

## Research Statement

# Modeling, Analysis and Simulation of Partial Differential Equations Describing Physical and Biological Phenomena

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## 1 General Objectives and Goals:

The mathematical modeling of physical and biological processes involves the description of the underlying science via partial differential equations (PDE's). Important aspects of problems in areas such as electromagnetics, acoustics, elasticity, and population dynamics include the ability to correctly model the physical process by appropriate PDE's, analyze them and accurately simulate the physical phenomena under investigation by using efficient numerical techniques. For most applications closed form solutions of the underlying PDE's either do not exist or are intractable. Thus, in many cases numerical approximation is the most convenient way to solve these PDE's.

My research goals encompass all of the intricacies described above: modeling various phenomena via PDE's, analyzing the wellposedness of the model by proving existence, uniqueness and continuous dependence of solutions, and using efficient numerical methods to accurately simulate the physical or biological process as well as make predictions about the process under investigation from simulations and analysis of the model. Mathematical modeling requires a thorough understanding of the specific physics or biology involved in order to make appropriate simplifying assumptions that are realistic, as well as to identify important variables and parameters, and to find relationships between them which can then be converted into (systems of) PDE's that describe the process completely. Once we have built a mathematical model we have to identify specific mathematical tools such as semigroup theory, homogenization, variational or mixed formulations, etc, to analyze the PDE's in order to obtain an understanding of properties of the model at the continuum level. This in turn is an aid to building accurate discrete methods that mimic properties of the continuum model, such as energy conservation, solenoidal properties, etc, to ensure that the numerical simulations of the model do indeed describe the correct physical or biological process. The availability of real data for comparison with simulations leads to improvements and/or additions to the mathematical model, which in turn leads to more accurate analysis and simulations therefore providing better agreement with the available data.

As a PhD student at the University of Houston, and as a summer graduate research assistant at Los Alamos National Laboratory, I studied numerical techniques for the simulation of wave propagation problems in the time domain using fictitious domain methods, finite element methods, finite difference schemes, operator splitting schemes and perfectly matched layer absorbing boundary conditions. As a postdoctoral research associate at the Center for Research in Scientific Computation at North Carolina State University, I have continued work on the numerical simulation of wave phenomena in dispersive media. We have built a model to simulate the modulation of electromagnetic fields by acoustic waves in dispersive dielectrics. I have used homogenization techniques to calculate the dielectric parameters of composite materials subjected to interrogating electromagnetic fields.

Recently, I have started work on building structured population models for marine species with viral infections.

## 2 Doctoral Research

As a PhD student, I have worked on different aspects involving the numerical modeling of wave propagation problems in the time domain. This area has been gaining momentum over the last few decades due to the broad range of applications that can be analyzed with this approach.

Under the guidance of Dr. James (Mac) Hyman and Dr. Michael Buksas I studied *perfectly matched layer (PML)* absorbing boundary conditions for Maxwell's equations, at the Mathematical Modeling and Analysis group at Los Alamos National Laboratory. Simulation of wave propagation often leads to problems defined on unbounded domains. This is the case, for example, in problems involving the scattering of electromagnetic and acoustic waves by a reflective object. In the PML approach, the numerical computation can be effectively restricted to a bounded domain by surrounding it with absorbing layers in which outgoing waves are trapped and attenuated. These layers are computationally easy to implement and perform significantly better than many competing techniques. During the course of this study, I developed and analyzed a uniaxial PML formulation for Maxwell's equations and then constructed the corresponding discrete PML model by employing Raviart-Thomas finite elements in two dimensions.

Under the guidance of Dr. Roland Glowinski at the University of Houston, I developed a *fictitious domain (domain imbedding)* approach along with operator splitting schemes for the solution of acoustic and electromagnetic scattering by obstacles. In a fictitious domain approach, the unbounded exterior problem is solved on a bounded domain, which has a simple shape, like a rectangle, and includes the scattering obstacles. The original initial-boundary value problem is then replaced by an equivalent problem on the extended domain, in which we enforce the boundary condition on the obstacle using distributed Lagrange multipliers. This approach is as efficient as the finite difference approach, but avoids the staircase approximation of the obstacles. I incorporated a PML model for the wave equation written as a first order system of PDE's into the fictitious domain technique. Nédélec mixed finite element as well as conforming finite element methods were used to discretize the models in space. I combined a novel *operator splitting scheme* for time discretization along with the fictitious domain approach to solve the wave scattering problem. My doctoral research [7] has led to two publications [2, 1]. Papers on PML models for finite element and finite difference schemes as well as a fictitious domain method for Maxwell's equations in two dimensions are in preparation.

