10:46:45 OCA PAD AMENDMENT - PROJECT HEADER INFORMATION 07/14/92

Active

Project #: B-06-681 Cost share #: Rev #: 14
Center # : R6590-0A0 Center shr #: OCA file #:
Work type : RES
Contract#: 70NANB8H0860 Mod #: BUD REV 920709 Document : GRANT
Prime #: Contract entity: GTRC

Subprojects ? : N CFDA:
Main project #: PE #:

Project unit: DDSC Unit code: 03.010.206
Project director(s):
CHOW S N MATH (404)894-8766

Sponsor/division names: US DEPT OF COMMERCE / NATL INST OF STDS & TECH
Sponsor/division codes: 110 / 005

Award period: 880901 to 930114 (performance) 930214 (reports)

Sponsor amount	New this change	Total to date
Contract value	0.00	889,561.00
Funded	0.00	889,561.00
Cost sharing amount		107,261.00

Does subcontracting plan apply ?: N

Title: DYNAMICAL PROBLEMS AND PHASE TRANSITIONS

PROJECT ADMINISTRATION DATA

OCA contact: Brian J. Lindberg 894-4820

Sponsor technical contact	Sponsor issuing office
DR. JOHN A. SIMMONS	SHARON D. GREEN
(301)975-6139	(301)975-6328
NAT INSTITUTE OF STANDARDS & TECH	NAT INSTITUTE OF STANDARDS & TECH
METALLURGY DIV. BLDG. 223, ROOM A164	GRANTS UNIT, BLDG. 301, ROOM B-128
GAITHERSBURG, MARYLAND 20899	GAITHERSBURG, MARYLAND 20899

Security class (U,C,S,TS) : U ONR resident rep. is ACO (Y/N): N
Defense priority rating : N/A N/A supplemental sheet
Equipment title vests with: Sponsor X GIT

Administrative comments -
ADMINISTRATIVE CORRECTION - BUDGET REVISED TO AGREE WITH BUDGET REVISION DATED 7/9/92.

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

SR 42687

Closeout Notice Date 03/24/93

Project No. B-06-681 Center No. R6590-0A0

Project Director CHOW S N School/Lab DDSC

Sponsor US DEPT OF COMMERCE/NATL INST OF STDS & TECH

Contract/Grant No. 70NANB8H0860 Contract Entity GTRC

Prime Contract No. ________

Title DYNAMICAL PROBLEMS AND PHASE TRANSITIONS

Effective Completion Date 930114 (Performance) 930214 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	
Final Report of Inventions and/or Subcontracts	Y	
Government Property Inventory & Related Certificate	Y	
Classified Material Certificate	N	
Release and Assignment	N	
Other	N	

CommentsEFFECTIVE DATE 9-1-88. CONTRACT VALUE $889,561.

Subproject Under Main Project No. ________

Continues Project No. ________

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other HARRY VANN-FMD	Y
FRED CAIN-OOD	Y

NOTE: Final Patent Questionnaire sent to PDPI.

B-10-681 [illegible]

Georgia Tech

Office of Grants and Contract Accounting

Georgia Institute of Technology
Lyman Hall/Emerson Building
Atlanta, Georgia 30332-0259
404•894•4624; 2629

October 18, 1989

U. S. Department of Commerce
National Bureau of Standards
Acquisition and Assistance Division
Attn: Richard E. de la Menardiere
Grants Unit, Bldg. 301, Room B-128
Gaithersburg, Maryland 20899

REFERENCE: Contract 70NANB8H0860

Dear Mr. de la Menardiere,

Attached are the Financial Status Report (SF-269) and the Federal Cash Transactions Report (SF-272) for U. S. Department of Commerce, National Bureau of Standards, Contract 70NANB8H0860, with Georgia Tech Research Corporation. The reports are for the period, July 1 - September 30, 1989. Enclosed also, is the Request for Advance or Reimbursement #7

Should you have questions, please contact Dale C. Turner of this office at (404) 894-5521.

Sincerely,

David V. Welch
Director

DVW/DCT/djt

Attachments

cc: Dr. S. N. Chow
Mr. Brian Lindberg ✓

National Bureau of Standards

3. RECIPIENT ORGANIZATION (Name and complete address, including ZIP code)	4. EMPLOYER IDENTIFICATION NUMBER	5. RECIPIENT ACCOUNT NUMBER OR IDENTIFYING NUMBER
GEORGIA TECH RESEARCH CORPORATION P. O. BOX 100117 ATLANTA, GA 30384	58-0603146	B-10-681/R6590-0A0

8. PROJECT/GRANT PERIOD (See instructions) FROM (Month, day, year)	TO (Month, day, year)	9. PERIO[D] FROM (Month, day, year)
09/01/88	09/30/89	07/01/89

10. STATUS OF FUNDS

PROGRAMS/FUNCTIONS/ACTIVITIES ►	(a)	(b)	(c)	(d)	(e)
a. Net outlays previously reported	$	$	$	$	$
b. Total outlays this report period					
c. *Less:* Program income credits					
d. Net outlays this report period (*Line b minus line c*)					
e. Net outlays to date (*Line a plus line d*)					
f. *Less:* Non-Federal share of outlays					
g. Total Federal share of outlays (*Line e minus line f*)					
h. Total unliquidated obligations					
i. *Less:* Non-Federal share of unliquidated obligations shown on line h					
j. Federal share of unliquidated obligations					
k. Total Federal share of outlays and unliquidated obligations					
l. Total cumulative amount of Federal funds authorized					
m. Unobligated balance of Federal funds					

11. INDIRECT EXPENSE

a. TYPE OF RATE (*Place "X" in appropriate box*) [1] PROVISIONAL [ ] PREDETERMINED [ ] FINAL [2] FIXED

	b. RATE	c. BASE	d. TOTAL AMOUNT	e. FEDERAL SHARE
1)	FY90 62.5%	MTDC	$70,910.80	$70,910.80

12. REMARKS: *Attach any explanations deemed necessary or information required by Federal sponsoring agency in compliance with governing legislation.*

2) FY89 60.0%

13. CERTIFICATION

I certify to the best of my knowledge and belief that this report is correct and complete and that all outlays and unliquidated obligations are for the purposes set forth in the award documents.

SIGNATURE OF AUTHORIZE[D] OFFICIAL

David V. W[elch]

TYPED OR PRINTED NAME

David V. Welch, Dir
Grants & Contracts

269-102

Questions pertaining to this report should be directed to: Dale Turner (404) 894-5521

FEDERAL CASH TRANSACTIONS REPORT

(See instructions on the back. If report is for more than one grant or assistance agreement, attach completed Standard Form 272-A.)

Approved by Office of Management and Budget, No. 80-

1. Federal sponsoring agency and organizational element to which [report] is submitted
U. S. Department of Commerce
Bureau of Standards

2. RECIPIENT ORGANIZATION

Name: GEORGIA TECH RESEARCH CORPORATION

Number and Street: P. O. BOX 100117

City, State and ZIP Code: ATLANTA, GA 30384

4. Federal grant or other identification number: 70NANB8H0860

5. Recipient's account number or identifying number: B-10-681

6. Letter of credit number: N/A

7. Last payment voucher number:

Give total number for this period

8. Payment Vouchers credited to your account:

9. Treasury checks received (or not deposited): -(

3. FEDERAL EMPLOYER IDENTIFICATION NO. 58-0603146

10. PERIOD COVERED BY THIS REPORT

FROM (month, day, year): 07/01/89

TO (month, day year): 09/30/89

11. STATUS OF FEDERAL CASH *(See specific instructions on the back)*		
	a. Cash on hand beginning of reporting period	$ (120,352.3
	b. Letter of credit withdrawals	
	c. Treasury check payments	-0-
	d. Total receipts *(Sum of lines b and c)*	-0-
	e. Total cash available *(Sum of lines a and d)*	(120,352.3
	f. Gross disbursements	153,264.0
	g. Federal share of program income	-0-
	h. Net disbursements *(Line f minus line g)*	153,264.04
	i. Adjustments of prior periods	-0-
	j. Cash on hand end of period	$ (273,616.3

12. THE AMOUNT SHOWN ON LINE 11J, ABOVE, REPRESENTS CASH REQUIREMENTS FOR THE ENSUING ___ Days	13. OTHER INFORMATION	
	a. Interest income	$
	b. Advances to subgrantees or subcontractors	$

14. REMARKS *(Attach additional sheets of plain paper, if more space is required)*

Questions pertaining to this report should be directed to:
Dale C. Turner (404) 894-5521

15. CERTIFICATION

I certify to the best of my knowledge and belief that this report is true in all respects and that all disbursements have been made for the purpose and conditions of the grant or agreement

AUTHORIZED CERTIFYING OFFICIAL

SIGNATURE:

