REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-02-

0343

1. REPORT DATE *(DD-MM-YYYY)*: 09/25/02

2. REPORT TYPE: FINAL

3. DATES COVERED *(From - To)*: Feb. 1996 - Oct. 2001

4. TITLE AND SUBTITLE
Mathematical and Numerical Methods for Analysis and Design of Electromagnetic Fields.

5a. CONTRACT NUMBER: F49620-96-1-0039

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

6. AUTHOR(S)
Angell, Thomas S.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Delaware
Mathematical Sciences
Newark, DE 19716

8. PERFORMING ORGANIZATION REPORT NUMBER
3-3-21-2553-03

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Dr. Arje Nachman, Manager
Program in Applied Mathematics
Air Force Office of Scientific Resch.
801 N. Randolph Street, Room 732
Arlington, VA 22203-1977

10. SPONSOR/MONITOR'S ACRONYM(S): AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

20021031 013

13. SUPPLEMENTARY NOTES

14. Absract: Report covers (4) specific areas. **(1) Wave Propagation and Scattering** which encompasses the essentials of direct scattering codes, new integral equation formulations, preconditioning, a posteriori error estimation, boundary and finite elements, finite difference methods, and parallelization. **(2) Inverse Scattering and Imaging** in which the forward codes play an essential role but where the emphasis is on target identification and non-destructive microwave imaging of structures including biological (dispersive) objects. **(3) Complex Media and Approximating Boundary Conditions**, which include various impedance, reactive and conductive conditions, which better, model the effects of dielectric, anisotropic or dispersive material or layers of such material with possible rough boundaries. **(4) Antenna Design** which not only includes calculation of radiation patterns from complex structures, including mutual coupling and near field interactions, but also the development and application of optimization methods for realistic design problems.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
U	U	U	UU		THOMAS S. ANGELL
					19b. TELEPHONE NUMBER (include area code) (302)831-2250

Mathematical & Numerical Methods for Analysis & Design of Electromagnetic Fields

Final Report

Thomas S. Angell, Principal Investigator

Department of Mathematical Sciences
University of Delaware
Newark, Delaware 19716

A Multidisciplinary University Research Initiative Project of the Defense Advanced Research Projects Agency
Monitored by: Arje Nachman
Air Force Office of Scientific Research
under Grant No. F49620-96-1-0039

September 25, 2002

1 Introduction

The MURI Grant to the University of Delaware and its associated institutions had as its mission the investigation and development of sound mathematical foundations for the development of effective codes for electromagnetic problems of direct concern to the Air Force. Under the auspices of the Air Force Office of Scientific Research, an interdisciplinary team was assembled involving scientists from fields of mathematics, electrical engineering, and computer science with the objective that such an interactive research program would accelerate the transition from mathematical model to practical numerical solution.

It was recognized at the outset that the thrust of this particular MURI research effort would be directed toward new formulations, the study of more realistic mathematical models, and the development of novel solution algorithms. It was believed that incremental refinements of existing methods would not suffice to handle problems of pressing concern to the Air Force representing, as they do, challenges for the next generation.

This understanding of Air Force needs led to a program which addressed basic problems inherent in accurately predicting the radiation and scattering from complex objects in a realistic environment, both from the point of view of design, control, and target signature, as well as the inverse problem of assessing the essential nature of objects, size, shape, location, internal configuration and constitutive parts from electromagnetic interactions.

The group was assembled, and was funded, starting in July, 1996, through the *Center for the Mathematics of Waves* at the University of Delaware, and under the direction of Ralph E. Kleinman[1] as Principal Investigator.

The following pages review selected accomplishments of this team, the results that have been obtained, and the contacts with Air Force programs and personnel which have been active and which promise to continue as mutually interactive points for the furtherance of the research program and of Air Force needs.

The overarching goal of research sponsored under the grant was the development of codes capable of resolving many of the computational electromagnetic problems of Air Force concern both present and future. As stated in the original grant proposal:

> *The bottom line question, from the Air Force point of view, is whether or not the electromagnetic community can provide codes which will be adequate to resolve long-standing problems in radar cross section, antenna design, and inverse scattering. At the present time, such codes are not available.*

To this end, a major portion of the research effort under this grant was directed toward new formulations, more realistic mathematical models, and novel solution algorithms in the belief that incremental refinements of existing methods would not suffice to handle either present large scale problems or future challenges.

The fact that, both in direct and inverse scattering, realistic targets are not perfectly conducting makes these problems particularly complicated. Instead of being adequately modeled by relatively simple boundary conditions, actual targets usually consist of inhomogeneous, anisotropic, dispersive material and/or layers of such material, with boundaries which may be rough. Mathematical modelling such materials, deriving useful approximate boundary or transmission conditions, and *incorporating these models in efficient direct solvers,* all serve to complicate the computational problem.

[1]Prof. Kleinman died suddenly in 1998

Likewise, in problems of antenna design which continue to be a subject of Air Force concern, the calculation of radiation patterns is equivalent to the calculation of scattered fields when mutual coupling is taken into account. This is true of dishes and of arrays as well as of *conformal antennas* where, for example, essentially the same codes may be used to compute both the radar cross section of an aircraft and the radiation pattern of a flush-mounted antenna; the material properties of the aircraft skin and the presence of layers will incur the same complications in scattering calculations as in radiation pattern calculations.

