Final Progress Report
1 January 95 - 30 June 98

[OBJECTIVES]

The problems and techniques addressed under the present contract deal with issues of mathematical modeling, analysis and computation that arise in the study of electromagnetic (EM) wave propagation and of the effects of internal surfaces in a variety of materials. The objectives proposed in the area of EM scattering relate to challenging applications of a new method -- the "Method of Variation of Boundaries", or MVB-- introduced by the principal investigator (in collaboration with O. P. Bruno) for the numerical solution of scattering problems. They include:

* the extension of the numerical algorithms based on analytic continuation from exactly solvable shapes to the case of EM scattering from two- and three-dimensional BOUNDED OBSTACLES;

* the search for alternative formulations of MVB that DO NOT rely on the EXACT solvability of the scattering corresponding to simple geometrical arrangements; and

* the development of an approach based on MVB for the solution of INVERSE scattering problems.

The plan proposed in connection with the study of the behavior of internal surfaces relates to polycrystalline and composite materials. It is concerned with the development and study of mathematical models that, though simplified,
This report describes accomplishments in the areas of electromagnetic scattering and smart materials achieved under Grant Nr. F49620-95-1-0113. With regards to problems of wave propagation, advances in the development of high-order perturbation methods are reported. These include the derivation and coding of algorithms for the numerical solution of the scalar and vector forward scattering problems for two- and three-dimensional configurations and the formulation of corresponding approaches to inverse scattering calculations and to the estimation of normal and quasi-normal cavity modes. Concurrent achievements in the study of smart materials are also recounted here. They include the development of nonlinear homogenization theories intended to capture overall elastic behaviors (e.g. of shape-memory alloys, SMA), or magnetic and rheological responses (such as those of magnetorheological fluids, MRF). The latter project was undertaken in collaboration with scientists at the Lord Corporation, the worldwide leader in MRF technology, and was geared towards the incorporation of advanced mathematical modeling and simulations into the design of MRF.
still remain useful for understanding the universal features of interfacial effects and, therefore, some of the overall characteristics of a given sample. The particular instances of such models to be investigated include:

* geometric and free-boundary models for the evolution of GRAIN BOUNDARIES;

* free-boundary models for the dynamics of solid-solid phase boundaries in SHAPE MEMORY (SM) ALLOYS; and,

* NONLINEAR HOMOGENIZATION theories within various contexts, such as (a) for SM alloys, like NiTi polycrystals: to calculate effective elastic responses; and (b) for particulate composites, e.g. electrorheological (ER) or magnetorheological (MR) fluids for applications involving active dampers: to predict effective magnetic and rheological signatures.

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STATUS OF EFFORT

Advances in the development of MVB include: 1) the extension of our algorithms to a rather general class of two-dimensional bounded obstacles; 2) the generalization of the theory to three-dimensional structures for both acoustic and EM wave propagation; 3) the proposition of an MVB based on integral-equation formulations rather than on the exact solvability of simple geometries; 4) the development of corresponding methods for the solution of eigenvalue-type problems; and, the implementation of algorithms for the numerical solution of 5) three-dimensional forward scattering problems (for the propagation of acoustic waves) and 6) two-dimensional inverse problems (for the reconstruction of rough periodic interfaces). A preliminary version of a code for normal mode calculations has also been accomplished; its comprehensive testing and its extension to the problem of identification of quasi-normal modes will be the focus of our near term efforts. In its two- and three-dimensional implementations, we have found that MVB may provide us, in many cases, with solutions to direct problems with an accuracy unparalleled by that given by other methods. These cases, we expect, will substantially broaden once we incorporate, in the next phase of our project, our newly devised integral-equation formulations. As for the inverse problem, our results on the minimization of the associated nonlinear least-squares cost functionals have shown that the analytic continuation ideas that are inherent to MVB may be used to design effective search strategies to overcome their non-convexity. Our program in this direction is to build around these ideas to attain a more comprehensive "globalization" of the minimization procedure.