DATE REPORT SUBMITTED: October 18, 1

TYPED OR PRINTED NAME AND TITLE: David V. Welch, Director, Grants & Contracts Accountin

TELEPHONE (Area Code) (Number) (Extension)

THIS SPACE FOR AGENCY USE

REQUEST FOR ADVANCE OR REIMBURSEMENT

(*See instructions on back*)

Approved by Office of Management and Budget, No. 80–R0183

PAGE 1 OF

1. TYPE OF PAYMENT REQUESTED

a. "X" one, or both boxes: ☐ ADVANCE ☒ REIMBURSEMENT

b. "X" the applicable box: ☐ FINAL ☒ PARTIAL

2. BASIS OF R

☒ CASH ☐ ACCRUAL

3. FEDERAL SPONSORING AGENCY AND ORGANIZATIONAL ELEMENT TO WHICH THIS REPORT IS SUBMITTED

U. S. Department of Commerce
National Bureau of Standards

4. FEDERAL GRANT OR OTHER IDENTIFYING NUMBER ASSIGNED BY FEDERAL AGENCY

70NANB8H0860

5. PARTIAL PAYMENT REQ NUMBER FOR THIS REQ

7

6. EMPLOYER IDENTIFICATION NUMBER

58-0603146

7. RECIPIENT'S ACCOUNT NUMBER OR IDENTIFYING NUMBER

B-10-681/R6590-0A0

8. PERIOD COVERED BY THIS REQUEST

FROM (*month, day, year*): 07/01/89

TO (*month, day, year*): 09/30/89

9. RECIPIENT ORGANIZATION

Name : GEORGIA TECH RESEARCH CORP.

Number and Street : P. O. BOX 100117

City, State and ZIP Code : ATLANTA, GA 30384

10. PAYEE (*Where check is to be sent is different than item 9*)

Name :

Number and Street :

City, State and ZIP Code :

11. COMPUTATION OF AMOUNT OF REIMBURSEMENTS/ADVANCES REQUESTED

PROGRAMS/FUNCTIONS/ACTIVITIES ▶		(a)	(b)	(c)	TOTAL
a. Total program outlays to date	(*As of date*) 09/30/89	$	$	$	$ 273,61
b. *Less:* Cumulative program income					
c. Net program outlays (*Line a minus line b*)					273,61
d. Estimated net cash outlays for advance period					
e. Total (*Sum of lines c & d*)					273,61
f. Non-Federal share of amount on line e					
g. Federal share of amount on line e					273,61
h. Federal payments previously requested					140,35
i. Federal share now requested (*Line g minus line h*)					133,26
j. Advances required by month, when requested by Federal grantor agency for use in making prescheduled ad-	1st month				
	2nd month				

Technical Report

NIST Project Number 70NANB8H0860

Performance Period: 9/1/88 - 9/30/89

Principal Investigator: Dr. Shui-Nee Chow
Co-Principal Investigator: Dr. Jack K. Hale

October 1989

Don Estep
Oct 1989

During the past summer, Estep concentrated on the development of the discontinuous Galerkin finite element method as a tool for the numerical analysis of pattern forming reaction diffusion equations. The work accomplished encompassed significant advances both in the theory and in the implementation.

Estep visited at Chalmers University in Sweden during June. Building on our previous work, we analyzed fully discrete schemes. We constructed fully implicit and partially implicit/partially explicit schemes which are adaptive in time and space and proved global error estimates of the type which suggest a mesh control strategy. These results hold for the case in which the space meshes at succeeding time levels "nest", that is, for the coarsening stage of the pattern formation. This work is being written into a paper now.

We also completed some preliminary calculations which indicate that the results extend to the case in which the space meshes do not nest, under some additional mild assumptions. This is necessary, of course, in order to guarantee accurate approximation of the metastable state while they evolve.

Later in the summer, we began several projects. Firstly, we studied alternate methods for the time discretization of the integral of the nonlinear term. Specifically, for the results above, we employ quadratic interpolation of the function values of he approximate at the previous three (implicit/explicit) or at the previous two plus the current (fully implicit) in order to approximate the time integrals. Alternatively, we can use quadratic interpolation computed using just two nodal values plus the midpoint value. In the first case, the scheme is cheaper, since those values need to be stored for the time step selection algorithm anyway, and the second case requires another function evaluation. However, it appears that the second method may have some advantage with respect to stability. Further analysis and experimentation is needed.

Another project begun is a detailed study of the work involved in using our methods and possible ways of improvement. The current scheme has significant advantages in terms of efficiency over previous versions of the method (both ours and Johnson's code for linear problems). The coefficient matrix is rearranged to put it into banded form, and specialized elimination routines keep the work count to O(M), in one dimension, and $O(M^3)$ in two dimensions, (M the number of mesh points in the interval or on a side respectively). Alternatively, the method can be so formed that matrices of the form: $I + aA + bA^2$, A a symmetric, banded, positive definite matrix, must be inverted at each time step. We will attempt to develop code to compute these matrices efficiently and then use iterative methods to reduce them. The goal is to reduce the work count in two dimensions to $O(IM^2)$ where I is the number of iterations.

Lastly, significant progress was made on an understanding of the superstability phenomena for stiffly stable methods for the time integration of semilinear parabolic problems. Stiffly stable methods (including the backward differentiation formulas of Gear found in the IMSL library and the discontinuous Galerkin methods) are those usually employed for adaptive time stepping. However, there is a drawback to these methods. In certain circumstances, these schemes may follow a "false solution" because the time steps have increased so much that the spectrum of the true solution is no longer modeled accurately. This phenomena is well known in methods for ODE's. We are exploring the possibility of its occurrence in methods for nonlinear parabolic equations. We have experiments to show that the global error strategies that the discontinuous Galerkin methods allow do not prevent this from happening. Next, we will try to demonstrate this problem for the method of lines. Finally, we will attempt to understand what happens in the case of an adaptive space mesh.

On the practical side, using the a priori estimates as a basis, we implemented the time step adaption strategy into our schemes. Extensive testing was performed on one dimensional problems. The order of convergence and the robustness and efficiency of the error estimators was confirmed.

Upon final testing of the two dimensional version with the rearrangement process described above, serious experimentation will begin. Two projects are being designed now. The first is the identification and classification of metastable states on a rectangular domain. This experiment will expand to include other shapes of domains as our experience grows. The second project is akin to the first. We are going to start with a thin domain, and consider the width of the thin side as variable. We are constructing a method, based on the discontinuous Galerkin scheme, which will take the width as a parameter and allow us to follow what happens to a solution, which reduces to a metastable state in one dimension when the width is zero, as the width changes.

JackK.Hale.
Oct 1989

Much of the effort has been devoted to reaction-diffusion equations on thin domains with Genevieve Raugel. This has taken much more time than originally expected due to complications that arose in the regularity theory of parabolic equations on nonsmooth domains and the regularity properties of inertial manifolds. At the present time, several results have been obtained and a manuscript is being prepared. We have been able to show that the attractors on this domain in R^3 reduce to attractors in R^2 as the thinness parameter goes to zero. For thin domains in R^2, we prove that the flow is equivalent to one on R^1.

Hale, Arrieta and Han are considering properties of eigenvalues and eigenfunctions of the Laplacian under irregular perturbations of the domain. This problem plays an important role in pattern formation.

Hale is also working with Sjoerd Verduyn Lunel on some problems related to averaging in delay equations when the system is subjected to rapidly oscillating nonautonomous terms.

Hale has also been attempting to formulate reasonable mathematical problems related to phase transitions in higher space dimensions and especially to understand the properties of the zero sets of equilibria and functions on their unstable manifolds.

Shui-Nee Chow
Oct 1989

Chow, Drachman and Wang have obtained a method of computing of normal forms for ordinary differential equations near an equilibrium. This is a user friendly program and can used easily with the symbolic manipulator system MACSYMA. We are planning to use other systems such as Mathematica, Maple, Reduce, Scratchpad.

Chow and Palmer have used ideas of the shadowing lemma to estimate how far a numerically computed orbit (which can be thought of as a pseudo-orbit) is from a true orbit. Our procedure is different from the one by Hammel, Yorke and Grebogi. Ours is based a concept of finite time hyperbolicity. Our procedure works forward. After N iterates we can decide whether our theorem applies and if it does, we can calculate the shadowing error. A comparison with the results of Hammel, Yorke and Grebogi was given.

Chow, Deng and Fieldler have completed a mayor work on a theory of homoclinic doubling bifurcation. This will be applied to phase transition and boundary layer problems. This work will be important in our numerical bifurcation problems for reaction diffusion equations.

