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13. ABSTRACT *(Maximum 200 words)*
The problems and techniques addressed under the present contract deal with issues of analysis and computation in electromagnetics. The primary goal consists of the development of efficient numerical tools for the prediction of scattered fields in a number of practical configurations. For this, substantial effort will be devoted to the extension and enhancement of the Method of Variation of Boundaries (MVB). Specific objectives in connection with MVB include: (1) advancement and implementation of algorithmic improvements for very high-order calculations (2) application to the solution of eigenvalue problems (related to cavities, resonators and waveguides); to the calculation of electromagnetic scattering from damaged objects and rough terrain; and to inverse scattering problems. (3) Concurrent with these endeavors the program will pursue the incorporation of the boundary-variation approach in more classical computational techniques, such as the finite-element methods (FEM). A first instance of such interactions will be sought through the implementation of high-order boundary perturbation approximations to computational radiation conditions (typically imposed on separable geometries). To enable and enhance such applications, the plan includes the development of new (high-order) discontinuous Galerkin (DG) finite element approach to electromagnetic scattering calculations which is expected to provide an advantageous setting for adaptivity and parallelization. Alternative high-order methods (e.g. based on integral equation formulations) wil also be considered.

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Electromagnetic Scattering
AFOSR Contract# F49620-99-1-0193

FINAL PROGRESS REPORT

1 April 99 - 30 November 01

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OBJECTIVES:

The problems and techniques addressed under the present contract deal with issues of analysis and computation in electromagnetics. The primary goal consists of the development of efficient numerical tools for the prediction of scattered fields in a number of practical configurations. For this, substantial effort will be devoted to the extension and enhancement of the Method of Variation of Boundaries (MVB). Specific objectives in connection with MVB include:

- advancement and implementation of algorithmic improvements for very high-order calculations

- application to the solution of eigenvalue problems (related to cavities, resonators and waveguides); to the calculation of electromagnetic scattering from damaged objects and rough terrain; and to inverse scattering problems.

Concurrent with these endeavors the program will pursue the incorporation of the boundary-variation approach in more classical computational techniques, such as the finite-element method (FEM). A first instance of such interactions will be sought through the

- implementation of high-order boundary perturbation approximations to computational radiation conditions (typically imposed on separable geometries).

To enable and enhance such applications, the plan includes the

- development of a new (high-order) discontinuous Galerkin (DG) finite element approach to electromagnetic scattering calculations

which is expected to provide an advantageous setting for adaptivity and parallelization. Alternative high-order methods (e.g. based on integral equation formulations) will also be considered.

STATUS OF EFFORT

Advances during the contract period recounted here include:

1) the demonstration of the joint analytic dependence of normal modes upon spatial variables and boundary perturbation parameters (see Refs. [3, 9, 16]). These results provided the theoretical foundation that allowed for

2) the implementation of an MVB algorithm for the estimation of eigenfrequencies and eigenfunctions of cavities and resonators [9], which is capable of dealing with the notoriously challenging problem of change in multiplicity.

As with previous MVB implementations a certain degree of ill-conditioning in the fundamental recursions was observed, which led to an investigation of possible ways to overcome it. Interestingly, a possible remedy emerged from a parallel effort to expand the domain of applicability of these methods to encompass free boundary problems [2, 5, 6, 11, 13]. As a result, a new approach (that of "Transformed Field Expansions" ---TFE---) to boundary variations has been devised whereby a change of variables is effected in advance of the derivation of the recursive formulas. This has the beneficial effect of bypassing the subtle cancellations that occur in the original recursions and which are partly responsible for the ill-conditioning. An initial application of this method resulted in

3) a new approach to the analyticity of Dirichlet-Neumann Operators (DNO) upon boundary variations [1, 4, 7]. In addition to providing a good testing ground for these new ideas, DNO have become instrumental in a variety of computational models, including scattering calculations (such is the case, for instance, with the "Operator Expansion" ---OE--- of Milder et al.).

