# EMSW21-RTG Mathematics of Materials
# Model Development, Analysis, Simulation and Control

## NSF Annual Progress Report for 2008-2009

The program "Mathematics of Materials" provides a wide range of interdisciplinary research and training opportunities for undergraduates, graduate students, and postdocs in the mathematical sciences. The research activities are organized around six topics that play a fundamental role in emerging technologies: multifunctional materials, polymers and composites including carbon nanotubes, orthopaedic biomaterials, dynamics of thin material layers, advanced material synthesis, and thermal interrogation of porous materials. Within each topic, investigations focus on fundamental model development, mathematical solution, numerical simulation, and control design. Each project involves substantial collaboration with experimental colleagues that provides interdisciplinary training opportunities to mathematics students and postdocs. The training component is designed to prepare students and postdocs for the varied roles of interdisciplinary research mathematicians. This includes training modules that introduce participants to research and career topics not typically covered in coursework, targeted courses on topics pertaining to research areas and national research agendas, and participation in summer internships and national conferences.

The activities for the time period July 1, 2008 – June 30, 2009 are summarized as follows.

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**Program Website:** `http://www4.ncsu.edu/~mahaider/NCSU_RTG_Site/RTG_Homepage.html`

# 1 Group Research Reports

The six topics comprising the research component of the program are Multifunctional Materials, Polymers and Composites, Orthopaedic Biomaterials, Dynamics of Thin Material Layers, Advanced Material Synthesis, and Thermal Interrogation of Porous Materials.

## 1.1 Multifunctional Materials

**Group Participants**

- *Faculty Leader:* Ralph Smith
- *RTG-Supported Postdoc:* Michael Stuebner
- *RTG-Supported Graduate Students:* Lisa Downen, Ryan Siskind and Donovan Shickley
- *RTG-Supported Undergraduate Students:* David Pate
- *REU-Supported Undergraduate Students:* Joel Shor (Princeton University), John Wallace (VA Tech), Travious Glover (Albany State) and Lee Hallock (University of Wisconsin, LaCrosse)
- *Externally-Supported Graduate Participants:* Jon Ernstberger, Xiang Fan, Heather Wilson, Francesca Reale-Levis
- *Externally-Supported Postdoctoral Participant:* Jayasimha Atulasimha
- *External Participating Faculty and Scientists:* Marcelo Dapino (OSU), Billy Oates (Florida State University), Zoubeida Ounaies (Texas A&M University), Chris Yakacki (MedShape Solutions Inc), and Rick Zrostlik (Etrema Products, Inc)

**Group Website:** `http://www4.ncsu.edu/%7ersmith/multifunctional.html`

**Group Report**

The Multifunctional Materials Group focuses on model development, full and reduced-order simulation techniques, parameter estimation, and control design for a range of materials including PZT, various ferromagnetic compounds, shape memory alloys, polymers and composites, and carbon nanotube-infused polymers.

*Model Development for Shape Memory Polymers*

Shape memory polymers (SMP) are similar to shape memory alloys (SMA) in the sense that they exhibit the shape memory effect and capability to generate and recover from large strains. However, they differ in the sense that these effects in SMP are due to complementary components at the molecular level including cross-links that determine permanent shape and switching segments that specify temporary configurations.

Shape memory polymers and composites provide the advantage of being lightweight, flexible, cost-effective, capable of generating larger deformations than SMA, and they can be tailored to meet specific control criteria. Due to the molecular basis for the shape memory effect in SMP, they can be controlled by light or chemicals as well as by heating. This provides the possibility for employing light as an input for deployment or shape control. It also makes the compounds viable candidates for use as biological or chemical sensors.

Ryan Siskind's dissertation research focused on the development and numerical simulation of constitutive and system models for shape memory polymers employed for high performance actuation. This involves experimental validation using data collected in collaboration with Chris Yakacki, MedShape Solutions, Inc.

*PZT-Based Actuators and Sensors*

Actuators and sensors employing the ferroelectric material lead zirconate titanate (PZT) are being widely investigated for applications requiring high set point accuracy, large input forces, and broadband capabilities. These properties make PZT transducers advantageous in applications ranging from laser positioning to vibration isolation platforms. However, due to its ceramic nature, initial PZT devices proved brittle and were not easily molded to underlying surfaces. This has recently been addressed through the development of actuators such as THUNDER (THin layer UNimorph Driver and sEnsoR), piezoceramic fiber composites (PFC) and Macro-Fiber Composites (MFC); e.g., see figure 1.

Michael Stuebner is investigating the development of models and simulation packages for MFC for subsequent control design. These models are being validated using experimental data collected by Billy Oates and his students (FSU). David Pate is investigating similarities and differences between the Homogenized Energy Model (HEM) and Prandtl-Ishlinskii models for these compounds.

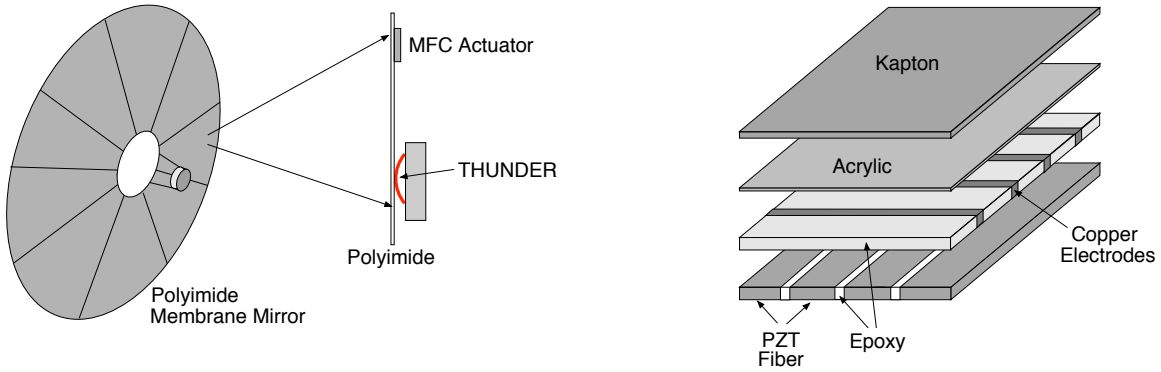



Figure 1: Membrane mirror employing MFC and PZT-based actuators and details regarding the construction of MFC.

*Model Development, Parameter Estimation and Control Design for Terfenol-D Transducers*

Terfenol-D actuators and sensors are presently being considered for a range of applications including sonar transduction, high speed milling, torque sensing, and high fidelity loudspeakers. For all of these applications, however, it is necessary to characterize the inherent material nonlinearities and hysteresis in a manner that facilitates design and real-time control implementation.

Lisa Downen is investigating the development of numerical techniques to reduce implementation times for algorithms. She is presently focusing on algorithms for ferroelectric and ferromagnetic materials but due to the universal nature of the modeling framework, resulting techniques will also likely apply to shape memory alloys. The REU team also investigated the development of algorithms that permit high speed implementation of physics-based hysteresis models.

Michael Stuebner and Jayasimha Atulasimha (VCU) are investigating the development and implementation of homogenized energy models (HEM) in collaboration with Billy Oates (FSU). They are also investigating the development of control algorithms that are being tested at Etrema Products, Inc. Xiang Fan's dissertation research focuses on the development and implementation of adaptive control algorithms for magnetic and ferroelectric actuators.

*Development of Statistical Emulators and Metamodels*

The homogenized energy model (HEM), used to characterize the nonlinear dynamics and hysteresis inherent to ferroic materials is based on energy analysis at the lattice level in combination with stochastic homogenization techniques that incorporate material and field nonhomogeneities.

Due to its energy basis, it incorporates a range of input behavior including stress, temperature and frequency dependencies. However, its incorporation of a range of underlying physics imbues it with a level of complexity that presently precludes real-time implementation at for very high speed applications (e.g., 10 Khz or above).

Graduate student Francesca Reale-Levis is investigating the development of Bayesian and Gaussian emulators that incorporate fundamental physics, are highly efficient to implement, and statistically quantify the uncertainty associated with the resulting reduced-order models.

*Model Development, Simulation and Analysis of Metamaterials*

Metamaterials are often defined as those that engineered to have properties not naturally occurring in nature. Examples include "left-handed" materials having negative indices of refraction. Applications under investigation include super lenses that surpass existing diffraction limits, stealth technology, magnetic resonance imaging, and improved antenna capabilities including the potential for arbitrarily small cell phones. Donovan Shickley is presently investigating model development for active metamaterial structures to improve the dynamic frequency response and bandwidth. An overview of some of these issues can be found in his AMGSS presentation.

*Model Development for Carbon Nanotube-Infused Polymers*

Polyimides are a class of polymers that are thermally and chemically stable, radiation resistant, and highly flexible. The inclusion or carbon nanotubes introduces conductivity and provides the compounds with the capability of becoming active structures. Hence they are being considered for a range of aerospace applications including gossamer mirrors and antennas. Heather Wilson is developing fundamental constitutive and system models for nanotube-infused polyimides and structures employing these compounds. The models are being validated using data collected by Sumanth Banda and Zoubeida Ounaies at Texas A&M University.

## 1.2 Polymers and Composites

**Group Participants**

- *Faculty Leader:* Negash Medhin
- *RTG-Supported Postdoc:* Michael Stuebner
- *RTG-Supported Undergraduate Students* Michael Dearman

**Group Website:** `http://www4.ncsu.edu/~mstuebn/RTG_Polymers_and_Composites/`

**Group Report**

The Polymer and Composites Group focuses on Molecular Dynamics (MD) simulations of molecular chains of polyethylene, carbon nanotubes and composite materials. This computational method calculates the time-dependent behavior of molecular systems based on physical and chemical potentials to describe the interaction between the particles. Because of the large number of particles, it is often impossible to find the properties of such extensive systems in an analytical way. Comprehensive software implementations are necessary to handle the complexity of the interactions.

In the first year, based on existing algorithms, an implementation algorithm was developed to compute the physical properties of a polyethylene chain. With the increasing requirement of modeling nanotubes and composites, it was necessary to apply different potentials and to develop new algorithms and code. Whereas in the first year we depended on second-party software to create

molecular chains and nanotubes, we can construct them now by our program. This increased the degree of freedom of possible constellations to model. Michael Stuebner's activities in the group focused on rewriting and improving the MD implementation. There exists now an object-oriented version which allows a simplified use and an easy extension for different types of molecules and composites for future challenges. Parts of the code is implemented using MPI to run in parallel on compute clusters. Thanks to new hardware funded by the RTG project, there is also work going on for a multithreaded version for improved performance. It also allows the simulation of larger particle systems.

Carbon nanotubes exhibit extraordinary strength, unique electrical properties and have an excellent heat conductivity. They are potentially useful in many applications in material science, nanotechnology, electronics and optics. With their enormous tensile strength, they can be used as reinforcements in light-weight materials. To understand their behavior, one has to be able to model the reinforced composite materials. With our MD simulation package, we can model carbon nanotubes packed in polyethylene layers. For this constellation, we are able to compute potential and kinetic energy, stress, strain and temperature over the period of picoseconds. Applying shear or tensile deformations, we can simulate the relaxation behavior of the composite material.

One of the rationales for pursuing the above computations is to help us explore the elastic properties of nanotube/polymer composites based on atomistic simulations. Thus we will consider a composite where single walled carbon nanotubes are embedded in polyethylene matrix. The carbon atoms of the nanotubes and monomers in the polymer chains are assumed to interact through van der Waals forces as are the carbon atoms on different nanotubes and monomers on different chains. However, we carry out full MD simulations on the polymer chains and the nanotubes. This procedure should give us a more accurate picture of the elastic properties of composites based on which we will eventually develop a continuum model.

We are also exploring how we can take advantage of our MD simulation and use it in conjunction with Rouse's model to study the dynamics of polydisperse polyethylene melts. We aim to compute the friction constant important in the Rouse model as well as the viscosity and stress tensor as a function of time. Then, one can explore the study of the viscoelastic behavior of the melt. The undergraduate RTG participant, Michael Dearman, is working primarily in this aspect of the group activities.

Finally, our effort will be directed at quantized molecular structural mechanics modeling of carbon nanotubes. The aim here is to have a more accurate guide to modeling the mechanical behavior under charge-induced strains.

## 1.3 Orthopaedic Biomaterials

**Group Participants**

- *Faculty Leader:* Mansoor Haider
- *RTG-Supported Postdoc:* Michael Stuebner
- *RTG-Supported Graduate Students:* Brandy Benedict, Janine Haugh
- *RTG-Supported Undergraduate Students:* Jeff Olander, Leslie Watkins
- *Externally-Supported Graduate Participants:* Eunjung Kim

**Group Website:** `http://www4.ncsu.edu/%7emahaider/NCSU_RTG_Site/OBGroupPage.html`

**Group Report**

In Year 2, the Orthopaedic Biomaterials group was comprised of the members listed above and held group meetings roughly once a month. In addition to the RTG-supported members of the group, one other graduate student working with the Faculty Leader in allied research areas participated in group activities. Of the RTG-supported graduate students, one (Brandy Benedict) successfully defended her doctoral thesis on 7/3/08 and is now employed as a tenure-track Assistant Professor in the Mathematics Department at Merrimack College. Another graduate student (Janine Haugh) commenced RA support on the RTG grant in July 2008.

As detailed on the group website, the research can be summarized as follows.

*Modeling the Dynamic Mechanical Environment of Cells in Articular Cartilage*

Cyclic loading of articular cartilage results in a complex microscale biomechanical environment that affects cellular metabolic activity. Cartilage cells (chondrocytes) are sparsely distributed throughout the extracellular matrix (ECM) and are encapsulated by a pericellular matrix (PCM) that is rich in a distinct type of collagen. A multiscale axisymmetric finite element model was developed for simulating biphasic fluid-solid mechanical interactions in a 3-zone domain subjected to confined compressive loading at varying frequencies. The model was used to conduct a parametric analysis evaluating the dual role of the PCM as both a protective and a transmissive layer around the cell. The protective role of the PCM is illustrated via a plot of traction normal to the cell at a loading frequency of 0.01 Hz.

*A Level Set Reaction-Diffusion Model for In Vitro Cartilage Regeneration*

A mathematical model and numerical solutions were developed for an interface problem that models an in vitro experiment for regeneration of articular cartilage in a localized defect region. In this experiment, a cylindrical tissue explant has a core region removed and replaced with a nutrient-rich hydrogel material. The gel-tissue aggregate is immersed in nutrient-rich media for several weeks. An axisymmetric reaction-diffusion model of this experiment was developed to capture coupling between cell-mediated nutrient absorption and matrix biosynthesis, and diffusive transport of nutrients and matrix constituents. The reaction at the gel-tissue interface was modeled via a level set method and potential effects of local interface curvature were also considered. A parametric analysis was conducted to simulate tissue regeneration times required to completely degrade the hydrogel. Advancement of the gel-tissue interface as the hydrogel degrades is governed by coupled effects of spatial gradients in nondimensional nutrient concentration and the local reaction along the gel-tissue interface.

A detailed summary of activities for each of the current RTG-supported participants is presented in the participant reports detailed in Section 2. Additionally, in Year 2 the following publications resulted from work by students supported in the prior year.

*Publications:*

- M.A. Haider, B.A. Benedict, E. Kim and F. Guilak, "Computational modeling of cell mechanics in articular cartilage," chapter in forthcoming book on *Computational Methods in Biomechanics*, Springer, New York, 28 pages, to appear.
- S.D. Olson and M.A. Haider, "A level set model for tissue regeneration in a cartilage-hydrogel aggregate," *International Journal of Pure and Applied Mathematics*, 18 pages, to appear.

## 1.4 Dynamics of Thin Material Layers

### Group Participants

- *Faculty Leaders:* Michael Shearer (Mathematics), Karen Daniels (Physics)
- *RTG-Supported Graduate Students:* Nick Giffen, Ellen Peterson
- *RTG-Supported Undergraduate Student:* Allison McAlister
- *Externally-Supported Graduate Participants:* Lindsay May (Mathematics), Dave Fallest (Physics)
- *Externally-Supported Undergraduate Participants:* Laura Golick (Physics), Chris Fox (Harvey-Mudd Mathematics)

**Group Website:** `http://www4.ncsu.edu/eos/users/s/shearer/www/RTG_DTML.html`

### Group Report

Two graduate students, Nick Giffen and Ellen Peterson, and undergraduate Allison McAlister are funded by the RTG project. A third student, Lindsay May, is working on a related project. In this report, we describe research projects in which the students have participated. The students work in collaboration with members of Karen Daniels' physics experimental lab, including undergraduates Laura Golick and Chris Fox, who visited from Harvey Mudd College during summer, 2008, and graduate student Dave Fallest. The entire group (including the rest of Daniels' graduate and undergraduate students working in her lab) meets regularly about four times a month, to discuss recent research developments, including experiments, and recent papers related to experimental and theoretical issues. Occasionally, a participant will make a presentation, partly to inform the group, and partly to practice for a seminar, conference or oral examination.