Gunter Meyer
Oct 1989

Phase transition problems often involve nonlocal boundary conditions on the free boundary. For example, in the Gibbs Thompson interface condition for the two phase Stefan problem the curvature term is, strictly speaking, a nonlocal boundary condition because spatial derivatives of the free boundary appear. In other applications, energy input to the free boundary may depend on the shape of the free boundary, as in the melting of an iceberg due to sunlight and shade. We have continued our examination of the applicability of a sequentially one dimensional method for multi dimensional free boundary problems by concentrating on formulations with global free boundary conditions. We show that this approach can handle such problems, including the Gibbs Thompson interface condition, without any change of the basic algorithm developed earlier for local free boundary conditions. Moreover, for a model problem involving an integral over the free boundary one can prove a priori convergence of the numerical method.

In connection with the study of diffusion problems with non convex free energy we have begun to study hysteresis phenomena. Of particular interest is the identification problem where the hysteresis operator is to be determined to fit measurements. So far we have considered the linear Preisach hysteresis operator which is based on the superposition of simple relays and which is suggested for ferromagnetism. A least squares identification algorithm and analysis has been provided to characterize the operation in the light of multiple and possible inconsistent data. Current work is focusing on nonlinear extensions of the Preisach operator which may be able to reproduce measured phenomena such as the drift of hysteresis loops which cannot be accounted for with the linear model.

Ron Shonkwiler
Oct 1989

Shonkwiler has worked on two projects in this connection. The first is on a deterministic method for finding the parameters of the IFS type discrete dynamical system giving rise to a given attractor. The method applies to a large class of attractors but is restricted to those having convex hulls consisting of finitely many hyperplanes. The principle attractors studied have been in the plane. Shonkwiler has worked out the necessary theory for the method in most of the cases which could be encountered (see below). Also Shonkwiler has a preliminary piece of software working for automated analysis.

The method is based on the vertex theorem for Iterated Function System attractors due to Marc Berger and upon a detailed eigenvalue analysis for those vertices which are fixed points of a map belonging to the function system. Such a vertex falls into one of three possible cases: either its corresponding map has equal eigenvalues (the similitude case) or of course the two eigenvalues are distinct. In this latter event there are two possibilities, the eigenvectors of the map (one or both) do not lie along the convex hull of the attractor the cusp case and they both do lie along the convex hull. It is this latter case that remains to be fully understood.

In order to automate the analysis of these two dimensional attractors, it is necessary to characterize geometrically those vertices which are fixed points and those which are not. It can be shown that the former type of vertex is the limit of boundary points of the attractor lying on an exponential curve of the form

$$u = u_0 e^{-\tau_1 t}, \qquad v = v_0 e^{-\tau_2 t}$$

with parameter t. Here u, v are coordinates in the direction of the eigenvectors and $\tau_1$and τ_2 are the corresponding eigenvalues. Vertices which are not fixed points are not the limit of boundary points lying on such curves. A local computational analysis at each vertex can decide whether or not there is such a boundary curve and if so, determine the parameters $\tau_1$and τ_2 as well as the eigen directions. In this way, those maps corresponding to fixed points which are also extreme points of the convex hull can be completely determined

The second project on which Shonkwiler has worked is the study of Monte Carlo methods for finding the parameters of attractors as discussed above. Mathematically this is the problem of minimizing a wildly varying scalar-valued error function of a modest number of real parameters. The error function is the Hausdoff distance between the given attractor and some test attractor generated by candidate solutions. Shonkwiler has developed fast algorithms (on the order of 15 minutes) converging to solutions for attractors generated by up to 12 parameters. These algorithms are based on biological evolution heuristics. Mathematically, the methods are in fact implementations of nonstationary Markov chains. It can be proved that the method will converge to an optimum given enough time

An interesting result which has been obtained from this study is that an mfold parallel implementation of such a Monte Carlo algorithm can be expected to achieve nearly an mfold speedup in convergence. Therefore theoretically it is possible to compute solutions in arbitrarily short times by using a sufficiently large number of processors.

TECHNICAL PROGRESS REPORT

NIST Grant 70NANB8H0860

Report Period 10/1/89-3/31-90

We have been very productive over the last few months. Progress has been made in both implementation of the problems and in our understanding of the numerical process involved. This is a good foundation for the next few months when Don Estep, one of our researchers, will go to Sweden.

We have codes for both Neumann and Dirichlet boundary conditions on a unit interval in one dimension and a unit square in two dimensions. Both of these codes use the "speed-up" rearrangement of the coefficient matrix which drops the work count for the direct solution of the system in $1-d$ from $O(n^3)$ to $O(n)$ and in $2-d$ from $O(n^6)$ to $O(n^4)$ for n the number of mesh points. In addition, a student at Georgia Tech has nearly completed a study of iterative methods to solve these systems. Our work gives a substantial advantage over previous implementations in terms of computational efficiency. In addition, we have made a study of various methods for computing the nonlinear integral which results from the discontinuous Galerkin method. After we complete some theoretical analysis, we will be able to make some judgements about which procedures to use. Our goal is to implement a scheme which is stable for all values of the diffusion constant which would provide some theoretical basis for trusting the numerical results as this constant tends to zero. Finally, we have spent time on graphics and have completed a video of some experiments in two dimensions.

In both one and two dimensions, the time step adaptation procedure has been coded and tested extensively. The results are striking in one dimension in particular, because of the exponentially slow motion of the solution. The global error control seems very robust; using large steps in metastable periods but quickly reducing the time steps well before the start of the 'fast' motion. In one dimension, we have made comparisons to LSODE implementation of the backward differentiation formulas (for which no theoretical foundation for optimal global error control exists). The global error estimator together with the slightly more stable discontinuous Galerkin schemes yield more conservative time sequences, however this pays off in terms of fending off the effects of superstability (see below) which tend to give false transition times.

The next goal is the incorporation of the space step adaptation procedure. It has become apparent through recent experimentation that a code either must sample at impractically large number of points or must be adaptive with refinement in the phase transition regions. In particular, a uniform spacing must be on the order of the diffusion constant or the time of transition is detected inconsistently. In one experiment in one dimension, the phase transition moves two orders of magnitude late if too few mesh points are used, and in two dimensions (with much faster motion) the time of transition is about 50% too late. We have measured a dependence on the transition time also in two dimensions. The implementation of the space adaption will follow the analysis performed last summer.

Over the last six months, we have conducted an exhaustive series of numerical experiments on some one-dimensional problems. The point was to determine the dynamical behavior of the numerical schemes – and whether this behavior models the behavior predicted in the true solution by the theoretical analysis of Hale and others. We found that the qualitative behavior of our numerical schemes follows the predictions of the theory. Namely, we found that the schemes correctly model the slow motion of the metastable states, the rate of collapse of the fronts and the motion of the zeroes. However, the constants governing this motion measured numerically were usually not the same as those predicted by theory, which poses some interesting questions. Of course, because of the discretization, it is not clear that the constants should be the same, and at this time, we do not understand how the discretization affects the dynamics (in particular, the mesh size does not tend to zero in practice and this certainly affects the dynamical behavior). Another point is that it is difficult to measure these qualities of the solution and we are designing new experiments. In two dimensions, we are building on the working code for a unit square domain in order to attack several problems such as more complicated domains, domains which increase in thickness, and systems of equations.

We continued to write our second paper on the theoretical foundation of the discontinuous Galerkin method. This paper will contain an a priori error analysis and some details of implementation for fully discrete and adaptive schemes. Moreover, we have begun to analyze the dynamical approximation properties of numerical methods for these problems. The first paper on superstability is nearly complete (ready for submission inside of a month). Superstability is a dangerous property of implicit schemes for stiff ODEs and parabolic PDEs which makes branches of solutions of the equations which are unstable appear numerically stable. One result of this is that a computation will remain on a metastable solution much too long. A related problem is the relation between the number of lines and an accurate determination of the dynamical behavior. Our experiments show that choosing too few lines can be disastrous and that a sufficient number of lines is on the order of the reciprocal of the diffusion constant for a uniform mesh. We conjecture that such a spacing is needed only in a small neighborhood of the phase transitions and have made some progress on such a result. Don Estep has begun to write a general paper on the practical aspects of our numerical work addressed to the metallurgy community.

PROGRESS REPORT

Period Covered: April 1, 1990 - July 31, 1990

Center for Dynamical Systems and Nonlinear Studies
Georgia Tech

Our objective has been to understand the development and movement of transition layers in reaction diffusion equations. The dynamics of the flow in the case of one space variable is well understood from the basic theory of Fusco, Hale, Carr and Pego which exploits invariant manifold theory and the gradient structure of the flow. In principle, the theory is valid in higher space dimensions, but very little is known about the possible structures of the equilibria and their unstable manifolds. Even good conjectures are not available. As a consequence, we have been attempting to attack the problem using both theory and numerics.

During the past year, we have spent considerable time with the personnel at NIST, especially with John Cahn and John Simmons. Having this contact has been important to help us to understand the basic models. Their experience also has been beneficial in the formulation of meaningful mathematical problems.