Based on these findings we were able to derive

4) a theoretical framework for a Transformed Field Expansion (TFE) approach to scattering calculations. These methods showed substantial promise in allowing for an understanding of the validity, advantages and limitations of perturbation methods. Indeed, to confirm our theoretical predictions we undertook

5) the implementation of TFE approximations for the solution of scattering problems, and their comparison with other, classical perturbative techniques. In particular, for instance, this study confirmed our prevision that the standard "Operator Expansion" method of Milder et. al is *not* appropriate for high-order approximations due to a pronounced numerical ill-conditioning. Further, this investigation also led to

6) the realization of a close relation between TFE approximations and so-called "preconditioned spectral techniques" [7]. In addition to providing further insight into the conditioning of boundary variation approaches, we expect that this relation will help guide the design of improved perturbative as well as spectral numerical methods.

Our latest advance relating to TFE, finally, concerns its application to other problems where shape deformations have been consistently used, mostly without regard to convergence and conditioning issues. Specifically, we have recently initiated a program aimed at

7) the derivation of a TFE approach for the analysis of models of resonant and/or bifurcation processes governed by geometric deformations [11, 13]. These models include both boundary value (e.g. open and closed resonant cavities) as well as free boundary problems (e.g. resonant traveling water waves) where moderate shape perturbations can have dramatic physical consequences. We expect that our new developments will not only shed light on these effects, but will also provide an alternative, constructive and stable means for their numerical simulation.

In connection with the development of DG schemes, on the other hand, recent work has focused on the continued development of a three-dimensional Maxwell solver. A preliminary version that incorporates discretizations of arbitrarily high order is now near completion. To achieve this goal several issues had to be resolved, including a proper choice of mathematical formulation, basis functions, quadrature rules and inter-element fluxes, their implementation within general unstructured meshes and the design of a stable high-order scheme for the time integration. The next immediate goal consists of the incorporation of (high-order) boundary conditions which will, in turn, allow for a thorough comparison of their performance and that of alternative numerical fluxes within scattering experiments. A final step in this phase of the program then will include the integration of adaptive error control strategies (starting with "p-adaptivity"), as well as parallelization mechanisms.

Concurrently with our work of DGFEM, we have also made significant advances in our program on integral equation techniques. Indeed we have recently completed

8) the development of an integrator for the simulation of scattering processes generated by (two-dimensional) "thin" penetrable bodies.

As we detail below, the relevance of such an integrator is twofold: on the one hand, it demonstrates the viability of our projected approach to the solution of three-dimensional scattering problems by thin structures (e.g. coatings) whose material characteristics (e.g. anisotropy) preclude the use of surface scattering solvers. On the other hand, we expect that these new integrators will also allow for the development of a general high-order volumetric scattering solver when combined with the "accurate Fourier methods" recently developed by O. Bruno et al. This latter solvers have been shown to exhibit spectral accuracy in the treatment of configurations that display *smoothly* varying material properties; the incorporation of our new thin volume integrators should extend the spectral convergence to realistic arrangements, with possibly discontinuous material features. Our future plans include such an incorporation which, when coupled with an appropriate acceleration scheme, we expect to deliver an efficient high-order code for volumetric scattering calculations.

Finally, our collaborative work with industry has continued in the general area of magnetics. Our contract with Lord Corporation has been completed, with the delivery of

9) a microscale simulator of the dynamic response of MRF samples on application of external fields [14, 17, 18].

Our work with Seagate Technology, on the other hand, is still ongoing. The project, jointly funded by Seagate and IMA, is geared towards the design of an efficient numerical code for the prediction of the magnetic response of GMR read heads. To this end we initially concentrated on

10) the implementation of a fast solver for the rapid evaluation of the energy associated with a given micromagnetic state

which incorporates, in particular, an efficient algorithm for the calculation of the induced magnetic potential and corresponding demagnetization energy (through an adaptive fast multipole scheme). Most recently, we have finalized

11) the integration of the fast energy calculator into a simulator of the dynamic response of a magnetic structure (as modeled by the LLG equation).

Within a new phase of this program (characterized by the incorporation of a new postdoctoral associate), current work is devoted to the extension of the code's capabilities, particularly those relating to admissible meshes, to enable the simulation of the response of complex designs. Projected work includes the development of analogous simulators for polycrystalline samples, the design and implementation of higher order integration techniques as well as of suitable interfaces that will facilitate the use of the simulators within an industrial environment.