In order to address some of these fundamental research problems, the MURI project was subdivided into four broad areas:

1. WAVE PROPAGATION AND SCATTERING which encompasses the essentials of direct scattering codes, new integral equation formulations, preconditioning, *a posteriori* error estimation, boundary and finite elements, finite difference methods, and parallelization;

2. INVERSE SCATTERING AND IMAGING in which the forward codes play an essential role but where the emphasis in on target identification and non-destructive microwave imaging of structures including biological (dispersive) objects;

3. COMPLEX MEDIA AND APPROXIMATING BOUNDARY CONDITIONS which include various impedance, reactive and conductive conditions which better model the effects of dielectric, anisotropic or dispersive material or layers of such material with possible rough boundaries;

and

4. ANTENNA DESIGN which not only includes calculation of radiation patterns from complex structures, including mutual coupling and near field interactions, but also the development and application of optimization methods for realistic design problems.

UNIVERSITY/RESEARCH LAB	WAVE PROPAGATION AND SCATTERING	INVERSE SCATTERING	COMPLEX MEDIA	ANTENNA DESIGN
University of Delaware Thomas S. Angell	• Colton • Hsiao • Kleinman • Monk • Dallas • Wang	• Angell • Colton • Coyle • Kleinman • Monk • Pelekanos	• Monk	• Angell • Kleinman • Lepelaars • Holston
University of Arizona Richard W. Ziolkowski			• Ziolkowski	
Colorado School of Mines John A. DeSanto	• DeSanto • Hereman • Misra			
A. J. Devaney Associates, Inc. Anthony J. Devaney	• Devaney • An	• Devaney		• Devaney • Heyman
Massachusetts Institute of Technology Jacob White	• White • Peraire			
New Jersey Institute of Technology G. A. Kriegsmann	• Hile • Kriegsmann • Luke		• Kriegsmann • Hile • Luke	• Kriegsmann
Virginia Polytechnic Institute State University Gary S. Brown	• Brown • Adams			

The table on the preceding page lists the participants and summarizes the various research efforts initially undertaken by them.

The subdivision made here is understandably arbitrary; the several research programs sponsored by the MURI grant fall most naturally under more than one umbrella. Certainly, most of the particular research efforts ultimately fall under the aegis of COMPUTATIONAL ELECTROMAGNETICS, the overarching theme of the grant. We make the divisions only for convenience of exposition.

2 Wave Propagation and Scattering

A major effort during the grant was devoted to the development of integral equation methods, hybrid methods involving disparate time and/or length scales, and wavelet based methods, all devoted to the description and calculation of scattered fields from various targets. Existing codes were analyzed, new iterative methods proposed and applied, in particular to problems of rough surface scattering and reconstruction from scattering data.

The research in this general area began with in-depth study of the boundary integral equations for the three dimensional electromagnetic scattering from smooth closed surfaces. The appropriate integral equations were derived, irregular frequencies were discussed along with Calderon projectors and all of the energy spaces needed to accurately describe the mapping properties of boundary integral operators were presented. These were employed to define the appropriate function spaces in which to seek approximate solutions via the Galerkin or moment method. This careful study led to a general investigation of the origin of instability in Galerkin methods, so often used in numerical work. This problem of instability was thoroughly investigated and led to a new analysis of wavelet methods applied to the solution of first-kind boundary integral equations which arise in inverse scattering.

Numerical experiments concerning the accuracy of approximate solutions in 3D electromagnetic scattering problems provided a validation of the rigorous proofs of convergence in terms of mesh sizes for the Magnetic Field Integral Equations (MFIE) applied to the electromagnetic scattering of a perfect conductor in three dimensional space. Likewise, the corresponding analysis for a transmission problem in 3D electromagnetics by using the approach of combined boundary element and finite volume methods was completed. For the MFIE, numerical experiments are performed and compared to those obtained from Mie series method and numerical results verify the theoretical error estimates.

In pursuit of several of these research objectives the group at MIT has developed a wide variety of results:

1. A dual-grid multipole projection algorithm that is nearly an order of magnitude faster for a given level of accuracy than standard multipole or grid monopoles. Experiments with the dual-grid multipole projection algorithm showed that not only is the method more efficient than standard multipole, it is much better conditioned than using grid monopoles. In addition, in three dimensions the dual grid multipole algorithm only requires fourth order expansions for single precision accuracy. This eliminates the need for kernel specific expansion or translation operator diagonalization.

2. A "Wavelet-like" approach to sparsifying integral operators which handles very irregular geometries and large numbers of interacting bodies. This "Wavelet-like" approach to sparsifying integral operators handles very irregular geometries and large numbers of interacting bodies. The approach also generates a diagonal preconditioner which insures Krylov-subspace method convergence in a number of iterations independent of discretization refinement.

3. A multigrid method for integral formulations for non-oscillatory kernels on very irregular geometries. The approach is nearly an order of magnitude faster than preconditioned Krylov-subspace methods combined with sparsification. This multigrid method for integral formulations with non-oscillatory kernels works for very irregular geometries. The method uses a local inversion smoothing combined with a tuned interpolation-projection scheme that avoids growth in low spatial frequency components during smoothing. When tested on a problem in substrate coupling, the approach is nearly an order of magnitude faster than preconditioned Krylov-subspace methods even when such methods are combined with sparsification.

4. A second-kind integral formulation for directly computing charge densities on multiple bodies.

5. A perturbation approach to handling dielectric interfaces with accuracy independent of dielectric constant ratio.

6. A precorrected-FFT accelerated solver for integral equations which allows for Green's functions derived from image principles. The precorrected-FFT accelerated solver for integral equations allows for Green's functions derived from image principles. The code has been used on a variety of 3-D structures associated with microsensors and electronic packaging and interconnect and is typically three to ten times faster than kernel specific fast multipole algorithms. For example, our code can analyze the force distribution on a micromachined comb drive, whose surface discretization requires more than 100,000 panels, in under five minutes on a desktop workstation.

