REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		FINAL 01 MAY 93 TO 30 APR 96

4. TITLE AND SUBTITLE
NUMERICAL MODELING FOR CRYSTAL GROWTH

5. FUNDING NUMBERS
F49620-93-1-0053
2304/CS 61102F

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AFOSR-TR-96
0382

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9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NM
110 DUNCAN AVE B115
BOLLING AFB DC 20332-8080

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
APPROVED FOR PUBLIC RELEASE;
DISTRIBUATION UNLIMITIED

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)
SEE REPORT FOR ABSTRACT

19960726 036

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR

Final Technical Report
1 May 1993—30 Apr 1996
AFOSR Grant F49620-93-1-0053

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25 May 1996

1. Objectives: Our research on moving boundary problems in crystal growth aims to develop and implement new numerical methods which produce better accuracy for a given cost.

2. Status of effort: We have developed efficient and accurate new methods in several subareas of crystal growth. These include spectral methods for phase field models, new vortex methods for convection in the melt, and related quadrature and interpolation techniques.

3. Accomplishments/New Findings: We have made substantial progress in two areas of our project; spectral methods for phase field models of phase transitions and vortex methods for computing convection in the melt. In the first area, we have developed two accurate and efficient new spectral methods for general parabolic systems of partial differential equations in periodic geometry and applied them to solve phase field models for crystal growth. In the second area, we have developed three new vortex methods for computing convection in the melt at high Reynolds numbers and tested them on flows without boundaries. We now summarize these results in more detail.

Phase field models for crystal growth

• We have developed new classes of accurate and efficient spectral methods for nonlinear parabolic systems of partial differential equations

$$U_t = F(t, x, U, \partial U, \partial^2 U)$$

with F a nonlinear elliptic operator in periodic geometry. Our methods discretize this problem—considered as an ODE in an infinite-dimensional space—in time with a high-order accurate, linearly-implicit, stiffly-stable ODE solver. This gives a sequence of linear variable-coefficient elliptic systems which are solved by a technique developed under support from this grant [3]. The technique of [3] is efficient, requiring only $O(N^d \log N)$ operations to obtain the numerical solution on a $N \times N \times \ldots \times N$ grid in d dimensions, and spectrally accurate in the sense that the error is $O(N^{-p})$ for every $p \geq 0$ if the solution is smooth. The basic idea is to transform the elliptic system into an equation involving only bounded operators, then discretize. The discrete problem has a condition number which is bounded as $N \to \infty$, hence can be efficiently solved by standard iterative methods such as GMRES.

• We have implemented a variable-step variable-order version of our method for parabolic systems and applied it to solve general crystal growth models of phase field type. Variable step sizes are vital to solving phase field models, because solutions vary on vastly different time scales during different regimes of the evolution. Typically initial fast transients give way to a front evolution problem, which is superseded at very long time spans by a slow geometric smoothing known as "ripening" in metallurgy. Similar phenomena occur in the increasingly significant phase field models of superconductivity.

Two major objectives of this work are parameter identification and model validation. Parameter identification addresses the question of how to set the various parameters in phase field models to correspond with a given physical experiment. In particular, does the interfacial thickness have to be the physical thickness of the interface between the solid and liquid phases? Model validation involves predicting experimentally verifiable differences between the various phase field models available for modelling the same physical experiment. This helps identify viable theories and eliminate duplication. Our numerical techniques have now reached the point where these two major objectives can be addressed.

A paper [4] based on this work has appeared in *J. Comput. Phys.* and a second paper [5] is in preparation. A summary of [4] follows.

Many physical problems are naturally formulated as systems of nonlinear parabolic partial differential equations. Phase field models for crystal growth and alloy solidification, Ginzburg-Landau models for superconductivity, reaction-diffusion systems for chemical processes and the Navier-Stokes equations of fluid mechanics are good examples. In some of these problems, periodic boundary conditions can be assumed for convenience.

Solving these problems numerically requires massive amounts of computer time and memory, making faster or more accurate methods extremely interesting. However, there are well-known dilemmas in constructing such methods. Explicit methods cost little per time step but require tiny time steps for stability. Implicit methods are less subject to stability restraints, but each step requires solution of a large system of equations. Low-order accurate methods are easy to program but require many degrees of freedom and many time steps. Highly accurate methods such as spectral methods can use fewer degrees of freedom and fewer time steps but require smooth solutions and are difficult to use efficiently.

