ONR Contract N00014-86-K-0691

RESEARCH IN COMPUTING AND APPLIED MATHEMATICS

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Co-principal Investigators: Christopher Anderson, Bjorn Engquist, Charles Lange, & Stanley Osher

FINAL REPORT*

Publications

This contract was awarded for research into the development of numerical and analytic techniques useful in solving problems arising in continuum mechanics, especially fluid mechanics, and particularly in areas in which the PI and co-PIs have special expertise. Projects that were pursued during tenure of the award including the following.

1. *Dynamical Processes in Freezing Materials.* Two main areas were attacked during the period of the contract: (a) the development of continuum theories of freezing processes, and (b) the solution of moving boundary problems connected with the freezing of materials. (a) *Continuum Theories.* A system near the melting/freezing point typically contains matter in three forms: solid, liquid and mush, the last being a mixture of solid and liquid phases. As a system evolves, it converts each of these forms into one of the others, i.e. the solid-liquid, solid-mush and liquid-mush fronts all move relative to the material. The objective is to develop a physically well-founded theory that will correctly describe the evolution of each domain and the motion of the interfaces separating them (see Hills & Roberts, 1987a,b 1988a,b,c; Loper & Roberts, 1987a,b; Roberts & Loper 1988). Complications that arise include coarsening (the increase in the mean size of the solid grains as the mush ages; see Hills & Roberts, 1990), coring (the fact that the material currently freezing onto the grains of an alloy does not have the same composition as that deeper in the grain, which froze earlier; see Hills & Roberts, 1988b,c), effects of surface tension (particularly the freezing temperature, which is depressed), and many other processes. Theories were developed that included the effects just specifically mentioned. These were tested by analytic solutions to simple situations, and the results gave

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*Prepared by the Principal Investigator, Paul H. Roberts, who thanks Christopher Anderson, Bjorn Engquist, Hans-Otto Kreiss, and Charles Lange for their assistance in preparing this report.

confidence that the theories were physically robust. Related ideas were applied to other mixture theories (Hills & Roberts, 1987c, 1989) (b) *Specific Solutions.* To determine the evolution of a system near the freezing point, requires that complicated Stefan problems be solved to determine the location and motion of the interfaces mentioned in (a) above. One challenging problem, to which previously only solutions involving such physical absurdities as superheated ice had been proposed, was solved at UCLA during the period of the contract (Hills & Roberts, 1991); it concerns the evolution of system cooled below the freezing point on its boundary but heated internally by (e.g. radioactive) sources.

2. *Nonlinear Waves.* A number of projects were undertaken concerning the interaction and evolution of a sea of small amplitude waves. A Fokker-Planck equation was developed that generalizes all known previous Focker-Planck equations, and with the help of which the frequency renormalization created by nonlinear interactions could be explicitly calculated in a first approximation (Putterman & Roberts, 1988). The particular case of acoustic turbulence was studied both for classical systems (so generalizing well-known Russian work) and quantum systems (so shedding more light onto the interface between classical and quantum physics). Large-scale numerical simulations were also undertaken (Haeri *et al.* 1992). Further work on ocean waves revealed the existence of a second sound phenomenon (Larraza 1987, Larraza *et al.* 1990).

Another project that still engages the attention of the PI includes three-dimensional integrations of the non-linear Schrödinger equation as a simple model of superfluid helium (the Bose condensate model) ; see Jones *et al.* (1986), Jones & Roberts (1987).

3. *Convection.* A number of investigations of MHD stability were completed. Magnetoconvection was studied, both for compressible and Boussinesq fluids (Jones & Roberts, 1990; Roberts, 1991). The well-known studies of the resistive instabilities of plasma equilibria was generalized to highly rotating systems (Kuang & Roberts 1990, 1991, 1992). A nonlinear study of the arotropic annulus (a crude model of the atmosphere of Jupiter) was undertaken: see Lin (1990). Mulder (1989) developed an new multigrid approach for the solution of convection problems.