7. A general multipole-accelerated Laplace solver, FastLap, which evaluates fields at arbitrary points using differentiated multipole expansions.

8. Both precorrected-FFT and fast multipole accelerated algorithms for generating reduced-order models from 3-D quasistatic and full wave analysis.

9. Sobolev-norm based adaptive gridding algorithms for discretized integral formulations. Adaptive gridding for discretized integral equations is much less well developed than techniques for discretized partial differential equations. Since integral operators associated with strongly elliptic kernels have bounded inverses in a fractional Sobolev norm, it is possible to get error estimates by computing Sobolev norms. Such strategies have been developed and it was demonstrated that they generate grids with small thin panels near exterior corners and correctly refine "shadows" of nearby bodies.

New approaches involving asymptotic methods were also studied and found useful in the analysis of engine inlets as well as in problems of antenna optimization for convex conformal objects.

2.1 Rough Surface Scattering

Rough surface scattering has long presented a challenge to analysts because, in general, all scales of roughness must be accounted for. Frequently, natural surfaces contain, simultaneously, roughness components that are either larger than, on the order of, and/or smaller than the electromagnetic wavelength. Asymptotic theories are available for certain classes of surfaces and these are useful for understanding and checking "exact" numerical calculations. It is imperative that numerical methods be developed for dealing with electromagnetic wave scattering from rough surfaces. It is essential that such methods be based on the physics of the scattering process, be well understood in so far as how they deal with the scattering, be well characterized from a numerical robustness standpoint, be numerically efficient, and be independent of the specific computer accomplishing the calculations.

There are various formalisms for the rough surface scattering problem. The exact treatment of the problem usually involves the solution of integral equations for the boundary unknowns. Most often they are solved using matrix inversion or iterative methods after some numerical discretization scheme has been employed. For matrix inversion, the various methods can be additionally characterized by the space in which the rows and columns are sampled. The usual scattering integral equations are described in state (or coordinate space) and both the rows and columns sampled in coordinate space. We refer to this as the coordinate-coordinate (CC) method. If the integral equations are written in terms of the scattering and transmission amplitudes in Fourier-transform (or spectral) space, we refer to the resulting representation spectral-spectral (SS) problem. There are two mixed representations, SC and CS, which have also proved useful in describing both the direct and inverse scattering problems.

These alternatives are summarized in the following table:

	METHOD		
PROPERTY	**SS**	**CC**	**SC**
Matrix Size	Relatively small	Relatively large	Relatively small
Conditioning	Well conditioned usually	Well conditioned always	Well conditioned usually
Matrix Structure	Sparse (diagonally dominant)	Dense	Diagonally dominant
Fill Time	Relatively slow (oscillating kernels)	Very slow	Extremely fast
Wavelet Transform	Helps for sparsification Inefficient for small problems	Particularly helpful for sparsification large matrices	Inefficient for small problems
Parallization	Helpful	Very helpful	Helpful
Limitations	Fails for grating with very large heights and slopes	Storage requirements large Very long run time	Fails for grating with very large heights and slopes
Advantages	New Approach for periodic surfaces	Highly reliable	Fastest code New for periodic surfaces 3-D code first choice

Additional efforts have been made for new code development including:

- A vectorized integration routine (here based on piecewise Gaussian quadrature) particularly useful for oscillatory integrands.
- A QR decomposition method using block matrix techniques to do Givens rotations more efficiently. The method works for both parallel and sequential implementation. Parallel implementations have been developed for the SGI PowerChallenge, as well as the Origin 2000.

A new iterative method has been developed to deal with electromagnetic wave scattering from perfectly electrically conducting (PEC) rough surfaces. This method is based on a physical re-ordering of the magnetic field integral equation for the current induced on such a surface. This new method is called MOMI for Method of Ordered Multiple Interactions because it modifies the original integral equation such that each iteration includes a summation of physically important multiple scattering interactions. The zero order iterate of the series provides sufficient precision for most applications. Inclusion of the first order iterate provides a result which is accurate enough to study the very sensitive problem of low grazing angle backscattering. While mathematical minimization techniques could be used in combination with the method to accelerate its convergence, this has been found to be unnecessary due to the rapid convergence of the method itself. Finally, we note that MOMI is completely complementary to matrix inversion methods whose goal is to reduce computational time involved in matrix-vector multiplication. It is felt that that a combination of these efforts yields a technique for simulating electromagnetic scattering problems which is better than either technique in isolation.
The research at Virginia Tech was focused on the development of a class of robust and efficient iterative methods for solving the boundary integral equations from finite targets in the vacinity of randomly rough surfaces. The study was based on the factorization of the kernel operator into a product of one-way wave operators, and a corresponding coupling operator which defines the interactions between forward and backward propagating waves on the surface of the scatterer.
The primary difficulty was to extend previous results to arbitrary scattering geometries and the application of accurate and numerically efficient approximations to the forward and backward scattering operators. The previous work under this grant produced iterative methods for closed body geometries and dielectric rough surfaces. However, the good convergence rates were dependent upon, for example, polarization or dielectric contrast ratios.
The latest results give methods which are independent of such parameters. This work can be viewed as complementing the efforts of others who have or are presently developing FMM-related techniques.
A significant part of the last phase of the work was the investigation of the development of an effective preconditioner for the electric field integral equation which will avoid the low-frequency breakdown problem associated with this eqation. The work on similar problems associated with the Galerkin procedures developed at Delaware has been crucial in the effective development of the preconditioners which have been shown to be effective in dealing with the breakdown problem.

1. The study of the general case of rough interfaces separating two dielectrics as well as special cases of perfectly reflecting surfaces and closed bodies.