We have been working on numerical schemes which follow the zero sets of solutions and exploit the abstract dynamics of the flow. Precise error bounds are being obtained. In addition, using the theory of exponential dichotomies and the shadowing lemma, we have been developing numerical schemes which can be used to assert that there is a true orbit of the flow near a numerically computed orbit and to estimate the error.

On the theoretical side, we are continuing our work on thin domains which contain a curve to determine the extent to which the flow for such PDE are equivalent to a lower dimension problem.

Papers on these topics are in the process of being completed.

During the next year, we intend to continue this type of investigation. More specifically, the numerical techniques will be applied first to two dimensional problems (and higher dimensions if time permits). One specific computation will be to take a domain which depends on a parameter ν with the property that it is a curve for $\nu = 0$. For ν small, it is a thin domain and we will have complete theoretical information about the dynamics of the flow. We will attempt to determine how the dynamics changes as ν becomes larger by exploiting homotopy methods. This should lead to a better understanding of the process underlying the development of complicated patterns.

We will continue to develop algorithms to determine when an exact orbit exists near a numerically computed one and develop this algorithm for problems involving large dimension.

Finally, for vector equations, we will determine the basic principles underlying the development of transition layers and investigate the movement of these layers in time. Attention will be given to the situation of smooth and nonsmooth layers (layers which may have self intersections).

DARPA Progress Report
Period covered: August 1, 1990 - October 31, 1990

Center for Dynamical Systems and Nonlinear Studies
Georgia Tech

We now have a program developed by Estep for a numerical scheme which follows the zero sets of solutions of reaction diffusion equations. We now should be able to use this program to gain information about the dynamics of the flow. We intend to make initial experimentation for thin domains over the arc of a curve. Beginning with the known dynamics on the curve, we will follow solutions to domains which are not thin and attempt to understand the manner in which the complications arise in the zero sets of the solutions.

Chow and Palmer have finished their work on exponential dichotomies and the shadowing lemma to obtain a theoretical way to assess that a true orbit of a flow or map exists in the neighborhood of a computed orbit. The implementation of the method is being pursued as well as extensions to the stochastic situation with the help of van Vleck.

Hale and Raugel have continued their efforts on the reduction of the dimension for the determination of dynamics for parabolic and hyperbolic equations. Two papers on this subject are in the process of being completed. One deals with the abstract theory of thin domains and the other with the limiting behavior of the solutions of gradient systems.

We are continuing our efforts to understand the basic principles involved in the development and movement of transition layers in reaction diffusion equations. Chen is in the process of obtaining a theory which will explain how the topology of smooth and nonsmooth layers (ones with self intersection) can change with time. In several space dimensions, he has defined a concept which seems to play the same role as the zero number or lap number does in one dimension. This should lead to a much better understanding of the dynamics.

Personnel from Ga. Tech. have spent considerable time with the personnel at NIST, especially with John Cahn and John Simmons. Dr. Cahn has developed a new model which is a system of ordinary differential equations on a lattice rather than partial differential equations. It is believed that this model is closer to reality. Chow and van Vleck have developed a computer program in color for the SUN which gives the steady states on cross sections of the lattice. The computations are very long for the SUN and it will be necessary to go to the supercomputer. The program is written to take advantage of parallel computations. The theoretical aspects of the model are beginning to be investigated by Chen, Chow and Hale.

We have been working on numerical schemes which follow the zero sets of solutions and exploit the abstract dynamics of the flow. Precise error bounds are being obtained. In addition, using the theory of exponential dichotomies and the shadowing lemma, we have been developing numerical schemes which can be used to assert that there is a true orbit of the flow near a numerically computed orbit and to estimate the error.

On the theoretical side, we are continuing our work on thin domains which contain a curve to determine the extent to which the flow for such PDE are equivalent to a lower dimension problem.

Papers on these topics are in the process of being completed.

During the next year, we intend to continue this type of investigation. More specifically, the numerical techniques will be applied first to two dimensional problems (and higher dimensions if time permits). One specific computation will be to take a domain which depends on a parameter ν with the property that it is a curve for $\nu = 0$. For ν small, it is a thin domain and we will have complete theoretical information about the dynamics of the flow. We will attempt to determine how the dynamics change as ν becomes larger by exploiting homotopy methods. This should lead to a better understanding of the process underlying the development of complicated patterns.

We will continue to develop algorithms to determine when an exact orbit exists near a numerically computed one and develop this algorithm for problems involving large dimension.

Finally, for vector equations, we will determine the basic principles underlying the development of transition layers and investigate the movement of these layers in time. Attention will be given to the situation of smooth and nonsmooth layers (layers which may have self intersections).

NIST Technical Report
Period: 8/1/90 - 12/31/90

We continued our efforts towards the analysis of numerical methods for the bistable and viscous Cahn–Hilliard problems in one and two dimensions. While simpler than the standard Cahn–Hilliard problem, our extensive testing has shown that second order semilinear parabolic problems offer many challenges to numerical analysis and pose serious difficulties in terms of getting accurate approximations. Some of the difficult phenomena are steep interfaces moving by mean curvature, metastability, quick reactions and locally complex solutions. We believe that the numerical analysis of these problems must be completed before satisfactory methods for the Cahn–Hillard equation can be developed.

We are seeking to develop numerical methods which follow a solution through all periods of its evolution and not just over a brief initial transient. In fact, the classical accuracy considerations of error control, which work well on linear problems, often fail to produce good approximations over this time span. Both the dynamical behavior and stability properties of the approximated solution and an understanding of the effects of discretization on the dynamics of the PDE will have to be incorporated in the error control of any rigorous theory. Moreover, it is simply impossible to use standard fixed mesh algorithms and get good approximation. For this reason, we study fully adaptive codes with mesh alignment.

Theoretically, we made more progress on a priori and a posteriori error analysis of the discontinuous Galerkin method [EL]. These estimates form the basis of the theory of error control for the d.G. schemes. Now, we are trying to overcome the difficulties posed by singularly perturbed problems. We have begun to study the special problems of error control. [DE] contains an explanation of the superstability phenomena in adaptive time integration of stiff ODEs, which is related to the question of whether a scheme can "miss" a transition period. Lastly, we have made serious experiments directed towards exposing the effects of discretization on the dynamics of the problem. We have made good progress in analyzing the one dimensional case and have introduced mesh alignment in our two dimension code.

We completed development of the fixed mesh code DGAL. DGAL implements the method of lines above a fixed mesh using the third order d.G. scheme for the adaptive time integration and piecewise continuous finite elements for the space approximation. The time steps are chosen by criteria based on our global a priori error analysis.

This code was actually just a development stage in the process of creating a fully adaptive code. We have implemented the first version of a fully adaptive scheme using a posteriori error control to govern the time step and the mesh in the FORTRAN code TRANSI. TRANSI uses the d.G. scheme for the adaptive time integration and the h–method for space mesh adaption (the current mesh is either subdivided or recomputed based on the current error estimate). The error control is derived from the residual–based a posteriori error estimate that holds for linear, nonhomogeneous problems. The time step adaptivity follows the same strategy as DGAL using the a posteriori estimate instead of the a priori estimate. In addition, at each time step the solution is computed on a predicted mesh and then this mesh is refined depending on the space error estimated locally on each triangle. The error estimate is only a conjecture, but we have good results. We continue to work on this aspect.

In space, the scheme uses isoparametric quadrilateral elements. A quadrilateral mesh is covered by a triangular mesh such that the diagonals of the quadrilaterals are chosen to lie as close as possible in the direction perpendicular to the gradient of the approximant. This gives an easily implemented mesh alignment. In addition, elements which form the border between refinement levels are treated specially in order to obtain regular meshes and to avoid constrained nodes. Only one extra node is allowed on each element side and only three on each element. Thus, each quadrilateral can be divided into at most five triangles.

In figures 2, 4 and 6, we present some solutions of the bistable equation in a square which exhibit the characteristics mentioned above. Next to the solutions, we give the meshes produced by TRANSI with contour levels superimposed. In these computations run on a SUN workstation, TRANSI was constrained to use only three to four sizes of quadrilateral elements. Nonetheless, these examples demonstrate the sharpness with which TRANSI distinguishes phase transitions.

We also thought the following experiment would make interesting reading.

It consisted of marking the time it takes for the numerical solution of the bistable equation in a square with the initial data shown in figure 7 to collapse to the steady state -1 versus the error tolerance. Hopefully, we expected to see that as we decreased the tolerance, these times would converge to the correct time. This does **not** happen with fixed mesh codes and that is why it is an interesting experiment.

The time of "collapse" of the solution to the steady–state versus the logarithm of the global error tolerance GTOL is plotted in figure 11. It is clear that there is little variance in the times as the tolerance is decreased (and the number of elements increased). The change in log(GTOL) averaged 5.6% while the average change in the time was 1.2%. Moreover, as the tolerance decreases, the variance decreases. Both of these traits are desirable.

