NAMT
92-033

Workshop on Computational Methods in Materials Science
(Abstracts)

September 16-18 1992

Carnegie Mellon University

Research Report No. 92-NA-033

September 1992

COMPUTATION OF CRYSTAL GROWTH IN TWO AND THREE DIMENSIONS

Robert Almgren

Dendritic crystal growth is one of the most fascinating pattern-forming processes in Nature. Examples range from the compelling beauty and symmetry of snowflakes to the technological importance of microstructure formation in metal casting, which can wreck the mechanical properties of the resulting material. A simple system of equations captures what is thought to be the relevant physics, but reproducing realistic structures and understanding the role of various physical parameters remain major challenges. I will present methods and results of an on-going program to model numerically this class of phenomena. Two-dimensional results are fairly complete, and I will discuss the beginnings of efforts in three dimensions.

THEORETICAL AND PRACTICAL PROBLEMS RELATED TO THE DESIGN OF CONSTITUTIVE LAW FOR PLASTICITY

Ivo Babuska

The major part of computational analysis of the plasticity problem relates to the formulation of consitutive law. There are many different laws proposed in the literature. They propose a special mathematical form, including a set of constants, to be determined, for example by experimentation.

The talk will elaborate on the constitutive law of aluminum alloy 5454 in the H32 condition. Results of experimental data will be presented together with the mathematical problems related to these experiments.

MACROSCOPIC MODELS OF SUPERCONDUCTIVITY

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We shall discuss some aspects of macroscopic models of superconductivity. Our approach is strongly influenced by analogies with the Stefan problem for melting/solidification of a pure material, at least for Type I superconductors, for which a model incorporating a sharp normal-superconducting interface is appropriate. We discuss the regularization of these problems by a Ginzburg-Landau approach, and we show how this suggests that Type II materials will not have sharp interfaces, but rather vortex arrays.

COMPUTATIONS OF TWINNING

Charles Collins
University of Michigan

Twinning is a fascinating phenomena in micromechanics. It is the result of a structural phase transition, where the phase change is marked by a change in the local symmetry of the material. In twinning, the material forms narrow bands in its interior, where in each band the material has a uniform orientation, but in adjacent bands it takes on different but symmetry-related orientations.

In this talk, I will start with a mathematical description of twinning and discuss the results of previous computational work. Then I will discuss a new approach based on the multigrid method.

NONLINEAR DIELECTRICS

Joseph P. Dougherty

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There are several types of nonlinearities common to high dielectric constant materials. The most well known is the P-E hysterisis loop that characterizes ferroelectric materials. Less studied, but technologically very important, is the reduction in dielectric constant that occurs when a ferroelectric capacitor is under dc bias. A third, and more interesting, dielectric nonlinearity is produced by electric field induced phase transitions. These phase transitions are usually induced between antiferroelectric to ferroelectric phases and are thought to be responsible for the high electro-mechanical efficiency in many compositions in the lanthanum doped lead zirconate titanate piezoelectric ceramics. Some practical devices utilizing the dielectric nonlinearities have been developed for fluorescent lighting circuits. The most difficult task on the project was the mathematical modeling of "simple" circuits containing nonlinear devices.

NUMERICAL MICROMAGNETICS

Donald R. Fredkin

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Micromagnetics is a continuum theory of magnetic materials. After reviewing the mathematical formulation of the theory, two numerical methods for solving realistic three dimentional problems in micromagnetics, both based on the finite element method, will be discussed. Some recent triumphs will be described and some major problems posed.

NUMERICAL SIMULATION OF NEMATIC LIQUID CRYSTAL FLOWS

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Numerical simulation of nematic liquid crystal flows have been the focus of many research projects during these last five years. This interest was motivated by the possibility of designing new materials possessingadvantageous processing and mechanical properties and also by the well-established continuum description in the Leslie-Ericksen (LE) theory.This theory describes the average orientation of molecules by a macroscopic unit vector called the director.

So far, most of the computations reported on complex geometries, use the special case of the Transversely Isotropic Fluids model. But this approach cannot accomodate many phenomena characteristic of liquid crystals such as wall-induced orientation, various boundary layers, and tumbling solutions. A finite-element method for computing liquid crystal flows using the full set of equations of LE theory, will be presented. The proposed algorithm decouples the computation of the velocity and the pressure from the director and reduces the calculations to two smaller elliptic problems. The non-convex constraint on the director (unit vector) is treated by a penalty approach combined with the fractional step method. Special features of the method are that it can be used to compute non-stationary solutions and also it allows the director field to be three-dimensional.