ACCOMPLISHMENTS/NEW FINDINGS

Our investigations in the area of electromagnetic scattering have focused on the development and implementation of high-order numerical methods. In particular, substantial effort was devoted to gaining a deeper understanding of geometric perturbation approaches, with a view to clarifying their validity and possibly extending their applicability. In this connection, and guided by our findings in a study of Dirichlet-to-Neumann Operators (DNO), we were able to identify the main source of numerical instabilities in classical perturbation methods for scattering problems. The investigation presented us with additional theoretical and computational challenges (e.g. unbounded domains, non-decaying solutions) that were not present in our DNO models. Their resolution then revealed that, in fact, the ill-conditioning associated with these approaches is intimately connected with our earlier realization, made also in connection with scattering problems under a previous AFOSR contract, that classical results on analyticity of solutions of PDEs (e.g. those of Calderon, Coifman el al, Craig et al, etc) *do not* suffice to guarantee the validity of a perturbative procedure. Indeed, our new results demonstrate that the actual plausibility of a perturbation scheme hinges on the validity of the underlying recursion (guaranteed, as we have shown, for instance, for very smooth—analytic—obstacles), rather than on a general result of analyticity of fields with respect to domain variations. Moreover, our most recent theoretical developments (and accompanying simulations) successfully identified previously observed numerical instabilities with cancellations within these recursions, which we showed to be pervasive in all classical implementations. Our specific findings include, for example, the recognition that the standard Operator Expansion Method of Milder et al. is particularly affected by these cancellations which, in fact, render a high-order implementation of this approach impractical, even for the smoothest of scattering interfaces. While still affected by them, the effect of cancellations in the MVB implementation is, however, significantly less pronounced.

In addition to clarifying the domains of applicability of classical approaches, our mathematical analysis also provided us with insight into possible improved implementations. Indeed, our investigation revealed that a simple change of independent variables allows for a recursive estimation of the terms in the perturbation series of the scattered field, a procedure that, as we have shown, *cannot* succeed in the original variables (where standard perturbative approaches are formulated). The possibility of recursively estimating the coefficients, in turn, suggested that a numerical implementation of such an approach would present significantly better conditioning properties. To confirm this conjecture, we developed, over the course of the present contract, a code based on these improved recursions, which indeed proved our expectation of enhanced stability to hold. Interestingly, we also realized that these new perturbative algorithms are closely related to the so-called "preconditioned spectral methods" and, in fact, they can be interpreted as a new, alternative implementation of these. The relevance of this interpretation lies in the possibilities it opens for improvements in both perturbative and spectral techniques that could be achieved by drawing from the advantages of one and applying to the other (e.g. exporting analytic continuation mechanisms into spectral approximations or incorporating ideas from Richardson iteration schemes into perturbative procedures).

As we have explained, our project in DG methods for electromagnetics, on the other hand, grew from our interest in the integration of geometric perturbation methods into more versatile computing strategies. This program, conducted in collaboration with B. Cockburn, involves the full-time assistance of a graduate student (supported by NSF) who is now finishing a preliminary code for the solution of Maxwell's equations with approximations of arbitrary order of convergence. This initial simulator uses Dubiner bases, Gaussian quadratures and upwinding schemes to deliver a high-order representation of the (local) variational equation. Goals for the immediate future include the incorporation of high-order boundary conditions, the development and implementation of p-adaptive capabilities and a first attempt at parallelization.

Still within the general area of high-order methods for computational electromagnetics, we have also advanced our program, in collaboration with O. Bruno, on accurate and efficient integral equation solvers. Our most recent accomplishment here consists of a successful completion of projected "thin volume" integrators for two-dimensional calculations. We recall that such solvers constitute the basis for our proposed improvement on the methods for volumetric scattering computations recently developed by Bruno et al. which we anticipate will exhibit high-order convergence even in the presence of material discontinuities. Moreover, these algorithms, when coupled with a suitable acceleration scheme, will likely be our method of choice for the treatment of certain specific thin structures, such as anisotropic coatings. The basic elements in these schemes for the evaluation of volume potentials consist of: 1) the splitting of the integration domain into two subdomains separated by the level set determined by the transverse coordinate of the target point (so that the two resulting integrals are themselves smooth functions of the field points); 2) a polynomial interpolation in the transverse direction to find additional values of the density as needed in a high-order quadrature of each of the two integrals; 3) in a tangential (non-transverse) direction, a Fourier interpolation to obtain additional values of the density for a subsequent local polynomial interpolation; 4) a change of tangential variables to deal with the singular and almost singular behavior of the fundamental solution near the target point; and 5) a trapezoidal approximation in the new tangential coordinate and a high-order quadrature rule in the transverse direction (e.g. with equispaced points). With this prescription, we have now confirmed our prediction of high-order convergence in the two-dimensional case. We expect that the experience gained in this instance will facilitate the three-dimensional implementation, as the basic ideas described above remain unchanged.