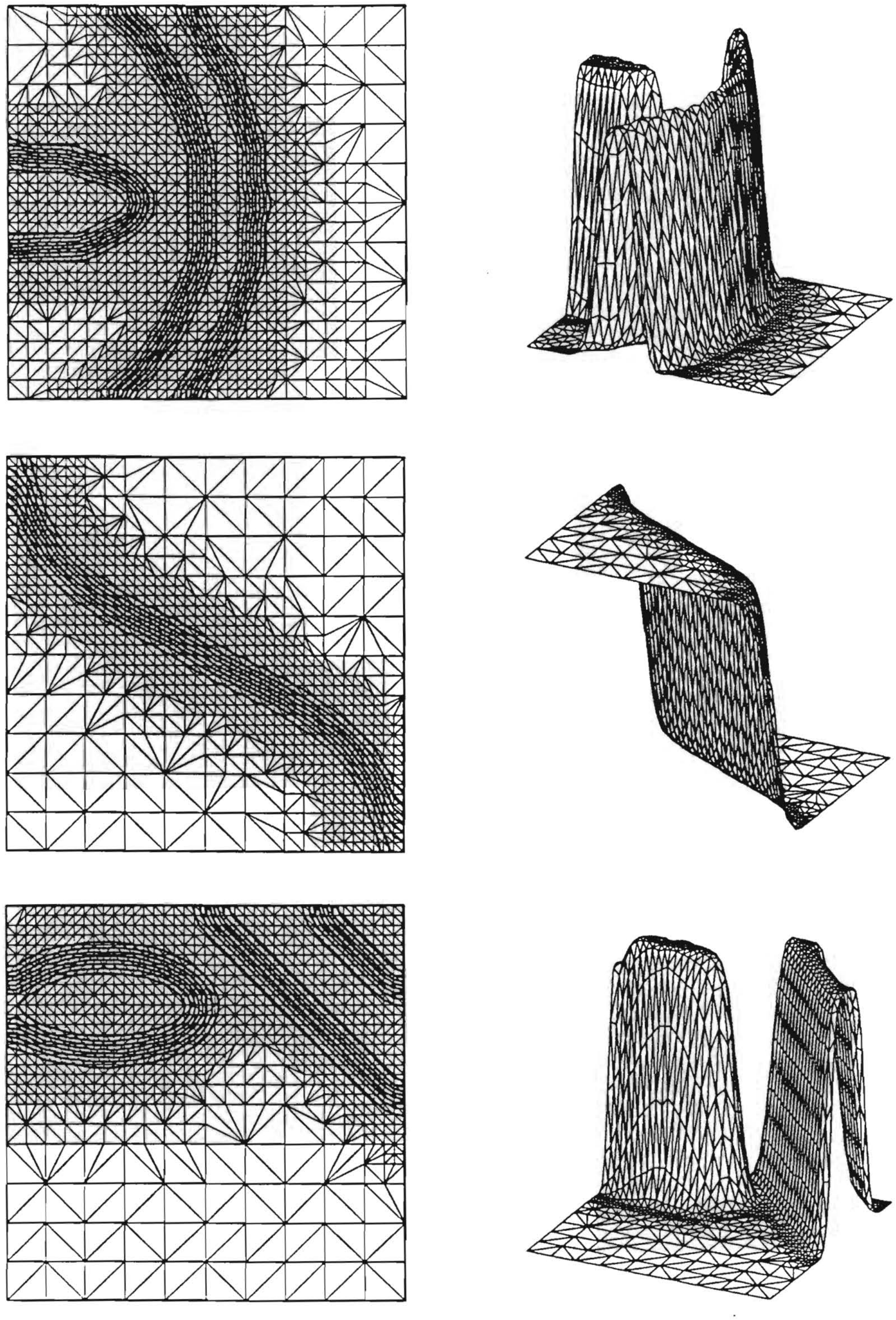
The number of elements and time steps vary with the time and GTOL. In figures 7 through 10, we show mesh and contour plots and the solutions for GTOL=.009. 7 and 8 are the solution and the mesh and contour levels for the first time step and 9 and 10 are the same views for time 2.59, three steps before the collapse of the solution to -1. The amount of refinement in the first step is clearly demonstrated. As the front dissipates and shrinks in height, TRANSI un–refines the mesh while preserving the same global error tolerance. Overall, TRANSI provides accuracy with much fewer number of elements than fixed mesh codes. The mesh alignment used in TRANSI certainly helps in this regard.

Next we plot $|| U + 1 ||_{L^2}$ (the "height" of U in L^2) and the time step size versus the time for GTOL=.001 in figure 13. This demonstrates how TRANSI adapts the time steps during the computation. In figure 14, we show the number of elements used by TRANSI for the same computation.

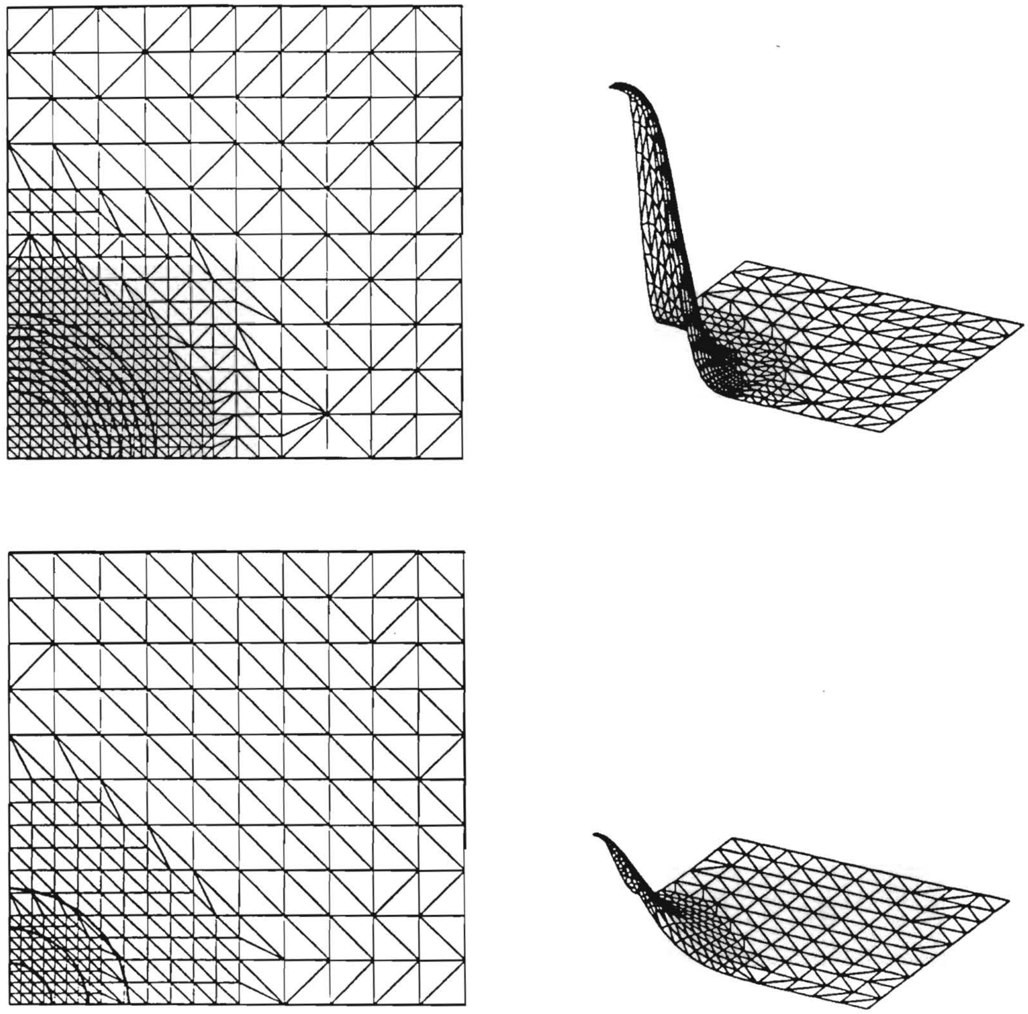
For the sake of comparison, we plot the results of the same experiment run with DGAL. In a fixed mesh code using a standard mesh (figure 15), different results are obtained when the initial data's peak is centered at different corners of the square. Figure 16 shows the initial data. Placing the peak at different corners affects the representation of the initial data. Figure 12 shows the times obtained for runs made using these two corners ($\times$ marks the data for the left hand corner and $\triangle$ that of the right). Clearly, the orientation of the front with respect to the mesh has a strong effect. It is also disturbing that in no sense do the times converge to a fixed value as the mesh size h decreases. In fact, by comparing the average percent change of $\log(h^2)$ which is 1.1% to the average percent change in the times, which is 5.3% for the computation made with the first initial data $(\times)$, and 8.6% for the second initial data $(\triangle)$, (almost the reverse of the results obtained with TRANSI!) we conclude that there is a complicated relationship between the motion of a front and its location with respect to the mesh.