The above algorithm has been applied to complex flows for both aligning and non-aligning nematic liquid crystals, subjected or not to an out of plane perturbations of the director Numerical results will be presented in various geometries exhibiting competition between shear and elongational rates. Comparisons with previous works will be adressed.

MODELS AND COMPUTATIONAL METHODS FOR TYPE-II SUPERCONDUCTIVITY

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Type-II superconductivity is characterized by the appearance of closely-spaced, vortex-like structures; these pose considerable difficulties when one attempts to effect a numerical simulation. We first consider Ginzburg-Landau type models for type-II superconductivity. In addition to the well-known homogenous, isotropic model of Ginzburg and Landau, we consider variants that account for inhomogenieties, anisotropies, variations in thickness, and periodic media. We then describe a computational algorithm based on a finite element discretization and present the results of some numerical simulations. We discuss the possible application of our techniques to studies of flux pinning and vortex motion phenomena,

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TITLE: NUMERICAL COMPUTATIONS OF THE DYNAMICS OF MARTENSITIC MICROSTRUCTURE

Mitchell Luskin
University of Minnesota

Coauthor: Petr Kloucek
University of Minnesota

We present numerical computations for the dynamics of the development of twinned microstructure and the propagation of the austenitic-martensitic interface.
Our computations approximated a three-dimensional model for the dynamics of the indium-thallium alloy which used a stress tensor computed from the Ericksen-James energy density and which included viscous dissipation.

Our first set of computations were initialized by the macroscopic deformation for the mixture of two variants. We obtained the dynamical development of fine-scale twinning when the deformation was prescribed on the crystal boundary (hard loading). However, when stress-free boundary conditions (soft loading) are prescribed we obtained the development of a time-periodic solution oscillating between two of the variants.

Our second set of computations were initialized by the deformation for the macroscopic deformation for the austenitic-martensitic interface. At a temperature below the transformation temperature, austenite was transformed into martensite near the interface and the interface moved into the austenitic region. At a temperature above the transformation temperature, martensite was transformed into austenite near the interface and the interface moved into the martensitic region.

EFFICIENT ALGORITHMS FOR MICROMAGNETICS

Ling Ma

Carnegie Mellon University
Department of Mathematics

The solution to nonconvex variational problems is often characterized by microstructure. The variational problem for the magnetization field in micromagnetics has a nonconvex pointwise constraint and a differential constraint of Maxwell's equation in the whole space. Energy minimizing sequences of magnetization fields can have oscillations whose scale converges to zero but whose amplitude remains finite. We will discuss the finite element approximation of the magnetization field for this variational problem, and present some analysis results. We will also discuss the computational issues induced by the nonconvexity and Maxwell's equation. Numerical strategies will be proposed and preliminary results will be presented. We will also present some recent experiments with a model for magnetostrictive materials.

HOW SHOULD WE COMPUTE MICROSTRUCTURES AND COMPOSITES?

Luc Tartar

Carnegie-Mellon University
Department of Mathematics
Center for Nonlinear Analysis

The talk will describe a few features which are understood at a theoretical level concerning oscillations in order to be able to answer the following important question: In a problem where we know that there are oscillations on a small scale, if a computation does show oscillations, are we sure that these computed oscillations have anything to do with the initial problem?

COMPUTATION OF MICROSTRUCTURE

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We discuss the numerical approximation of non--convex variational problems. These problems concern the behavior of shape memory alloys and other materials with a high degree of crystalline order which develop complicated and poorly understood microstructures in response to loading and thermal gradients.

In order to avoid representing highly oscillatory functions (i.e. the fine scale microstructure) on a mesh, an algorithm is proposed which computes a Young measure characterizing such oscillations. In a finite element context, this results in additional computations associated with the Young measure on each element. These computations are local to each element, so the associated subproblem of constructing a Young measure for each element can done in parallel. (For example, on a single instruction -- multiple

data architecture.) These ideas can be extended to approximate associated evolution equations.