This paper presents a numerical method for computing smooth solutions of the general second-order nonlinear parabolic system of partial differential equations

$$\partial_t u = \mathcal{F}(t, x, u, \partial u, \partial^2 u) \tag{1}$$

in the box $B = [0,1]^d$ in R^d, with periodic boundary conditions on the boundary ∂B. Here the solution $u : R \times B \to R^q$ is a smooth vector function of time t and space x, and

$$\mathcal{F} : R \times B \times R^q \times R^{dq} \times R^{d^2 q} \to R^q \tag{2}$$

is a smooth vector function of time, space, u and the collection of first and second partial derivatives $(\partial u, \partial^2 u)$. We assume $\mathcal{F}$ is periodic with period 1 in x and satisfies a linearized ellipticity condition. Since this does not guarantee well-posedness, we assume our system has a unique smooth solution on the time interval of interest.

Our method combines an extrapolated linearly implicit Euler time discretization with a fast spectrally-accurate method for solving linear variable-coefficient elliptic systems. This gives arbitrary order accuracy in time and spectral accuracy in space at optimal cost. We validate the method with

numerical results, including mean curvature systems and phase field models of solidification.

2-D vortex methods for incompressible flow

• We have studied vortex methods for incompressible 2-D flows both as the simplest examples of level-set-based moving boundary techniques and as solvers for the convection in the melt around a growing crystal. In 1992-4, we developed a new second-order accurate "triangulated" vortex method which solved the long-standing problem of long-time inaccuracy in traditional vortex methods [6]. A summary of [6] follows.

Vortex methods for inviscid incompressible two-dimensional fluid flow are usually based on blob approximations. This paper presents a vortex method in which the vorticity is approximated by a piecewise polynomial interpolant on a Delaunay triangulation of the vortices. An efficient reconstruction of the Delaunay triangulation at each step makes the method accurate for long times. The vertices of the triangulation move with the fluid velocity, which is reconstructed from the vorticity via a simplified fast multipole method for the Biot-Savart law with a continuous source distribution. The initial distribution of vortices is constructed from the initial vorticity field by an adaptive approximation method which produces good accuracy even for discontinuous initial data.

Numerical results show that the method is highly accurate over long time intervals. Experiments with single and multiple circular and elliptical rotating patches of both piecewise constant and smooth vorticity indicate that the method produces much smaller errors than blob methods with the same number of degrees of freedom, at little additional cost.

Generalizations to domains with boundaries, viscous flow and three space dimensions are discussed.

• In 1994-5, we carried this line of research further. First, we developed an important tool for constructing quadrature formulas for singular integral operators in several dimensions, as reported in [8]; a summary follows.

Many numerical problems require the evaluation of integrals

$$\int_B f(x)dx, \tag{3}$$

where B is a D-dimensional subset of R^d and f is an integrable function on B. Many methods have been devised for the numerical calculation of such

integrals, each useful for certain values of D and d and certain classes of B and f. In the case $d = D = 1$ an extensive literature exists, while in $d > 1$ dimensions much less work has been done.

This paper focuses on the evaluation of such integrals in the following common situation.

(a) B is a rectangle $[a, b] := [a_1, b_1] \times \ldots \times [a_d, b_d]$.

(b) We are given values $f(x_j)$ of f at N points x_j not of our choosing.

(c) We are given an integrable but singular function $\sigma : B \to R^s$, which is C^k away from a lower-dimensional subset S of B, and f has the form

$$f(x) = \varphi(x) \cdot \sigma(x) + \psi(x), \tag{4}$$

where $\varphi : B \to R^s$ and $\psi : B \to R$ are unknown C^k functions on B.

We construct two rules for numerical integration. First, we construct a rule W with weights W_j, $1 \leq j \leq N$, which integrates smooth functions accurately:

$$\sum_{j=1}^{N} W_j g(x_j) = \int_B g(x)dx + E_N, \tag{5}$$

where E_N decreases rapidly as $N \to \infty$ if g is smooth enough and the points x_j happen to be distributed appropriately. For example, $E_N = O(N^{-k/d})$ if g is C^k and the points are uniformly distributed on B, where k is the order of accuracy of the rule. The computation of W requires $O(N(k^{2d} + \log^2 N))$ time and $O(k^{2d} + N)$ space. Precise error bounds are proven and numerical examples are given.

