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6. AUTHOR(S)
Roy A. Nicolaides

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Carnegie Mellon University
Dept. of Mathematical Sciences
Pittsburgh, PA 15213

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Computational algorithms for electromagnetic scattering and structured phase transitions are investigated. For scattering, three contributions are presented: (i) Analysis of spurious offset fields, (ii) the use of divergence boundary conditions, (iii) analysis of covolume (unstructured FDTD) algorithms with estimates of convergence rates. For structural phase transitions adaptive mesh techniques are combined with finite dimensional optimization algorithms to compute new global minimizers for martensitic phase transformations.

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Final Technical Report
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Roy Nicolaides
Department of Mathematical Sciences
Carnegie Mellon University
Pittsburgh
PA15213

1 Computational Methods for Structural Phase Transitions

For microstructure computations based on the Ericksen-James model, the main focus has been on the application of adaptive mesh methods. Adaptive computation is necessitated by the extremely fine meshes that seem to be required for accurate solutions to microstructure problems. These fine meshes are needed to prevent certain unphysical solutions to the discretized models from appearing. Above a critical meshsize, minimizers of the discretized energy are not related to any physical minimizer of the continuous energy functional. The critical meshsize is relatively fine and this fact severely limits the number of interesting computations that can be carried out. In the adaptive approach, very high degrees of local refinement are performed but only in regions of the crystal in which large energy contributions are present. Typically, these are in boundary layers. In the boundary layers, very fine meshes can appear whereas in the main part of the domain the meshes remain relatively coarse. We have had very satisfactory results with this approach, compared with the fixed grid approach. A very complex layer structure has been successfully computed; to compute this solution with a fixed mesh would be all but impossible.

The adaptive mesh structure is derived from a quadtree approach. In previous work we showed how erroneous 'solutions' could arise from the use of rectangular meshes coupled with numerical integration. For this reason, a further adaptation of the quadtree mesh is used. It consists of an aditional refinement of the quadtree mesh into triangles. Each square element of the mesh is split into two triangles using a positive slope diagonal. In each triangle a linear approximation is assumed as in the usual piecewise linear finite element method. The advantage of this is that since the derivatives of the linear displacement fields are all constant, the bulk energy function is computed without the use of approximate integration. Optimization of the discrete system is peformed using a step by step relaxation type algorithm in which variables are subjected to a fixed perturbation until no further reduction in the bulk energy function is obtained. Then the size of the fixed perturbation is reduced and the energy reduction phase is repeated. Once the size of the perturbation is sufficiently small the iteration is terminated and the (near) minimizer is accepted. This procedure was found to work well and it was used in all the optimization computations.

The work reported above is described in detail in the following thesis:
"*Numerical Solution of a Nonconvex Optimization Problem Modeling Martensitic Microstructure*" by Han Wang, Department of Mathematical Sciences, Carnegie Mellon University. (Available from University Microfilms, Ann Arbor, Michigan)

In addition, the following paper (supported in part under AFOSR F49620-92-J-0133) has appeared:
R. A. Nicolaides, N. Walkington & H. Wang *Numerical Methods for a Nonconvex Optimization Problem Modeling Martensitic Microstructure* Siam Journal of Scientific Computing, 18, 4, p1122–1141 (1997)

As part of the mesh generation aspects of our work a new algorithm for the generation of Voronoi–Delaunay meshes was developed. This work is
R. A. Nicolaides & H. Wang *Intersecting Half Planes to Generate Voronoi–Delaunay Mesh Pairs in Three Dimensions* (will be submitted to the Journal of Algorithms)

2 Computational Methods for Electromagnetic Scattering

The research on electromagnetic scattering has several distinct aspects. In the first place we have worked on avoiding erroneous solutions when time harmonic solutions of Maxwell's are computed by marching the time dependent equations to a periodic state. Second, we have investigated the use of divergence boundary conditions as a replacement for interior divergence constraints. Last, the covolume method for discretizing Maxwell's equations was investigated and its convergence characteristics were obtained by rigorous mathematical techniques.