Our investigations of material interfaces, on the other hand, have focused on the development of mathematical formulations of grain boundary dynamics that are amenable to effective numerical simulations and on the advancement of nonlinear homogenization theories to capture overall elastic behavior (as in shape-memory alloys), or magnetic and rheological responses (as in magnetorheological fluids). Our work on grain boundary motion motivated the conception of a level-set approach to the simulation of interfacial evolution capable of handling multi-phase junctions and the complex topological rearrangements they undergo in simple metallic alloys. For SM polycrystals, however, the calculation of their elastic properties already poses a challenging problem, due to the nature of the underlying strain-induced phase transformations. In this regard we have developed a general method for the evaluation of the effective elastic energy of SM polycrystalline specimens. This method will, in the future, be exported to the realm of particulate suspensions, where it shall be incorporated in the calculation of the overall magnetic properties of MR fluids. On the other hand, we have recently shown that these properties can be estimated by adapting some rather classical ideas of nonlinear homogenization provided the particles can be treated as magnetic continua e.g. if they support a great number of magnetic domains. For this case, we have
devised a numerical algorithm whose predictions show very good agreement with experimental data collected at Lord Corporation (Cary, NC), our industrial partner in the MR composites venture. Also, over the last year, our project in this area has advanced towards the goal of providing Lord with the first realistic simulations of the dynamic agglomeration of particles within their patented fluids upon application of an external magnetic field. Our approach combines particle dynamics simulations with fast field calculations (fast multipole methods).

ACCOMPLISHMENTS/NEW FINDINGS

The focus of our research in computational electromagnetics has been on the extension of our MVB algorithms to bounded obstacle configurations [3, 7, 11], on the development of corresponding methods for the solution of inverse scattering problems [1] and, more recently, for the determination of the resonant modes of cavities. We have also made advances towards a reformulation of MVB in terms of appropriate integral equations which, as we said, we expect to broaden the applicability of our methods.

In [3, 7, 11] we demonstrated, through a number of numerical examples, that MVB can produce highly accurate solutions to problems of acoustic wave propagation (Helmholtz equations) for a wide variety of two- and three-dimensional geometries. Moreover, we showed that the very nature of our method allows for the reduction of the FULL three-dimensional Maxwell problem of EM scattering to that of a sequence of iterated pairs of Helmholtz equations. Indeed, our new analytic approach breaks down the problem of computing the reflected and transmitted fields for an arbitrary obstacle into a series of field calculations for a SPHERE which, in turn, permits us to effectively utilize the corresponding Debye potentials.

Our most recent accomplishments in this area, on the other hand, relate to another problem of great interest in electromagnetics, namely that of predicting the normal and quasi-normal modes associated to arbitrarily shaped resonators. For our boundary variation methods these problems are significantly removed from the scattering problems we considered previously. Indeed, the non-uniqueness of solutions to the corresponding differential equations could cast some doubt on whether they can be continued analytically. Establishing that the eigenmodes can be chosen to depend analytically in BOTH spatial and perturbation variables simultaneously is the subject of our current work. Under the assumption that this is the case, we have developed and implemented a numerical algorithm to compute normal modes for LARGE (two-dimensional) perturbations of a circular (cylindrical) cavity. In contrast with the aforementioned scattering configurations, serious difficulties had to be overcome to derive suitable recursive relations for the successive terms in the perturbation series. These difficulties arose as a result of the possible existence of multiple eigenvalues for the unperturbed configuration which continue analytically as separated, distinct eigenvalues. Our newly developed formulas allow us to detect and appropriately handle such "splittings" and, when implemented numerically, they can deliver accurate estimates of eigenfrequencies and eigenfunctions for rather dramatic perturbations of circular resonators. Our plan for the near term is to focus on the completion of our theory, on a comprehensive testing of our working code and on the extension of these ideas to quasi-normal mode calculations.

The results in [3, 11] clearly establish that, much as in the two-dimensional case [7], MVB has the potential to provide us, in many cases, with highly ACCURATE BENCHMARK SOLUTIONS. Indeed, our examples show that, for scatterers whose boundaries are not highly oscillatory (i.e. where no large contributions arise from high order Fourier modes in its parameterization) MVB produces solutions of exceptional quality. Such solutions are obviously desirable even for simple configurations that may not lend themselves to exact calculations (as is
the case, for instance, with the EM scattering problem from a perfectly conducting spheroid, whose exact solution involves the inversion of infinite matrices, see [3]). For more complex three-dimensional configurations, on the other hand, the current limitations of MVB are mostly tied to our insistence on the EXACT solvability of the unperturbed geometry. Indeed, the instabilities in the calculation of the Taylor coefficients, which become discernible at very large values of the perturbation parameter, can be enhanced if more than a few Fourier modes are needed to accurately represent the target obstacle. We expect, however, that this will be largely remedied by considering an INTEGRAL-EQUATION FORMULATION of MVB. In this formulation densities are sought in the form of a Taylor series and the resulting succession of problems on the basic scatterer are solved NUMERICALLY. As it turns out, this opens the door to a number of effective applications of MVB. Our most immediate investigations in this area will concentrate on the development of such an approach for the calculation of EM signatures of damaged projectiles, where the axisymmetric nature of the undamaged object can be exploited through our analytic continuation methods.