2. The research effort includes theoretical development of the integral equations for electromagnetic scattering,

3. The development of approximation methods using both wavelet-based analysis, iterative (MOMI) methods and other analytical tools including the recent use of preconditioners,

4. The large-scale computational implementation of the results, and the minimization of computation times.

Applications of the above include the following.

1. The scattering from aircraft and missiles,

2. The behavior of radar scattering from various obstacles situated at or near a rough surface on land, and

3. The analysis of data useful in processing satellite imagery.

2.2 Hybrid Methods

Although recent advances in computer technology have increased the speed at which engineers and scientists routinely perform large scale scientific computations, there are certain classes of technological problems which can not be efficiently solved by a direct computational approach. These problems typically contain disparate length and/or time scales which make their governing equations ill-conditioned from a numerical point of view. In many cases these disparate scales can be exploited, using asymptotic methods, to yield new approximate equations and boundary conditions which are well suited for numerical methods. This combination of asymptotic and numerical techniques often provides an efficient hybrid method to study the original problem. The primary objective of this sub-project is to construct such hybrid methods to attack and understand electromagnetic scattering by electrically large structures with local fine structure and by large slowly changing cavities, and also the electromagnetic propagation of short pulses in highly dispersive media.
The work done during the grant included:

1. Developing hybrid methods for numerically simulating the scattering of time harmonic electromagnetic waves by electrically large structures with locally periodic surface coatings. The period of this surface structure is the order of the incident wavelength.

2. Developing hybrid methods for numerically simulating the scattering of time harmonic electromagnetic waves by large slowly changing cavities.

3. Developing Dirichlet-to-Neumann boundary operators which accurately model the contents of a cavity and adapting these conditions to be used with general purpose electromagnetic scattering codes.

4. Developing and analyzing efficient numerical methods for simulating the propagation of short electromagnetic pulses in dispersive media whose characteristic relaxation time scales are very short.

This work included specific applications which involved scattering from electrically large, periodically coated targets, scattering from large, slowly changing cavities loaded with linear material, the numerical implementation of an accurate Dirichlet-to-Neumann boundary condition map for a large, slowly changing, loaded cavity, and the modelling of propagation of short pulses through models of biological media and absorbing layers.

2.3 Error Control and Conditioning

The Galerkin method is one of the most widely used and effective schemes for generating approximate solutions of operator equations (as well as variational formulations of such equations). For example, the Galerkin method provides the foundation for the finite-element and boundary-element methods, as well as the method of moments used so frequently in electromagnetic computations. However it is not uncommon for a particular implementation of the Galerkin method to converge theoretically yet be numerically unstable. Here, "numerical instability" means unboundedness of the sequence of condition numbers of the linear systems that must be solved to construct the Galerkin approximants. Unless the data are known very accurately and the system to be solved is not too large, such a numerical instability may seriously erode the accuracy of the numerical results.

There were few systematic guidelines available to assist in the design of stable Galerkin schemes or the stabilization of existing unstable schemes. This deficiency was probably explained by noting that, like the question of error analysis, the matter of stability is essentially mathematical. That is, nothing short of a fundamental mathematical analysis of the Galerkin method will serve as the basis for a systematic attack on the problem of designing numerically stable procedures. On the other hand, it appears that decisions presently made during the design of a Galerkin procedure are frequently based on considerations such as speed and simplicity alone; too often the result is numerical instability.

More generally, a significant number of the methods employed for the approximate solution of operator problems ultimately reduce, in one way or another, either to the need for accurate direct solution of large systems of linear algebraic equations or to an iterative computation involving such systems. An understanding of stabilization techniques for the Galerkin procedures may also lead to insight into the same questions in these other settings.

2.3.1 Objectives for Convergence Study:

This research effort, carried out at Delaware was directed toward

1. The formulation of practical guidelines and methods for the design of numerically stable Galerkin procedures.

2. The production of usable techniques to be applied in the stabilization of presently existing unstable Galerkin schemes.

3. The use of appropriately chosen preconditioners as determined by the use of appropriate spaces of trial and test functions.

4. The production of numerical examples showing the particular rate of convergence for these procedures *as determined by the choice of trial and test functions.*

5. The investigation of the use of wavelet bases appropriate for boundary spaces for the boundary integral equations of the first kind and tests for convergence.

The requirements of practicality and usability are of central importance. Indeed, it happens frequently that one or more approaches are known that will, in principle, ensure the numerical stability of a computation, but a method for implementing the strategy is either lacking or too expensive. The research here gives significant insights into the choice of settings which produce both stable and usable Galerkin schemes for the boundary integral equations which arise in scattering theory.

2.4 Non-radiating Sources

Another goal is to fully develop the theory of *non-radiating sources* (NR sources). Such sources generate fields that vanish identically outside their spatial support and play extremely important roles in both direct and inverse scattering. In particular, these NR sources provide a certain freedom that allows the forward problem to be solved in an optimally efficient manner in cases where only the scattering amplitude of the object is desired. It follows that the scattering amplitude is invariant under the addition of an NR source component and this invariance can be used to minimize the computational effort required by the forward solver. With specific reference to the tomographic based forward solver devised by one member of the MURI team, A. J. Devaney, theoretical estimates indicate a considerable time savings for computing fields generated by very large ($ka >> 1$) penetrable scatterers.

2.4.1 Objectives for Non-radiating Source Models

In this area the principle goals were as follows.

1. The development of an efficient forward Helmholtz equation solver that works in the large to very large ka range.

2. The development of a tomographic based forward solver that reduces the 3-D Lippmann Schwinger integral equation satisfied by the field to a set of coupled 1-D equations that are individually satisfied by the tomographic projections of the 3-D field.

