it reaches the well. In contrast, a slightly perturbed initial free boundary will develop cusps and break down long before it reaches the well.

We have shown that a general purpose algorithm for one-phase free boundary problems can reasonably well reproduce the free surface in a model problem for which an analytic test solution is available. The numerical experiments indicate that only a time implicit method merits consideration for such problems and that special attention must be paid to the discretization of derivatives in the method of lines. As in earlier work the system of ordinary differential equations resulting from the method of lines approximation is solved iteratively. Since non-smooth free boundaries require more discretization lines than a Stefan type problem, fairly long computing times are to be expected. An adaptive updating of the relaxation parameter proves to be effective for reducing the number of iteration, and hence the run times, required for convergence. More promising yet is the application of a multi-grid technique, although the results obtained so far do not yet show the dramatic improvement anticipated. Further research into the multi-grid aspects of the method of lines is planned.

Two reports were prepared during this period. Report 1. below discusses the numerical aspects of the Hele-Shaw suction problem. Report 2. below contains a derivation of a family of analytic solutions for a specific Hele-Shaw problem based on conformal mapping techniques.

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7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:
published: SINUM 18 (1981), pp. 150-164
SINUM 18 (1981), pp. 165-177
Int. J. Heat Mass Transfer 24 (1981), pp. 778-781
(reprints sent to ARO)
8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

None

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BRIEF OUTLINE OF RESEARCH FINDINGS

The fixed point arguments used in a recent paper (SINUM 18 (1981), 165-177) for a convergence proof for front-tracking appear to allow no significant extension of the published result. However, a classical monotonicity argument as given, e.g., in Courant and Hilbert, Vol. II for the nonlinear Poisson equation also was found to be applicable to elliptic free boundary problems. When coupled with the moving-hyperplane version of the maximum principle a new method of analysis of front tracking results which eliminates some of the ad-hoc assumptions necessary in the above paper, and which is applicable to a general class of nonlinear field equations.

These results were presented at the symposium on Moving Boundary Problems in Montecatini, Italy in June 1981 and are presently being prepared for publication.

PROGRESS REPORT

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1. ARO PROPOSAL NUMBER: P-16373-M
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4. CONTRACT OR GRANT NUMBER: DAAG29-79-C-0145
5. NAME OF INSTITUTION: Georgia Institute of Technology
6. AUTHOR(S) OF REPORT: Gunter H. Meyer
7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

Numerical methods for free boundary problems - 1981 survey,
Proceedings of the Montecatini Conference on Free Boundary
Problems, to appear.
8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

none

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BRIEF OUTLINE OF RESEARCH FINDINGS

We have begun to study free boundary problems where the free boundary no longer is a level set. One dimensional problems of this type can be handled effectively with the sweep method used in our work (see, e.g., our work on binary solidification). Multi dimensional problems remain largely unexplored. We have now begun experiments with the Reynolds equation for the pressure p in a hydrodynamic journal bearing where the usual cavitation condition $p = \partial p / \partial n = 0$ is replaced by $p = -s/R$, $\partial p / \partial n = 0$. Here s is the surface tension in the lubricant and R denotes the radius of curvature of the free boundary. For these conditions the free surface is expected to destabilize and develop oscillations (for a discussion of the model and some qualitative results see C. Cuvelier, A free boundary problem in hydrodynamic lubrication including surface tension, Springer Lecture Notes No. 90, New York 1979). The method of lines remains applicable in principle to such problems but requires great care in approximating the free boundary. Numerical results for this problem so far are disappointing. However, we hope for better success in porous medium flow problems where the surface tension and curvature terms are expected to stabilize the free boundary.

Concurrently, the application of monotone methods to reaction-diffusion problems of the type $Lu = f(u, x, t)$ was examined, where L is a linear parabolic operator and where f denotes a Michaelis-Menten reaction or a first order reaction with a stationary reactant. The method of lines is quite effective numerically for such problems, and monotone methods can be used to establish the mathematical convergence of the numerical algorithm, at least at discrete time levels. The application of our methods to systems of reaction-diffusion equations is the next step to be examined.

Finally, in examining the method of lines for elliptic problems we noted that standard SOR methods for elliptic problems can be interpreted as special numerical integrators for an associated parabolic problem which depends on the relaxation parameter and whose equilibrium solution also solves the elliptic problem. On the basis of the Lax stability theory we hope to find the optimum relaxation factor for the elliptic problem by minimizing the amplification factors for the parabolic problem. The spectral radius of the SOR iteration matrix would not enter into this calculation. Numerical results indicate that this approach is promising. The computed and known optimum relaxation factors for the Laplace model problem are close (they differ by less than 10^{-2} for a 10×10 mesh and are indistinguishable for much larger meshes). Theoretical error bounds to explain this numerical agreement are not yet available.