[DE] Dieci, L. and Estep, D., *Some stability aspects of schemes for the adaptive integration of stiff initial value problems*,to appear in SIAM J. Sci. Stat. Comput.

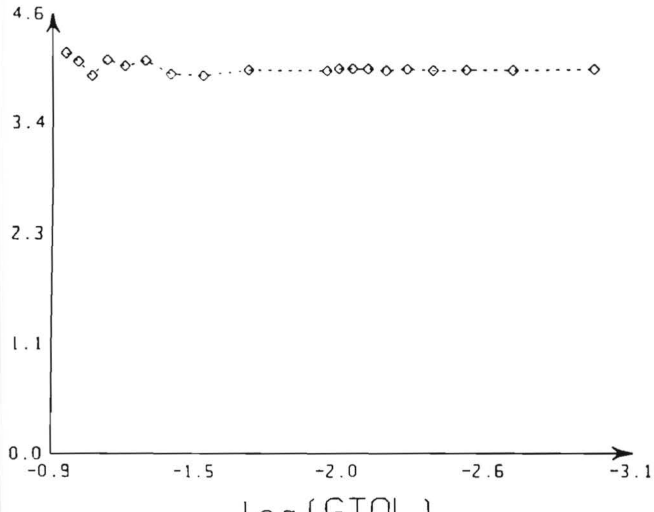
[EL] Estep, D. and Larsson, S., *Fully discrete discontinuous Galerkin schemes for semilinear parabolic problems*, in preparation.



Figures 1–6. Examples of steep transition layers in solutions of $u_t - \Delta u = u - u^3$ in the unit square with Neumann boundary conditions. On the left are the meshes generated by TRANSI with contour levels superimposed. On the right are projections of the solutions.



Figures 7–10. 7–8 show the initial data and initial mesh for the experiment. The "radius" of the data is approximately .25. 9–10 show the solution at time 2.59, three steps before the solution becomes -1. Here, GTOL=.009.



igure 11. Plotted is the time it took for the TRANSI solution become -1 versus the log of the global error tolerance. creasing accuracy goes to the right. *Linear interpolation as used to get accurate times.*

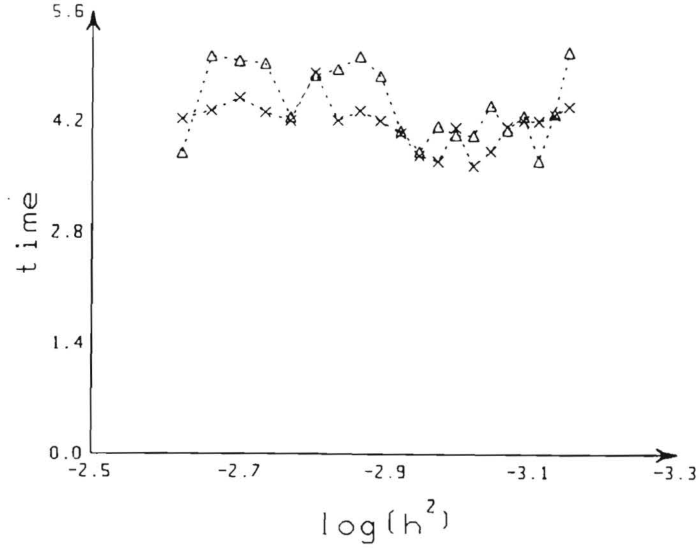
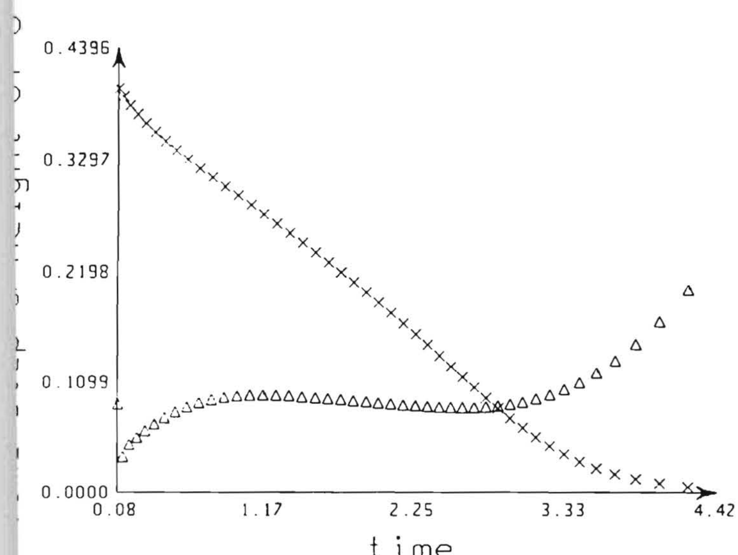


Figure 12. Plotted is the time it took for the DGAL solution to become -1 versus the log of the mesh size. Increasing accuracy goes to the right. × marks the data for the peak centered at (0,0). △ marks the data for the peak centered at (1,0).



igure 13. TRANSI Adaptivity: × marks the height $U + 1 ||_{L^2}$ as time progresses. △ marks the time steps.

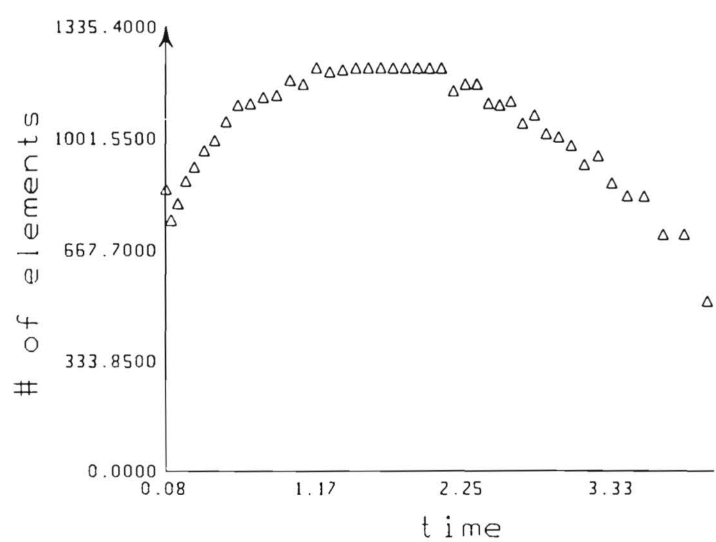


Figure 14. TRANSI Adaptivity: a plot of the number elements used by TRANSI as time progresses.

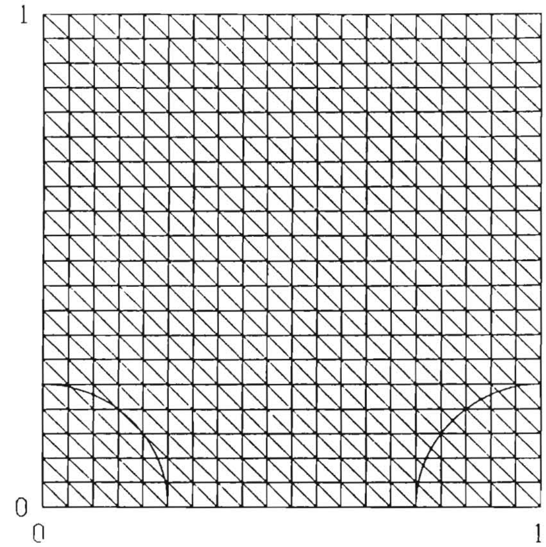


Figure 15. The standard fixed mesh used in the experiment. The semicircles mark the transition layer of the initial data.

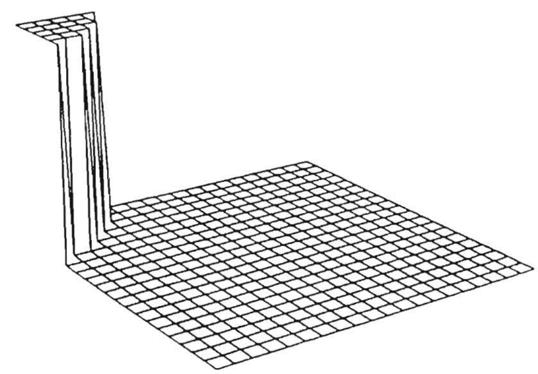


Figure 16. The initial data above a 20x20 mesh.

