EORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ____

roject No. G-37-603 GTRI/~~GIT~~ DATE 6/17/83

roject Director: G. H. MEYER School/~~GSM~~ MATH

ponsor: National Science Foundation
Washington, D.C. 20550

ype Agreement: Grant No. MCS-8302548 2/28/86

ward Period: From 6-15-83 To ~~11-30-84~~ (Performance) ~~2-28-85~~ (Reports)
11/30/85

ponsor Amount: This Change Total to Date

Estimated: $ ____ $ 20,446

Funded: $ ____ $ 20,446

ost Sharing Amount: $ 6729 (first year) Cost Sharing No: G-37-312

itle: Mathematical Sciences: The Method of Lines for Multi-Dimensional Free Boundary Problems

DMINISTRATIVE DATA OCA Contact Don Hasty

Sponsor Technical Contact: 2) Sponsor Admin/Contractual Matters:

MS MYRA B. GALINN

DR ANDRZEJ MANITIUS (202) 357-9671

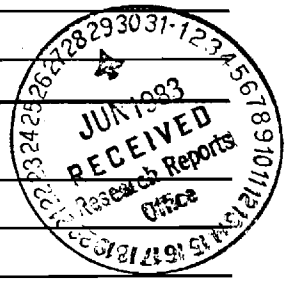
Military Security Classification: N/A

(or) Company/Industrial Proprietary: N/A

lemental Information Sheet for Additional Requirements.

– Contact OCA in each case. Domestic travel requires sponsor of $500 or 125% of approved proposal budget category.

quipment: Title vests with GIT; however None proposed –



OMMENTS:

OPIES TO:

roject Director
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Procurement/EES Supply Services
Research Security Services
Reports Coordinator (OCA)
Research Communications (2)
GTRI
Library
Project File
Other ____

EORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 9/12/86

ject No. G-37-603 School/~~Lab~~ MATH

ludes Subproject No.(s) N/A

ject Director(s) G. H. Meyer GTRC /~~XXX~~

nsor National Science Foundation

e Mathematical Sciences: The method of lines for Multi-Dimensional Free Boundary Problems

ective Completion Date: 11/30/85 (Performance) 2/28/86 (Reports)

nt/Contract Closeout Actions Remaining:

- [ ] None
- [ ] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [X] Final Report of Inventions - Questionnaire sent to P.I.
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other _____

tinues Project No. _____ Continued by Project No. _____

PIES TO:

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A Progress Report on Grant No. MCS-8302548

The Method of Lines for Multi-Dimensional Free Boundary Problems

Work on the numerical solution of free boundary problems with the method of lines has progressed in several directions.

Domain restrictions inherent in the method of lines in previous applications can be relaxed by mapping the physical domain to a more convenient computational domain. Extensive numerical experiments indicate that the method of lines will perform well in the presence of cross derivatives. The importance of the proper choice of coordinates is brought out for a filtration problem in [1].

Building on the monotone convergence results of [2] a program has been written to solve multi-dimensional diffusion-reaction equations. The numerical experiments with a heat/mass transfer problem coupled through an Arrhenius reaction and a free boundary look promising. We hope to provide a convergence theory analogous to [2] using variational inequalities for vector valued functions.

A mathematical and numerical analysis of a one dimensional parabolic problem without variational structure arising in polymer diffusion has been completed in collaboration with A. Fasano and M. Primicerio from the University of Florence.

Finally, the method of lines has seen preliminary testing on problems with curvature terms on the free boundary. So far, the results indicate no discernible change in the solution for small curvature terms, and no convergence of the algorithm for large curvature terms. As predicted by the referees, this problem proves to be quite a challenge.

1. The Method of Lines, Line SOR and Free Boundaries, to appear in the SIAM Proceedings of the Special Year in Energy Mathematics.

2. Free Boundary Problems with Nonlinear Source Terms, to appear in Numerische Mathematik.

NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I–PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
Georgia Institute of Technology Atlanta, GA 30332	Applied Mathematics	MCS 8302597/48
	4. Award Period From 6/1/83 To 11/30/85	5. Cumulative Award Amount $51,725

6. Project Title

The Method of Lines for Multi-Dimensional Free Boundary Problems

PART II–SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

The method of lines is established as a simple numerical method for multi-dimensional free boundary problems for elliptic and parabolic equations. When the approximating ordinary differential equations are solved in line iterative fashion with a sweep method, a flexible sequentially one-dimensional front tracking algorithm results which can accommodate a variety of free boundary conditions. Moreover, for steady-state and time-dependent obstable problems this approach is shown to converge to the unique solution of the underlying variational inequality. The method is also effective for elliptic operators with cross derivatives and thus can be used for front tracking along non-orthogonal directions. The extension of this approach to systems of equations with multiple free boundaries appears possible. First results with reaction-diffusion systems are encouraging.