In addition to our advances in the solution of the forward scattering problem, our efforts towards the development of an inverse solver based on the MVB ideas of high-order perturbation have met with initial success, as we have been able to produce the first set of numerical results [1]. Indeed, and for the sake of simplicity, we have initially tested our schemes on the problem of reconstruction of rough (periodic) interfaces. For the numerical implementation, we considered a nonlinear least-squares cost functional J on the set of scattering amplitudes corresponding to non-evanescent modes, supplemented with a Tikhonov regularization term. We showed that analytic continuation may be used to GLOBALLY evaluate such cost functionals along ANY line in the space of admissible profiles. In fact, our algorithms calculate the field scattered by "points" along such lines through an appropriate analytic extension of the fields corresponding to dilations (in function space) of the WHOLE LINE. As in the case of the original MVB, these dilations then allow us to resort to the RAYLEIGH HYPOTHESIS to recursively calculate the Taylor series of the diffracted amplitudes. Our results on the analytic dependence of the fields on the dilation and line parameters then guarantee the possibility of continuation via Pade approximation.

Upon writing the recursive formulas and Pade approximation operator in the form of matrix equations of constraints, we coded a conjugate gradient algorithm for the (constrained) minimization of J. For the line search we compared the performance of our "global" model with that of local linear and quadratic ones. Also, the gradient computations were performed EXACTLY by taking advantage of the explicit dependence of the continuation formulas upon the interface profiles and combining them with the use of the "adjoint equations". A number of conclusions can be drawn from these experimental results [1], namely:
(a) In general, the cost functional J will present several local minima (depending, of course, on the wavelength and angle of radiation). Therefore, if no additional information about the profile is available, ANY local minimization algorithm may fail to yield its reconstruction in a single run.
(b) The local minima may persist as additional information on the scattering at different frequencies is added to the cost functional. In fact, our examples show that the non-convexity may persist even after the incorporation of efficiency data corresponding to a number of wavelengths that is (theoretically) sufficient to completely determine the structure from far-field measurements.
(c) Due to (a) and (b), algorithms that claim success in inversion through local minimization (e.g. gradient methods) must contain safeguards (explicit or implicit) against local versus global convergence. Indeed, the most common remedy to this problem consists of simply running the optimization code for a number of initial guesses in the parameter space that describes the family of admissible profiles.
(d) The use of analytic continuation through Pade approximation for the "line search" in the directional minimization steps may reveal the existence of non-
convex regions thereby partially "globalizing" the search and, therefore, accelerating its convergence.

(e) The demonstrated ability of rational approximations to capture the global behavior of a cost functional along any line may provide us with the starting point for the development of a truly global minimization procedure. It is also worth noting here that the integral-equation formulation described above should prove particularly relevant to the development of effective algorithms for optimal design based on MVB, as it could greatly enlarge their domain of applicability.

Regarding our research on material interfaces, we have concentrated our effort on the study of the dynamical behavior of grain boundaries in metals. Our current work in this area has grown out of our earlier accomplishment, under the present contract, of a mathematical formulation of the idealized motion of these interfaces [8] and it relates to a newly proposed level-set method for their numerical simulation (H. K. Zhao, T. Chan, B. Merriman and S. Osher, J. Comput. Phys. 127, 1996, 179-195). Although based on our own variational formulation of the problem, this algorithm departs from our approach as it introduces TWO level-set functions for the description of a single grain in order to deal with the tri-junctions. The numerical results that have been reported do seem to present the general characteristics of the evolution of ideal grain boundaries (curvature-driven, constant angles at triple points, etc) but whether they represent solutions to the actual equations of motion remains to be investigated. Indeed, our own theoretical considerations and preliminary numerical results suggest that the algorithm should indeed be modified to correctly account for the physical model, even away from triple junctions. We believe, for instance, that the numerical value of the surface energies as enforced by the algorithm are only HALF of their true value.