FINAL REPORT
(TWENTY COPIES REQUIRED)

1. ARO PROPOSAL NUMBER: _____
2. PERIOD COVERED BY REPORT: 8/1/79 - 12/31/82
3. TITLE OF PROPOSAL: Locally one dimensional numerical methods for multi-dimensional
free surface problems
4. CONTRACT OR GRANT NUMBER: DAAG 29-79-C-0145
5. NAME OF INSTITUTION: Georgia Institute of Technology
6. AUTHOR(S) OF REPORT: Gunter H. Meyer
7. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP
DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES:

Attached

8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED
DURING THIS REPORTING PERIOD:

Final Report on research performed under Contract DAAG29-79-C-0145 on "Locally one dimensional numerical methods for multi-dimensional free surface problem."

Research on the numerical solution of free boundary problems for partial differential equations with locally or sequentially one-dimensional methods has been supported by the U.S. Army Research Office through two consecutive 3-year research contracts. The time and resources provided have made it possible to develop a reasonably comprehensive mathematical theory and flexible numerical algorithms on which to base current computational methods and future research.

During the first 3-year period, the method of fractional steps and the method of lines were applied to elliptic and parabolic free boundary problems. Both methods lead to sequentially one-dimensional algorithms for multi-dimensional partial differential equations. They are judged to be conceptually simple, easily coded, and little affected by complex free boundary conditions. A more detailed account of this phase of the research is contained in the final report on Grant DAAG-29-76-G-0261 (copy attached).

During the past three years work was directed toward demonstrating the flexibility of the method of lines for increasingly complex problems, on examining the behavior of certain ill-posed elliptic free boundary problems, and on establishing a mathematical theory for sequentially one-dimensional algorithms. In particular, the locally one-dimensional solver was applied to coupled heat and mass transport during alloy solidification [4]. This work is preparatory to applying locally one-dimensional methods to multi-dimensional reaction-diffusion systems. With the same goal in mind monotone

iterations were applied to elliptic free boundary problems with nonlinear source terms. In this setting a complete convergence analysis can be given for the method of lines when applied to free boundary problems which are equivalent to variational inequalities.

At the same time Hele-Shaw flow in a porous medium was examined. The Hele-Shaw injection problem is readily solvable and completely analyzable with variational inequalities. In contrast, the suction problem is ill-posed, has no variational structure and has not yielded to analysis. Our numerical method, on the other hand, remains applicable but requires careful attention to implementation [5]. An attack on the suction problem with conformal mapping [6] yielded some special analytic solutions against which numerical results can be compared.

Among our current projects we are examining whether surface tension effects can stabilize the suction problem. This work requires extensive numerical experiments on a Cyber-type computer. At the same time, we have begun work on implementing locally one-dimensional methods on a micro-computer.

Reports and papers prepared during the contract period:

G. H. Meyer, On the computational solution of elliptic and parabolic free boundary problems, in Free Boundary Problems, E. Magenes, edt., Istituto Francesco Severi, Rom 1980.

_____, The method of lines and invariant imbedding for elliptic and parabolic free boundary problems, SIAM J. Num. Anal. 18 (1981), 150-164.

_____, An analysis of the method of lines for the Reynolds equation in hydrodynamic lubrication, SIAM J. Num. Anal. 18 (1981), 165-177.

_____, A numerical method for the solidification of a binary alloy, Int. J. Heat Mass Transfer 24 (1981), 778-781.

_____, Hele-Shaw flow with a cusping free boundary, J. Comp. Phys. 44 (1981), 262-276.

- _____, Test solutions for a one-phase problem through conformal transformations, in Numerical Treatment of Free Boundary Problems, T. Albrecht et al., eds., Birkhäuser, Basel, 1982.
- _____, Anfangs-und Randwertaufgaben bei der Linienmethode für elliptische Gleichungen, Seminar über die Linienmethode und Anwendungen, K. J. Schwenzfeger, ed., Hochschule der Bundeswehr Munich, 1982.
- _____, Numerical methods for free boundary problems -- 1981 survey, Proceedings of the 1981 Montecatini Conference, to appear.
- _____, Free boundary problems with nonlinear source terms, submitted to Numerische Mathematik.