*Models of Granular Flow*

Nick Giffen is working on a model for particle size segregation in granular avalanches. When the particles are fully segregated, all the large particles are above the small particles, with a sharp interface between. However, due to shear in the avalanche, the interface can steepen and break, thereby becoming unstable. The subsequent mixing can be viewed in finite difference simulations of the governing first order nonlinear PDE. NickâĂŹs results this year include an analysis of shock steepening. We formulated an ODE system that completely characterizes when an interior shock forms in finite time. The ODE results are confirmed by PDE simulations with sample initial conditions to probe different cases arising in the analysis. Allison McAlister is working to generalize the ODE analysis to circumstances in which the ODE is non-autonomous, for which analytic results are more limited.

To understand the evolution immediately after breaking, we found an explicit solution in the generic case of a smooth vertical interface with a cubic singularity at a point. However, the solution breaks down at a predictable time, after which the solution structure is clear, but highly implicit. Numerical solutions involve a complicated iteration, and this has been carried out for a short time. As the evolution proceeds, even this structure breaks down in a predictable way, and the subsequent propagation of a mixing zone has a simple structure that nonetheless has to be calculated numerically. In a special case, of a piecewise quadratic initial interface, the beginning structure can persist for all time, if the initial curvature is sufficiently large, but for smaller curvature, the solution more closely resembles the final stage of the generic evolution, but this structure appears immediately and persists. This research has been written up in a paper that is currently in the final stages of completion before submission.

A segregation and mixing model is being tested in the lab of physicist Karen Daniels, part of our RTG team. This is joint work between Daniels, Shearer, Lindsay May and undergraduate Kasey Phillips, and is related to experiments of physics undergraduate Laura Golick. In the experiment, glass beads of two sizes are sheared in a Couette cell. That is, the beads fill the space between concentric cylinders, with a heavy top plate that can move vertically, and a bottom plate that can be rotated, providing shear to the material. To test the basic idea of the segregation model, it is modified to suit the experiment. In particular, in contrast to avalanches, the shear rate is not uniform across the material. This complicates solving the PDE, but a simplification is that we can take layers of different size beads, to eliminate one spatial variable. The analytic solution of the model equation is compared to the experimental data through a packing fraction density, that quantifies the local volume occupied by a mixture of small and large beads. This leads to a prediction of the height of the top plate as a function of time. The height is measured in the experiment using an accelerometer.

Two papers relating the model to the experiment are being prepared for journal submission. The first paper treats the theory of the PDE solutions. This is of independent interest, since the coefficients are non-constant in space, and we also treat the case of discontinuous coefficients, the topic of several recent papers in connection with porous media flow. The second paper will give all the details of the experiment, data processing and comparison to theory. Lindsay presented a poster at the SIAM Annual Meeting, in July, 2008, and gave a talk at the Joint Mathematics Meeting in Baltimore in January, 2009. Lindsay expects to graduate in August, 2009, and she begins work in a research group at Northrup-Grummon in September 2009.

*Flow of Thin Liquid Films*

Coating flows can be modeled by the lubrication approximation, leading to a nonlinear PDE. Ellen Peterson's project, in collaboration with physics graduate student Dave Fallest, is to investigate flow down an incline, when the free surface has a distribution of surfactant, which modifies its shape. There are several computational and analysis issues to be explored. Recent progress includes analysis of stability of a traveling wave, numerical simulations of the effect of a small amount of surfactant on an initially flat film, and multiple time-scale analysis of the evolution. The latter shows that the surfactant stimulates the free surface to send off a fast wave, carrying no surfactant, leaving behind, at roughly half the speed, a wave carrying surfactant that continues to deform the free surface. Additional collaborators on this project include Rachel Levy (an NCSU graduate now at Harvey Mudd College), and Tom Witelski (Duke and Oxford Universities). One paper was submitted in Fall, 2008 and has been accepted for publication in the proceedings of Hyp2008, the biennial conference on hyperbolic conservation laws:

- E. Peterson, M. Shearer, T. Witelski, R. Levy, "Stability of Traveling Waves in Thin Liquid Films Driven by Gravity and Surfactant," Proceedings, 12th International Conference on Hyperbolic Problems: Theory, Numerics, Applications, Hyp2008.

Experimental results show an expanding droplet of surfactant, with the thin film distorted into a ridge at the leading edge of surfactant. The spreading rate of the surfactant agrees with scale invariance in the equation, and PDE simulations with rotational symmetry show convergence to the corresponding similarity solution.

We held a one-day conference on January 10th, 2009 entitled "Thin Films Day" at which students from Duke and UNC-Chapel Hill, as well as from our group and Rachel Levy (Harvey-Mudd) gave presentations.

Ellen Peterson gave multiple presentations over the past year, including poster presentations. She attended an IMA workshop on Higher Order Geometric Evolution Equations: Theory and Appli-

cations from Microfluidics to Image Understanding, March 23-26, 2009 and Promoting Diversity at the Graduate Level in Mathematics: a National Forum, MSRI, October 2008.

## 1.5 Advanced Material Synthesis

### Group Participants

- *Faculty Leaders:* Pierre Gremaud (Mathematics) and Jay Tu (Mech and Aero Engineering (MAE))
- *RTG-Supported Graduate Students:* Jeb Collins (7/1/08-12/31/08), William Cousins (6/1/09-Present)
- *RTG-Supported Undergraduate Student:* Rachael Gordon-Wright
- *Externally-Supported Graduate Participant:* A. Paleocrassas (MAE)

**Group Website:** `http://www4.ncsu.edu/eos/users/g/gremaud/WWW/laser.html`

### Group Report

The group conducts has conducted research in two RTG related fields.

*Laser Drilling*

Laser drilling is an important industrial process by which laser pulses are used to drill holes in hard materials. It presents several advantages over conventional techniques such as low heat input into the material, accuracy, consistency, ease to automate and ability to drill very small holes of the order of 10 microns in diameter. This technique is used either with single or multiple pulses.

One of the difficulties in this field is that several different regimes are encountered. During drilling, material is removed from the workpiece through two mechanisms: vaporization and melt ejection. The relative importance of each mechanism has been the object of several theoretical studies. In the case of thermal ablation (roughly the lower left part of Figure 2, left), the interaction of the laser with the material surface creates a molten pool. As some of the material vaporizes, the pressure of the vapor (recoil pressure) is large enough to push the melt radially outward from the center

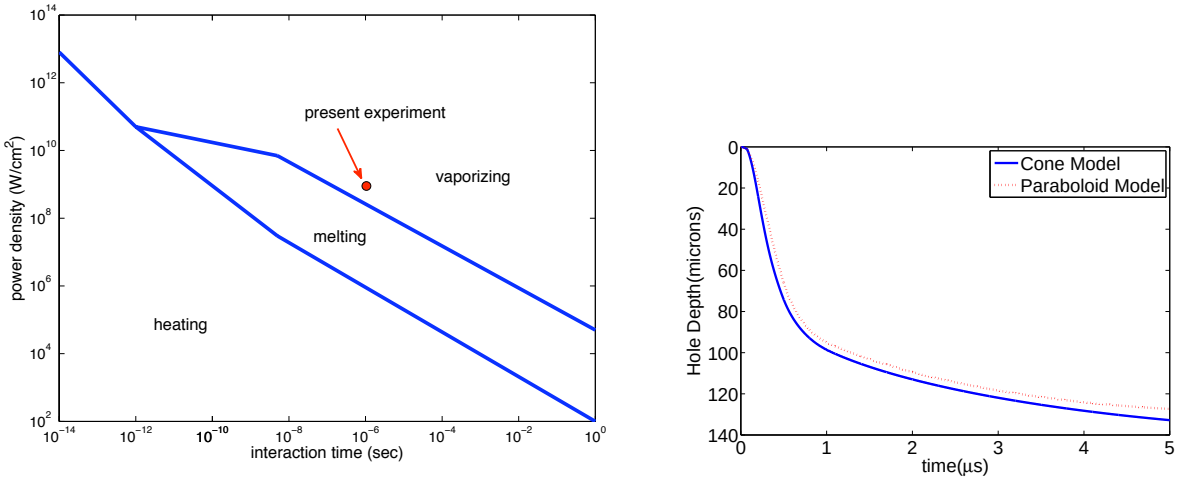



Figure 2: Left: Approximate range of various regimes for laser ablation; right: penetration depth versus time.

| | Hole Depth | Hole Radius |
|---|---|---|
| Experimental Data | 136 $\mu$m | 11.5 $\mu$m |
| One-d. profile ($\ell \to \infty$) | 80 $\mu$m | |
| Conical profile ($\ell = 1$) | 133 $\mu$m | 11.1 $\mu$m |
| Parabolic profile ($\ell = 2$) | 127 $\mu$m | 10.5 $\mu$m |

Table 1: Experimental and numerical results.

of the beam, leading to melt ejection. In this study, done in collaboration with the Precision Processing Lab of Jay Tu, Mechanical Engineering, NCSU, a mathematical model is derived, implemented and validated for drilling using lasers with intensities in the GW/cm$^2$ range and microsecond pulses. The present study corresponds to non-thermal ablation (roughly the upper right part of Figure 2), left, which corresponds to higher melt surface temperature, the main process by which melt is removed is through evaporation instead of convection as the material vaporizes before it can get convected in any significant way.

The present study retains simplified one-dimensional formulations, obtained through cross-sectional averages, but combines these with the possibility of describing the shape of the drilled hole, a novel feature for this type of models. The model itself relies on classical thermodynamical arguments, careful description of the rapid evaporation process through kinetic theory and classical gas dynamics. As can be seen from Table 1, the model provides a fast, inexpensive and accurate way to predict penetration depth, the most important variable with respect to applications. Figure 2, right, displays the time behavior of the penetration depth.

The present work is a first step toward the design of a fully controlled laser drilling system to be developed in collaboration with Prof. Tu's group.

These results were presented at the AMS Sectional meeting at NCSU, April 4, 5, 2009 and will be presented at the SIAM annual conference in Denver, CO, July 6–10, 2009.

*Publications:*

- J. Collins and P. Gremaud, "A simple model for laser drilling," em Mathematics and Computers in Simulation, submitted.

*Granular Free Surfaces*

Precision agriculture is a fast developing research field which aims at optimizing all aspects of agricultural production. The combined use of GPS technology and on the ground sensors will allow farmers to take into account variations within fields. We investigate the behavior of agricultural spreaders which play a key role in the application of seeds, fertilizers and pesticides. The grain spreading process consists of two distinct phases: first, a mechanical phase, in which the grains are accelerated by rotating arms, see Figure 3, left, and second, a ballistic phase in which the grains/particles fly through the air. Our offers a new mathematical model of the above mechanical phase. So far, we have done study of the steady state equations of centrifuged granular systems. The resulting equations are akin to the St-Venant equations but where the driving external force is the centrifugal force instead of gravity. This work is done in collaboration with Rachael Gordon-Wright. A time dependent model has also been developed, see Figure 3, right. This latter model is being developed in collaboration with François Rioual, CEMAGREF, France, in whose lab experimental as well as discrete mechanical data are being gathered. These results were presented at the 7th Euromech FLuid Mechanics Conference, Sep. 14–18, Manchester UK, 2008.

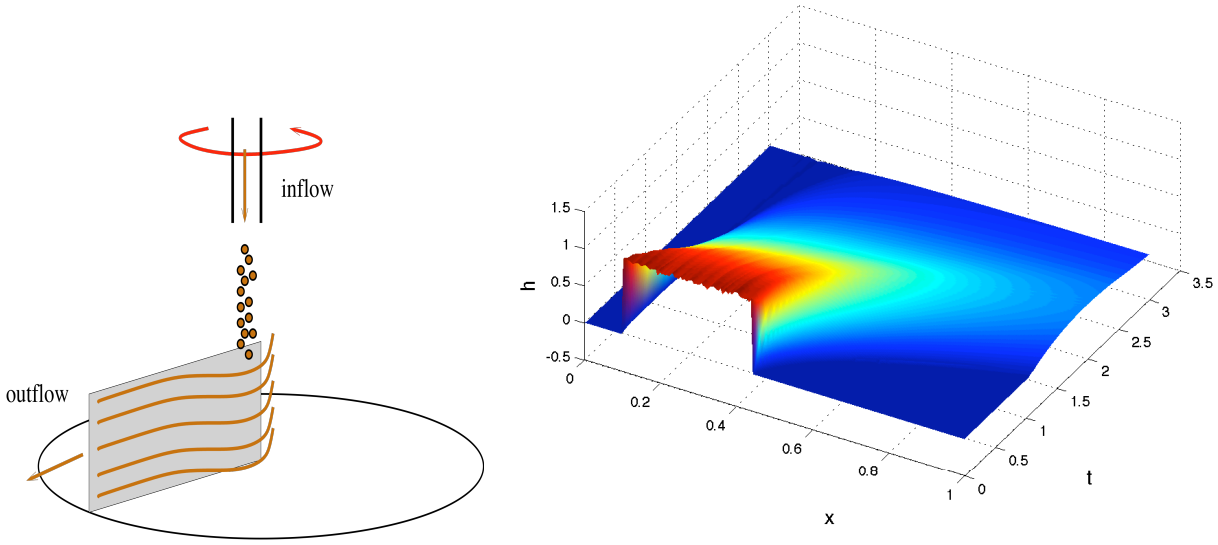



Figure 3: *Left: General experimental setup of the spreader system with one rotating arm and grain inflow through a funnel, right: evolution of the profile under rotation.*

*Publications:*

- P. Gremaud, "Granular free surfaces," *SIAM Review*, submitted.
- P. Gremaud and F. Rioual, "Depth averaged model for grains spreaders," in preparation.
- R. Gordon-Wright and P. Gremaud, "Determination of granular free surfaces under rotation," in preparation.

*Future Work*

William Cousins, graduate student, will start working on mathematical modeling of blood perfusion. The issue here is distinct from classical hemodynamics problems where fluid dynamics models are appropriate. As part of the project, we will revisit some not full understood models of circulations in capillaries and their influence on the overall blood flow (structured tree boundary conditions). We will also develop new models how blood cerebral perfusion per se (i.e., away from any major vessels). In the spirit of homogenization theory, porous medium like models will be investigated.

## 1.6 Thermal Interrogation of Porous Materials

### Group Participants

- *Faculty Leader:* H.T. Banks
- *RTG-Supported Graduate Students:* Amanda Criner
- *External Participating Scientist:* William Winfree (NASA Langley Research Center)

**Group Report**

The goal of our research is to develop an efficient method to thermally interrogate porous materials for both damage detection and characterization. Nondestructive evaluation (NDE) is a very useful tool that enjoys widespread use in testing structures, especially as they age beyond their design life. Proper use of NDE can increase the safety and service life of components in aircraft, spacecraft, automobiles, trains, and piping. There are numerous viable NDE methods including ultrasound, magnetic particle imaging, eddy current, acoustic emission, and radiology to mention a few [8]. These methods have been successfully developed for a large range of problems, particularly for homogeneous metallic structures [2–5]. Composite materials are lighter and stronger than metallic materials, however, are inherently nonhomogenous and often are fabricated with acceptable levels of porosity. These materials are used in many critical structures including aeronautical and aerospace vehicles, so there is a need to develop and evaluate NDE techniques for these materials [7, 11]. Particular advantages of thermal NDE are that it is a single sided, noncontacting and a large area technique making in-service evaluation feasible. It is also possible to embed temperature sensors in the material [9] for continuous structural heath monitoring. We treat here the problem of thermal NDE in porous materials.

In [1], we developed simulations to represent the physical problem with a $L_1$ by $L_2$ rectangle, where $L_2 = 2L_1$, with randomly placed pores. Let $\Omega$ denote the rectangle minus $N$ pores, which are given by $\Omega_1, \Omega_2, \ldots \Omega_N$. The entire region is then $\hat{\Omega} = \Omega \cup (\cup_{i=1}^{N} \Omega_i)$. The exterior boundary of $\Omega$ has 4 edges, which we denote by $\omega_j$ where $j$=1, 2, 3, 4. Each pore $\Omega_i$ has a smooth boundary with $\Omega$ given by $\partial\Omega_i$, as depicted in Figure 4. In this procedure, a damage is represented by an unusually large pore, which is consistent with damage due to oxidation.

We developed many different algorithms to generate porous domains. These algorithms use different probability distributions to choose the major and minor semi-axes of the pores. These algorithms were used to simulate examples with different percent porosity (2%, 5%, and 10%). We used MatLab's PDEtoolbox to solve the heat equation on these domains. We would then place a damage (a large ellipse) on the same domain, again solve the heat equation and then compare the temperature results.

We varied damage size, considering elliptical damages with widths 0.7 mm, 1.05 mm, and 1.4 mm at different locations within the 2 mm by 1 mm sample. We demonstrated that we could detect certain damages, depending on the percent porosity of the sample, size and location of the damage, as well as the resolution and location of the temperature sensor.