New forward solvers were developed and applied to several problems of importance to the resolution of high ka .

2.5 Electromagnetic Interference Codes

This phase of the research program was concerned with modelling the complicated interactions within micromachined sensors as well as to analyze electromagnetic interference in electronic systems. These problems are characterized by the presence of geometrically complicated three-dimensional structures consisting of materials of different constitutive parameters and, possibly, of multiple bodies. Codes capable of, for example, analyzing electrostatic forces in an entire microsensor have been based on a combination of a discretized integral formulation, a preconditioned iterative solver, and a sparse representation of the integral operator. They are now in use. The overall goal of this aspect of the MURI effort was to extend these codes to such areas as full-wave electromagnetics and layered media.

2.5.1 Objectives for Electromagnetic Interference Codes

The specific goals for the work included:

1. Developing a precorrected-FFT program for General Green's functions and complicated 3-D geometries.

2. Investigation of Multilevel Methods for Integral Equations in irregular geometries.

3. Investigation of Fundamental Aspects of Sparsification Techniques, including the connection between wavelets and multipole expansions, grid and dual-grid multipole algorithms, and difficulties in grid projection.

4. Investigation of Integral formulations for multiple materials and to generate desired engineering quantities.

5. Developed Arnoldi based model-order reduction techniques for full wave problems.

3 Inverse Scattering

The work in the area of inverse scattering was devoted to an investigation of optimization algorithms, coupled with boundary and volume integral equations, to develop both the mathematical foundation and the practical implementation of numerical methods for various inverse problems including shape identification and profile inversion from scattered data. The goal of the work is to develop working codes for realistic ATR problems; the strategy is to incorporate advances in direct solvers into various approaches which already have proved to be successful in nontrivial examples.
Research efforts in such problems pervaded much of the work done under this MURI Grant. There is considerable interaction among various subteams concerning such important areas as, for example Hybrid Methods or Rough Surfaces. Here we are concerned with the subject of inverse methods *per se*.
Specific goals of the work can be summarized as:

1. **Modified Green's Functions.** Investigate the usefulness of combining the complete family approach with the modified Green's function approach to inverse scattering particularly for problems in which only backscattered data is available.

2. **3–D Electromagnetics.** Provide the theoretical groundwork on which a full 3–D electromagnetic inversion code can be based.

3. **Shape Identification.** Continue and expand the revised complete family approach to shape reconstruction by establishing convergence, testing stability, incorporating modified Green's functions, and extending to time domain.

4. **Non-radiating Sources.** Investigate the role of non-radiating sources in the development of tomographic methods as well as in the broader context of identification of penetrable objects from scattered data.

5. **Modified Gradient Methods.** Expand the modified gradient approach to inverse scattering by seeking better initial choices in the minimization algorithm, deriving a comparable algorithm for discontinuous fields at the boundary, extending the method to multifrequency spatially limited data.

6. **Real Data.** Develop together with AFRL/SN (Hanscom AFB) a data bank of canonical inverse scattering problems including experimental data sets and reconstructions.

7. **Total Variation.** Incorporate the total variation as a penalty term in the functionals of all methods.

8. **Dispersive Media.** Derive an algorithm for imaging biological tissue within the human body at microwave frequencies in collaboration with AFRL/HED (Brooks AFB).

3.1 Complete Families

Of the many methods available one method, a variant of the complete family approach in which a set of linearly independent set of solutions of the underlying partial differential equation is chosen as a set of basis functions, has been of particular interest. Such methods, not in the context of inverse problems but in that of the solution of boundary value problems for known domains, have been used at least since the early 1950's in numerical analysis by, for example, L. Collatz and his students. A new variant is the idea of applying the method to inverse problems in which the boundary of the scattering domain is *unknown*. This consists in the attempt to optimize, over a suitable class of "candidate" surfaces, a cost functional consisting of two terms, the first measuring the error in matching the complete family expansion of the scattered field with the measured far field, and the second measuring the degree to which the assumed representation fails to satisfy known boundary conditions by appropriate choice of the coefficients and the unknown surface. Related to these methods is the study of non-radiating sources mentioned above in regard to the development of tomographic based forward solvers. The NR sources form the null space for linearized inverse scattering and determine hard bounds on the degree to which a penetrable scatterer such as a real airplane can be determined from scattering data.

A working code was developed that alternates between two optimization problems, one which minimizes the defect in the boundary conditions and one which minimizes the deviation between the far-field pattern for the trial surface and the observed far-field pattern. The code has been tested on canonical shapes used by other investigators and has proved very rapid in the 2D case. The method has likewise been tested on problems in waveguides. However in that case we have found that there are serious questions regarding the well-posedness of the boundary value problems in that setting. In particular, there are serious questions concerning the uniqueness of solutions of the original boundary value problem which is crucial to the development of any inverse method. We have developed a new way to formulate the radiation condition which allows a uniform way to characterize scattering problems in free space as well as in spatially restricted domains. These characterizations which involve the notion of reciprocity and radiation conditions are likewise of interest for problems of layered media.

3.2 Modified Gradient Methods

It is also possible to represent the scattered field as a solution of an integral equation rather than a superposition of members of a complete family. The methods are similar in that the field and the unknown contrast or refractive index are simultaneously reconstructed by iterative minimization of a functional containing two terms the second of which represents the residual error in satisfying the integral equation rather than the boundary condition. The optimization method used here is a conjugate gradient method and the efficiency of the method depends on how the step sizes are chosen at each iteration.