2.1 Time marching to a periodic state

An efficient and popular approach to computing time harmonic solutions of Maxwell's equations consists of time marching the discretized equations to a steady state. Typically, the FDTD method is used for the discretization. When using this approach it is frequently observed that while the computed solutions are periodic they may not be time harmonic. The usual approach to this difficulty is purely empirical, and consists of an ad hoc postprocessing operation to subtract off the so-called "spurious offset" field(s) to leave a time harmonic field. Prior to our work, there was no precise mathematical explanation of the appearance of the spurious fields. In our work we obtained a set of partial differential equations which are satisfied by the spurious fields. An analysis of these equations reveals the properties of the spurious fields. Based on the results of this analysis, we have shown how to perform the time marching so that no spurious field ever appears in the solution (thereby avoiding the need for postprocessing). The resulting solutions are just the ones that were desired in the first place. Associated with the computational aspects of this topic are a number of mathematical issues. We have provided a detailed and rigorous mathematical analysis of the issues which arise. In particular we have proved that by following our algorithms it can be guaranteed that no spurious offset fields will arise. In addition, we have proved that the time domain approach to computing the periodic solution (with radiation conditions applied a finite distance from the scatterer) does indeed provide a solution which asymptotically approaches the periodic solution. This work is mathematically rigorous.

Our work on spurious fields is published in the following two papers:
U. Kangro & R. A. Nicolaides: *Spurious Fields in Time Domain Computations of Scattering Problems* IEEE Transactions on Antennas and Propagation 45, 2, p228–234 (1997)
U. Kangro & R. A. Nicolaides: *Asymptotic Behavior of Solutions of Two Dimensional Periodic Scattering Problems* SIAM Journal of Mathematical Analysis 28, 6, (1997) (to appear)

For the three dimensional case see the doctoral thesis: "*Spurious Fields in Computational Electromagnetics*" by U. Kangro, Department of Mathematical Sciences, Carnegie Mellon University. (Available from University Microfilms, Ann Arbor, Michigan)

2.2 Divergence boundary conditions

A well known problem in computational electromagnetics is the appearance of "spurious modes" resulting from the incorrect imposition of divergence constraints. To avoid imposing these constraints directly it has been suggested to enforce them only on the boundary of the domain. The main advantage of this approach is to permit the use of standard finite elements to solve the vector Helmholtz form of Maxwell's equations. This is vastly more efficient than the use of edge elements, which is the current practice. Mathematically, in order to use the divergence boundary condition it is necessary to prove that it leads to the same solution as the interior application of the divergence equation called for by Maxwell's equations. This part of our work investigates whether and when the solutions computed by the two formulations are the same.

We have shown that the formulations are *not* always equivalent–in fact they are not equivalent in some of the most important situations in which they would be useful. We proved that for interior problems the following simple criterion can be used to decide the equivalence: equivalence holds if and only if the scalar Poisson equation with any smooth right hand side and Dirichlet boundary conditions has a solution in H^2. When this is not true a simple minded application of divergence boundary conditions will normally give incorrect solutions having a *nonzero* divergence. This simple criterion shows that the underlying issue is really one of regularity of the domain. In particular, for domains with reentrant edges the divergence boundary condition cannot be safely used without additional precautions. The necessary precautions would require building singular functions into the finite element basis. Unfortunately, what these functions should be is not known in general.

The work on divergence boundary conditions is presented in:
U. Kangro and R. A. Nicolaides: *Divergence Boundary Conditions for the Vector Helmholtz Equation with a Divergence Constraint* (to appear in Mathematical Modeling and Numerical Analysis)

2.3 Covolume methods for computational electromagnetics

Discretization of electromagnetic scattering problems is an area of extensive current activity. Our approach has been to use an unstructured version of the well known Yee scheme. The unstructured approach is applied on Voronoi-Delaunay type meshes; it is the electromagnetics version of the covolume approach that we introduced in fluid mechanics. In addition to setting up the covolume approach for use with scattering problems we have performed theoretical and practical work using it. On the theory side we have proved the convergence of the method and obtained the rate of convergence. As a side product, our results apply to the classical Yee scheme and provide the best results so far obtained for that algorithm. Our results show that the covolume approach is first order accurate on arbitrary meshes and second order accurate on smoothly varying (for instance, uniform) meshes. We have also worked on higher order versions of the covolume algorithm, mainly although not exclusively for statics problems. A fourth order algorithm has been derived and its convergence has been proved.

The following publications have been prepared on this area:
R. A. Nicolaides & D. Q. Wang: *Convergence Analysis of a Covolume Scheme for Maxwell's Equations in Three Dimensions* (to appear in Mathematics of Computation July 1998).
R. A. Nicolaides & D. Q. Wang: *A higher order covolume method for planar div–curl equations* (Submitted to Journal of Numerical Analysis (IMA))

Additional results may be found in the doctoral thesis: "*Applications of the Covolume Method in Computational Electromagnetics*" by D. Q. Wang, Department of Mathematical Sciences, Carnegie Mellon University. (Available from University Microfilms, Ann Arbor, Michigan)