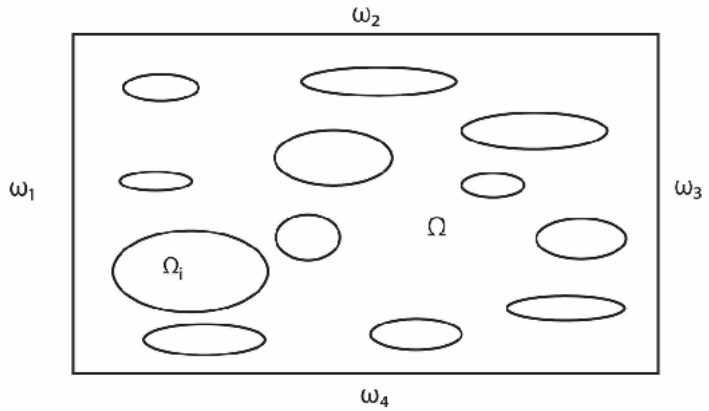


Figure 4: A typical example of a 2-D specimen

The simulations presented in [1] are convenient to investigate different porosity schemes and damage sizes but are too computationally intensive for the iterations required in parameter estimation algorithms, so damage characterization is not achievable with this scheme. Furthermore, the methodology used in [1] would not be appropriate in a 3-D setting. However, we can use these simulations to evaluate approximations of the porous domain which would be appropriate in damage characterization and parameter estimation. We improved these simulations by using a result in [10] to better approximate the distance between two ellipses, which improved the generation of the random porous domain. This change allows us to carry out sufficiently many simulations to have large sample sizes so we can make conclusive statements regarding the efficacy of our approximation of the porous domain.

Our goal is to find approximations of the effect of the porous domain which are feasible for the inverse problem and thus damage characterization. So we replace the typical porous domain, which has over 70 ellipses and over 75000 mesh points in the finite element routine, with a homogeneous domain on which we solve a limiting or homogenized heat equation with an "effective" thermal diffusivity. We suspect homogenization theory will provide a good approximation of the porous domain.

Homogenization theory assumes periodicity in the coefficients of the partial differential equation. This is physically justified; porosity of composite materials is typically periodic because it is a product of periodicity in the manufacturing process. The usual homogenization theory [6] requires that periodicity go to zero in some sense. The periodicity of the coefficients is a result of periodic geometry (for instance we could have a geometry with an infinite number of infinitely small circles within a rectangle, see Figure 5) though homogenization can be applied to much more complex geometries.

Homogenization also has a rigorous mathematical foundation. Recall the heat equation, below,

$$\frac{\partial u}{\partial t} - k\Delta u = 0, \quad \text{in } \Omega, \tag{1}$$

with boundary conditions,

$$\left.\frac{\partial u}{\partial \eta}\right|_{\cup_i \Omega_i} = 0, \quad \left.\frac{\partial u}{\partial \eta}\right|_{\cup_{i=1}^3 \omega_i} = 0, \left.\frac{\partial u}{\partial \eta}\right|_{\omega_4} = S_o \chi_{[t_o,t_s]}(t), \tag{2}$$

and initial condition

$$u(x,0) = u_o. \tag{3}$$

The above formulation has one distinct problem, the boundary conditions do not give a unique solution in $H^1(\mathbb{R}^2)$. We will restrict solutions to $\tilde{H}_0^1(\mathbb{R}^2)$ by replacing (2) with

$$\left.\frac{\partial u}{\partial \eta}\right|_{\cup_i \Omega_i} = 0, \quad \left.\frac{\partial u}{\partial \eta}\right|_{\cup_{i=1}^3 \omega_i \setminus \omega_5} = 0, \quad u\big|_{\omega_5} = 0, \quad \left.\frac{\partial u}{\partial \eta}\right|_{\omega_4} = S_o \chi_{[t_o,t_s]}(t), \tag{4}$$

where $\omega_5$ is a small portion of the back boundary.

We approximate (1), (3)–(4) on the porous domain by considering a related problem on a domain composed of the disjoint union of compressed reference cells, as in Figure 5. The reference cell is given by a 2 by 1 rectangle with pores $\Omega_i$ and material $\Omega$. The reference cell is composed of much fewer pores (an order of magnitude) than in the original problem. The limit problem is formulated on a geometry composed of rectangles, $2\epsilon$ by $\epsilon$, where $\epsilon \to 0$. Within each rectangle are the pores $\Omega_i^\epsilon = \epsilon\Omega_i$ depicted in Figure 5.

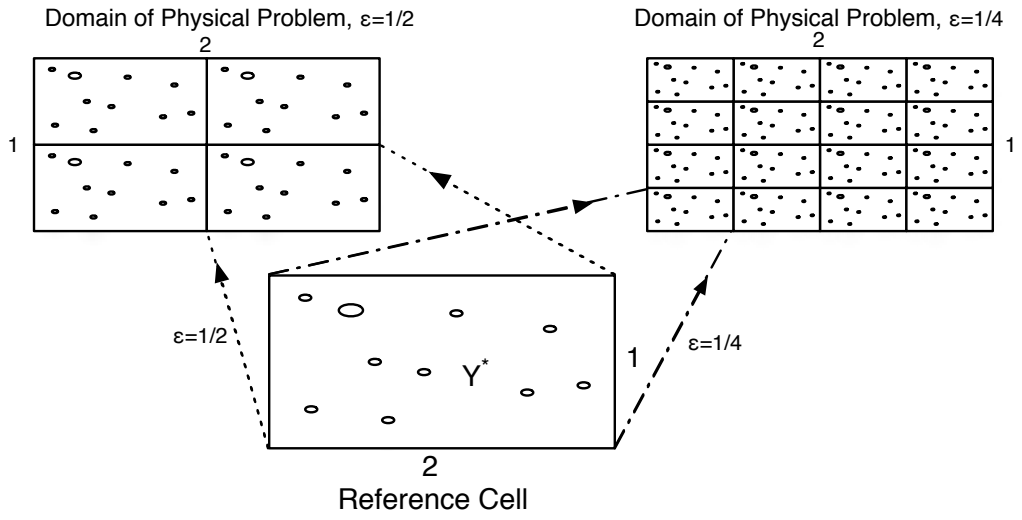



Figure 5: The reference cell and the physical domain with $\epsilon = \frac{1}{2}$ and $\epsilon = \frac{1}{4}$.

On this domain the following partial differential equation,

$$\frac{\partial u_\epsilon}{\partial t} - k\Delta u_\epsilon = 0, \quad \text{in } \Omega^\epsilon, \tag{5}$$

converges weakly to

$$u_\epsilon \rightharpoonup \theta \hat{u},$$

where $\theta = \frac{|Y^*|}{|Y|}$, $|Y^*|$ is the area occupied by material in the reference cell and $|Y|$ is the area of the whole rectangle. The limit $\hat{u}$ is given by the solution of

$$\theta \frac{\partial \hat{u}}{\partial t} - k\nabla \cdot (A^0 \nabla \hat{u}) = 0 \tag{6}$$

$$\hat{u}(x,0) = \theta u_o$$

$$\left.\frac{\partial \hat{u}}{\partial \eta_{A^0}}\right|_{\cup_{i=1}^3 \omega_i \setminus \omega_5} = 0, \quad \hat{u}\Big|_{\omega_5} = 0, \quad \left.\frac{\partial \hat{u}}{\partial \eta_{A^0}}\right|_{\omega_4} = \theta S_o \chi_{[t_o,t_s]}(t). \tag{7}$$

The matrix $A^0$ is a matrix with constant coefficients. The coefficients of $A^0$ are found by solving two elliptic partial differential equations on the reference cell and represent (along with $k$) an "effective" thermal diffusivity.

This approximation reduces the number of mesh points used in [1] by an order of magnitude but the reference cell must be generated only once (which takes about 20 seconds) to obtain $A^0$ and then (6) is easily solved with classical techniques. The parabolic problem on very a complicated domain becomes a less complicated elliptic problem on one reference cell and a parabolic problem with constant effective diffusivity on a homogeneous domain.

We believe that homogenization will also be useful in detecting damage in porous material. If we replace the homogeneous domain in (6) with a homogeneous domain that has one void that represents potential damage, then we can readily carry out an inverse problem to estimate $k$ in (6) to identify the damage in the sample. We plan to pursue this direction of research in the coming months. We plan to validate this approach with data obtained from the NASA NDE Branch labs' (W. Winfree) experiments designed and carried specifically in support of our research.

# 2 Individual Postdoc, Graduate and Undergraduate Reports

During the reporting period, 1 postdoc, 7 graduate students, and 6 undergraduate students were supported by the RTG. In this section, we summarize their research activities, presentations, conferences and workshops attended, papers, and personal statements.

| **Postdoc** | **Graduate Students** | **Undergraduate Students** |
|---|---|---|
| Michael Stuebner | Jeb Collins (4th year) | Michael Dearman (Senior) |
| | Amanda Criner (2nd year) | Rachael Gordon-Wright (Junior) |
| | Lisa Downen (2nd Year) | Allison McAlister (Junior) |
| | Nicholas Giffen (4th Year) | Jeff Olander (Senior) |
| | Janine Haugh (4th Year) | David Pate (Junior) |
| | Ellen Peterson (3rd Year) | Leslie Watkins (Senior) |
| | Donovan Shickley (1st Year) | |

## 2.1 Postdoc Reports

### 2.1.1 Michael Stuebner

**Summary of Research Activities**

In my second year as a postdoctoral associate in the Research Training Group “Mathematics of Materials," I continued my research in three of the subgroups. In the areas of *Polymers and Composites*, I advanced the molecular dynamics simulation software. Besides simulations of polyethylene chains we are also able now to carry out computations for carbon nanotubes and composite materials made out of nanotubes and polyethylene chains. In the *Multifunctional Materials Group*, I continued working on the homogenized energy model and did modeling and parameter identification for Macrofiber composite and PZT patches. In the field of *Orthopaedic Biomaterials*, I started implementing biphasic poroviscoelastic models for articular cartilage and investigate alternate approaches for computing an expensive stress-strain integral which is part of the model.

*Polymers and Composites*

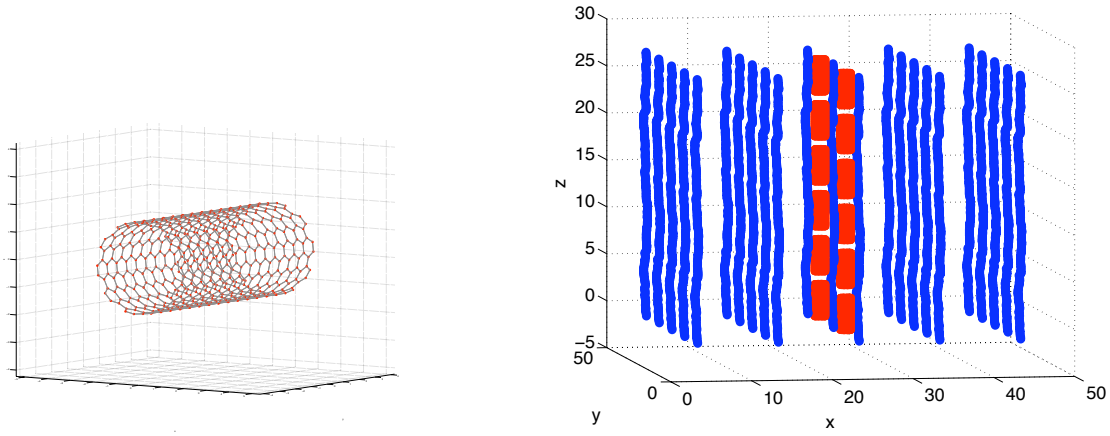
My focus in this group is on simulations which can be used to study the mechanical and physical properties of proteins and polymers as well as the electronic properties of nanoscale devices and nanomaterials. The goal is to accomplish parametric studies of the influence of material and geometry to understand the effects of loading on specific regions of polymer-nanotube composites. To achieve that goal, it is necessary to have a thorough understanding of the mechanical and electrical behavior of molecules and nanotubes. Unfortunately, it is often not practical to go to a laboratory and do experiments. Some of the properties are hard to obtain whereas others are impossible to measure. A way around this problem is to use Molecular dynamics simulations. It is a multidisciplinary method and includes laws and theories from mathematics, physics, chemistry, as well as algorithms from computer science and information theory. Atoms and molecules are allowed to interact for a period of time by approximations of known physics, giving a view of the motion of the atoms. The simulations describe the relationship between molecular structure, movement and function. From a numerical perspective, it is the problem of solving Newton’s equation of motion for a system of particles. Efficient and reliable simulation techniques are needed. It is very important to carry out the simulation long enough to characterize the molecular relaxation process. Last year I implemented the molecular dynamics algorithm for a single polyethylene chain. This year I extended

the computations for layers of polyethylene chains which give a more realistic view on the properties of the material.

A next step was to start studying the properties of carbon nanotubes. First synthesized in 1991 by vaporization of graphite, carbon nanotubes have great strength while being very light. They have a diameter of 1-5 nm, while the length is in the range of microns. Carbon nanotubes are superb conductors of heat and electricity. Potential applications of carbon nanotubes are the use as field emitters, for energy storage and as electrodes in batteries. With the ability to attach essentially any chemical species to their sidewalls, they can be used for catalyst support. Further applications are the use as nanoscale devices like sensors, actuators, electrostatic switches and to reinforce light-weight materials (composites).

Based on this application, our group considered composite structures made out of polyethylene chains reinforced with carbon nanotubes as shown in Figure 6. For this new challenge I had to extend our software. Starting with the creation of the nanotubes, I also added an implementation of the Tersoff potential and the interaction with the molecules. Having complete control over the structure increases the degree of freedom in modeling. The nanotubes can now easily placed in the polyethylene matrix and all interactions are simulated.

For practical application of molecular dynamics simulation, one has to generate an appropriate starting configuration. This requires searching for a global minimum of the potential energy while enforcing the constraints on the system that arise from the bonded interaction potentials. To obtain a starting configuration in a state of equilibrium, a differential evolution algorithm was used. The method is more likely to produce a global minimum while taking into account the constraints inherent in the geometry of the molecule. It is able to extend the search outside of the initialized range of the search space which is a beneficial property in problems with no boundary constraints. In boundary constrained problems, it is essential to ensure that parameter values lie inside the allowed ranges which will be guaranteed by replacing parameter values that violate boundary constraints with random values generated within the feasible range. Differential evolution is inherently parallel and hence is suitable for implementations on multi-processor machines. Thus, we can handle a molecular chain with a large number of monomers or composite materials consisting of multiple chains and nanotubes. I have carried out a simulation on a single processor as well as an MPI version for multiple processors. The parallel version shows a greatly improved speed in finding the configuration with the minimal potential energy.




(a) (b)

Figure 6: (a) Carbon nanotube and (b) composite material.

For the simulation of the polyethylene chains, we considered bonded and non-bonded interactions. Nonbonded interactions model flexible interaction between particle pairs. A well known non-bonded interaction potential is the Lenard-Jones potential. This potential consists of a short-range repulsion and a long-range attraction term. Particles cannot occupy the same position resulting in repulsion between the monomers. On the other hand, because of polarization, electrostatic attraction between the particles is created. Bonded interactions model strong chemical bonds and are not created or broken during simulations. Such interactions impose constraints that have to hold during the simulation. The most common interactions employed in molecular dynamics simulations are the covalent interactions and the bond angle interactions. The bonds will typically involve the separation between adjacent pairs of monomers. The bend angles are between successive bond vectors and therefore involve three monomer coordinates. The last interaction potential we consider is a four-particle torsional interaction potential. The torsion angles are defined in terms of three connected bonds, hence four monomer coordinates. The molecular model is then given by

$$\begin{aligned} U &= 4\varepsilon \sum_i \sum_{\substack{j \\ j>i}} \left[ \left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} \right] + \tfrac{1}{2} \sum_{bonds} k^r_{ij}(r_{ij} - r_0)^2 + \tfrac{1}{2} \sum_{\substack{bend \\ angles}} k^\theta_{ijk}(\theta_{ijk} - \theta_0)^2 \\ &\quad + \tfrac{1}{2} \sum_{\substack{torsion \\ angles}} \sum_m k^{\phi,m}_{ijkl}(1 + \cos m\phi_{ijkl}). \end{aligned} \tag{8}$$