Recent work has shown that striking improvement in the fidelity of the reconstructions in this modified gradient method was achieved by incorporating into the functional that is to be minimized a penalty term consisting of the total variation of the contrast. The choice of penalty parameter and the efficacy of the penalty term in cases of high contrast and in other algorithms are but some of the questions that are proposed for further investigation.

As with all ill-posed problems, it is crucial to incorporate *a priori* information whenever possible. In several striking examples when the algorithm was modified to incorporate the information that the scatterer was perfectly conducting, it successfully reconstructed shapes in a "blind test" from experimental data supplied by AFRL/SN (Hanscom AFB).

The iterative gradient methods are available for the reconstruction of the profile of an inhomogeneous penetrable scatterer. These methods have applicability in particular, in the realm of medical imaging. There are also other methods which have initially shown promise, in particular, the dual space method which was effective in the reconstruction of two dimensional inhomogeneous media. The objective is to image structures inside the human head using microwave radiation, a task which will require a 3 dimensional algorithm for dispersive media. Essential to this task was the use of efficient 3D

electromagnetic forward solvers, also a priority of the MURI effort.
These methods, which fall under the classification of modified gradient methods have also been used to analyze the inverse problem for TE mode which leads to a domain singular equation. The method has proved effective in numerical experiments to determine the basic features of a scattering object such as shape, location, and index of refraction.

3.3 Regularized Sampling Methods

The study of inverse scattering problems related to detecting buried objects has also been pursued on two fronts. The problem of detection of shape and location of an object embedded in a homogeneous half space has been considered using variants of the modified gradient method. Multifrequency data has also been used and various results from different inversion algorithms compared. Much of the work has been summarized in the Ph.D. dissertation of J. Coyle at Delaware, and in subsequent papers of Colton and Monk and others including a major review article appearing in SIAM Review.
On another front, the problem of detection of an object embedded in a medium consisting of one of two layers (air and earth) has been investigated. Here, the objects are assumed to be anisotropic, inhomogeneous and possibly conducting and the inversion is carried out from measurements of the field scattered into the upper layer when the system is illuminated at microwave frequencies. No *a priori* assumptions are made here regarding the number of buried objects.
Traditional optimization approaches to this problem are difficult to implement. Instead we simply wish to find the location and size of the buried objects and not their precise properties. We have shown that this is possible from the given data, although this problem is very sensitive to measurement noise. This "ill-posedness" needs to be handled carefully.
The previously mentioned considerations have led us to use the "regularized sampling method" originally introduced for isotropic media. Our work extends these results to the case of a buried anisotropic scatterer. Numerical tests of the method have been carried out and show that the algorithm can detect buried objects.

4 Complex Media

The primary objective of this part of the research effort, carried out primarily at the University of Arizona, but also at MIT, was to develop an understanding of the physical processes involved with the interactions of ultrafast electromagnetic pulses with complex materials and structures. The project developed the analytical and numerical modeling techniques that will allow the self-consistent coupling of macroscopic phenomenological macroscopic material models and microscopic, nonresonant and resonant quantum mechanical material models with macroscopic Maxwell's equation electromagnetic field solvers. Emphasis was given to developing the techniques required to model the diverse space and time scales associated with these large-scale electromagnetic structures. The resulting simulators can be applied to a variety of propagation and scattering problems of relevance to EMI/EMC; vulnerability and susceptibility which speaks to the role of HPM and new remote sensing; and communications applications.
Some of the original tasks addressed were:

1. to develop the tools and techniques for modeling the interaction of ultrafast intense fields with two and three dimensional structures and materials;

2. to further develop and validate phenomenological linear and nonlinear material models;
3. further development of multi-level atomic quantum mechanical material models;
4. integration of these material models in propagation and scattering studies dealing with continuous-wave and ultrafast-pulse interactions with resonant and nonresonant materials and structures to understand their impact on military and commercial remote sensing and communications systems; and
5. the integration these materials into a variety of integrated electromagnetic structures to design and develop novel electromagnetic communications components and systems.

Specific applications include:

1. propagation in complex materials including linear and nonlinear electric and magnetic coatings,
2. scattering from passive and active corrugated surfaces (frequency, polarization, and amplitude selective structures), and
3. aperture coupling into highly resonant cavities loaded with linear and nonlinear passive and active materials and devices.

These applications are clearly closely related to the work discussed previously, e.g. in the development of direct solvers using absorbing boundary conditions. This modeling tool set can also be used to investigate the design of ultrafast electromagnetic pulses to optimize the interactions with and the performance of these systems.
Specific developments persued were:

1. linear passive artificial material models to realize, for example,
   (a) time-domain Debye materials for polarization and magnetization fields;
   (b) time-domain Lorentz materials for polarization and magnetization fields;
   (c) time-domain time derivative Lorentz materials for polarization and magnetization fields;
   (d) time-domain two time derivative Lorentz materials for polarization and magnetization fields.

   These artificial materials are realized by connecting an electrically small electric dipole and magnetic loop antennas to complex passive loads.
2. Active, nonlinear artificial material models to realize, for example,
   (a) differentiators;
   (b) negative impedance compensators;
   (c) phase shifters; and
   (d) curve shapers.

   These artificial materials are realized by connecting an electrically small electric dipole and magnetic loop antennas to complex active loads.