Second, we construct a rule w with weights w_j which integrates singular functions accurately. The singular rule w has the "local correction" property that $w_j = W_j$ except for a small number of j's, those for which x_j is near the singular set. This property is important in the application of fast algorithms to the efficient evaluation of families of singular integrals. The computation of those w_j's differing from W_j requires $O(k^{3d})$ time. Error bounds are proved and numerical results are given .

These general rules are constructed with certain specific classes of applications in mind, including computational fluid dynamics, potential theory and crystal growth. These applications require the application of integral operators

$$u(x) = \int_B K(x, x')\omega(x')dx' \tag{6}$$

where K has known singular behavior on a lower-dimensional set but ω is (at least piecewise) smooth. Typically K is singular at a single point, we know $\omega(s_j)$ at N points s_j, and we would like to approximate M values $u(t_i)$ at points $t_i \in R^d$. We have no control over the location of the s_j and would like to avoid the artificial viscosity produced by interpolating, so we take the s_j's as given.

A classical approach to this problem is product integration. Here we approximate $u(t_i)$ by a rule of the form

$$u_i = \sum_{j=1}^{N} K_{ij}\omega(s_j) \tag{7}$$

with K_{ij} chosen to integrate some class of ω exactly for each i. This is a $M \times N$ matrix multiplication, so it costs $O(MN)$ work, which is very expensive when M and N are large. This has been a stumbling block in computational fluid dynamics, potential theory for the Laplace equation, and crystal growth. Product integration also tends to require difficult, expensive, and sometimes impossible algebraic manipulations and evaluation of integrals in closed form. A major objective of this paper is to eliminate the calculations required by product integration, and replace them with a single general-purpose method which produces locally corrected quadrature rules of arbitrary order for any given singularity.

More recently, fast summation methods have been developed for several kernels K. These methods evaluate the discrete sum

$$u_i = \sum_{j=1}^{N} K(t_i, s_j)W_j\omega(s_j) \qquad 1 \le i \le M \tag{8}$$

to accuracy ϵ, in $O((N+M)\log\epsilon)$ work. Such methods have been developed for vortex methods, potential theory and Gaussian kernels. However, these methods cannot be combined with product integration, where the weights depend on the point of evaluation t_i.

Another class of recently-developed fast methods is aimed more directly at the continuous problem. These methods are related to product integration in some cases, usually have a fixed and not too high order of accuracy, and tend to be slower than fast methods for discrete sums. Like product integration, they sometimes require difficult and expensive algebraic manipulations and evaluation of integrals which can be carried out only in special cases.

Singular quadrature rules of the type developed in this paper allow the application of fast algorithms for discrete sums to the continuous problem, because w_j are independent of the point of evaluation t_i except for a few points near the singularity. Thus fast methods can be applied to the sum with weights W_j, and then u_i can be corrected locally to get an accurate and inexpensive approximation of $u(t_i)$. This observation was apparently first made by Rokhlin, who developed one-dimensional singular endpoint-corrected trapezoidal rules. It has been applied to one-dimensional integral equations by Starr.

Our method requires knowledge of the singularity $\sigma(x)$ only in the weak sense that we need modified moments

$$\int_{B \cap C} P_\alpha(x)\sigma(x)dx \tag{9}$$

over rectangles C, with P_α a suitable family of multidimensional orthogonal polynomials. Obtaining these moments is itself a highly nontrivial task in this generality, with many possibilities depending on the singularity and on B. We have implemented, as part of our method, a general multidimensional adaptive Gaussian quadrature code, with a novel error estimator, which may be of some independent interest. It is sufficient for vortex methods and for volume potentials in potential theory, and hence for the solution of variable-coefficient elliptic partial differential equations as in [3]. Numerical results indicate that it is competitive with standard codes in dimensions $d = 2$ and $d = 3$.

The techniques presented in this paper generalize immediately to solve several other problems of considerable interest. We can approximate and differentiate functions known at arbitrary points, a technique which is useful in many computational problems. We can integrate singular functions over more general domains, such as curves and surfaces. Several such generalizations, along with several refinements of the basic method, are discussed in [8].