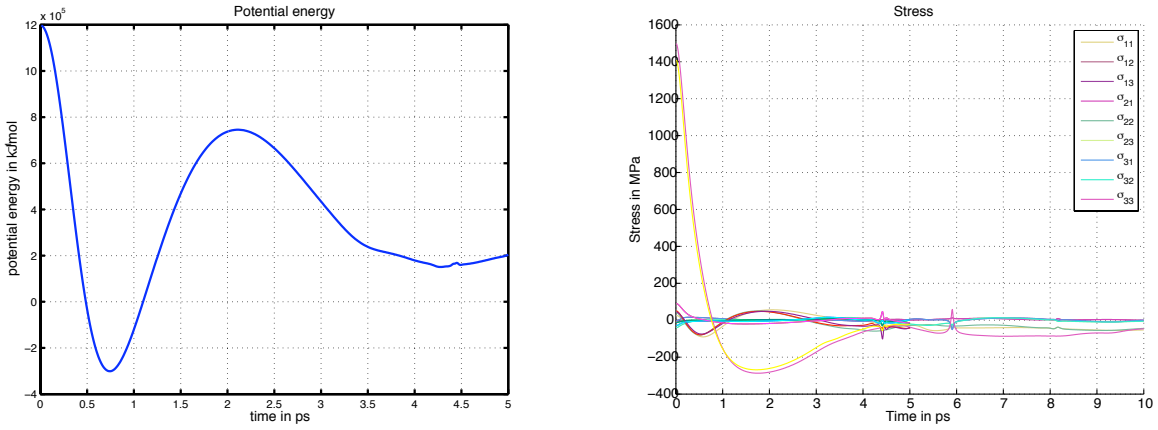
For the simulation of the nanotube, the Tersoff potential is used. It is a three-body potential functional which explicitly includes an angular contribution of the force. The strength of a bond between two atoms is not constant, but depends on the local environment. A bond between an atom $i$ and another atom is weakened by the presence of other bonds involving atom $i$. The Tersoff potential is widely used in various applications for silicon, carbon and germanium. The potential between two atoms $i$ and $j$ is given as

$$\hat{U}_{ij}(\hat{r}_{ij}, \theta_{ijk}) = A_{ij} e^{-\lambda_{ij}\hat{r}_{ij}} - \frac{B_{ij}}{\left(1 + \beta_i^{n_i} \left( \sum_{k \neq i,j} \left( 1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{d_i^2 + (h_i - \cos\theta_{ijk})^2} \right) \right)^{n_i} \right)^{\frac{1}{2n_i}}} e^{-\mu_{ij}\hat{r}_{ij}} \tag{9}$$

with $A_{ij}$, $B_{ij}$, $\beta_i$, $n_i$, $c_i$, $d_i$, $h_i$, $\lambda_{ij}$, $\mu_{ij}$ element-specific parameters and $k$ a bonded atom of either $i$ or $j$. Simulations are also accomplished for a composite material made out of nanotubes and polyethylene. The composite consist of five layers of polyethylene chains. In the middle layer, carbon nanotubes are embedded. Besides the potential mentioned above for the polyethylene chains and nanotubes, the Lenard-Jones potential was used for nanotube-nanotube, polyethylene-polyethylene and nanotube-polyethylene interactions. In one case, a tensile deformation and in another case a shear deformation was applied. The composite was given time for relaxation. The potential energy was computed by summing up all the used potentials. The stress at a monomer/atom $k$ was computed using the virial theorem

$$\sigma^k_{ij} = -\frac{1}{V} \left( m^k \mathbf{v}^k_i \mathbf{v}^k_j + \sum_{n=1}^{N} \mathbf{f}^{kn}_i \mathbf{r}^{kn}_j \right) \tag{10}$$

where $V$ is the volume of the composite, $m^k$ the atomic mass, $\mathbf{v}_k$ the velocity vector and $\mathbf{f}$ the force vector between atoms $k$ and $n$. The results are shown in Figure 7.




(a) (b)

Figure 7: (a) Potential energy and (b) stress for the composite.

*Multifunctional Materials*

In the Multifunctional Materials group, I continued studying the effects of hysteresis and nonlinear behavior of ferroelectric and ferromagnetic materials. The focus was on modeling the response of piezoelectric patches and Macro Fiber Composite (MFC) actuators using a beam model with polarization quantified by the homogenized energy model. The model was validated by data collected in the NCSU CRSC/Math Instructional and Research Laboratory and the Department of Engineering at Florida State University.

Piezoelectric materials such as PZT are increasingly considered for use as actuators and sensors due to their broadband drive capabilities and their relatively high energy densities. They are presently employed in essentially all nanoposition systems such as atomic force microscopes (AFM) due to their high set point accuracy. This property also makes them advantageous for use in the focusing mechanisms for miniature cameras and ultrasonic motors. Macro Fiber Composites (MFC) are planar actuators comprised of PZT fibers embedded in an epoxy matrix that is sandwiched between electrodes. Due to their construction, they exhibit significant durability and flexibility in addition to being lightweight and providing broadband inputs. They are presently being considered for a range of applications including positioning and control of membrane mirrors and configurable aerospace structures.

However, the advantages provided by piezoelectric compounds come at the cost of hysteresis and constitutive nonlinearities at all drive levels. This behavior must be incorporated in models to achieve the full potential of the devices.

The homogenized energy model [15] was chosen to characterize the dynamic behavior of piezoelectric materials due to its capability for characterizing a range of minor loop behavior under highly varied operating conditions. It is a multiscale approach based on energy relations and stochastic homogenization techniques. The macroscopic model quantifies the bulk polarization P by

$$[P(E)](t) = \int_0^\infty \int_{-\infty}^\infty \nu_1(E_c)\nu_2(E_I)[\bar{P}(E+E_I;E_c,\xi)](t)\,dE_I\,dE_c$$

where $\nu_1$ and $\nu_2$ are density distributions, $E_I$ the interaction field and $E_c$ the coercive field. For negligible thermal relaxation the kernel $\bar{P}$ is given by

$$\bar{P}(E) = \frac{1}{\eta}E + P_R\delta(E;E_c,E_I),$$

where $P_R$ is the remanence polarization and $\delta = 1$ if dipoles are positively oriented and $\delta = -1$ if they are negative. If thermal relaxation mechanisms are considered the kernel changes to

$$\bar{P} = x_+ \langle P_+ \rangle + x_- \langle P_- \rangle.$$

The evolution of dipole fractions is quantified by the differential equations

$$\begin{aligned} \dot{x}_+ &= -p_{+-} x_+ + p_{-+} x_- \\ \dot{x}_- &= -p_{-+} x_- + p_{+-} x_+ \end{aligned}$$

where $\langle P_+ \rangle$ and $\langle P_- \rangle$ are the expected polarizations and $p_{+-}$ and $p_{-+}$ the transition likelihoods. These quantities can be expressed in terms of error functions. The parameters of the homogenized energy model have to be identified using experimental data. The identification process yields the minimization problem

$$\min_p \sum_{i=1}^{N} |w^N(t_i, \bar{x}; p) - \hat{w}(t_i)|^2 \tag{11}$$

where $p$ are the parameters, $w^N(t_i, \bar{x}; p)$ is the displacement computed by the model depending on the parameters and $\hat{w}(t_i)$ is the experimental data.

Motivated by the experimental setup shown in Figure 8, we consider a thin cantilever beam of length $\ell$, width $b$ and thickness $h$ that is clamped at $x = 0$ and free at $x = \ell$. We let $\rho, YI, cI$ and $\gamma$ respectively denote the effective linear density, stiffness, Kelvin-Voigt damping and air damping coefficients and we let $w(t, x)$ denote the transverse displacement of the beam.

Force and moment balancing yield the strong model formulation

$$\begin{aligned} &\rho \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0 \\ &w(t,0) = \frac{\partial w}{\partial x}(t,0) = 0 \\ &M(t,\ell) = \frac{\partial M}{\partial x}(t,\ell) = 0 \\ &w(0,x) = w_0(x) \quad , \quad \frac{\partial w}{\partial t}(0,x) = w_1(x) \end{aligned} \tag{12}$$

where the moment is

$$M(t,x) = -YI \frac{\partial^2 w}{dx^2} - cI \frac{\partial^3 w}{dx^2 \partial t} + k_1 [P(E(t)) - P_R] \chi_{pe}(x).$$

For numerical implementation, (12) is employed in weak formulation. The solution is approximated using cubic B-splines. One obtains a second order semi-discrete system which can be rewritten as a first order system that facilitates implementation using standard ODE routines.

In the CRSC/Math Instructional and Research Laboratory at NC State University, I participated in experiments done by Grace Kepler, Adam Attarian and Hien Tran to validate the numerical computations. The experimental setup (see Figure 8) consisted of an aluminum cantilever beam, driven by two surface-mounted piezoceramic patches QP10N [12]. The beam was fixed at one end and the acceleration was measured using an accelerometer located close to the opposite end. Experiments showed that the first fundamental harmonic was at 4.5 Hz. To demonstrate the effect of the coupling between the cantilever structure and the nonlinear response of the ferroelectric material, the beam was driven with different frequencies. An interesting case is an input driving frequency of 2.25 Hz, which is half the value of the resonance frequency of the structure. The expectation is that the

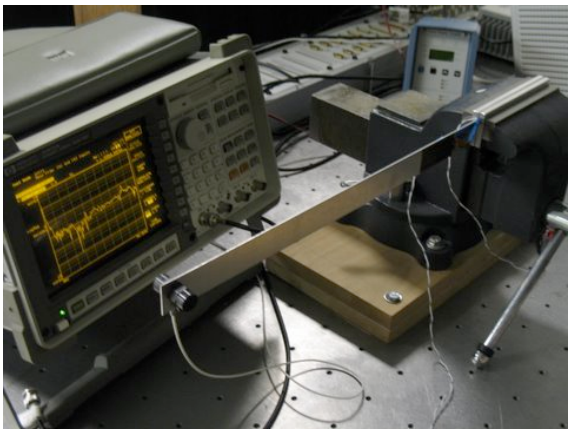
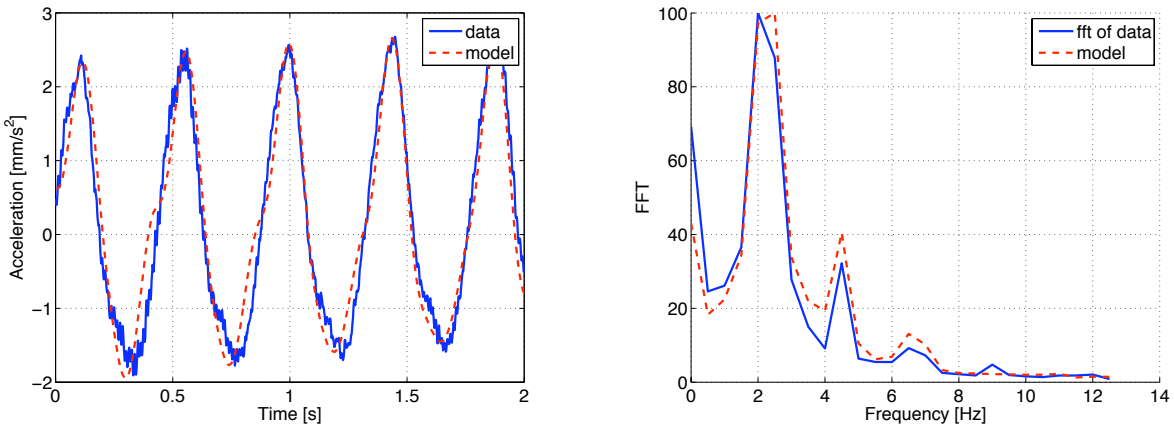


Figure 8: Experimental setup in the CRSC/Math Instructional and Research Laboratory.

second harmonic (4.5 Hz) produced due to the nonlinear response of the piezoelectric material is selectively amplified by the cantilever structure as it coincides with its resonance frequency. Therefore, the second harmonic is expected to have a strong presence in the vibrations of the cantilever beam. It can be observed in Figure 9 that both the experimental data and model simulation show the presence of a strong second harmonic as was expected.

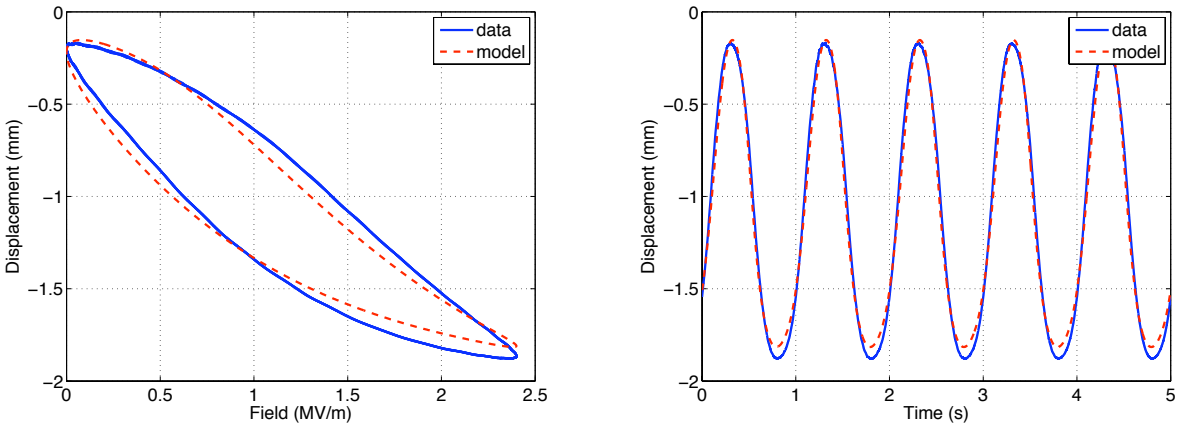
A second set of data results from experiments done by Michael Hays and William S. Oates at Florida State University. In this experimental setup, an aluminum cantilever was compressed between two aluminum blocks for full rigidity. At one side, a Macro Fiber Composite actuator of type M-4010-P1 [14] with lateral, expanding motion was attached. The driving patch has the same width as the beam and covered the region from 25–50 mm measured from the fixed end. In three experiments, an input voltage in the range of 0–200 VDC, 0–400 VDC, and 0–1200 VDC was applied. The driving frequency was 1 Hz. The displacement was measured at a capacitor probe $\bar{x} = 70$ mm away from the fixed end.

The results of the numerical simulations show that the beam model in combination with the homogenized energy model is able to describe the nonlinear behavior of piezoelectric patches. As




(a) (b)

Figure 9: (a) Time domain response and (b) frequency domain response of the PZT patch and model predictions for a driving frequency of 2.25 Hz.




(a) (b)

Figure 10: (a) Phase space and (b) time-domain comparison of experimental MFC data and model prediction for 400 V input.

shown in Figure 10, the predicted results fit the experimental data in both time domain as well as frequency domain. In continuation of my work the successful collaboration with William Oates at Florida State University will be extended. I have already received additional data sets to further validate the model.

*Orthopaedic Biomaterials*

In this group, I started working on development of an accelerated numerical method for the biphasic poroviscoelastic model of articular cartilage biomechanics. In the model, stress is expressed as a function of strain history. There are several approaches of avoiding the high cost of evaluating the stress-strain integral. The focus of my work is on an alternate approach for improved accuracy using Gauss-Legendre quadrature.

Articular cartilage is modeled by the linear biphasic poroviscoelastic (BPVE) model as a mixture of a solid and a fluid phase. The model incorporates a diffusive drag term between the phases (flow-dependent) and intrinsic dissipation mechanisms (flow-independent). The intrinsic dissipation is described using a constitutive relation in which the solid matrix stress depends on the strain rate via a time integral with a continuous relaxation spectrum. In the case of the one-dimensional confined compression stress relaxation problem in small strain, the reduced momentum equation is given by

$$\frac{\partial \sigma}{\partial z} = \frac{1}{\kappa}\frac{\partial u}{\partial t}, \quad 0 < z < h,\ 0 < t < t_f \tag{13}$$

where $u(t,z)$ is the axial displacement, $h$ is the tissue layer thickness, $\kappa$ is the hydraulic permeability and $t_f$ is the duration of the experiment. The solid matrix stress is viscoelastic and of the form

$$\sigma(t,z) = H_A \int_{-\infty}^{t} G(t-\tau)\frac{\partial}{\partial \tau}\left(\frac{\partial u(\tau,z)}{\partial z}\right) d\tau \tag{14}$$

where $H_A$ is the drained aggregate modulus of the solid phase. The reduced continuous stress-relaxation function is formulated as

$$G(t) = 1 + c\int_{\tau_1}^{\tau_2} \frac{e^{-\frac{t}{\tau}}}{\tau}\, d\tau. \tag{15}$$

The governing equations (13)-(14) can be solved by using finite difference or finite element methods and numerical integration techniques. In each time step $n$, $n = 1 \ldots N$ the integral (14) has to be evaluated which leads to a cost of $O(N^2)$. To overcome the prohibitive cost, it is common to use a discrete spectrum approximation of the continuous spectrum relaxation function in terms of an exponential series [16]. A primary advantage of this decomposition is that separability of the exponential kernel leads to an update rule. The full $O(N^2)$ computation can be reduced to a $O(N)$ computation, at the expense of inaccuracies introduced via the discrete series re-approximation. The displacement and surface stress are shown in Figure 11.