For each one dimensional problem a new sweep method called continuous orthonormalization is suggested which can adaptively resolve boundary layers and turning points. The value of this method is demonstrated with an obstacle problem for a highly loaded beam.

PART III–TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (√)	Approx. Date
a. Abstracts of Theses					
b. Publication Citations					
c. Data on Scientific Collaborators					
d. Information on Inventions					
e. Technical Description of Project and Results		x	(from follow-up proposal)		
f. Other *(specify)*					

2. Principal Investigator/Project Director Name *(Typed)*	3. Principal Investigator/Project Director Signature	4. Date
Gunter H. Meyer		7/2/86

NSF Form 98A (5-78) Supersedes All Previous Editions

Form Approved OMB No. 99R001

IV. Recent and Ongoing Sponsored Research

The proposed research presents a natural evolution of earlier research on free boundary problems for a single one- or multi-dimensional parabolic equation. Recent research in this area has been funded by the National Science Foundation with a two-year grant and a supercomputer supplement since the summer of 1984. The specific topics described in our previous proposal were investigated during this period, and the results were mixed. Several publications resulted from this work.

1) Many numerical tests were run on a Cray with Hele-Shaw problems when the free boundary condition involved surface tension. Formally, the method of lines-SOR algorithm readily permits higher derivatives of the free boundary, but the line-SOR consistently diverged as the number of lines increased. We are currently experimenting with a pseudo-spectral approximation for the free boundary to define a more Newton-like iteration.

2) Convergence of the method of lines for time dependent problems is the thesis subject of D. E. Womble who should complete his Ph.D. research by next summer.

3) The possibility of combining the method of lines with domain mapping methods was explored to remove some of the geometric restrictions inherent in this approach. Cross derivatives arising from such mappings do not degrade the numerical performance of the method of lines. The importance

of the proper choice of coordinates is brought out in [1].

4) The power of the one-dimensional sweep method was exploited in a detailed study of a one-dimensional polymer swelling problem for which a complete mathematical analysis could be given [2].

5) The method of continuous orthonormalization for linear two point systems was analyzed and adapted to free boundary problems [3]. A fourth order obstacle problem with singular perturbation behaviour and bifurcation was analyzed and readily solved with this method [4].

6) A first application of the method of lines to diffusion systems is described in [5] for a problem which can be written as a variational inequality for $\bar{u}$. In this case monotone convergence of the sequentially one-dimensional method can be shown. This setting does not include the exothermic reaction problem (3.2).

7) An analysis of the sweep method for the one-dimensional dead core problem $u'' = \sqrt{u}$, $u(0) = 1$, $u(s) = \varepsilon$, $u'(s) = 0$ was carried out. It was shown that the position of the free boundary s is changed by $O(\varepsilon^{1/4})$ when $u(s) = 0$ is replaced by $u(s) = \varepsilon$. The results were presented in September 1985 at a free boundary conference in Oberwolfach. Moreover, the computer code for (3.2) depended on this study.

Literature References Acknowledging NSF Grant MCS 8302547/48

1. G. H. Meyer, The method of lines, line SOR and free boundaries, in Mathematical Methods in Energy Research, K. I. Gross, edt., SIAM, Philadelphia, 1984.

2. A. Fasano, G. H. Meyer, and M. Primicerio, On a problem in the polymer industry: Theoretical and numerical investigation of swelling, to appear in SIAM Journal on Math. Anal.

3. G. H. Meyer, Continuous orthonormalization for boundary values problems, to appear in Journal of Comp. Phys.

4. G. H. Meyer, Continuous orthonormalization for stiff free boundary problems, to appear in the proceedings of the 1984 Maubuisson conference on free boundaries, Pitman Research Notes in Mathematics.

5. G. H. Meyer, On the numerical solution of free boundary problems for reaction-diffusion systems, to appear in Advances in Free Boundary Problems (tentative title), M. Niezgodka, edt.