## 3 Postdoctoral and Current Work

At the Center for Research in Scientific Computation (CRSC), North Carolina State University (NCSSU), I have worked on problems in computational electromagnetics as well as mathematical biology under the guidance of Dr. H. T. Banks. The study of transient electromagnetic waves in lossy dispersive dielectrics are important in areas such as microwave imaging for noninvasive medical applications in which one seeks to investigate the internal structure of an object by means of electromagnetic fields at microwave frequencies. This is done for example, to detect cancer or

other anomalies by studying changes in the dielectric properties (such as permittivity, conductivity, relaxation times, etc.) of tissues. Other potential applications for such interrogation techniques are nondestructive damage detection in aircraft and spacecraft where very high frequency electromagnetic pulses can be used to detect the location and width of cracks that may be present. I have studied the numerical simulation of electromagnetic waves in dispersive media in which the dielectric polarization is described by first and second order polarization models like the Debye and Lorentz models, respectively. My colleagues and I have built a model that features modulation of the material polarization, and thus the behavior of the electromagnetic pulse, by pressure waves. Traveling acoustic pressure waves are generated in the dispersive medium and serve as virtual reflectors for an interrogating microwave electromagnetic pulse propagating in free space and impinging on a dielectric slab. Inverse problems involving electromagnetic interrogation techniques in two dimensions for identifying the dielectric parameters of a Debye medium were performed along with statistical error analysis. This analysis is used to obtain confidence intervals for all the estimated parameters, thereby providing levels of confidence that can be associated with estimates obtained with our methodology. This project is part of ongoing work in collaboration with Dr. R. Albanese of Brooks Air Force Base, Dr. H. T. Banks and Dr. G. M. Kepler of the CRSC at NCSU. The model, along with numerical results and statistical analysis, has been published in [3, 6]. A paper analyzing the wellposedness of our model via energy methods is in preparation. Dr. G. M. Kepler has built an antenna to conduct experiments in the laboratory which verified that very high amplitude pressure waves are required in order to generate detectable acousto-electromagnetic reflections. Her observations agree with numerical simulations that I performed using realistic estimates of acoustic and dielectric parameters that are available in the literature. A summary of experimental and numerical procedures and results will be presented in a forthcoming paper [5].

Another problem that I have considered is the behavior of the electromagnetic field in a material presenting heterogeneous micro structures (composite materials) which are described by spatially periodic parameters. The motivation for this study is the use of electromagnetic interrogating signals (possibly in the Terahertz range) for detection of defects in the insulating foam on the fuel tanks of the NASA space shuttles. Defects in the foam are believed to contribute to the problem of separation of the foam during liftoff, resulting in significant damage to and possibly subsequent destruction of the space vehicle itself. These composite materials are subjected to electromagnetic fields generated by currents of varying frequencies. When the period of the structure is small compared to the wavelength, the coefficients in Maxwell's equations oscillate rapidly. These oscillating coefficients are difficult to treat numerically in simulations. My colleagues and I used the process of homogenization in which the composite material having a microscopic structure is replaced with an equivalent material having macroscopic, homogeneous properties. Hence a system of PDE's with periodically varying coefficients which oscillate rapidly is replaced by a limiting homogeneous system with new effective constant coefficients. The primary purpose here is that the new homogeneous system facilitates computation. Our numerical approximation to this approach involved a recursive convolution method to approximate the integral term. Our results for this study agree well with other techniques that are available in the literature. In addition, our results are valid for general micro structure geometries and afford flexibility in assumptions about material polarization laws. Also, with our approach we can compute homogenized versions of the dielectric response function, which is the kernel of the hysteretic term that describes the material polarization. We have not seen any comparable results related to the dielectric response function in the literature. This work has led to a publication [4] and is an ongoing project in collaboration with Dr. H. T. Banks,

Dr. N. L. Gibson and Dr. D. Cioranescu and her associates at the University Pierre and Marie Curie, Paris VI in France.

Part of my current research also involves discussions of stability, dispersion and phase error analysis for finite element and finite difference schemes in Debye and Lorentz media. In these models, in addition to dispersion, dissipation also plays an important role in long term simulations in which the propagating waves lose energy traveling over long distances. Hence such analyses are very important to identify accurate numerical schemes and suitable discretization variables that simulate the correct physics of the problem. This work is being prepared to be submitted shortly.