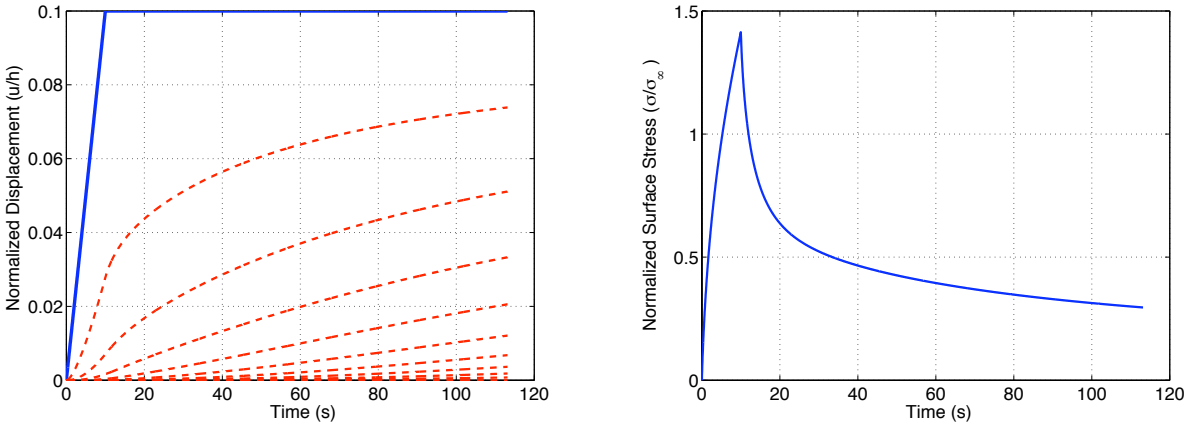
Another approach uses a mathematical error estimate that allows truncation of the history integral [13]. Nondimensionalization of the governing equations and integration by parts in (14) lead to an alternate formulation. After sufficient time has passed, retention of only a fixed portion of the strain history is necessary to preserve accuracy to the specified tolerance. This approach provides excellent accuracy at a fraction of the cost of the full continuous spectrum model, but is significantly more computationally intensive than the discrete spectrum method.

Motivated by the previous techniques described above, I am developing alternate efficient methods for accurate numerical evaluation of the BPVE model. First, I implemented my own versions of the existing methods. Next, I formulated and tested different computational and mathematical approaches with the aim of achieving a significant speed-up in computation time. One computational improvement is the use of a look-up table for the exponential kernel (15) when a fixed time grid is employed. With the number of time steps known one can compute the value of the exponential functions upfront for each time step. This avoids the recurrent evaluation in the computation of (14) and leads to a speed-up in the continuous spectrum model of a factor of 10.

I also focused on developing and implementing a discrete spectrum model with higher accuracy than the existing ones. Our idea is to approximate the continuous spectrum relaxation function by a numerical integration rule using weights and integration points (Gaussian quadrature)

$$\int_b^a \omega(x) f(x)\, dx \approx \sum_{i=1}^{K} w_i f(x_i). \tag{16}$$

Finding the weights and integration points is closely related to the theory of orthogonal polynomials. There exist a system of orthogonal polynomials $p_k(x)$ associated with the weight function $\omega(x)$. For




(a) (b)

Figure 11: (a) Displacement and (b) surface stress at different values of $z$.

the most common weight function $\omega(x) \equiv 1$ and the interval $[-1,1]$, the corresponding orthogonal polynomials are

$$p_k(x) = \frac{k!}{(2k)!}\frac{d^k}{dx^k}(x^2-1)^k, \quad k = 0,1,2,\ldots. \tag{17}$$

Up to a factor these are the Legendre polynomials. The integration points $x_i$ are determined by the roots of the polynomials and the weights are given by

$$w_i = \frac{2}{(1-x_i^2)\left(\frac{p_k'(x_i))}{p_k(1)}\right)^2}. \tag{18}$$

There are different ways of employing this approximation. One could use a higher order quadrature rule in the interval $[\tau_1,\tau_2]$ or partition the interval into either equally or non-equally spaced subintervals and use a lower order quadrature rule.

Table 2 suggests that use of a lower order quadrature on non-equally spaced intervals may be the best approach. Applying the quadrature of order $K$ with $M$ intervals of length $l_i$, $i = 1\ldots M$ we obtain the following scheme for numerical integration of (14)

$$\sigma(t,z) = H_A \int_{-\infty}^{t} \left(1 + c\sum_{i=1}^{M}\sum_{j=1}^{K} w_j \frac{e^{-\frac{t-\tau}{x_{ij}}}}{x_{ij}}\frac{l_i}{2}\right)\frac{\partial}{\partial\tau}\left(\frac{\partial u(\tau,z)}{\partial z}\right)d\tau \tag{19}$$

$$= H_A\frac{\partial u(t,z)}{\partial z} + H_A c\sum_{i=1}^{M}\sum_{j=1}^{K}\int_{-\infty}^{t} w_j \frac{e^{-\frac{t-\tau}{x_{ij}}}}{x_{ij}}\frac{l_i}{2}\frac{\partial}{\partial\tau}\left(\frac{\partial u(\tau,z)}{\partial z}\right)d\tau \tag{20}$$

$$= H_A\frac{\partial u(t,z)}{\partial z} + H_A c\sum_{i=1}^{M}\sum_{j=1}^{K} I_{ij}(t,z) \tag{21}$$

A key idea of this new technique is that the kernel in the integral is also a separable discrete exponential series. Thus, for $\sigma(t+\Delta t,z)$ we obtain an update rule

$$\sigma(t+\Delta t,z) = H_A\frac{\partial u(t+\Delta t,z)}{\partial z} + H_A c\sum_{i=1}^{M}\sum_{j=1}^{K} e^{-\frac{\Delta t}{x_{ij}}} I_{ij}(t,z) \tag{22}$$

$$+H_A\int_{t}^{t+\Delta t}\left(1 + c\sum_{i=1}^{M}\sum_{j=1}^{K} e^{-\frac{\Delta t}{x_{ij}}} w_j \frac{e^{-\frac{t-\tau}{x_{ij}}}}{x_{ij}}\frac{l_i}{2}\right)\frac{\partial}{\partial\tau}\left(\frac{\partial u(\tau,z)}{\partial z}\right)d\tau. \tag{23}$$

| 1 interval | | 5 intervals equally | | 5 intervals non-equally | |
|---|---|---|---|---|---|
| order | error | order | error | order | error |
| 5 | 2.3083191277369376 | 1 | 3.2615179259374761 | 1 | 0.8889919612476676 |
| 10 | 1.1775508239223217 | 2 | 2.2706255897873480 | 2 | 0.1048005320551259 |
| 15 | 0.6282657858695053 | 3 | 1.6650391118617858 | 3 | 0.0117633221084374 |
| 20 | 0.3363040124575639 | 4 | 1.2439579179524185 | 4 | 0.0012973298997107 |
| 25 | 0.1788648666933885 | 5 | 0.9372283019067211 | 5 | 0.0001420827568369 |
| 30 | 0.0943815974522646 | 6 | 0.7086494382176450 | 6 | 0.0000155131520280 |

Table 2: Comparison of different quadrature rules and intervals for $\tau_1 = 0.1$, $\tau_2 = 100$ and $t = 0.01$. The value of the integral is 6.8103007461553148.

The cost of this approach is of order $O(N)$. The accuracy can easily improved by finding an optimal spacing of the intervals or using more quadrature points. Currently, I am working on incorporating this scheme into existing programs for simulating BPVE cartilage mechanics as well as the derivation of error estimates.

**Presentations**

- "Frequency Response of Piezoelectric and Magnetostrictive Hysteretic Nonlinear Systems," ASME Conference on Smart Materials, Adaptive Structures and Intelligent Systems, Ellicott City, MD, October 2008.
- "Modeling the nonlinear behavior of macro fiber composite actuators," SPIE Conference on Smart Structures/Nondestructive Evaluation for Health Monitoring and Diagnostics, San Diego, CA, March 2009.
- "Frequency Response of Ferroelectric and Ferromagnetic Hysteretic Systems," 33rd SIAM Southeastern Atlantic Section Conference, Columbia, SC, April 2009.

**Papers**

- N.G. Medhin and M. Stuebner, "An evolutionary algorithm for molecular dynamics simulation," in preparation.
- M. Stuebner, J. Atulasimha and R.C. Smith, "Frequency response of piezoelectric and magnetostrictive materials based hysteretic nonlinear systems," Proceedings of SMASIS08, ASME 2008 Conference on Smart Materials, Ellicott City, MD, October 28-30, 2008.
- M. Stuebner, J. Atulasimha and R.C. Smith, "Quantification of Hysteresis and Nonlinear Effects on the Frequency Response of Ferroelectric and Ferromagnetic Materials," CRSC Technical Report CRSC-TR09-06; *Smart Materials and Structures*, submitted.
- M. Stuebner, R.C. Smith, M. Hays and W.S. Oates, "Modeling the Nonlinear Behavior of Macro-Fiber Composite Actuators," CRSC-TR09-08; Proceedings of the SPIE, Smart Structures and Materials 2009.

**Personal Statement**

The aquisition of a multi-core workstation from grant money allowed me to start developing multithreaded implementations of the software used in the different groups. It greatly improved the speed of the computations and enables me to tackle larger problems. The financial support made it possible for me to participate in conferences and present my research. I am thankful for all the support I obtained in the group during the last year.

## 2.2 Graduate Student Reports

### 2.2.1 Jeb Collins

**Summary of Research Activities**

Our research consists of finding a simple model for laser drilling. This is a process where a laser is used to create a precision hole in a metal workpiece. The regime of laser we are trying to model has a microsecond pulse with a power density in the GW/cm$^2$ range. We work in this laser regime because it is the regime our collaborator, Dr. J. Tu uses in his lab [18]. We compare our model against

his data. We use a radial averaging method to model the heat transfer problem within the solid, and we solve the Knudsen layer problem to obtain the state of the vapor being created. All this is used to calculate the speed of the solid/vapor interface. Using this information we calculate the depth of the hole drilled and compare to experimental data.

*Heat Transfer Problem*

Solving the heat transfer problem determines the temperature of the solid being drilled into. We do this using the heat equation

$$\rho_s c_s \frac{\partial T}{\partial t} = k_s \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right] \qquad r > 0, z > 0, t > 0, \tag{24}$$

where we are assuming axisymmetric behavior due to the fact the laser has an axisymmetric profile. The solid is at ambient temperature initially. We determined from nondimensionalization that the radial diffusion plays a secondary role. This leads us to simplify (24) by assuming a radius profile for the hole being drilled. The two profiles we chose we a cone and a paraboloid, as shown in Figure 12. These profiles, combined with the boundary condition at the solid/vapor boundary

$$k \nabla T \cdot n = -W n_z + \rho_s L_v u \cdot n$$

gives the following one-dimensional heat equation,

$$\begin{aligned} \frac{\partial \bar{T}}{\partial t} = \alpha \left( \frac{\partial^2 \bar{T}}{\partial z^2} - \frac{4 s s'}{R^2 - s^2} \left( \frac{\partial \bar{T}}{\partial z} + \frac{1}{k} (W - \rho_s L_v u_z) \right) \right), & \quad z > 0, t > 0, \\ k \frac{\partial \bar{T}}{\partial z} = -W + \rho_s L_v u_z, & \quad z = 0, t > 0, \\ \lim_{z \to \infty} \bar{T} = T_0, & \quad t > 0, \\ \bar{T}(\cdot, 0) = T_0, & \quad z > 0, \end{aligned} \tag{25}$$

where $\bar{T}$ is the radially averaged temperature. This simplified problem is solved to determine the temperature of the solid.

*Knudsen Layer Problem*

The Knudsen layer problem consists of determining the state of the vapor using the state of the solid via the following jump conditions [17],

$$T_g = f(m) T_s \rho_g = g(m) \rho_{sat}(T_s) \tag{26}$$

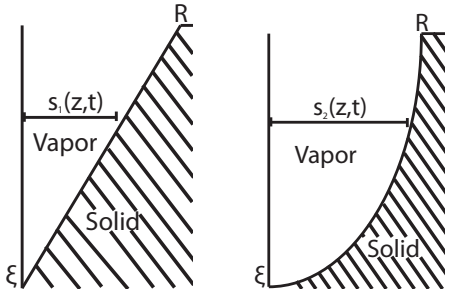



Figure 12: Conic and parabolic cross sections for the hole being drilled.

where $T_g, \rho_g$ are the temperature and density of the vapor, $T_s$ is the temperature of the solid and $m$ is a dimensionless evaporation rate. These jump conditions are derived from kinetic theory. To close the above system of three unknowns, we use the Rankine-Hugoniot jump conditions from the Euler gas dynamics equations, which are relatively simply since we are working in one dimension. Combining these three equations gives us a highly nonlinear scalar equation for $m$. We solve for $m$ numerically and then plug it back into the jump conditions to determine the state of the vapor.

*Results*

Taking all the states calculated we are able to compute the speed of the solid/vapor interface [19], which as we evolve over time tells us how deep a hole our model drills. We are able to obtain hole depths experimentally from Dr. Tu's lab. The radius of the hole at the surface is assumed to be proportional to hole depth. The proportionality constant was determined using parameter estimation techniques, fitting our model to hole depth and hole radius data from Dr. Tu's lab. Here we present the comparison of our various models with the experimental data.

| | Hole Depth | Hole Radius |
|---|---|---|
| Experimental Data | 136 $\mu$m | 11.5 $\mu$m |
| One-d. profile ($\ell \to \infty$) | 80 $\mu$m | |
| Conical profile ($\ell = 1$) | 133 $\mu$m | 11.1 $\mu$m |
| Parabolic profile ($\ell = 2$) | 127 $\mu$m | 10.5 $\mu$m |

Table 3: Experimental and numerical results.

**Presentations**

- "A Simple Model for Laser Drilling," Numerical Analysis Seminar, North Carolina State University, (February 23, 2009).
- "A Simple Model for Laser Drilling," AMS Spring Southeastern Section Meeting, North Carolina State University, Raleigh, NC, (April 5, 2009).

**Papers**

- J. Collins and P. Gremaud, "A simple model for laser drilling," *Mathematics and Computers in Simulation*, submitted.

**Personal Statement**

This program has been very helpful to me. It has allowed me to pursue interesting research and learn good researching techniques. The Research Training Modules have continued to be informative and helpful. I have enjoyed having younger graduate students in the program. Passing along advice to them about graduate school and research has helped solidify my understanding better. All in all I have enjoyed this program.

### 2.2.2 Amanda Criner

#### Summary of Research Activities

Details regarding my research activities are provided in the group report of Section 1.6.

#### Presentations

- "Fundamentals of LaTeX," Research Training Module, North Carolina State University, (September 2008).
- "Thermal Interrogation of Porous Materials," Applied Mathematics Graduate Student Seminar, North Carolina State University, (January 2009).
- "Thermal Interrogation of Porous Materials," Research Training Module, North Carolina State University, (April 2009).

#### Papers

- "H.T. Banks, B. Boudreaux, A.K. Criner, K. Foster, C. Uttal, T. Vogel, W.P. Winfree, "Thermal Based Damage Detection in Porous Materials," *Inverse Problems in Science and Engineering*, accepted with revision.

#### Personal Statement

I have benefited from the RTG program several ways. My research, professional collaborations and communication skills have all developed significantly from the RTG program. The research that I have done this year will play an important role in my Ph.D. thesis. My research has also given me a good understanding of the importance of composite materials and the need to for more development in the area of advanced materials. During our "Group Research Updates", I learned valuable information about the frontiers of advanced materials research. I also developed connections outside of my institution. I further developed my collaboration Dr. William Winfree at NASA Langley Research Center and hope to work with data that he can provide to test my results against volumetric data. I also met and worked with Dr. Cioranescu who has developed many homogenization techniques. I gave a brief presentation about LaTeX during one of the Research Training Modules and brief presentation of our research progress this year. These presentations helped me develop my professional communication skills. I have also improved my communication skills by attending the Research Training Modules including presentations on using XFIG (Dr. Smith, Oct 31, 2009), and poster presentations (Adam Attarian, Jan. 30, 2009).

### 2.2.3 Lisa Downen

#### Summary of Research Activities

My research has focused on background review and initial programming of models quantifying hysteresis in ferromagnetic materials. These models build upon the homogenized energy framework that combines energy analysis at the lattice level with stochastic homogenization techniques to construct macroscopic characterization techniques having the potential for real-time design and control implementation. The numerical component of the research has focused on the development of MATLAB programs to simulate material behavior and provide a basis for subsequent model validation with experimental data.

**Papers**

- L. Downen, T. Glover, L. Hallock, S. King, J. Shor, J. Wallace and R.C. Smith, "Efficient Algorithms for Implementation of Hysteresis Models," Proceedings of the SPIE, Smart Structures and Materials 2009.

**Personal Statement**

Since entering the RTG program, I have primarily been concentrating on my classes, which were selected primarily to provide a mathematical foundation in my research area (ferromagnetic shape memory alloys), and attending RTM meetings regularly. More recently, I have been analyzing MATLAB code that models ferromagnetic and other similarly behaved materials. Since my background is in chemical engineering, where highly specialized programs are often used for simulations, and pure mathematics and chemistry, where neither program emphasized numerical approaches to problem solving, this provides me with an opportunity to build my mathematical programming skills that was not available to me previously. Given that my background is outside of applied mathematics, attending RTM meetings has given me the opportunity to be introduced to topics that are important to me now but were not particularly relevant in my previous areas of study.

### 2.2.4 Nicholas Giffen

**Summary of Research Activities**

For the past year, I have been studying particle-size segregation in granular materials, specifically related to avalanches. My research has been focused on two main areas in this field: shock formation, and shock wave breaking. A third field of study I have more recently undertaken is determining scaling properties of the PDE model that is used. The research has been supplemented by reading recent literature on avalanche models and segregation. A paper with Dr. Shearer is in the final stages of preparation [20].