3. A polarization and magnetization field based numerical absorbing boundary condition (ABC) in 1D, 2D, and 3D FDTD simulators for lossy media based on the two time derivative Lorentz materials;

4. The numerical simulation capability to model all of these artificial linear and nonlinear materials;

5. Continued development of a two-dimensional two-level and three-level Maxwell-Bloch equation FDTD simulator;

6. The capability to model photonic band gap structures;

7. Use of 1D and 2D FDTD simulators to model ultrafast pulse interactions with a variety of waveguide grating structures;

8. Integrating photonic band gap structures with waveguide grating structures to achieve enhanced output couplers;

9. Demonstrating the feasibility of optical diode and triode configurations based upon scattering gratings loaded with two-level atom materials;

10. A discrete differential form approach to the numerical simulation of Maxwell's equations on unstructured meshes.

In addition, persuit of these accomplishments led to a number of new results some of which are listed below:

1. The development of Maxwellian-based absorbing boundary conditions (ABCs for 1D, 2D, and 3D FDTD simulators for both lossless and lossy materials. These ABCs were demonstrated to be as effective as the now-popular Berenger PML ABC, but more cost effective to implement. The artificial material work was a spin-off of the successful numerical-based ABC efforts.

2. The design of highly absorbent matched materials with the passive molecules. These have a number of practical applications including radar cross section mitigation and the design of anechoic chambers. Artificial magnetic walls with the passive molecules which may have applications to shielding from power lines and to magnetic insulation for particle beam transport have also been designed. The active molecules can be used to have a surface actively respond to an interrogating signal. These "smart skins" can have a number of manufacturing and target identification applications involving civilian and military cars, ships, and airplanes.

3. The 1D and 2D FDTD simulators have been used to study the effects of ultrafast pulses on grating assisted output couplers and mode converters. Further, an approach to designing gratings for use in mode converters in planar integrated optics systems as been developed. Enhanced waveguide grating assisted output couplers using photonic bandgap materials have also been successfully designed. These enhanced couplers can be used as switches between guided and radiation modes. Enhanced radiation mode couplers that can be used to interconnect two distant waveguides has also been designed.

4. Photonic bandgap materials have been carefully studied. These are synthetically realized materials which make use of dielectric and magnetic materials placed in a periodic fashion. We have studied micron-sized waveguiding structures and vertical cavity surface emitting lasers

(VCSELs) with our simulators. Active regions in these structures with our Maxwell-Bloch solver were included.

5. The usefulness of the two-level FDTD Maxwell-Bloch simulator was established. We have used it to model in detail gratings loaded with resonant two-level atom materials. These loaded gratings lead to gain in and beam steering of the scattered field. Such optical diode and triode configurations may have significant impact on all-optical switching schemes for civilian and military integrated photonic systems.

6. A discrete differential form approach to obtaining the numerical update equations for solving Maxwell's equations on an unstructured mesh was also analyzed. The analysis has revealed defects in the discrete surface integral (DSI) algorithm. These defects may explain why the DSI algorithm develops instabilities at late times for some meshes.

5 Antenna Design

? Antennas, which are devices for transmitting or receiving ? electromagnetic energy, can take on a variety of physical forms. They ? can be as simple as a single radiating dipole, or far more complicated ? structures consisting of nets of wires, two–dimensional patches of ? various geometric shapes, or solid conducting surfaces. Regardless of ? the particular nature of the device, the desire is always to transmit or ? receive electromagnetic signals in a desirable and efficient manner. ?
Air Force interests in the area of antenna design are motivated by ? the need to optimize the efficiency of these devices for ? communication, target identification and HPM. They typically involve the ? optimization and control of both radiated and scattered field either ? by the manipulation of feedings to the various elements of the ? antenna, or by actual on-line control of the geometry of the antenna ? structure or even of the constitutive parameters of the radiating ? surfaces that constitute the antenna. Problems of interest include ? beam forming, null-placement, various synthesis or pattern matching ? problems and the analysis of antenna/platform interactions. ?
Optimization methods in antenna design have a long history. A published ? overview of some of the mathematical problems involved, studied a number of such practical problems in a functionals defined in the appropriate functions spaces. Methods of functional analysis and optimization theory can be used to study the existence and properties of optimal solutions, and to develop computational procedure for the numerical approximation of these solutions in concrete cases. These considerations formed part of the motivation in the original proposal. Part of the effort under the MURI grant was devoted to a number of extensions of both computational and theoretical results. A good portion of the grant effort in this particular area was devoted to the preparation of a monograph which is to appear in 2003 published by Springer-Verlag.
In summary, several lines of research were addressed:

1. The expansion of the number of examples treated with multicriteria optimization methods with particular emphasis on comparison of results for optimal antenna synthesis problems which appear in the literature.

2. The development of efficient algorithms for the computation and display of Pareto surfaces.

3. The investigation of the use of conductivity, resistivity, and higher order impedances as controls for optimizing radiation and scattering characteristics.

4. The investigation, both in the time and frequency domains, of techniques of adaptive control in the detection and steering of electromagnetic signals.