NIST Technical Report

January 1, 1991 - June 30, 1991

"Dynamical Problems and Phase Transitions"

Dr. Shui-Nee Chow and Dr. Jack Hale
Principal Investigators

July 31, 1991

Report

Xu-Yan Chen

July 26, 1991

Much of my research during the saty in the NIST is concerned with the study of spatial-temporal structures of solutions to nonlinear partial differential equations, basically from dynamical systems point of view. Topics I considered spread over A-D below:

A. Nonlinear Diffusion Problems (extinction and free-boundaries)

A gas flow in porous media with strong absorption effect is described by a degenerate parabolic equation with singular nonlinear term. The boundaries of the gas flow exhibit some interesting dynamical behaviors such as expansion, shrinking and extinction. I obtained several qualitative properties of these boundaries, in a joint work with Hiroshi Matano and Masayasu Mimura. We proved that as the gas fades away, not only the density of the gas flow tends to 0 but also the volume of the gas will become infinitesimal. We also demonstrated the continuity of the boundaries and the possibility of splitting of the gas flow. A paper will appear in J. Reine Angew. Math.

B. Time-Periodic Nonlinear Parabolic Equations (structural stability)

A biological wave in a media with seasonal changes can be described by nonlinear partial differential equations of parabolic type:

$$u_t = u_{xx} + f(t, x, u, u_x),$$

where the nonlinear term f depends on time t periodically. Other physical phenomena such as heat conduction in the earth are also modeled by the above equation.

In a joint work with Mingxiang Chen and Jack Hale, I proved the Morse-Smale property of Dirichlet initial-bounadary value problem of time-periodic semilinear parabolic equations. One important consequence of this result is the structural stability of the equation, in other words, a small perturbation of the nonlinear term does not change the dynamic structure of the attractor. A paper is in preparation.

C. Mean Curvature Flow (singularities)

The mean curvature flow is one of basic mathematical models of interfacial dynamics and is extensively studied by a large number of scientists. Its law of motion can simply be stated as that the normal velocity V of the interface is given by the mean curvature K of the interface: $V = -K$.

One of major difficulties in studying the motion by curvature comes from the fact that the topological type of interface may change significantly in the intermediate stage of the dynamic process. Recently, I considered symmetric interfaces which are the hypersurfaces of bodies of rotation in high (more than three) dimensional Euclidean spaces and succeeded in obtaining a complete classification of qualitative behavior of the interfacial motion. Assuming only the smoothness of the initial data, I proved that as the interface becomes singular, it can develop only finitely many singularities. The asymptotic form of these singularities is classified in detail. Using these results, I was also able to show (jointly with M. Soner and T. Souganidis) that the interface regains its smoothness immediately after singularities have been formed. Two papers are in preparation.

D. Reaction Diffusion Systems (free-boundary problem)

Interfacial patterns like rotating spiral waves and expanding target fronts are observed in the famous Belouzov-Zhabotinski reaction. The propagation of such chemical waves is phenomenologically described by a system of singularly perturbed reaction diffusion equations. In my Ph.D. thesis I studied some general features of the interfacial dynamics in the system. Among other things, I considered the singular limiting problem of the system, which is a free-boundary problem whose interface equation involves the curvature effect and the time-history of the interface. As in the case of mean curvature flow, the global classical solutions do not exist in general, because of the possiblity of topological changes of interfaces. I proved in thesis the local (in time) existence of classical solution of the free boundary problem. Recently, I was able to further construct a global weak solution by applying the theory of viscosity solution. A paper is in preparation.

Research at NIST by Erik S. Van Vleck

During my visit to the metallurgy division of NIST in the fall of 1990 it was suggested by John Cahn that I look at two papers on differential-difference equations by L. Hillert and Cook, de Fontaine and Hilliard. In these papers equations were derived in an effort to model a binary solid-solution over a finite lattice. In accordance with these ideas we considered differential-difference equations over three-dimensional primitive, face centered, and body centered cubic lattices with periodic boundary conditions so that at each lattice point p we had an equation of the form:

$$\frac{dc(p)}{dt} = \sum_r \{f'(c(p+r)) - f'(c(p)) + (c(p+r) - c(p))f'' \\ -\beta(c(p+r))\Delta c(p+r) + \beta(c(p))\Delta c(p)\}$$

where the summation is over all nearest neighbors and $\Delta c(p)$ is the finite difference analogue of the laplacian, depending on the lattice structure, centered at $c(p)$. This is analogous to a finite difference approximation in space with a large spacing between the mesh points. We set the free energy function $f(c) = c^3 - c$ and the function $\beta(c) = c^2 - 1$. The values at the lattice points are such that $-1 \leq c(p) \leq 1$. A value of -1 at a lattice point corresponds to the site being occupied by an A atom with probabitity one, while a value of 1 corresponds to the site being occupied by a B atom with probability one.

Numerical experiments were performed initially using a forward Euler approximation and subsequently using higher order explicit and implicit methods. The initial data was produced using a random number generator with values in the interval $[-1, 1]$. The results of our experiments were visualized using bit mapped images by displaying two dimensional slices of the data side by side and using a spectrum of color to denote the probabilities at each lattice point. The evolution was observed by animating the images as time is increased, and the images were recorded on video tape.

Since my initial visit I have begun to work on a slightly different equation. Consider a partial differential equation of the form

$$\begin{cases} u_t = \Delta\{f(u) + \epsilon g(\nabla u)\Delta u\} \quad \text{in} \quad \Omega \\ n \cdot \nabla\{f(u) + \epsilon g(\nabla u)\Delta u\} = 0 \quad \text{on} \quad \partial\Omega \end{cases}$$

where Ω is a smooth bounded domain in $\mathbb{R}^k$, $k \leq 3$. Here $f(u) = u^3 - u$, $g(\nabla u) = \gamma_1 - \epsilon\gamma_2|\nabla u|^2$. We consider $\gamma_1, \gamma_2 > 0$. This equation has a good Liapunov function of the form

$$L(u) = \int_\Omega (F(u) + \epsilon G(|\nabla u|^2)dx$$

where $G(|\nabla u|^2) = -\gamma_1/2|\nabla u|^2 + \epsilon\gamma_2/12|\nabla u|^4$.

Currently in one space dimension I am working on analyzing the structure of the steady-state solutions, and I am exploring the possible connections between steady-state solutions. Numerically my focus is in three space dimensions, where as before I consider coarse discretizations that depend on the lattice structure. Since the discretization is coarse stiffness is not a problem. I have begun to solve the resulting differential-difference equation using multistep variable order, variable time step, Adams formula codes due to Hindmarsh. I am developing codes and a graphical interface to explore the affects of different lattice structures on the behavior of the solution.

NIST TECHNICAL REPORT

July 1, 1991 - October 31, 1991

Dynamical Problems and Phase Transitions

Dr. Shui-Nee Chow and Dr. Jack Hale
Principal Investigators

October 31, 1991

NIST Quarterly Technical Report

Period Covered: 7/1/91 - 10/31/91

Submitted by Jack Hale and Shui-Nee Chow

Keng Huat Kwek, a graduate researcher, worked at NIST on the research project. During this time he managed to complete the proof of global existence of a Cahn-Hilliard type equation. He also did some numerical experiments on this equation in one space dimension and two space dimension by using a relatively new numerical method, i.e., discontinuous Galerkin finite element method. Moreover, these visits were a motivation for some of the work in the thesis of Kwek at Georgia Tech, where he considered the Cahn-Hilliard equation with dispersion from the theoretical and computational point of view. These models are perhaps more realistic in plasma physics than in alloys.

Study of spatial-temporal structures of solutions to nonlinear partial differential equations, basically from dynamical systems point of view, were carried out by Xu-Yen Chen, Post Doctoral Fellow in the Center for Dynamical Systems and Nonlinear Studies. Topics considered were the following:

A. Nonlinear Diffusion Problems (extinction and free-boundaries)

A gas flow in porous media with strong absorption effect is described by a degenerate parabolic equation with singular nonlinear term. The boundaries of the gas flow exhibit some interesting dynamical behaviors such as expansion, shrinking and extinction. Chen obtained several qualitative properties of these boundaries in a joint work with Hiroshi Matano and Masayasu Mimura. They proved that as the gas fades away, not only the density of the gas flow tends to 0 but also the volume of the gas will become infinitesimal. Also demonstrated was the continuity of the boundaries and the possibility of splitting of the gas flow. A paper will appear in J. Reine Angew. Math.

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NIST Quarterly Technical Report

Period Covered: 8/1/91 - 10/31/91

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NIST TECHNICAL REPORT

November 1, 1991 - December 31, 1991

Dynamical Problems and Phase Transitions

Dr. Shui-Nee Chow and Dr. Jack Hale
Principal Investigators

January 31, 1992

NIST Quarterly Technical Report

Period Covered: 11/1/91 - 12/31/91

Submitted by Jack Hale and Shui-Nee Chow

Xu-Yan Chen has continued his study of mean curvature flow and is concentrating on completing two papers on the manner in which the singularities of these surfaces can develop and how smoothness develops immediately afterwards.