A simple model, formulated by Savage and Lun [23], and later simplified by Gray and Thornton [21], is a nonlinear, scalar, first order PDE. Given a smooth initial condition in a set two-dimensional region along with the PDE, it is possible to determine if and when a shock will form on the interior of this region. By taking partial derivatives of the PDE and analyzing the resulting ODE system and its corresponding phase portrait, we can fully determine the behavior of the system.

In granular flow, a shock separating large particles above from smaller particles below is stable. However, unless the interface is horizontal, then it is possible during shear flow for it to become vertical at a point and lose stability. Under a linear velocity profile, typical of avalanche flow, the subsequent motion is known to produce a mixing zone; mathematically, this develops from a singularity in the PDE solution. My research problem is to resolve the structure of this mixing zone both analytically and numerically.

PDE simulations of the model suggest a general structure for the mixing zone. This involves a combination of rarefaction waves and shock waves. Such a solution was formulated in an idealized case of an initially straight vertical interface [22]; my challenge is to understand the structure in the more general case of a breaking interface that has a vertical tangent at a single point. I have resolved the structure in the generic case of a smooth interface with a vertical tangent and cubic singularity.

I have also looked at a piecewise quadratic initial interface, where the structure simplifies significantly. I discovered that the structure of the mixing zone solution is different under different linear velocity profiles and determined a condition on the model to determine which structure would fit the solution. This suggested a scaling to determine the structure of the mixing zone.

Lab meetings are held together with Dr. Karen Daniels' physics research group of undergraduate and graduate students, as well Dr. Shearer's students. In lab meetings, we discuss progress on experiments in granular materials and liquid films, and often focus on papers relating to a specific topic or experiment.

**Presentations**

- "Particle size segregation in granular avalanches: shock formation and shock breaking," Applied Mathematics Graduate Student Seminar, North Carolina State University, (October 2008, April 2009).
- "Particle size segregation in granular avalanches: shock formation and shock breaking," Research Training Module, North Carolina State University, (March 2009).

**Papers**

- N. Giffen and M. Shearer, "Shock formation and shock breaking in models of particle size segregation," in preparation.

**Personal Statement**

In the past year I have gone from an understanding of particle-size segregation in granular materials to really grasping the ideas and concepts that combine all areas of study in this field. As last year, literature searches have helped improve my overall knowledge of the subject, but more importantly are the lab meetings that I have had with my lab group. Understanding how each piece of the puzzle fits together, from shock formation, to pressure affecting mixing and segregation rates, to scaling of the PDE, all of these pieces fit together, and this is where I have gone from just an understanding of the concepts to fitting the concepts together as a story in a bigger picture.

This research has greatly improved my individual analytic skills. My advisor and I have relied less on numerical simulations this year, and have done more analytic work to obtain our results. Many of the ideas we have come up with, have come from my own line of thought and work, and it is rewarding to be able to bounce ideas back and forth with Dr. Shearer so that the individual and team concept are both reinforced. My Latex skills once again have improved to the point where I feel it is a natural computing language for me, just like Microsoft Word has been in the past.

Finally, the RTM program has helped me become a more well rounded student. I have learned about laser welding, carbon nano-tubes, smart materials, and more, as well as the mathematical concepts that accompany each idea. The modules have also given me a greater technical background in Latex and photo editing programs so that I can give nicer looking and flowing talks, as well as writing neater looking papers.

### 2.2.5 Janine Haugh

**Summary of Research Activities**

Articular cartilage is a connective tissue lining the surfaces of bones in diarthrodial joints such as hips, knees, and shoulders. As a natural biomaterial, cartilage is important for load support, energy distribution, and lubrication of joints, but can become damaged due to injury or osteoarthritis. Cartilage has a limited capacity for repair and growth which is regulated by cells, called chondrocytes, that are sparsely distributed throughout the tissue's extracellular matrix (ECM).

In recent years, the potential use of nutrient-rich hydrogels seeded with cartilage cells as biomaterials for tissue regeneration and repair has seen wide interest. In this study, I am developing mathematical models for cartilage regeneration in the local environment of a single cell seeded in a hydrogel scaffold. A spherical geometry is employed with three concentric regions: the cell, its extracellular matrix, and the hydrogel — see Figure 13).

Radially symmetric reaction-diffusion equations are used to describe the coupling of nutrient and synthesized (unlinked) matrix concentrations in the three regions. Several models are considered to describe the process by which unlinked matrix proteins react with the hydrogel to form linked extracellular matrix. Numerical solutions are based on finite difference methods and capture motion of the evolving gel-tissue interface. The resulting models are used to conduct a parametric analysis that quantifies tissue regeneration times in terms of underlying biophysical parameters in the models.

*Level Set Reaction-Diffusion Model*

The following set of reaction-diffusion equations are used to model evolution of nutrient concentration $N(r,t)$ and unlinked matrix protein concentration $M(r,t)$ in the cell ($0 < r < a$):

$$\frac{\partial N}{\partial t} = D_N^{(1)}\left(\nabla^2 N\right) - k_N\left(N - N_*\right) \tag{27}$$

$$\frac{\partial M}{\partial t} = D_M^{(1)}\left(\nabla^2 M\right) + k_M\left(N - N_*\right) \tag{28}$$

This model assumes that transport is exclusively diffusive and that nutrients are absorbed by the cell in order to synthesize unlinked matrix proteins.

The region outside of the cell is modeled as a domain with two zones accounting for the transition of the hydrogel to ECM as the unlinked proteins diffuse outward from the cell and react with the hydrogel to form linked ECM. Hence, in this region ($a < r < R$), there is diffusion of nutrients and unlinked matrix but no absorption or synthesis occurring, so that:

$$\frac{\partial N}{\partial t} = \nabla \cdot \left(D_N^{(2,3)}(r)\nabla N\right) \tag{29}$$

$$\frac{\partial M}{\partial t} = \nabla \cdot \left(D_M^{(2,3)}(r)\nabla M\right). \tag{30}$$

$D_N^{(2,3)}(r)$ and $D_M^{(2,3)}(r)$ are continuous functions modeling the sharp transition between diffusion coefficients for the ECM and hydrogel regions via the relation:

$$D_i^{(2,3)}(r) = \frac{D_i^{(3)} - D_i^{(2)}}{2}\tanh\left(\frac{\phi}{\epsilon}\right) + \frac{D_i^{(3)} + D_i^{(2)}}{2}, \tag{31}$$

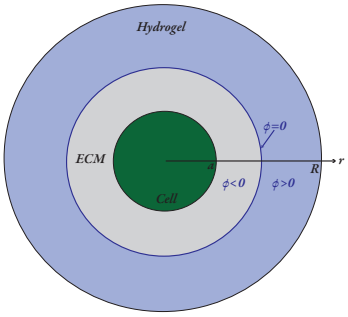



Figure 13: A radially symmetric spherical geometry with three zones (cell, ECM and hydrogel) is used to model cartilage regeneration in the local environment of a single cell (chondrocyte).

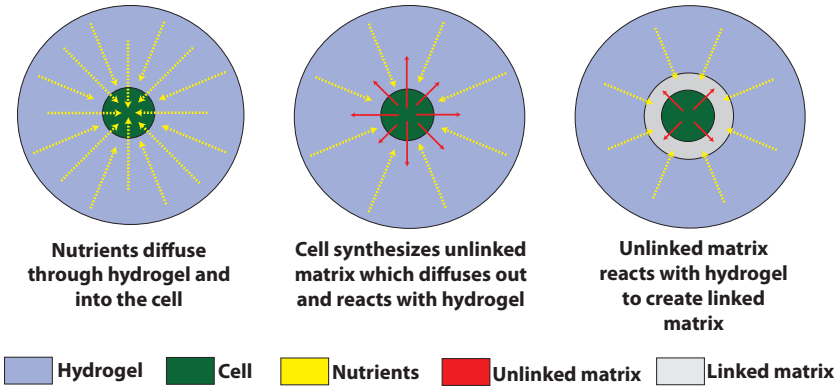



Figure 14: Illustration of the reaction-diffusion model for cartilage regeneration in the local environment of a single cell. Nutrients diffuse through the hydrogel into the cell where they are absorbed and utilized to create unlinked matrix proteins. These unlinked matrix proteins diffuse out of the cell and create linked extracellular matrix (ECM) when they react with the hydrogel, resulting in an advancing interface.

where $\epsilon << 1$ is prescribed. Lastly, as unlinked matrix proteins reach the hydrogel, the process by which these proteins interact with the hydrogel to create linked ECM is idealized as a local reaction along an (advancing) interface between ECM and hydrogel. We assume that the cell can detect the extent to which further ECM synthesis is required in order to achieve a target volume $V_T$ of ECM. The resulting interface reaction equation is modeled as:

$$\frac{\partial \phi}{\partial t} + F\,|\nabla \phi| = 0, \quad F = k\,[V_T - V_M(t)]\,M(r,t) \tag{32}$$

where $V_M(t)$ is the volume of the cell and ECM layers at time $t$ and the ECM-hydrogel interface is located along the level set $\phi = 0$. A visual representation of this entire process is seen in Figure 14, and all equations were nondimensionalized prior to application of the model.

*Preliminary Results*

The nutrient and matrix reaction-diffusion equations were solved numerically using first-order implicit Backward Euler schemes on time derivatives and second-order implicit Backward Euler schemes on spatial derivatives. The level set equation was discretized using a first-order entropy-satisfying upwind viscosity scheme. Values and ranges for diffusion coefficients and other physical

| Case | $\frac{N_H}{N_*}$ | $k_N$ | $k_M$ | $k$ | Time (days) |
|---|---|---|---|---|---|
| I | 10 | 0.1 | 0.01 | 0.1 | 0.4837 |
| II | 10 | 0.1 | 0.01 | 0.01 | 4.8520 |
| III | 10 | 0.1 | 0.01 | 0.005 | 9.6957 |
| IV | 10 | 0.1 | 0.01 | 0.001 | 48.5135 |
| V | 10 | 0.1 | 0.01 | 0.0001 | 484.7854 |

Table 4: Parametric analysis of regeneration time required to achieve target volume $V_T$. The model was most sensitive to the nondimensional gel-tissue reaction rate $k$, and the order of magnitude of the regeneration time varies inversely with the value of $k$.

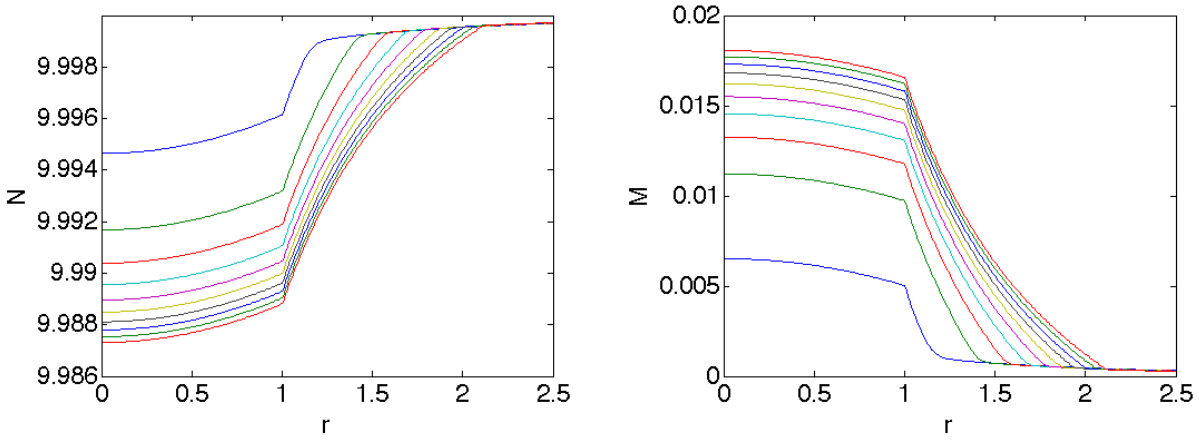



Figure 15: Nondimensionalized nutrient and unlinked matrix profiles for Case IV. $r = 1$ is the cell boundary.

parameters were chosen based on the literature. For example, nutrients are generally much smaller than matrix proteins and therefore diffuse more quickly, whereas the ECM is a dense fibrous matrix with diffusion coefficients that are significantly smaller than those for the hydrogel or the cell. Typical profiles of nutrient and unlinked matrix protein concentrations are shown in Figure 15. An example of regeneration curves demonstrating the accumulation of synthesized ECM volume, until the target volume $V_T$ is reached, are shown in Figure 16. A parametric analysis was conducted to gain an understanding of coupling between the nutrient absorption, matrix synthesis, and gel-tissue reaction rates, as well as to see what impact the hydrogel nutrient concentration has on regeneration time required to achieve the target volume $V_T$.

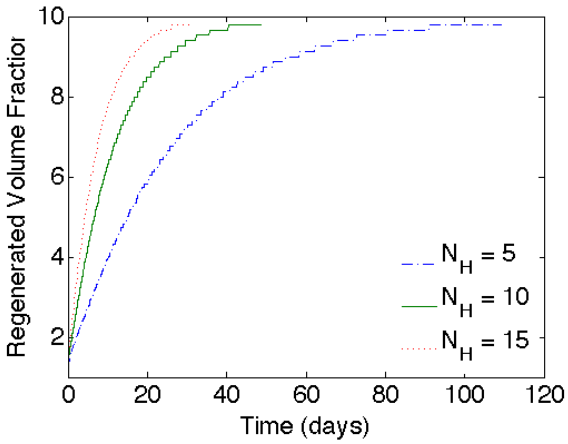



Figure 16: ECM regeneration curves showing the time required to reach target volume when initial volume fraction is 10% for three hydrogel concentrations. All other parameters are the same as in Case IV.

**Presentations**

- "Your Hips Don't Lie: Modeling Cartilage Regeneration," poster, Department of Mathematics Alumni & Friends Brunch, North Carolina State University, (October 2008).
- "A Reaction-Diffusion Model for Extracellular Matrix Regeneration in a Cell-Seeded Hydrogel," Applied Mathematics Graduate Student Seminar, North Carolina State University (December 2008).
- "Modeling Cartilage Regeneration in the Extracellular Environment of a Cell-Seeded Hydrogel", 2009 Graduate Student Research Symposium, North Carolina State University, (March 2009).
- "Modeling Cartilage Regeneration in the Extracellular Environment of a Cell-Seeded Hydrogel", poster, Mathematics and Statistics Building Dedication, North Carolina State University, (May 2009).

**Additional Conferences of Workshops**

- *The Twenty-Fifth Annual Workshop on Mathematical Problems in Industry*, University of Delaware, (June 2009).
- *Graduate Student Mathematical Modeling (GSMM) Camp*, Rensselaer Polytechnic Institute, June 2009).

**Papers**

- J.M. Haugh and M.A. Haider, "A reaction-diffusion model for extracellular matrix regeneration in the local environment of a chondrocyte seeded in a hydrogel," in preparation.
- J. Olander, R.F. Arnold, D.F. Marous, A.J. McLamb, K.C. Thompson, W.R. Woodruff, J.M. Haugh and M.A. Haider, "A mathematical model for cartilage growth in a cell-seeded hydrogel scaffold," in preparation.

**Personal Statement**

While I really love teaching, the RTG has been wonderful since it has allowed me to focus completely on my research instead of being distracted by other responsibilities. I've also learned a lot through the RTMs and the coursework. My favorite RTM was easily the Job Panel. It was extremely helpful to talk to people who currently have jobs and some who were going through the interview process at the time so that I will know what to expect in the fall when I begin the search myself. Especially in today's economy, searching for employment is very stressful. I'm glad to know I have people I can go to for advice here, and I already have a list of places to look for job listings and of things to expect from that module!

I have taken three of the RTG courses, and each of them has been beneficial for me. In the Fall 2007 semester I took *Asymptotic Analysis and Perturbation Methods* which has been very helpful in my research by expanded my knowledge of nondimensionalization, asymptotic approximations, and boundary layer methods. These have all come up to varying extents during my work. In the Spring 2008 semester I took *Validation, Verification, and Uncertainty Quantification* which was especially valuable because a class of that type is so rare. It is important to know the difference between validation and verification and both should be done to convince others your results are worthwhile.

Lastly in Spring 2009 I took *Continuum Mechanics of Elastic and Viscoelastic Solids* which was helpful by both refreshing some concepts I haven't used in a while and by introducing many new ones. Another interesting aspect of these classes is that they frequently weren't only full of math students. Depending on the nature of the course, there may have been statistics and biomathematics students, various engineers, physicists, or others. These students offered a perspective and background unique from my own which made class more interesting and even seem more relevant!