Finally, funding for our program in computational micromagnetics has been renewed and a new postdoctoral associate, Dr. Santiago Betelu, has joined our collaborative effort with Seagate Technology. His current work is focused on the extension of the recently finalized simulator of the (Landau-Lifshitz-Gilbert, LLG) dynamics of a magnetic structure, which was completed within the previous phase of the program. For practical reasons, particular attention will be given to extensions that allow for simulations on complex designs (i.e. by allowing for the treatment of general unstructured meshes), as well as to those that will ease the use of the solver (e.g. by interfacing it, at least partially, with automated design tools). Future plans include the development of higher-order, more efficient schemes that will also allow for the investigation of polycrystalline specimens.

PERSONNEL SUPPORTED

- *Faculty/Industrial Collaborators (NOT SUPPORTED BY THIS GRANT)*
  - H. Thomas Banks (Department of Mathematics, North Carolina State University).
  - Oscar Bruno (Applied Mathematics, California Institute of Technology).
  - Bernardo Cockburn (School of Mathematics, University of Minnesota).
  - Avner Friedman (School of Mathematics, University of Minnesota).
  - Kazufumi Ito (Department of Mathematics, North Carolina State University).
  - Mark Jolly (Advanced Technologies Research Group, Lord Corporation)
  - Hung Ly (Department of Mathematics, California State University)
  - Lei Wang (Seagate Recording Heads, Seagate Technology)

- Post-Docs *(NOT SUPPORTED BY THIS GRANT)*
  - Santiago Betelu (Institute for Mathematics and its Applications, University of Minnesota)
  - David Nicholls (Department of Mathematics, University of Notre Dame)
  - Nilima Nigam (Department of Mathematics and Statistics, McGill University)

- Graduate Students *(NOT SUPPORTED BY THIS GRANT)*
  - Fatih Ecevit (School of Mathematics, University of Minnesota).
  - YoungAe Han (School of Mathematics, University of Minnesota).
  - Gerardo Ortigoza (School of Mathematics, University of Minnesota).
  - Paul Castillo (Center for Applied Scientific Computing, Lawrence Livermore National Laboratory)

PUBLICATIONS

- *SUBMITTED*
  - *Journals*

[1] D. Nicholls and F. Reitich, "Analytic continuation of Dirichlet-Neumann operators", submitted (2000).

[2] A. Friedman and F. Reitich, "Quasi-static motion of a capillary drop, II: the three-dimensional case", submitted (2001).

- *ACCEPTED*
  - *Books/Book Chapters*

[3] O. P. Bruno and F. Reitich, "High-order boundary perturbation methods", Book Chapter, in Mathematical Modeling in Optical Science, Frontiers in Applied Mathematics Series, Gang Bao et al., ed., SIAM (2001), 71-109.

➢ *Journals*

[4] D. Nicholls and F. Reitich, "A new approach to analyticity of Dirichlet-Neumann operators", Proc. R. Soc. Edinburgh, to appear.

[5] A. Friedman and F. Reitich, "Nonlinear stability of a quasi-static Stefan problem with surface tension: a continuation approach", Ann. Sc. Norm. Sup. Pisa, to appear.

[6] A. Friedman and F. Reitich, "Quasi-static motion of a capillary drop, I: the two-dimensional case", J. Diff. Equations, to appear.

[7] D. Nicholls and F. Reitich, "Stability of high-order perturbative methods for the computation of Dirichlet-Neumann operators", J. Comput. Phys. 170 (2001), 276-298.

[8] T. M. Simon, F. Reitich, M. R. Jolly, K. Ito and H. T. Banks, "The effective magnetic properties of magnetorheological fluids", Math. Comput. Modelling 33 (2001), 273-284.

[9] O. P. Bruno and F. Reitich, "Boundary-variation solution of eigenvalue problems for elliptic operators", J. Fourier Anal. Applic. 7 (2001), 169-187.

[10] C. H. Lee, F. Reitich, M. R. Jolly, H. T. Banks and K. Ito, "Piecewise linear model for field-responsive fluids", IEEE Trans. on Magnetics 37 (2001), 558-560.