New initiatives are concerned with how stable subharmonic solutions of reaction diffusion equations can arise. The theory developed by M. Chen, X.-Y. Chen and Hale for time periodic equations will play a major role.

Chris Grant, a new postdoc at the Center, is attempting to show that the solutions of the Cahn-Hilliard equation in one-space dimension exhibit exponentially slow motion, a phenomena that had been previously observed by Carr-Pego and Fusco-Hale for reaction diffusion equations. The methods to be employed are extensions of the procedures of Broussard-Kohn and Alikakos-McKinney. It is relatively easy to obtain slow motion of order ϵ^n, for any n, but the slow exponential motion requires new ideas.

TECHNICAL REPORT ON CAHN-HILLIARD-MORRAL SYSTEMS

National Institute of Standards and Technology
DARPA 70NANB8H0860

Shui-Nee Chow
Jack K. Hale
Co-Principal Investigators

Period Covered: 1/1/92 - 3/30/92

May 1992

TECHNICAL REPORT ON CAHN-HILLIARD-MORRAL SYSTEMS

CHRISTOPHER P. GRANT*

One of the leading continuum models for the dynamics of phase separation and coarsening in a binary mixture is the Cahn-Hilliard equation, which in the one-dimensional case can be written as

$$\begin{aligned} u_t &= (-\varepsilon^2 u_{xx} + W'(u))_{xx}, & x &\in (0,1) \\ u_x &= u_{xxx} = 0, & x &\in \{0,1\}. \end{aligned} \tag{1}$$

Here W represents the bulk free energy density of the mixture as a function of the concentration u of one of its two components. The parameter ε represents an interaction length and is assumed to be a small positive constant. This equation was derived in [6] based on the free energy functional of van der Waals [18]

$$\mathcal{E}_\varepsilon[u] \equiv \int_0^1 \left(W(u) + \frac{\varepsilon^2}{2}|u_x|^2 \right) dx. \tag{2}$$

In the early 1970s, Cahn and Morral [16] and DeFontaine [10] [11] initiated the study of systems of partial differential equations that model the phase separation of mixtures of three or more components in essentially the same way that the Cahn-Hilliard equation models the separation of binary mixtures. (See Eyre [13] for a comprehensive survey of such systems.) If the domain is again taken to be $[0,1]$, then, after a change of variables, such systems can be written in the form

$$\begin{aligned} u_t &= (-\varepsilon^2 u_{xx} + DW(u))_{xx}, & x &\in (0,1) \\ u_x &= u_{xxx} = 0, & x &\in \{0,1\}, \end{aligned} \tag{3}$$

where u is now an n-vector (for an $(n+1)$-component mixture), and W maps a subset of $\mathbf{R}^n$ into $\mathbf{R}$. Again, $\mathcal{E}_\varepsilon$ defined by (2) represents the total free energy of the mixture, and it is easy to check that it provides a Lyapunov functional for (3). Also, the mass $\int_0^1 u\,dx$ of a solution is conserved.

Note that any constant is an equilibrium solution to (3). A linear analysis of the equation about an unstable constant equilibrium suggests that typical solutions that start near such a constant undergo fine-grained decomposition with a characteristic length scale that is $O(\varepsilon)$. (See [14] for a precise mathematical formulation and rigorous verification of this in the two-component case.) This fine-grained decomposition of initially homogeneous mixtures has also been frequently observed in physical experiments [7]. Therefore, if one is interested in the later stages of evolution for a typical solution of (3) it makes sense to start with initial data $u(x,0)$ that is close to the *phases* (preferred homogeneous states) of W through most of the domain, with sharp transition layers separating the various intervals where u is nearly constant.

Consider when $n = 1$ (i.e., the original Cahn-Hilliard equation (1)), the case for which the most work has been done. Carr, Gurtin, and Slemrod [8] showed that all of the local minimizers of $\mathcal{E}_\varepsilon$ with any specified mass are monotone, so, in general, we would expect that the fine-grained structure of u would coarsen as $t \to \infty$. Numerical

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work by Elliott and French [12] indicates that this evolution occurs very slowly. (Such slowly evolving states are sometimes said to be *metastable.*) Bronsard and Hilhorst [4] have shown that, in the dual Sobolev space $H^{-1}[0,1]$, this evolution occurs at a rate that is $O(\varepsilon^k)$ for any power k. Using completely different techniques, Alikakos, Bates, and Fusco [1] constructed a portion of the unstable manifold of a two-layer equilibrium which intersects a small neighborhood of a monotone equilibrium and showed that the speed of the flow along this connecting orbit is $O(\exp(-C/\varepsilon))$ for some constant C. Recently, Bates and Xun [3] have found exponentially slow motion for the n-layer states of (1) by combining the methods of [1] with those used by Carr and Pego [9] to study reaction-diffusion equations.

In [15], we have obtained results similar to those of Bates and Xun in that we also obtain exponentially slow motion, but the methods we use are much simpler, and they are valid not only for the two-component Cahn-Hilliard equation (1) but for the multi-component Cahn-Morral system (3), as well. It should be mentioned, however, that our results deal only with the speed of motion and say nothing about the geometric structure of the attractor. Our main result is summarized in the following theorem.

THEOREM 0.1. *Let v be a step function whose range is confined to the phases of W. Then there exist positive constants C and δ (depending only on the location and type of the discontinuities of v) and an ε-parametrized family $u^\varepsilon(x,t)$ of solutions of* (3) *such that*

$$\|u^\varepsilon(\cdot,0) - v\|_{H^{-1}} \leq \delta$$

and

$$\lim_{\varepsilon\to 0}\left\{\sup_{0\leq t\leq M\exp(C/\varepsilon)} \|u^\varepsilon(\cdot,0) - u^\varepsilon(\cdot,t)\|_{H^{-1}}\right\} = 0,$$

for any $M > 0$.

In words, if a solution starts off near the phases of W and has "efficient" transitions between the phases then it moves extremely slowly in $H^{-1}[0,1]$. This also implies that that the motion of the interfaces along the interval $[0,1]$ is extremely slow.

Our results are based on the approach introduced by Bronsard and Kohn [5] in their study of slow motion for reaction-diffusion equations. The improvement from superpolynomial to exponential speed is made possible by incorporating some ideas of Alikakos and McKinney [2] about the profile of constrained minimizers of (2). Use is also made of techniques of Sternberg [17] for describing the nature of globally stable steady-state solutions of (3) in the limit as $\varepsilon \to 0$.

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NIST Technical Report

Period Covered: April 1, 1992-June 30, 1992

Our report this period consists of a listing of preprints by researchers in the Center for Dynamical Systems whose work was supported wholly or in-part by DARPA Grant 70NANB8H0860 during the period September 1989 through June 1992. Please find the attached list on the following five pages.

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79 *On the global dynamics of attractors for scalar delay equations*, C. McCord and K. Mischaikow.

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81 *Algebraic rank tests for complete controllability of non-autonomous linear systems*, H. Leiva and B. Lehman.

NIST Technical Report

Period Covered: July 1, 1992-September 30, 1992

Jack K. Hale

Work-in-Progress

We are studying the stability of simple motions in lattice models on nonequilibrium media and existence of smooth foliations near equilibria of finite and infinite dynamical systems. We are also investigating pattern formation and invariant measures in coupled lattice maps.

FINAL REPORT - DARPA 70NANB8H0860

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November 1, 1992 - January 14, 1993

In our study of dynamic systems and phase transitions, we have been concerned with both continuous and discrete models.

One of the primary objectives has been to try to understand the mechanism for the creation of complicated patterns in the systems and then to see how these patterns evolve into simpler systems with the rate of the motions of boundaries. In the latter problem, we have been particularly interested in the rate at which the phase boundaries move. These problems are being attacked from both the numerical and theoretical sides.

Specific numerical techniques have been devised by G. Meyer, D. Estep and E. van Vleck. The goal here has been to develop methods which will follow a solution through all periods of its evolution and not just over a brief initial instant. This involves a theoretical understanding of some of the dynamics and then a development of the numerical scheme with this in mind.

For the continuous models, we have studied mean curvature flow (X.-Y. Chen) and the exponentially slow motion of transition curves for reaction diffusion equations (J. Hale), the Cahn-Hilliard equation and systems of Cahn-Hilliard-Morral (C. Grant). The methods developed here seem to provide new information about global dynamics even when the motion is not so slow.

We also have been trying to determine the effect of the shape of the domain in a PDE on the global dynamics. Due to the complexity of the problem, we have concentrated on problems on thin domains in reaction diffusion equations and damped hyperbolic equations (J. Hale and G. Raugel). The shape of the domain is reflected in dispersive terms on the reduced domain and several situations have been analyzed showing how the shape can create stable patterns.

Some of our recent work has been devoted to lattice models of nonequilibrium media. We are investigating pattern formation, stability and invariant measures in coupled lattice maps.