### 2.2.6 Ellen Petterson

**Summary of Research Activities**

In collaboration with Rachel Levy and Tom Witelski, we are studying the evolution of the height of a thin liquid film under the effects of surfactant. We consider two geometries: a horizontal substrate, where surfactant is the primary driving force and the inclined plane, where surfactant and gravity are both driving forces. A system of fourth order nonlinear PDE can be derived from the Navier-Stokes equation and applying the lubrication approximation to analyze the behavior of the film

$$h_t + \left(\tfrac{1}{3}h^3\right)_x - \nabla.\left(\tfrac{1}{2}h^2\nabla\Gamma\right) = \beta\nabla.\left(\tfrac{1}{3}h^3\nabla h\right) - \kappa\nabla.\left(\tfrac{1}{3}h^3\nabla\Delta h\right) \quad (33)$$

$$\Gamma_t + \left(\tfrac{1}{2}h^2\Gamma\right)_x - \nabla.(h\Gamma\nabla\Gamma) = \beta\nabla.\left(\tfrac{1}{2}h^2\Gamma\nabla h\right) - \kappa\nabla.\left(\tfrac{1}{2}h^2\Gamma\nabla\Delta h\right) + \delta\,\Delta\Gamma. \quad (34)$$

In these equations, $h(x,t)$ is the height, $\Gamma(x,t)$ represents the surfactant concentration, $\beta$ is related to gravity, $\kappa$ surface tension, and $\delta$ to the molecular diffusion of surfactant molecules. The parameters $\beta,\kappa,\delta$ control the regularizing terms on the right hand side. The system for the horizontal surface differs by the absence of the terms $\left(\tfrac{1}{3}h^3\right)_x$ in (33) and $\left(\tfrac{1}{2}h^2\Gamma\right)_x$ in (34).

*Inclinded Plane*

In [27] and [26] traveling waves were identified and studied, both with and without regularizing terms. The structure of the height profile is piecewise constant with four steps, and the surfactant concentration is a continuous piecewise linear structure. The traveling waves exist only when the upstream and downstream heights are well-separated. We examine the stability of the traveling wave solutions both analytically and numerically.

*One-dimensional analysis without regularization*

We consider the one-dimensional case with no regularization, $\beta = \kappa = \delta = 0$. The behavior of a perturbation on each step of the traveling wave solution must be examined separately. Using the dispersion relation, we are able to determine the growth rate and velocity of a perturbation placed on each step. This analysis suggests that the unregularized one-dimensional system is stable.

*One-dimension without regularization numerical simulations*

We have implemented various numerical methods in order to examine the behavior of a perturbation on each step of the traveling wave. These methods include both finite volume methods and finite difference implicit and explicit methods. The numerical results support the analytical findings in the behavior of the perturbations.

*One-dimensional analysis with regularization*

We examine the spectral stability of the linearized PDE system. We consider the traveling wave $h(x,t) = \bar{h}(x), \Gamma(x,t) = 0$. Using the asymptotic equations we are able to show that there exists a solution that decays at $\infty$ and one that decays at $-\infty$. We then use the Evans function and stability indicator function to examine the stability of the system [25]. This analysis is consistent with stability.

*Multi-dimensional analysis with regularization*

We have a preliminary analysis near $\Gamma = 0$ that shows that the smooth traveling wave (i.e., with $\beta$, $\kappa$, $\delta$ all positive) is unstable in two dimensions. As in [24], the analysis reduces to determining the sign of an integral of the upstream and downstream heights. Rather than flowing as a planar wave, the film travels down the incline with a corrugated front.

*Horizontal Substrate*

We consider an initially uniform thin film with a droplet of insoluble surfactant deposited on the surface. We assume the droplet is radially symmetric, thus the system that describes this behavior is

$$h_t = \frac{1}{r}\frac{\partial}{\partial r}\left\{ r\left[ \frac{1}{3}\frac{\partial}{\partial r}\left( \beta h - \kappa\left[ \frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r}\right]\right) h^3 + \tfrac{1}{2}h^2\frac{\partial \Gamma}{\partial r}\right]\right\} \tag{35}$$

$$\Gamma_t = \frac{1}{r}\frac{\partial}{\partial r}\left\{ r\left[ (\delta + \Gamma h)\frac{\partial \Gamma}{\partial r} + \tfrac{1}{2}\Gamma h^2\frac{\partial}{\partial r}\left( \beta h - \kappa\left[ \frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r}\right]\right)\right]\right\}. \tag{36}$$

*Numerical simulations – Unregularized System*

We first consider the unregularized system, $\beta = \kappa = \delta = 0$ with the surfactant in a compact region. The point where the surfactant concentration goes from zero to positive causes a shock to develop in the height profile. From the jump conditions of (35) and (36) we determine the size of this jump. We are then able to implement this jump as a boundary condition in the numerical simulations. We found that the edge of the surfactant travels with a speed of $t^{\frac{1}{4}}$.

*Experiment*

In collaboration with Karen Daniels' lab at NCSU, we are experimentally investigating the evolution of the film height driven by a surfactant. We are using an insoluble fluorescent surfactant, NBD-PC which enables us to visualize the location of the surfactant and thus make connections between the height of the film and the location of the surfactant. We are examining the rate that the edge of the surfactant propagates and the evolution of the height profile. These results will then be compared to the numerical simulations.

**Presentations**

- "Thin Fluid Films with Surfactant", Triangle Soft Matter Workshop, North Carolina State University, poster and soundbite, (May 2009).
- "Thin Fluid Films with Surfactant", SAS Hall Dedication, North Carolina State University, poster, (May 2009).
- "An Overview of Thin Fluid Films Research," Research Training Module, North Carolina State University, (March 2009).
- "Thin Fluid Films Under the Influence of Surfactant," Applied Mathematics Graduate Student Seminar, North Carolina State University, (March 2009).
- "Thin Fluid Films with Surfactant," Higher Order Geometric Evolution Equations: Theory and Applications from Microfluidics to Image Understanding, IMA-University of Minnesota, poster, partially funded by RTG (March 2009).

- "Shock Waves: Flow of Thin Liquid Films," North Carolina State Graduate Recruitment Day, (February 2009).
- "Flow of Thin Films with Surfactant: Behavior of Perturbations," Thin Films Day, North Carolina State University, (January 2009).
- "Flow of Thin Films with Surfactant: Behavior of Perturbations," Applied Mathematics Graduate Student Seminar, North Carolina State University, (November 2008).
- "Flow of Thin Films with Surfactant: BeginningStability Analysis," EDGE Cluster Meeting, North Carolina State University, (October 2008).

**Additional Conferences and Workshops**

- Promoting Diversity at the Graduate Level in Mathematics: a National Forum, MSRI, partially funded by RTG (October 2008).
- Enhancing Diversity in Graduate Education (EDGE) Reunion, Pomona College, panelist, (June 2008).

**Papers**

- E. Peterson, M. Shearer, T. Witelski, R. Levy, "Stability of Traveling Waves in Thin Liquid Films Driven by Gravity and Surfactant," Proceedings, 12th International Conference on Hyperbolic Problems: Theory, Numerics, Applications, Hyp 2008, To appear.

**Personal Statement**

The RTG offers students opportunities that may not have been available to us without the program. For example, students are encouraged to build a well-rounded framework for our careers through the connections each group has with either an industrial group or an academic lab group. We are led to see beyond the mathematics field and develop a comprehensive view rather than just a mathematical one. Also, by having each RTG group report on their work we were able to learn from other students' experiences. Building a foundation for good collaboration and understanding how different fields work is a great experience to be having as a graduate student. Also, the travel fund enables us to attend conferences where we experience a different aspect of the mathematical field. These conferences offer an opportunity to be exposed to other current research interests/areas, attend presentations by respected mathematicians, present our own work, and network. These experiences are an important aspect of developing into a mathematician.

### 2.2.7 Donovan Shickley

**Summary of Research Activities**

I have been researching potential active metamaterial structures. Metamaterials are materials designed to have properties not found in nature and have a negative index of refraction. The applications of metamaterials include a lens that can surpass the diffraction limit, novel stealth technology by invisibility cloak, and the improvement of antennae and medical imaging capabilities.

Creating a material with a negative refraction index is done by making the effective electric permittivity and magnetic permeability of the material negative. An invisibility cloak is made by

surrounding the object to be hidden with concentric cylinders of periodically arranged split-ring resonators (SRRs), which can be considered a unit cell of a metamaterial. The dimensions of the SRRs determine the resonant wavelength of the material, which is the wavelength of light at which the object is invisible. This has been experimentally verified at microwave frequency. Since the dimensions of the SRRs are fixed, the invisibility cloak is theoretically limited to interacting with only the resonant wavelength determined at the time of fabrication.

Current work in the field includes extending the capability of cloaking to multiple wavelengths with the ramification of making objects invisible with respect to visible light. My research goal is to create a model for an SRR that could dynamically change dimension by incorporating adaptive materials such as piezoelectrics. I have surveyed papers dealing with passive metamaterial structures and their limitations with applications to active structures and am currently working on finding a model for SRRs that describes the magnetic permeability as a function of the dimension.

**Presentations**

- "Passive Metamaterial Structures, Applied Mathematics Graduate Student Seminar, North Carolina State University, (April 20, 2009).

**Personal Statement**

The RTG program is exciting because I am able to research novel materials that have wide and significant applications. I am learning much about not only metamaterials but also how to begin to study a specific field and the methodology of finding a research problem. My curiosity for math that compelled me to go to graduate school has been continually satisfied by this opportunity. The ability to start early on what could be my doctoral research is invaluable and will no doubt make me more efficient later as my focus turns more from classes to research.

**Awards**

- *Provost Research Fellowship:* Received a single year $5000 award upon admittance to the NCSU Applied Mathematics doctoral program.

## 2.3 Undergraduate Reports

### 2.3.1 Michael Dearman

**Summary of Research Activities**

Polymers and composites have many practical and useful applications, like plastic, which is widely used today. In order to better understand how polymers and composites work, and how to maximize their ability, it is important to study their dynamics and understand how they act under certain conditions. I have learned the basics of polymer and composite research this semester under the guidance of Dr. Medhin in the RTG Polymer and Composites group.

I began my research by gaining a solid understanding of the different kinds of polymers and the energies associated with polymers. A polymer chain is a string of repeating large molecules, called monomers. To simulate a polymer chain we begin by using the molecular dynamics method (MD). By computing the interaction between several monomers, we found the chain closely resembled a bead-spring model, so we simplified our MD by assuming the chain acted like a bead-spring model. Also, we assumed the chain was not entangled, and our computations were at a constant pressure and temperature. The different potential energies that were considered in the MD method

for our chain were a Lennard-Jones potential that depends on the distance between monomers, a bond-bending potential that depends on the angle of the monomer bond, and torsional potential that depends on the dihedral angle between monomers. MD discretized these potential energies to compute forces, and in turn computed an update in position for each monomer in discrete steps. In order to accurately simulate the chain using MD, we used picoseconds as our time increment. From our simulation we can compute quantities such as the relaxation time of the chain. MD accurately simulates our polymer chain, but takes a long time to compute through a long time increment or for chains with a large number of monomers.

The Rouse model can simulate a polymer chain faster than MD, and still keep much of the accuracy. The Rouse model treats the polymer chain like a bead-spring model, and notes that correlation between two monomers drops to zero as the number of monomers between them increase. For the polyethylene chain I used as my example, about twenty monomers are needed for this correlation to be nearly zero. Using this fact, we normalized the monomers into groups called beads, and simulated the chain based on the interaction of the beads. From this approximation we computed values such as relaxation time and stress on the chain faster than MD. The Rouse model decreased the amount of computations, but still approximated the chain closely to MD simulation.

The Rouse model assumed there are no hydrodynamic interactions however. To continue my understanding and research in polymer and composite dynamics, I will study the Zimm model, which also accounts for hydrodynamic interactions.

**Personal Statement**

I have learned a great deal about the mathematical research process this semester by being a part of the Polymer and Composite research group. I learned that it is best to start with simple assumptions and add one condition at a time. After adding each condition it is good to compare the results to experimental data, if it is available. Through the RTM seminars I have learned that a proper presentation should summarize the important parts of your research paper on the powerpoint slides, while you explain the details. Too many details on a slide may confuse the audience and lose their attention. The RTM also taught me that the same ideas apply to presentation posters: include the important information such as formulas and graphs, without all the derivations. Whoever is viewing your poster should be able to read for a few minutes and walk away with a fairly solid understanding of your research. From the seminars by the other RTG groups, I have seen how the research process is very similar for each group, even if the research areas are very different.

This research experience has given me understanding about the mathematical research process, a great head start in a future career in mathematical research, and will give me an edge over other students in getting a research assistantship at Texas A&M University as a graduate student in the next couple of years.

**Future Plans:** Attend graduate school in Mathematics at Texas A&M in Fall 2009.

### 2.3.2 Rachael Gordon-Wright

**Summary of Research Activities**

This semester I worked with Dr. Pierre Gremaud modeling granular surfaces. Our goal was to model the behavior of the surface of some amount of granular material being rotated about a fixed axis, using a cylindrical coordinate system. The forces acting on a single particle in this surface layer of material are the gravitational force, a reaction force between the particles, and a friction force

between the particles that acts parallel to the surface. Using Newton's Laws and Coulomb's Law of Friction, we obtained a single first order partial differential equation for our model

$$(1+\mu)^2(Fr\partial_r h+1)^2-(F^2r^2+1)\left(1+(\partial_r h)^2+\left(\frac{1}{r}\partial_\varphi h\right)^2\right)=0 \tag{37}$$

where $\mu$ is the coefficient of internal friction and the Froude number $F$ is defined by

$$F=\frac{\omega^2 L}{g}.$$

Here $L$ is a characteristic length, $\omega$ is the angular velocity, and $g$ is the acceleration due to gravity. Equation (37) describes the yield surface shown in Figure 17. In fact, however, a continuum of admissible states are possible and correspond to the "interior" of the yield surface. Permissible values of the gradient of the height $h$ are determined using this equation. Figure 17 is a graph of the above yield surface in terms of the radius. For a fixed value of the radius, if the calculated values of the gradient fall outside the surface, the values must be adjusted to the closest allowable value. This is an optimization problem with one constraint, to minimize the distance between the point corresponding to the calculated values of the gradient and equation (37).

We have developed a three dimensional program. The program accepts as inputs the values of the radius of the container, coefficient of friction, angular velocity, and a set of data points representing the initial height of the material. The mass of the material and values of the gradient are calculated. Values of the gradient falling outside the permissible range are projected onto the surface of the above figure based on the optimization problem described in the preceding paragraph. Based on a flat initial height profile and a fixed angular velocity, the result shown in Figure 18 was obtained.

A paper describing the above method and further results is in preparation. We will analyze the effects of changing the shape of the container as well as removing the outer walls of the container altogether. In addition, we will study the history of retention. Specifically, how will the surface

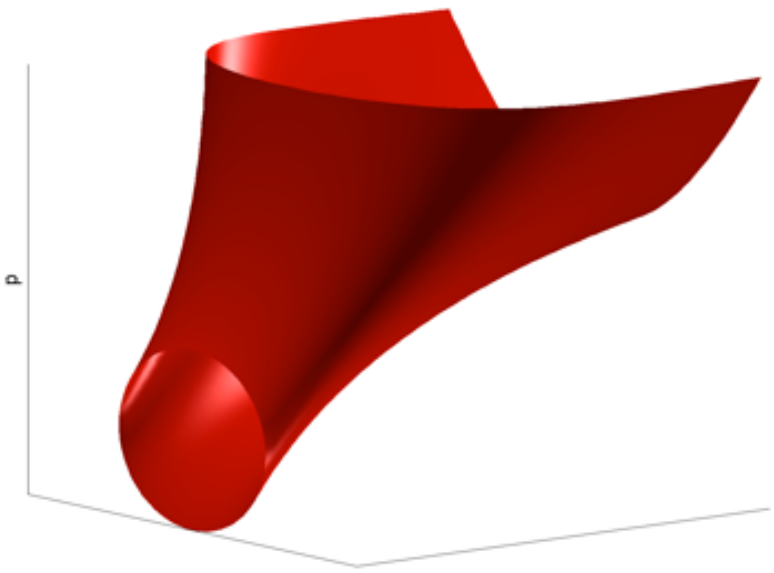


Figure 17: Yield surface determined by (37).

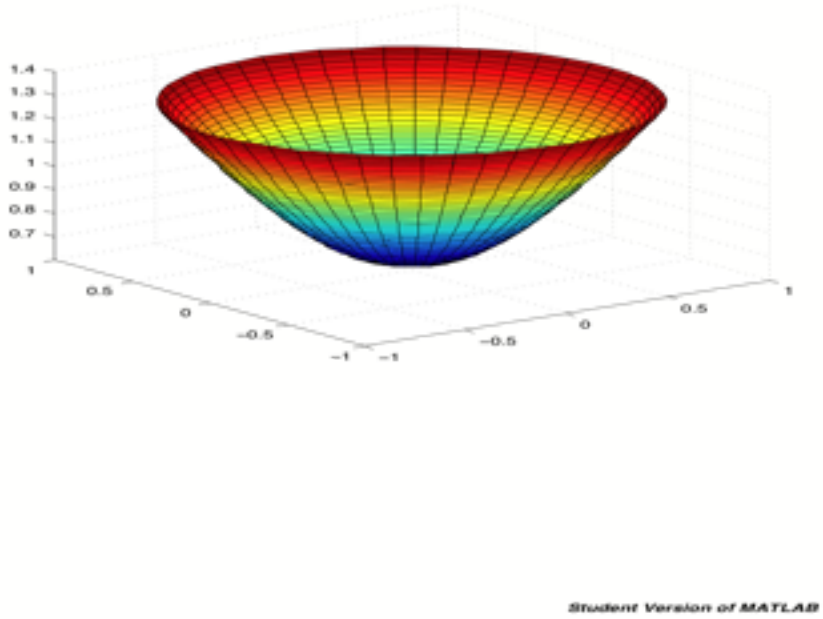



Figure 18: Optimized results based on a flat initial height profile and fixed angular velocity.

features of this rotating cylinder of granular material change if the angular velocity is decreased? Hysteresis effects are expected. In the future, one goal is to add a time component to our model.