I have recently started studying structured population models in viral epidemiology. My colleagues and I have considered a novel approach for developing a stable operational platform for the rapid production of large quantities of therapeutic and/or preventative countermeasures. The ideas that we have developed can also serve as the foundations in designing an economical platform for the production of complex protein therapeutics to replace mammalian cell culture production methods used in the pharmaceutical industry. In [8] we use an approach that involves recruiting the biochemical machinery in shrimp for the production of a vaccine or antibody by infection using a virus carrying a passenger gene for the desired countermeasure. In such a system one might first stock shrimp postlarvae and allow them to grow normally in a controlled environment. Then one infects them with a specific virus, resulting in vaccine production. To mathematically demonstrate the feasibility of this approach we consider a hybrid model of the shrimp biomass/countermeasure production system which has two components: biomass production, and production of countermeasure (antibody/vaccine). We feed the output of the biomass production model as input to the vaccine production model. For initial investigations the amount of vaccine produced is assumed equal to the total infected biomass. Thus, the vaccine production model will be equivalently described by the course of the viral dynamics in shrimp. We have built size and class-age structured population models for the spread of viral diseases in shrimp populations. These models divide the population into compartments in various stages of the disease. Each subcategory is modeled as a (Sinko/Steifer) structured population model with mass (size) and residency times in the compartment (class-age) as the structure variables. In [8] we describe the derivation of our model from first principles as well as conduct simulations of the model using parameter values based on available knowledge about the disease life cycles of specific species. This work is an ongoing project with Dr. H. T. Banks and Dr. S. Hu of the CRSC, Dr. T. Allnut, Dr. R. Bullis and Dr. A. K. Dhar of Advanced Bionutrition Corporation in Maryland and Dr. C. Browdy of the Marine Resources Research Institute in South Carolina. Two papers analyzing the wellposedness of similar nonlinear size and class-age structured epidemic models with compartments using weak formulations and semigroup theory, as well as comparison principles and monotone approximations, to prove existence, uniqueness and continuous dependence of solutions are in preparation [9, 10].

## 4 Future Work

In the future I plan to continue my work in modeling, analysis and simulations in the areas of computational electromagnetics, acoustics and mathematical biology. Specifically, in the area of fictitious domain methods, I am planning to extend my approach to solving scattering problems in three dimensions using PML's, and Nédélec finite elements, along with appropriate operator splitting schemes. Analysis of the resulting mixed-hybrid formulations via the derivation of inf-sup conditions

for the continuous as well as discrete models is required in order to prove existence and uniqueness of solutions. The ideas developed in my PhD thesis can be extended to wave phenomena in other fields like elastodynamics, for example. In the area of dispersive wave phenomena, discussions of stability, dispersion and phase error as well as simulations of dispersive models such as the Cole-Cole model and higher order dispersive media is of interest for biological applications. In the homogenization of periodic materials, we used a recursive method to solve the discrete homogenized equations. A more effective method would be to use an auxiliary differential equation approach for the polarization to obtain a homogenized model. This will enable us to consider inverse problems to estimate dielectric parameters of foam and other materials that exhibit periodic micro structures. In the field of viral epidemiology, analysis and simulations of structured epidemic models for modeling the spread of viral diseases in different populations is important to predict ways in which the disease can be controlled and contained.

As a mathematician it is very important that I continue exploring different theoretical and numerical methods, and keep up with, as well as contribute to, the state of the art in techniques for the analysis and discretization of PDE's. I am interested in collaborating with experts working in different disciplines to explore how mathematics can contribute to solving real world problems via the process of modeling. Interdisciplinary work leads to better understanding of the applications as well as helps in creating new mathematical techniques. Also, as history has frequently demonstrated, methods created and used for one scientific application over time find themselves useful in other fields. Thus it is very important to keep abreast of techniques used in a wide variety of scientific areas and I will continue to expand the various fields of applications that I can contribute to as they become available to me. Lastly, I am interested in further exploring the statistical and probabilistic aspect involved in the process of modeling. Errors enter naturally in laboratory settings leading to data uncertainty. When comparing estimates obtained from numerical simulations to such noisy estimates obtained experimentally, we must provide appropriate measures of uncertainty in order to demonstrate how much confidence we have in our results and thus how successful we are in our attempts to model the given problem. It is this analysis of numerical solutions to a wellposed model formulation that feeds back into model development to close the loop on the entire process of mathematical modeling of physical and biological processes.

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