CONTRIBUTED SESSIONS

DYNAMICS OF PARTICLES IN TYPE III SUPERCOMPUTERS

Weinan E

NUMERICAL MINIMIZATION OF THE LANDAU-DE GENNES FREE ENERGY FOR LIQUID CRYSTAL

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We are developing a numerical package to compute equilibrium configurations of the order-parameter tensor field for nematic liquid crystals confined to finite cylinders by minimizing the Landau-deGennes free-energy functional subject to combinations of strong and weak surface anchoring and to external electric and magnetic fields.

The problem is discretized by a finite-element method using piecewise-linear approximating functions on tetrahedral elements. The resulting discrete free-energy functional is minimized using large-sparse optimization techniques. The program will allow for continuation in the parameters, path following, identification of bifurcation points and phase transitions, and branch switching. The large-scale simulations are performed on the Cray Y-MP8/864 at the Ohio Supercomputer Center (OSC), and the equilibrium director fields are visualized using three-dimensional graphics generated by the apE graphics package developed at the OSC.

A NONLINEAR EIGENVALUE EQUATION FOR MODULATED STRUCTURES

Robert B. Griffiths
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Carnegie-Mellon University

There are a number of crystalline materials which exhibit a one-dimensional modulation whose period can depend on the temperature. The Frenkel-Kontorova model, a collection of particles in a periodic potential in one dimension, with springs connecting neighboring particles, provides a simplified description of this state of affairs. Looking for the ground state of this model leads rather naturally to an eigenvalue problem:

$$V(u) + \min[W(u - u') + R(u')] = \lambda + R(u)$$

where V is a given periodic function of u, W is the potential of the spring, and the unknown eigenfunction and eigenvalue are R, with the same period as V, and λ, respectively.

The best numerical method presently available for solving the eigenvalue problem consists in replacing the unit interval of u with a grid of N equally spaced points, and solving the discretized problem numerically using a procedure whose running time is roughly proportional to N^2. One should be able to do better than a simple discretization, but we have not succeeded: a basic difficulty is that even when V and W are smooth functions, R, while continuous, can be quite unsmooth.

HOMOGENIZATION OF REACTIVE TRANSPORT THROUGH POROUS MEDIA

Ulrich Hornung

There are several models describing diffusion, convection, adsorption, and reaction of chemical species through porous media. Depending upon the major aspect of application - such as soil chemistry, heterogeneous catalysis, or chromatography - different assumptions are made on the dynamics and kinetics on the pore scale. It is shown that

various models can be put into a common framework and can be homogenized for deriving the models on the macro-scale. The notion of {\em two-scale convergence} will be explained and its usefulness for the convergence proofs will be demonstrated. Examples of numerical simulations will also be given.

HOMOGENIZATION PROBLEM FOR BLOCKY MEDIA WITH PERIODICAL MICROSTRUCTURE

B.A. Shoykhet

The homogenization problem is considered for layered and blocky media with periodical structure. The interaction of blocks is modeled by conditions of unilateral contact with friction. The macroproperties are derived from solution of the special contact problem for cell of microstructure.

The method was worked out to determine the boundaries of statistically admissible macrostresses under macrohomogenous loading. As an example, curves of theoretical strength of large specimens were constructed for block packing of brickwork type and for regular hexagon-shaped cells.

Problems of homogenization of an elastic layered medium and some blocky media that are without binding of blocks were solved in closed form.

The case of rigid blocks with elastic layers at the contacts was considered. The homogenization problem is reduced to a finite-dimensional non-linear system of equations and inequalities. General methods were developed to investigate similar systems, and applied to the brickwork type of packing.

The obtained averaged equations reveal some properties of anisotropic plasticity with hardening and non-associate law of plastic flow.

NOVEL APPROACHES TO LANDAU-GINZBURG MODELING OF SOLIDIFICATION

Eduardo A. Socolovsky

Center for Nonlinear Analysis
Hampton University

We present a Landau-Ginzburg approach to solidification of a material from its melt and some of the phenomena reproduced. These include: traveling waves, Mullings-Sekerka type instabilities giving rise to needle crystal growth and tip-splitting, motion by mean curvature, and anisotropic capillary length or mobility giving rise to needle or faceted crystal growth. We also show that simulating real materials requires long-time high performance computations, which coupled with the fact that the equations have inertial sets leads to Nonlinear-Galerkin Methods with wavelet hierarchical bases.

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