As for our efforts in composite materials, we initially concentrated on the study of the overall elastic energy in SM polycrystals [2, 6, 10]. These are polycrystalline materials whose constituent crystallites can undergo shape deforming phase transitions as a response to stress, strain or temperature changes; they constitute the most common form in which SM alloys are found. Under a given overall solicitation, say prescribed boundary deformations, the crystallites in the structure collectively follow certain patterns of transformation. This collective behavior determines the useful and unusual properties of polycrystalline SM alloys: pseudelasticity (large recoverable deformations) and shape-memory effect (recovery of shape upon heating). In the ideal non-dissipative context considered in [2, 6], the patterns of transformation induced by an overall deformation are such that the total elastic energy in the material is minimized. Thus the goal of our work: numerical calculation and estimation by means of rigorous bounds of such minimum values. As we describe there, bounds are useful as they provide rigorous benchmarks for numerical simulations and approximations. Such comparisons allowed us, for instance, to demonstrate the accuracy of a set of numerical calculations of effective energy values for some geometrically simplified grain arrangements. These values were obtained with the aid of a new statistical optimization approach which involved the solution of a sequence of linear elasticity problems [6]. To deal with general microgeometries we later introduced, in [2], a tensorial parameter that contains information about the microstructure and disorder of the polycrystal. Under an assumption of isotropy of both elastic constants and microgeometry, we showed that this parameter allows for the explicit calculation of rigorous and stringent upper bounds on the effective energy for both two- and three-dimensional polycrystals. Moreover, by consideration of some particular cases, we demonstrated that our bounds can yield improvements of as much as 50% over those obtained under Taylor's constant strain hypothesis.

Nonlinear effective medium theories, such as those described above, are also playing a central role in our continuing collaborative research project with the
Advanced Technologies Group at the Lord Corporation (Cary, NC). The goal of the project is to develop mathematical models and numerical algorithms that will aid in the design of magnetorheological fluids. These constitute examples of CONTROLLAI ("smart") fluids: their rheological properties vary in response to an applied magnetic field. In fact, the essential characteristic of MR fluids is that they may be continuously and reversibly varied from a state of free flowing liquids in the absence of an applied magnetic field to that of stiff semi-solids in a moderate field. This feature has inspired the design of a great variety of devices based on the use of MR composites, including semi-active dampers, clutches, brakes, hydraulic valves and robotic control systems of various sorts (see http://www.mrfluid.com). However, a number of practical issues (e.g. low power demand, high achievable yield stresses, low sensitivity to impurities, etc) had to be resolved before such devices could become industrially viable. Their patented choice of materials has recently allowed Lord to become the first (and so far, the only) company to commercialize MR devices (their products can be found, for instance, in a number of exercise machines --stair climbers, stationary bicycles, etc--, and will soon be prevalent as active suspension controllers in truck driver seats).

As it has often been the case in technological applications, Lord's success resulted from a great deal of experimentation and little mathematical and/or numerical work (generally in the form of oversimplified models). However, it has now become apparent that, in order to retain the leadership in this area, the company should strive to optimize the macroscopic characteristics of their product. As their researchers recognize, this task could vastly benefit from the use of advanced mathematical and numerical techniques. Their interests are mainly concerned with the determination of effective magnetic and rheological properties of MR suspensions and, particularly, with their dependence on design parameters (such as particle shape, size, distribution and volume fraction).

We are, therefore, pursuing this goal on two parallel though complementing fronts: on the one hand, we are guiding a postdoctoral associate (co-funded, since August 1997, by Lord and the National Science Foundation) in the implementation of fast magnetic field calculations on particulate geometries to be incorporated into dynamic simulations of the magnetic response of MR fluids. Some preliminary results have already proven fruitful as they have duplicated the experimentally observed two-time scale evolution of microstructure formation. Concurrently, we have integrated the efforts of a graduate student at NC State University whose task is to develop, under our direction, an effective medium theory applicable to the NONLINEAR saturable nature of magnetizable media, see [12]. In this regard, we have recently completed the implementation of a numerical algorithm for the calculation of overall nonlinear magnetization curves for periodically arranged magnetic particle chains within a carrier fluid. The particles are treated as magnetic continua, a hypothesis that can be substantiated within our context due to the relative size of magnetic domains (on the order of tens of nanometers) to that of the ferromagnetic particles themselves (a few microns). Interestingly, despite the approximations involved, our numerical results show very good agreement with experimental data from the linear to the saturation regimes.