5.1 Multicriteria Optimization

A significant part of the research on antenna optimization has been in the area of MULTICRITERIA OPTIMIZATION. It has long been recognized that the narrow focusing of the main beam of an antenna has the concomitant effect of increasing unwanted side lobe power thereby decreasing the efficiency of the antenna. The design of such an antenna leads to a typical optimization problem with conflicting goals as was recognized by Dolph. The approach used by Dolph and used ever since, has been to control one criterion with an inequality constraint, while optimizing the other. In contrast we have introduced here the techniques of multicriteria optimization for these problems. We considered both Dolph's problem of finding a current distribution which simultaneously maximizes the half–power beam width in the main lobe while minimizing the height of the side lobes and the problem usually treated as the optimization of the signal–to–noise ratio. The problems were posed as as multicriteria problems and we reported numerical results showing that the optimal currents, here called Pareto points, can be computed and give trade–off curves, the curves illustrating the price exacted for improving one criterion in terms of degrading the other, in a form useful to design engineers.
Results during the grant included work with a post-doctoral student concerning such problems for circular antennas, a doctoral thesis developing new theoretical results of direct interest to computation of Pareto points in specific applications, and a series of reports, related to and extending the fundamental work of Smale, and, in particular, studying crucial topological questions concerning the way in which boundaries of regions are mapped into the range space. As Pareto points must show up on the boundary of regions, these questions are crucial to the understanding of a variety of problems not the least of which is the development of effective numerical procedures for the computation of Pareto points which avoid randomization as, for example, in current applications of genetic algorithms. The work has recently been extended by colleagues in Germany to deal with problems in which near-field intensity as well as far-field directivity need to be considered. Applications of these results have been made to problems of interest to manufacturers of cellular telephones. This work suggests that similar techniques may have application to problems of Air Force concern regarding near-field effects on the human body in highly intensive electromagnetic environments as, for example, cockpits of fighter aircraft.
We likewise considered the application of these multicriteria techniques to problems of control of electromagnetic signals and scattering characteristics as well as for inverse (shape and profile identification) problems. It is important in the investigation of these methods, to expand the number of particular examples treated, to compare the new results with constrained optimization results already found in the literature, and to develop effective numerical codes for the solution of these problems.

5.2 Ultra-wide Band Antennas

Concurrent research within this area was driven by the need for a theory and associated performance criteria for ultrawide-band (UWB) antennas. Conventional frequency domain tools and performance measures do not adequately describe UWB antennas in a number of applications which include high-range resolution (HRR) imaging and automatic target recognition (ATR). Of particular interest are sources (antennas) that generate well-collimated pulsed fields (pulsed beams) and extended (three-dimensional) antennas. One overall goal of the project has been the development of a time-domain (TD) antenna theory that can be efficiently implemented for short-pulse fields. The work in 3-D antennas has been motivated by the 3D antenna developed at AFRL/SN (Hanscom AFB). This antenna formed the focus for much of the research devoted to antenna design and synthesis for UWB antennas during the grant period.

5.3 Time-Domain Formulations

A fully time-domain (TD) formulation of the antenna synthesis problem has been generated and applied in extensive computer simulations. An associated frequency domain theory has also been developed and both approaches have been employed to aid in the development of the 3-D optically excited antenna being developed at AFRL/SN (Hanscom AFB). Recent experiments conducted at AFRL/SN (Hanscom AFB) indicate a good agreement between theory and experiment.
Progress has been made in understanding the role of *non-radiating sources* in optimal extended (3-D) antennas and of determining their role in the inverse scattering problem. This work has led to the development of a procedure for mathematically constructing an orthonormal basis of NR sources and of a procedure for determining the spatial support of a scatterer or antenna from (measured) far field data.

6 Dissertations

The following students defended their theses during the period of the grant. We list them by institution

6.1 Colorado School of Mines

1. Boleg, Jeff, *Parallel QR Decomposition for Electromagnetic Scattering Problems*, June 1997, MS Thesis, Dept. of MCS, Colorado School of Mines.

2. Yang, Lihua, *Parallel Algorithms for Multi-Dimensional Wavelet Transforms on Shared and Distributed Memory Machines*, June 1997, MS Thesis, Dept. of MCS, Colorado School of Mines.

6.2 University of Arizona

1. Rose, Tom, *Finite-difference Time-domain Modeling with Bioelectromagnetic Applications*, December 1996, MSEE Thesis, ECE Dept., University of Arizona.

2. Liang, Tao, *Design and Modeling of Grating Assisted Devices for Microwave and Optical Applications*, July 1997, Ph. D. EE, ECE Dept., University of Arizona.

3. Kaus, Cindy, *Topological and Geometrical Considerations for Maxwell's Equations on Unstructured Meshes*, August 1997, Ph. D. Math, Dept. of Mathematics, University of Arizona.

6.3 MIT

1. Phillips, Joel, *Rapid Solution of Potential Integral Equations in Complicated 3-dimensional Geometries*, June 1997, PhD Thesis, EECS Dept., MIT

2. Kamon, Matt, *Fast Parasitic Extraction and Simulation of Three-dimensional Interconnect via Quasistatic Analysis*, January 1998, PhD Thesis, EECS Dept., MIT

3. Chou, Mike Chuan, *Fast Algorithms for Ill-Conditioned Dense-Matrix Problems in VLSI Interconnect and Substrate Modeling*, June 1998, PhD Thesis, EECS Dept., MIT

6.4 University of Delaware

1. Pelakanos, George, *Direct and Inverse Scattering by an Elastic Inclusion*, June, 1997, Ph.D. Thesis, Dept. of Mathematical Sciences, University of Delaware.

2. Coyle, Joe, *Direct and Inverse Problems in Electromagnetic Scattering from Anisotropic Objects*, June, 1998, Ph.D. Thesis, Dept. of Mathematical Sciences, University of Delaware.

3. Nigam, Nilima, *Variational Methods for a Class of Boundary Value Problems Exterior to a Thin Domain*, June, 1999, Ph.D. Thesis, Department of Mathematical Sciences, University of Delaware.

4. Wen, Lixin, *A Two-Dimensional Electromagnetic Inverse Scattering Problem for* **TE** *Irradiation*, December, 1999, Ph.D. Thesis, Department of Mathematical Sciences, University of Delaware.

7 Publications Listing

7.1 Books

1. R. Tolimieri, M. An, and C. Lu *Algorithms for Discrete Fourier Transform and Convolution*, 2'nd ed., Springer-Verlag, New York, 1997.

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3. G. Dassios and R. Kleinman, *Low Frequency Scattering*, Oxford Science Publications, Clarendon Press, Oxford, 2000.

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7.2 Book Contributions

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