• The quadrature rules developed in [8] allowed us to produce new 2-D vortex methods of arbitrary order with excellent long-time accuracy properties, as reported in [7]; a summary follows.

Vortex methods are powerful and sophisticated numerical methods for computing incompressible turbulent flows Because they are grid-free and naturally adaptive, they create little or no numerical diffusion and preserve

features which other methods may distort. Vortex methods are particularly useful when computing free-surface, free-space and external flows, because only the support of the vorticity need be discretized.

A typical vortex method involves several steps; velocity evaluation, vortex motion, diffusion and boundary conditions. In this paper, we focus on the most expensive and difficult step, the velocity evaluation. We employ standard techniques for the vortex motion and consider inviscid free-space flow to eliminate diffusion and boundary conditions. General background material on vortex methods is presented in Section 2.

The standard velocity evaluation approximates the Biot-Savart law by a fixed quadrature rule, with weights conserved by incompressibility and independent of the singularity in the Biot-Savart kernel. Smoothing is required to make the quadrature rule accurate.

There are three major and interrelated difficulties with the standard approach. First, the use of fixed quadrature weights loses accuracy as the flow becomes disorganized. Perlman and Beale and Majda observed large oscillations in the error during long-time integrations. These oscillations are not present in triangulated vortex methods, regridded methods, or Beale's method, which generate new weights at each step. Second, smoothing is required because the quadrature weights ignore the singularity; this lowers the order of convergence. Third, if any product integration or similar techniques are used to treat the singularity, the variable weights preclude the use of the fast multipole method on which the practicality of the method depends.

This paper presents a different velocity evaluation method which overcomes these difficulties. A new quadrature rule at each step preserves long-time accuracy. Smoothing is unnecessary since the method integrates the Biot-Savart law with order-q accuracy for any fixed q. Only the nearby weights vary with the singularity, so the fast multipole method can still be applied.

Our method is described in Section 3. It is based on locally-corrected quadrature rules for multidimensional singular kernels as developed in [8] and proceeds in stages. First a data structure groups the N vortices into cells convenient for integration. Then a global order-q quadrature rule which ignores the singularity is built. The fast multipole method evaluates this rule efficiently (yielding a regridded vortex method if smoothing is used). Finally, we correct the weights of vortices near the evaluation point and the appropriate terms of the velocity, using the detailed calculations from

Appendix A.

Numerical results presented in Section 4 show that this method has several nice features. It runs in $O(N \log N)$ CPU time with N vortices and achieves essentially qth order accuracy for any specified q. It deals effectively with arbitrary initial distributions of vortices. Long-time accuracy is preserved. The method is naturally parallel since each point is corrected independently.

The method extends naturally to 3-D calculations, Navier-Stokes equations, and flows in bounded domains. It is equipped with a natural interpolation which gives the vorticity at any point.

• In 1995-6, we developed new methods based on the smooth quadrature rules developed under prior support from this grant [8]. A summary of the results presented in [9] follows.

We present a new approach to vortex methods for the 2D Euler equations. We obtain long-time high-order accuracy at almost optimal cost by using three tools: fast adaptive quadrature rules, a free-Lagrangian formulation, and a nonstandard error analysis. Our error analysis halves the differentiability required of the flow, suggests an efficient new balance of smoothing parameters, and combines naturally with fast summation schemes. Numerical experiments with our methods confirm our theoretical predictions and display excellent long-time accuracy.

Vortex methods solve the 2D incompressible Euler equations in the vorticity formulation by discretizing the Biot-Savart law with the aid of the flow map. They have been extensively studied, widely generalized and applied to complex high-Reynolds-number flows.

Vortex methods involve several components: velocity evaluation, vortex motion, diffusion, boundary conditions and regridding. In this paper, we improve the speed, accuracy and robustness of the velocity evaluation. We eliminate the flow map, improve the quadrature used for the Biot-Savart law, and analyze the error in a nonstandard way, requiring less differentiability of the flow and obtaining efficient new parameter balances. We employ standard techniques for the vortex motion and consider inviscid free-space flow to eliminate diffusion and boundary conditions. Our approach combines naturally with regridding and fast summation methods.