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[ *
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* Graduate Students (NOT SUPPORTED BY THIS GRANT)
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* Other (please list role):

PUBLICATIONS

[ SUBMITTED ]

* Books/Book Chapters

 [ Journals ]

* Conferences

[ ACCEPTED ]

* Books/Book Chapters


* Journals

* Conferences

INTERACTIONS/TRANSITIONS
* Participation/Presentations At Meetings, Conferences, Seminars, Etc
--- Mathematical Modeling in Industry - A Workshop for Graduate Students
(organizer), Institute for Mathematics and its Applications, University of Minnesota, July 22-31, 1998
--- Minisymposium on Triple Junctions, Third International Conference on
Grain Growth, Pittsburgh, 16 June 1998
--- Workshop on Continuum Mechanics and Non-linear Partial Differential
Equations (in honor of John Ball's 50th birthday), Minneapolis, 11 June 1998
--- Minisymposium on Emerging Methods in Electromagnetic and Acoustic
Scattering, Fourth International Conference on Mathematical and Numerical
Aspects of Wave Propagation, Golden, 2 June 1998
--- Oberwolfach Meeting on Phase Transitions, Oberwolfach, Germany, 14 May 1998
--- Contractors Meeting, US Air Force Office of Scientific Research, San Antonio,
January 8-10, 1998
--- Reunion de Analisis y Ecuaciones No Lineales, Buenos Aires, Argentina,
19 December 1997
--- Research Seminar in the Mechanics of Materials, Aerospace Engineering and
Mechanics, University of Minnesota, Minneapolis, 4 November 1997
--- Workshop on Numerical Analysis of Free Boundary Problems, Ittingen,
Switzerland, 13 October 1997
--- Fifth Industrial Mathematics Modeling Workshop for Graduate Students
(organizer), North Carolina State University, Raleigh, August 4-12, 1997
--- Collaborative Research Visit to the Computational Science Laboratory,
Eastman Kodak Company, Rochester, June 22-24, 1997
--- Minisymposium on Mathematical Issues in Smart or Active Material Structures
and Devices, Second SIAM Conference on Mathematical Aspects of Materials Science,
Philadelphia, 12 May 1997
--- Workshop on Mathematics and Materials, Brockhouse Institute for Materials
Research, Hamilton, Canada, 23 April 1997
--- Materials Seminar, National Institute of Standards and Technology (NIST),
3 April 1997
--- Collaborative Research Visit to the Institute for Mathematics and its
Applications, Minneapolis, March 27-30, 1997
--- PDE Seminar, Worcester Polytechnic Institute, 21 February 1997
--- Colloquium, University of Minnesota, Minneapolis, 30 January 1997
--- Contractors Meeting, US Air Force Office of Scientific Research, San Antonio,
January 5-7, 1997
--- PDE Seminar, University of Buenos Aires, Argentina, 30 December 1996
--- Colloquium, Pennsylvania State University, State College, 19 November 1996
--- PDE Seminar, Rutgers University, Newark, 29 October 1996
--- Fourth Industrial Mathematics Modeling Workshop for Graduate Students
(organizer and group leader), North Carolina State University, Raleigh,
August 5-13, 1996
--- Third European Conference on Underwater Acoustics, Heraklion, Crete,
Greece, June 24-28, 1996
--- Center for the Mathematics of Waves Seminar, University of Delaware, Newark,
10 May 1996
--- Center for Nonlinear Analysis Seminar, Carnegie Mellon University, Pittsburgh,
24 April 1996
--- PDE Seminar, University of Minnesota, Minneapolis, 13 March 1996
--- Real Analysis Seminar, University of Minnesota, Minneapolis, 11 March 1996
--- Post-Doc Seminar, Institute for Mathematics and its Applications, Minneapolis,
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NEW DISCOVERIES, INVENTIONS, OR PATENT DISCLOSURES
[None]
HONORS/AWARDS
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