Final report on work performed under Grant DAAG 29-76-G-0261 on
"Locally one dimensional numerical methods for multidimensional
free surface problems"

The applicability of locally one dimensional methods to multidimensional free boundary problems was examined. Such problems require the solution of an elliptic or parabolic field equation over a domain which is unknown a priori and which must be determined from over-prescribed boundary data. Our main objective was to identify a numerical method for such problems which is widely and easily applicable, but which at the same time has a solid mathematical foundation.

Initially, we examined the method of fractional steps which for a multidimensional diffusion equation leads to a sequence of loosely coupled one dimensional free boundary problems in alternating orthogonal directions. In a report prepared just prior to the grant period this method is introduced and used together with invariant imbedding to solve a variety of Stefan type free boundary problems. The method works well and allows comparable numerical resolution in all space directions. However, it does impose certain restrictions on the shape of the free boundary which severely limit the applicability of the ADI method.

To overcome this limitation we began working with the method of lines based on a simple finite difference discretization of time and of all but one space variable. The original multidimensional equation is thus replaced by a system of one dimensional problems along parallel lines. This system is solved in line SOR fashion so that again a sequence of uncoupled one dimensional problems results. As above we apply invariant imbedding to each one dimensional problem. A description of this approach appears in [1]. A comparison with the fractional step method for a two dimensional

ablation problem [2] shows that only relatively few lines compared to the number of such points along each line should be used and hence that the numerical resolution is not equally fine in all directions. Nonetheless, even in this severe test problem the method of lines performs as well as the ADI method. Because free surfaces of more general shape are admissible further work has concentrated on the method of lines/SOR/invariant imbedding.

The success of this method, even in the crude implementation employed as far, was good motivation to establish the mathematical validity of the algorithm. As a first step convergence of the iterative numerical method and the discretization was established for Poisson's equation subject to nonlinear boundary data on a fixed domain [3]. Recently, the arguments were extended to establish convergence for an elliptic free boundary problem arising in hydrodynamic lubrication [4]. As far as we are aware this is the first time that a multidimensional front tracking algorithm can be completely analyzed. Current work is concerned with convergence for the equations arising in fluid flow through a porous dam. This problem is characterized by considerably more complicated boundary conditions than present in the lubrication problem.

Although we are primarily concerned with multidimensional problem the one dimensional solver is at the heart of our method and we continue to gather experience with the invariant imbedding method. An application to a problem with distributed boundary conditions is described in [7].

During the grant period we participated in two conferences dedicated to free and moving boundary problems. A survey over numerical methods for Stefan problems and a comparison with the method of lines was presented in [5], while an application of our methods to a variety of practical problems including heat and mass transfer, Hele-Shaw flow, and three dimensional ablation is described in [6].

Two additional publications were prepared for the 1977 and 1978 Army Numerical Analysis Conferences. A revision of the first report was published as [2] while the material of the second is contained in [6].

Colloquium talks on our work were presented during the past three years of several universities and laboratories in the U.S., Canada, Austria, Germany and Great Britain.

In summary, the basic premise that sequential one dimensional methods provide a useful tool for multidimensional free boundary problems has proved to be correct. It remains to establish firmly the limits of their applicability and to provide an analysis for a wider class of problems than was possible so far. First and foremost, however, the software aspects of our methods deserve attention in order to improve the efficiency of our methods.

During the grant period the following graduate student assisted in our project.

L. Kramarz, Ph.D. from Georgia Tech, 1977, [8]
F. Gerwig, M.S. from Georgia Tech, 1977
D. Dvorak, graduate student in mathematics

Papers and reports prepared during the grant period

1. G. H. Meyer, An application of the method of lines to multi-dimensional free boundary problems, J. Inst. Maths. Applcs. 20 (1977), 317-329.
2. , Direct and iterative one dimensional front tracking methods for the two dimensional Stefan problem, Numerical Heat Transfer 1 (1978), 351-369.
3. , The method of lines for Poisson's equation with non-linear or free boundary conditions, Numer. Math. 29 (1978), 329-344.
4. , The method of lines for the Reynolds equation in hydrodynamic lubrication, Brunel Inst. of Comp. Maths. Tech. Report TR 21, 1978, submitted for publication.
5. , The numerical solution of multidimensional Stefan problems - a survey, in Moving Boundary Problems, D. G. Wilson, A. D. Solomon, P. T. Boggs, eds., Academic Press, N. Y. 1978.
6. , Invariant imbedding for elliptic and parabolic free boundary problems, Brunel Inst. of Comp. Maths. Tech Report TR 13, 1978, submitted for publication.
7. , A numerical method for heat transfer in an expanding rod, Int. J. Heat Mass Transfer 21 (1978), 824-826.
8. L. Kramarz, Global approximations to solutions of initial value problems, Math. Comp. 32 (1978), 35-59.