First, we review Lagrangian vortex methods. These move the nodes of a fixed quadrature rule with the computed fluid velocity, preserving the weights of the rule by incompressibility. This procedure loses accuracy when the flow

becomes disorganized, motivating many regridding techniques. Even before the flow becomes disorganized, however, obtaining high-order accuracy with a fixed quadrature rule requires smoothing of the singular Biot-Savart kernel. Smoothing gives high-order accuracy for short times but slows down fast velocity evaluation techniques and halves the order of accuracy relative to the differentiability of the flow. We review two free-Lagrangian vortex methods, the triangulated vortex method we developed in 1993-4 and our quadrature-based method of 1994-5. Triangulated vortex methods are robust, practical and efficient but limited to second-order accuracy. Quadrature-based methods compute adaptive quadratures tailored to the Biot-Savart kernel at each time step, yielding long-time high-order accuracy at asymptotically optimal cost.

The present paper develops a free-Lagrangian method which couples kernel smoothing with adaptive quadrature rules *not* tailored to the Biot-Savart kernel, producing long-time high-order accuracy. The asymptotic slowdown produced by kernel smoothing is almost eliminated by a careful choice of smoothing functions and parameters, based on a new error analysis of the velocity evaluation. This analysis requires about half as many derivatives of the solution as the standard approach.

The structure of our method is standard: At each time step, the smoothed velocity is evaluated once and the vortices are moved with an explicit multistep method. The velocity evaluation is nonstandard: First, a data structure groups the N vortices into cells convenient for integration. Then a global order-q quadrature rule is built. Finally, the fast multipole method is used with this rule to evaluate the smoothed velocity field.

The error is measured for standard test problems and our theoretical predictions are fully verified. Then more complex flows are computed.

4. Personnel Supported: This grant has supported one faculty member, the PI, for the summer months of each academic year. The associated AASERT grant has supported one graduate student per academic year, Ricardo Cortez, Hans Johansen and Brandoch Calef.

5. Publications:

[1] J. Strain. Fast adaptive methods for the free-space heat equation. *SIAM J. Sci. Comput.*, 15:185-206, 1994.

[2] D. W. McLaughlin and J. Strain. Computing the weak limit of KdV. *Comm. Pure Appl. Math.*, XLVII:1319-1364, 1994.

[3] J. Strain. Efficient spectrally-accurate solution of variable-coefficient

elliptic problems. *Proc. Amer. Math. Soc.*, 122:843-850, 1995.

[4] J. Strain. Spectral methods for nonlinear parabolic systems. *J. Comput. Phys.*, 122:1-12, 1995.

[5] J. Strain. Analysis of phase field models with spectral methods. *J. Comput. Phys.*, to be submitted June 1996.

[6] G. Russo and J. Strain. Fast triangulated vortex methods for the 2-D Euler equations. *J. Comput. Phys.*, 111:291-323, 1994.

[7] J. Strain. 2-D vortex methods and singular quadrature rules. *J. Comput. Phys.*, 124:131-145, 1996.

[8] J. Strain. Locally-corrected multidimensional quadrature rules for singular functions. *SIAM J. Sci. Comput.*, 16:1-26, 1995.

[9] J. Strain. Fast adaptive 2-D vortex methods. *J. Comput. Phys.*, submitted March 1996.

6. Interactions/Transitions:

a. Participation/presentations at meetings, conferences, seminars, etc:

Our work on triangulation, quadrature and vortex methods has been presented in lectures, colloquia and seminars at Arizona, Boulder, Brown, Davis, Grenoble, MIT, Stanford, Lawrence Berkeley Laboratory, NASA-Ames Research Center, the 1995 AMS-SIAM Summer Seminar on the Mathematics of Numerical Analysis, Park City, Utah, the 6th International Symposium in Computational Fluid Dynamics, Incline Village, Nevada, the 2nd International Workshop on Vortex Flows and Related Numerical Methods, Montréal, Canada, and the ASME Conference on Computational Fluid Dynamics, San Diego, California.

b. Consultative and advisory functions to other laboratories and agencies: The PI served on the NSF Applied Mathematics Panel for Materials Science during January 1996.

c. Transitions: The triangulated vortex method we developed has been adopted by Dr. John Grant's group at the Naval Undersea Weapons Center, Newport, RI. They have applied the method to calculate moderate-Reynolds-number flows around various bodies of DoD interest and are currently extending the method to three-dimensional flows.

7. New discoveries, inventions, or patent disclosures: None.

8. Honors/Awards: Received NSF Young Investigator Award, September 1992.