4. *Singular Perturbation Methods.* Lange continued his long term collaboration with Robert Miura on perturbation methods, and

published an investigation of the asymptotics of differential-difference equations (Lange & Miura, 1991). Lange has also continued his collaboration with Don Smith on integral equations involving a small parameter. Together, they have completed a lengthy study of the application of singular perturbation methods to such problems (Lange & Smith, 1988). Unusual kind difficulties arise from the theory of elasticity of elastic membranes and shells. These have significant technological applications to tubular chemical reactors. Lange & Weinitschke (1991a, b) have developed the necessary mathematical apparatus to solve these problems.

5. *Vorticity*. During tenure of the award, Anderson continued his investigations into the creation, interaction and merging of vorticity. The results of such study are technilogically significant, since vorticity creation and shedding has a significant bearing on the lift and drag of a moving body. It can also be argued that the vorticity contains the physics, and that the primary task in integrating the equations of motion is that of solving the vorticity equation, and subsequently deriving the flow subsequently from the relevant Poisson equation, perhaps by domain decomposition methods (Anderson 1988a). The direct solution of the vorticity encounters difficulties in satisfying the boundary conditions. Anderson has developed new techniques for overcoming these (Anderson 1988b, 1989a), and has applied the resulting methods to problems involving vortex shedding (Anderson *et al.* 1990; see also Anderson *et al.*, 1988a) as well as to the interaction of vortex rings (Anderson *et al.*, 1988b; see also Anderson, 1989b). Anderson (1990) also made a number of suggestions concerning fast particle simulations, as well as alternative implementations (Anderson, 1992) of the multipole method of Greengard & Rokhlin (1991). Cottet (1990a, b) also added to the theory of deterministic vortex methods for the Navier-Stokes equations, with particular reference to implementation of the boundary conditions, through a particle-grid superposition method.

6. *Shocks*. During tenure of the award, many applications have been made by Osher and his collaborators of essentially non-oscillatory schemes for shock capture: Fatemi *et al.* (1991a,b), Harten (1988, 1990), Harten & Chakravarthy (1992), Harten *et al.* (1987), Mao (1989a,b, 1990), Marquina (1992), Osher & Shu (1989, 1991), Shu & Osher (1989), Shu *et al.* (1992), Yang (1990). These can be used to compute the motion of shocks whose speed depends on their curvature, for which a Hamilton-Jacobi formulation is particularly convenient (Bardi & Osher, 1991; Osher, 1989, 1991; Osher & Shu,

1991). This has applications to solving problems involving crystal growth and those involving the propagation of flames or detonations (Ton *et al.*, 1992). The general problem of calculating the motion of an interface is a challenging one; other contributions have been made by Mao (1991a,b), Mulder *et al.* (1991). Chu & Wu (1991) developed the theory of magnetohydrodynamic shocks further. Engquist *et al.* (1989b) developed nonlinear numerical filters for shock calculations. Mostrel (1988) developed new numerical schemes for transonic flow problems. Sjogreen (1988) reported on shock calculations using algorithms developed for parallel computation. Engquist & Huynh (1989) developed iterative pre-conditioned Newton-type methods for shock calculations.

Several investigations were made of problems encountered when conservation laws are solved computationally. Lafon & Osher (1991) explored high order filtering methods for the solution of high order systems of hyperbolic conservation laws. Donat & Osher (1990) investigated the propagation of errors in nonlinear approximations to conservation laws. Marquina (1990) used a local piecewise hyperbolic reconstruction of numerical fluxes in the solution of nonlinear conservation equations. Durlofsky *et al.* (1990) developed a triangle-based TVD scheme for the solution of hyperbolic conservation laws. The incorporation of a maximum principle into a triangular stencil was implemented by Liu (1992).

Engquist & Sjogreen (1990) gave new methods for solving stiff hyperbolic systems. Brenier (1991) added to the theory of hyperbolic differential equations that have oscillatory coefficients. Papageorgiou & Smyrlis (1991) studied the route to chaos for the Kuramoto-Sivashinsky equation.

7. *Turbulence*. Henshaw has almost completed a fourth order accurate difference code for Navier-Stokes equations, using overlapping grid techniques. One can use rather general boundary conditions. Adaptivity will be added. As part of her thesis Jennifer Hou (neé Chang) has compared finite differences and spectral methods for model problems. She has also implemented the methods on the connection machine. Henshaw and Kreiss have made perturbation calculations for 2D turbulent flows. The following results are interesting:

(a) The effect of the perturbations depend very much on the frequency of the perturbation;
(b) Fully turbulent flows are stable against perturbations in short time intervals;

(c) In long time intervals the effect of a change in Reynolds number is large. For example, changing R from 10^5 to 2.10^5 changes the large scale by O(1). To be able to make the calculations more efficient D. Brown has implemented our code on the connection machine at Los Alamos National Labratory.

