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Final Report: AFOSR Proposal 91-0165 on Numerical Modelling of Crystal Growth

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1 Summary

A code which solves the two-dimensional Euler equations for inviscid incompressible fluid flow was developed. It is based on a) adaptive triangulation of initial data, b) fast summation of the velocity field induced by a piecewise linear vorticity distribution, and c) Delaunay triangulation of the vortices at each step. The Euler equations were chosen as a model problem for crystal growth because they share the numerical structure of moving points without the added difficulties of finding curvature and normal; instead, the velocity field is simply found from the Biot-Savart law. The code was tested on multiple rotating patches of constant and smooth vorticity. It is second-order in space and fourth-order in time, even on piecewise constant solutions. The errors are much smaller than standard blob-based vortex methods with the same number of degrees of freedom.

2 Final Report

The research objective of this grant was to develop accurate and efficient adaptive numerical methods for solving the moving boundary problems which arise in crystal growth and unstable solidification. The methods under development use adaptive triangulation schemes to speed up level set methods and fast algorithms to speed up potential theory for the heat and Laplace equations.

The grant was terminated after one year, due to a change of institution by the PI. During that year, a model problem was solved, consisting of the Euler equation for two-dimensional inviscid incompressible fluid flow in free space. This problem, in vorticity formulation, has the same structure as crystal growth, but a simpler velocity functional. The common structure is that of a collection of points moving under a velocity function which is a functional of the points and of information associated with them. In crystal growth, the velocity function is found by computing the crystal-melt interface as the level set of a function known on the points (using Delaunay triangulation and linear interpolation, for example), solving an integral equation on the interface (which comes from heat potential theory and requires fast summation schemes for its efficient solution), and evaluating an integral formula for the velocity of each point. The Euler equations are much simpler, and require only interpolation of the vorticity values to a continuous vorticity field followed by evaluation of the Biot-Savart integral for each velocity.

An algorithm was developed and a Fortran code has been produced, in collaboration with Dr. Giovanni Russo of the University of L'Aquila, Italy. A paper (Title: Fast triangulated vortex methods for the 2-d Euler equations) is now in preparation, and will be submitted to SIAM J. Sci. Stat. Comput. shortly. The work was presented in seminars during spring 1992 at the Consiglio Nazionale delle Ricerche, Rome, Italy, at the Institute for Advanced Study, at the Mathematics Department, Carnegie-Mellon University, at the Mathematics Department, Duke University, at the Applied Mathematics Group, MIT, and as part of an invited address at the SEAS-SIAM Regional Meeting in Huntsville, Alabama.

The method developed represents a significant advance over classical blob vortex methods in several ways. The initial adaptive triangulation scheme allows complete freedom in the choice of initial data. In particular, the piecewise constant initial vorticity fields which have attracted so much in-

terest lately can be modelled with no additional effort. The code handles piecewise constant or smooth initial vorticity fields with equal facility. Furthermore, a very small number of degrees of freedom are required to represent the solution, because the method is adaptive.

The Delaunay triangulation at each step overcomes the mesh tangling which had hitherto afflicted such Lagrangian methods. The Delaunay triangulation is in many ways the nicest possible triangulation of given points, hence natural for this application. In the course of this work, a new method for constructing the Delaunay triangulation was invented and coded, and works extremely well. It is based on quadtree spatial data structures combined with circumcircle criteria.

Evaluating the velocity at each step from a piecewise linear vorticity field via the Biot-Savart law was the bottleneck in previous methods of this type; a direct calculation runs in quadratic time and prevents the use of more than a few hundred vortices, a number insufficient for practical applications. During this research, a fast summation code was developed which speeds up the velocity evaluation by several orders of magnitude. It is a modification of the fast multipole method which deals with continuous source distributions rather than point sources. Accordingly, numerical experiments with tens of thousands of vortices were carried out on an ordinary workstation.

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