[11] A. Friedman and F. Reitich, "Symmetry-breaking bifurcation of analytic solutions to free-boundary problems: an application to a model of tumor growth", Trans. Amer. Math. Soc. 353 (2001), 1587-1634.

[12] T. M. Simon, F. Reitich, M. R. Jolly, K. Ito and H. T. Banks, "Estimation of the effective permeability in magnetorheological fluids", J. Intell. Mat. Sys. Struct. 10 (2000), 872-879.

[13] A. Friedman and F. Reitich, "On the existence of spatially patterned dormant malignancies in a model for the growth of non-necrotic vascular tumors", Math. Models and Meth. Appl. Sci. 11 (2001), 601-625.

[14] H. V. Ly, F. Reitich, M. R. Jolly, H. T. Banks and K. Ito, "Simulations of particle dynamics in magnetorheological fluids", J. Comput. Phys.155 (1999), 160-177.

[15] K. Ito and F. Reitich, "A high-order perturbation approach to profile reconstruction. I: Perfectly conducting gratings", Inverse Problems 15 (1999), 1067-1085.

➢ *Conferences*

[16] O. P. Bruno and F. Reitich, "Solution of Laplace-eigenvalue problems via variation of the boundary into the complex domain", in Mathematical

and Numerical Aspects of Wave Propagation, A. Bermudez et al., ed., SIAM (2000), 471-476.

[17] H. T. Banks, K. Ito, M. Jolly, H. V. Ly, F. Reitich and T. M. Simon, "Dynamic simulations and nonlinear homogenization study for magnetorheological fluids", in Proceedings of SPIE's 6th International Symposium on Smart Structures and Materials, vol. 3667 (1999), Mathematics and Control in Smart Structures, Vasundara V. Varadan, ed., 92-100.

[18] H. V. Ly, M. R. Jolly, K. Ito, F. Reitich and H.T. Banks, "Dynamic simulations of the temporal response of microstructure formation in magnetorheological fluids", in Proceedings of the Seventh International Conference on Electrorheological Fluids and Magnetorheological Suspensions, Honolulu, July 19-23, 1999.

INTERACTIONS/TRANSITIONS

- *Participation/Presentations At Meetings, Conferences, Seminars, Etc*
  - Georgia Institute of Technology, Atlanta, February 5, 2001.
  - State University of New York at Buffalo, Buffalo, November 2, 2000.
  - Minisymposium on Surface Scattering, Fifth International Conference on Mathematical and Numerical Aspects of Wave Propagation, Santiago de Compostela, Spain, July 13, 2000
  - Minisymposium on Low-Frequency Nondestructive Evaluation of Conductive Structures, Progress in Electromagnetics Research Symposium (PIERS 2000), Boston, July 6, 2000
  - Minisymposium on Magnetic Materials, Third SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 24, 2000
  - University of Utah, Salt Lake City, April 10, 2000
  - IMA Workshop on Analysis and Modeling of Optical Devices, Minneapolis, September 10, 1999
  - Lawrence Livermore National Laboratory, Lawrence Livermore, July 23, 1999
  - University of Augsburg, Augsburg, Germany, July 13, 1999
  - Minisymposium on Micromagnetics and Magnetic Materials, ICIAM 99, Edinburgh, Scotland, July 8, 1999
  - University of Minnesota (Aerospace Engineering and Mechanics), Minneapolis, May 25, 1999

- *Consultative And Advisory Functions To Other Laboratories And Agencies*
  - Member of the Review Panel on Materials and Mechanics, Applied and Computational Mathematics, National Science Foundation, February 17-19, 2000
  - Member of the Preproposal Review Panel for the "Knowledge and Distributed Intelligence (KDI) initiative on New Computational Challenges", National Science Foundation, March 15-16, 1999

- *Transitions*

  The effort of our research on magnetorheological fluids was geared towards the development of advanced controllable materials for commercialization by the Lord Corporation (Cary, NC); our collaborator at Lord was Dr. Mark R. Jolly of the Advanced Technologies Research Group. Past and ongoing research on micromagnetics, on the other hand, seeks the development of a simulator for the operation of GMR read heads, for potential use in the design process at Seagate Technology (Minneapolis, MN); our collaborator at Seagate is Dr. Lei Wang of the Recording Heads Group.