8. *Systems having Two Widely Different Time Scales.* Kreiss & Lorenz (1992) have completed a paper on slow solutions for highly oscillatory problems". They succeeded in connecting the bounded derivative principle with asymptotic expansions and the existence of a slow manifolds. Also, sharp estimates of the effect of the fast scale on the slow time scale were obtained. Kreiss (1992) has completed a large survey article on problems with different time scales. It discusses the connection between ordinary and partial differential equations and also treats applications in Geophysics and Plasma physics. Kreiss *et al.* (1991) have presented a new discussion of convergence of the solutions of the equations governing a compressible fluid to the solutions of the incompressible Navier-Stokes equations. Browning *et al.* (1992) have made a comparison of the differential systems and the numerical methods used in the computation of smooth oceanographic flows. For highly oscillatory problems the time integrator is still an obstacle. Some of these difficulties are discussed in a forthcoming paper by Kreiss & Abrahamsson (1992). A paper by Kreiss & Scherer (1992) on the method of lines for hyperbolic differential equations wil appear shortly. B. Gustafsson, J. Oliger & H.-O. Kreiss have started work on a book on *Numerical Methods for Time Dependent Problems.*

9. *Initial boundary value problems.* Lixin Wu has defended his thesis: "Stability of difference approximations for initial boundary value problems." Kreiss has worked on a new definition of wellposedness for initial boundary value problems. It is based on the resolvent condition and it is the weakest definition, which is stable against lower order perturbations. Also, the discrete analog of this definition is very effective for the method of lines.

10. *Far-field Boundary Conditions.* When the solution of hyperbolic equations are required in infinite domains, it is necessary in practice to cut off the domain at great distance and to add boundary conditions at the cut-off that preserve the essential condition that the waves are outgoing. Reflection in the far field would lead to a return of the waves to the source regions and to the corruption of the

solution. The implementation of far-field boundary conditions had been of special interest to Engquist and his collaborators for several years, and further progress was made during the period of this award. The main contributions were applications to fluid dynamics and steady problems. See Engquist (1989), Engquist & Gustafsson (1987) and Engquist & Halpern (1988, 1990). Global boundary conditions for use with fast Helmholtz solvers were studied by Engquist *et al.* (1989a).

11. *Other Computationally-Oriented Work.* Bamberger *et al.* (1988a,b) developed methods for solving parabolic equations in heterogeneous media. Rizzi & Engquist (1987) surveyed the theory and practice of computaional fluid mechanics, concentrating mainly on specially selected topics.

Conferences

The *UCLA Workshop on Vortex Methods* was held at UCLA during May 20 through May 22, 1987 and was supported by this Contract. It was organized by Chris Anderson and brought together people investigating, by computational and analytic methods, the evolution of vortical structures. It resulted in a book in the Springer series Lecture Notes in Mathematics; see Anderson & Greengard (1988).

The Workshop on the Nonlinear Dynamics of Rotating Magnetic Systems was held at UCLA during August 4 through 8, 1987 and was supported by this Contract. It was organized by Paul Roberts and brought together 41 people interested in this interesting branch of MHD, one that has wide significance in planetary and extra-terrestrial magnetism. The report on the meeting (Roberts, 1987) was widely distributed.

The Second International Symposium on Domain Decomposition Methods was held in UCLA during January 14 through 16, 1988 and was partially supported by this Contract. Tony Chan was the organizer on site and one of the editors of the final published proceedings (Chan *et al*, 1989). Nearly 100 people attended the meeting, and 40 featured lectures presented state-of-the-art reviews, covering theory, algorithms, parallel implementations, and applications.

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† Authors supported by the Grant (which include the Principal Investigator, the Co-principal investigators, other faculty members, visitors and students) are shown in bold face type. The phrase "CAM Report" refers to the Series of reports on *Computational and Applied Mathematics* produced by the Department of Mathematics at UCLA.

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