**Presentations**

- "Free Granular Surfaces," Math Undergraduate Research Presentations, North Carolina State University, April 22.

**Workshops Attended**

- 2009 SAMSI/CRSC Undergraduate Workshop, May 18-22.

**Personal Statement**

Working with the Mathematics of Materials group this year has been a unique educational experience. When I first arrived at NC State, I had only a vague idea of what applied mathematics was and even less knowledge about what it meant to do research in mathematics. I applied to the RTG group to learn about applied mathematics and get a feel for what it is like to do research. After my first semester working with Dr. Gremaud, I have met those goals and more. It has helped shape my plans for the future.

I have learned a great deal about applied mathematics working for the RTG group. I beginning to learn how the theory taught in class is applied to complicated real world problems. It is different from anything I have done before. The math was familiar, but figuring out how to make it work for our problem was new. Working with the RTG group has also given me a better understanding of what it means to do research. I thought you had to be an expert in a subject before you could do research in it. But it turns out you pick up knowledge along the way and you learn how to do research by actually doing it. As a student, I had become used to succeeding right away, but in research the first method you try is frequently wrong. Even if something you try is wrong, you learn from making mistakes.

Graduate school in mathematics has been part of my long-term plans since entering college. Coming to NC State, I did not know what kind of math I wanted to focus on, and to be honest I still don't. Working with the RTG group has helped me narrow my interest to applied mathematics. I would like to use my problem-solving skills and have a chance to work in wide variety of fields. Continuing with the RTG group will help me hone those skills.

### 2.3.3 Allison McAlister

**Summary of Research Activities**

The Gray-Thornton Model for particle segregation yields the conservation law

$$\frac{\partial \phi}{\partial t} + u(z)\frac{\partial \phi}{\partial x} + \frac{\partial}{\partial z}\left(f(\phi)\right) = 0 \tag{38}$$

where $\phi$ is the volume fraction of small particles in the whole and u(z) is the velocity parallel to the surface. Differentiating the PDE with respect to $x, z$, we get thhe system of ODEs,

$$\frac{dv}{dt} = -2vw \tag{39}$$

$$\frac{dw}{dt} = -2w^2 - u'(z)v \tag{40}$$

in which $v = \frac{\partial \phi}{\partial x}$, $w = \frac{\partial \phi}{\partial z}$ and $d/dt$ is differentiation along a characteristic on which $\phi$ is constant. Graduate student Nick Giffen has considered the conditions of $\frac{\partial \phi}{\partial x}$ versus $\frac{\partial \phi}{\partial z}$, where u'(z) is constant, that lead to shock formation. We get a solution similar to Figure 19.

The trajectories that go to infinity in finite time indicate that the gradient of $\phi$ is approaching infinity as well. Those trajectories that do not approach infinity all approach zero tangent to the limiting parabola, indicated by the red parabola.

However, what happens if u'(z) is a non-constant function of z? This semester, I have spent the bulk of my time constructing an analogous MATLAB model illustrating this scenario. This necessitated the construction of a three-dimensional model with axes: $v = \frac{\partial \phi}{\partial x}$ on one horizontal axis,

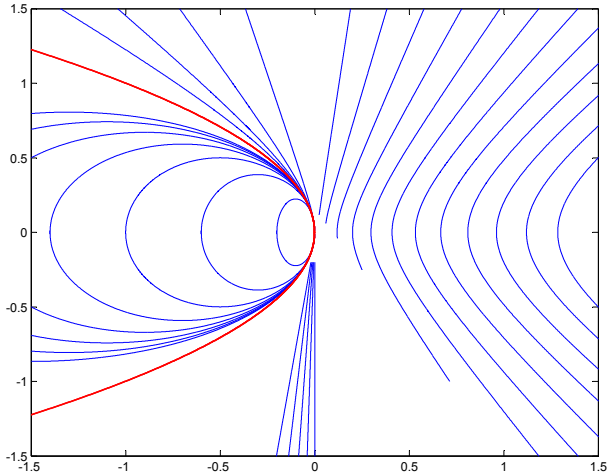



Figure 19: Phase portrait in the autonomous case.

$w = \frac{\partial \phi}{\partial z}$ on the other horizontal axis, and $t = time$ on the vertical axis. Given a condition as above, we can obtain a diagram similar to Figure 19 (in this case, I have kept $\phi$ constant at 0.75, z varies as the following: $z = (2\phi - 1)t + z0$, and $u'(z) = 1 + tanh(z)$.

Each time marker ($t_0$, $t_1$, etc.) corresponds to a different limiting parabola. Each of these parabolas corresponds to one trajectory. When the corresponding trajectory crosses the parabola, the slope as viewed from above is zero. These parabolas are shown below in red. In Figure 20(a), the view shows each parabola at its respective time marker. Figure 20(b) is a view from above, showing the $v$ and $w$ axes. This figure shows the intersection of the trajectories and the parabolas.

Currently, I am investigating initial conditions of $\phi$ that lead to shock wave formations.

**Presentations**

- Progress report at lab meeting, (May 2009).

**Personal Statement**

As a part of the RTG program at NCSU this year, I have truly felt as if I am in a training process. Upon entering the program, when people would ask me what research in mathematics entailed, I could only make a guess (and not a very good one at that). After only one semester of cooperation with this program, I have learned a good deal about the research process and its parts, and this new knowledge has impressed upon me the amount that I still have left to learn. I have experienced inter-departmental collaboration through our weekly lab meetings with our counterparts in the physics department. Through separate weekly meetings with Dr. Shearer, I have gained a bit of understanding of the broad scope of our particular focus.

This experience has contributed a good deal to the achievement of my educational and career goals. My immediate goal after receiving my bachelor's degree is to teach at the high school level for a while, and every high school teacher dreads the question, "But how are we ever going to use this?" As a part of the RTG, I have become much more confident in the answers that I will give to this particular challenge. I now possess a better understanding of the role that mathematics plays in the way we view the world around us. My education has been enriched by my participation in the RTG program, and looking back on the experience as a whole, I cannot think of a better way to have spent the second semester of my junior year.

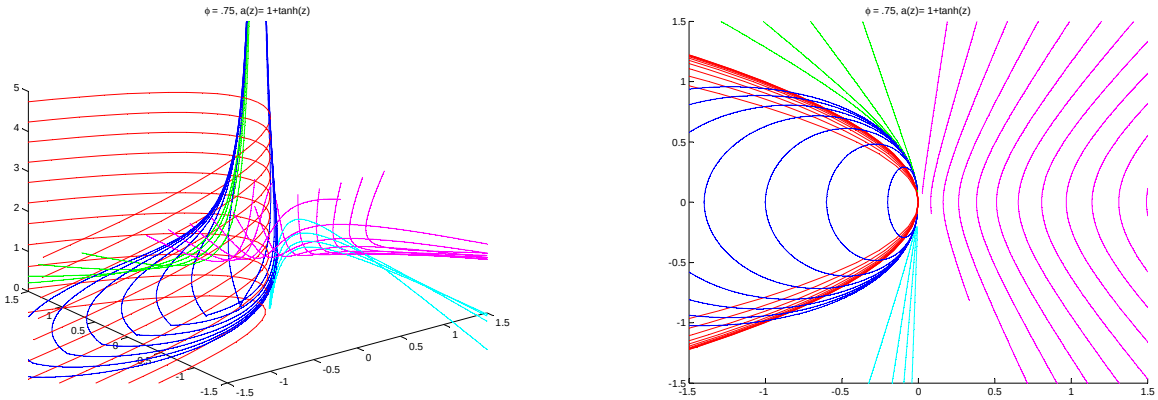



Figure 20: Trajectories and phase portrait in the non-autonomous case; (a) parabolas at their respective time markers and (b) views from above.

### 2.3.4 Jeff Olander

**Summary of Research Activities**

With over 20 million people suffering from osteoarthritis, cartilage regeneration procedures may provide a much-needed and efficient alternative to treatments like exercise, medication, and surgery. This is because researchers have regenerated cartilage in joint defects, where newly grown, healthy cartilage is seamlessly merged with the surrounding tissue in several weeks or a few months. In one such procedure, a nutrient-rich biocompatible scaffolding polymer material is injected directly into the defect. This hydrogel material is seeded with chondrocytes, or cartilage cells. Over time, these cells produce healthy cartilage, which accumulates around the chondrocyte. Finally, the cartilage replaces the hydrogel to completely fill the defect. This new cartilage remains in homeostasis, able to self-repair any minor damages that it may incur. Development of these procedures through laboratory experimentation alone is costly. ODE models can mediate some of this cost by simulating the evolution of a cell-seeded system with only a handful of unknowns. Although it doesn't account for the spatial behavior of the growing cartilage, an ODE model contains measurable parameters and is speedily solved using software like MATLAB.

In my research, I have developed an ODE model for cartilage regeneration based on extending an earlier ODE model developed by students in the 2008 NCSU Mathematics REU program. In particular the previous model neglected several key aspects that are required to ensure that nutrients and matrix proteins were regulated down to baseline levels associated with a state of homeostasis in the tissue. This summer, I am in the midst of applying the extended model in a parametric analysis of the dependence of tissue regeneration times on the underlying model parameters.

*ODE Cartilage Regeneration Model*

The ODE cartilage regeneration model employs four dependent variables, that are concentrations, for simulation of cartilage growth in a cell-seeded hydrogel scaffold assumed to have an infinite supply of nutrients. These variables are unlinked extracellular matrix, $M_u(t)$, linked extracellular matrix, $M_L(t)$, nutrient level inside the cell, $N(t)$, and hydrogel concentration, $H(t)$. The growth rate of each variable is explained by one of four coupled ordinary differential equations

$$\dot{M}_u = c_1(N - N_c)(M^* - M_L) - c_2 H M_u - c_3 M_u \tag{41}$$

$$\dot{M}_L = c_4 H M_u \tag{42}$$

$$\dot{N} = c_5(H_s - H)(M^* - M_L) - c_6(N - N_c) \tag{43}$$

$$\dot{H} = -c_7 H M_u \tag{44}$$

subject to the initial conditions:

$$M_u(0) = 0, \quad M_L(0) = 0, \quad N(0) = N_c, \quad H(0) = H_0. \tag{45}$$

In the above model, $N_c$ is the minimum nutrient concentration necessary for cell survival, $H_0$ is the initial concentration (polymer density) of the hydrogel, $H_s$ is the saturating concentration (polymer density) of the hydrogel, and $M^*$ is the target level of linked extracellular matrix in the healthy, homeostatic state.

The aspects of the cartilage regeneration problem accounted for in this model are now described. Equations (42), (44) and the second term in (41) model the reaction that converts unlinked matrix to linked matrix as the unlinked matrix comes into contact with the hydrogel. The last term in (41) and the last term in (43) model rates at which the cells would naturally regulate excess unlinked matrix proteins or excess nutrients back down to their homeostatic levels $M_u = 0$ and $N = N_c$,

respectively. The first term in (41) models aspects of the cellular physiology that require access to nutrients to synthesize unlinked matrix proteins, as well as the inherent ability of the cell to detect and regulate protein synthesis until the target level of linked matrix $M_L = M^*$ is achieved in the extracellular environment. Similarly, the first term in (43) also contains a cell regulatory term $(M^* - M_L)$, but is now multiplied by a term accounting for the fact that transport of nutrients to the cell may be inhibited by a dense hydrogel.Overall, this model accounts for coupling between several key mechanisms in the cartilage regeneration problem, and is consistent with a homeostatic state corresponding to the values $M_u^\infty = 0, M_L^\infty = M^*, N^\infty = N_c$ and $H^\infty = 0$.

*Preliminary Results*

The model was nondimensionalized by scaling $M_u$ and $M_L$ by $M^*$, $N$ by $N_c$, $H$ by $H_s$, by taking $1/c_6$ as the unit of time, and was implemented in MATLAB using the routine 'ode45'. Typical results, as shown in Figure 21, illustrate the wide variation in evolution of model variables with parameters such as initial hydrogel polymer concentration. These varied responses will have a significant effect of times required for the linked matrix concentration $M_L(t)$ to reach within a specified tolerance of the target value of $M^*$ (or 1 in the nondimensional case). Presently, I am using the model to conduct a detailed parametric analysis of the effects of model parameter variations on the time $t_R$ require to achieve 95% of the target value of linked matrix concentration; i.e. $M_L(t_R) = 0.95M^*$. Many cases exhibit a nonlinear, non-monotonic parametric dependence indicating the presence of optimal parametric states for minimization of tissue regeneration times.

**Presentations**

- 'ODE Modeling of Cartilage Regeneration in a Cell-Seeded Scaffold," 2009 Spring Math Undergraduate Research Presentations, North Carolina State University, (April 2009).

**Papers**

- J. Olander, R.F. Arnold, D.F. Marous, A.J. McLamb, K.C. Thompson, W.R. Woodruff, J.M. Haugh and M.A. Haider, "A mathematical model for cartilage growth in a cell-seeded hydrogel scaffold," in preparation.

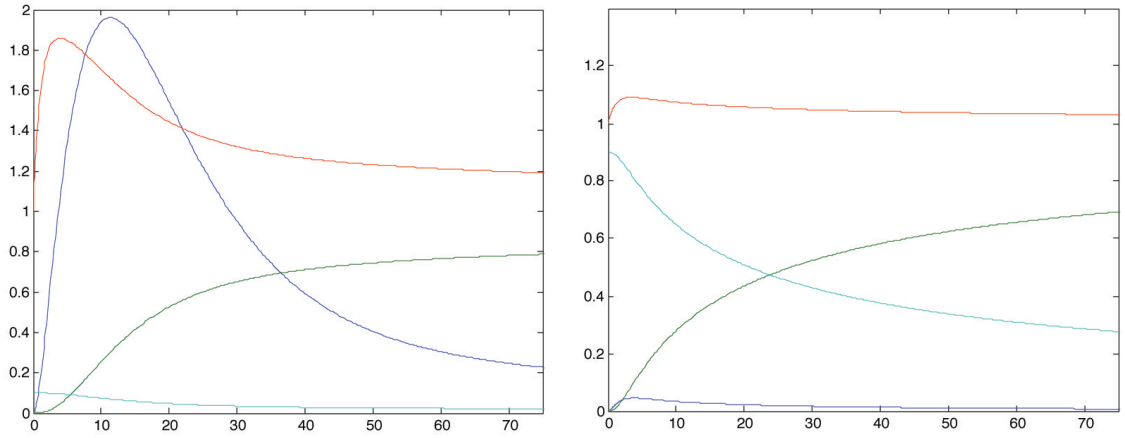



Figure 21: Simulations of cartilage regeneration using the ODE model showing $H(t)$ (cyan), $M_L(t)$ (green), $N(t)$ (red) and $M_u(t)$ (blue) for the cases of initial hydrogel polymer of: (a) a lower density, (b) a higher density.

**Personal statement**

I was very excited to become involved with Dr. Haider's research. As a disabled person, I have a deep appreciation for the work being done in medicine to help people with challenges to their mobility. While advances in cartilage replacement will not directly help me, I take pleasure in knowing that I'm involved in a project that can someday reduce the impact of disability on people's lives.

### 2.3.5 David Pate

**Summary of Research Activities**

My goal is to compare the homogenized energy model to the Prandtl-Islinskii (P-I) model for hysteresis. So far I have researched and explored the Prandtl-Ishlinskii almost completely. I focused on the main version of the P-I model, the symmetric generalized model.

The symmetric-generalized P-I model is versatile, demonstrated experimentally, and has an analytically obtained inverse. Its versatility comes from being able to easily define the density function and model coefficients. It has been demonstrated experimentally with shape-memory alloys, piezoceramics, and magnetostrictive materials, to name a few. The inverse is itself a P-I model that has analytical formulas to determine all the proper coefficients.

The P-I model is based on a play operator and envelope function. The play operator is the source of the hysteresis loops. Using a hyperbolic tangent envelope function

$$y(v(t)) = a_1 \tanh(a_2 v(t) + a_3) + a_4$$

allows the model to saturate as illustrated in Figure 22.

Most of my time has been spent researching and understanding the model, coding the model and inverse model in MATLAB, exploring the abilities and limitations, and developing an easy-to-use implementation algorithm. I have extensively documented the effect of different density functions on the model and the behavior of minor loops. I have also documented the inverse model and its implementation.

My goal in the future is to better understand the derivation of the inverse model and improve on the implementation procedure for the model. Ultimately the goal is still to compare all of this information to the homogenized energy model.

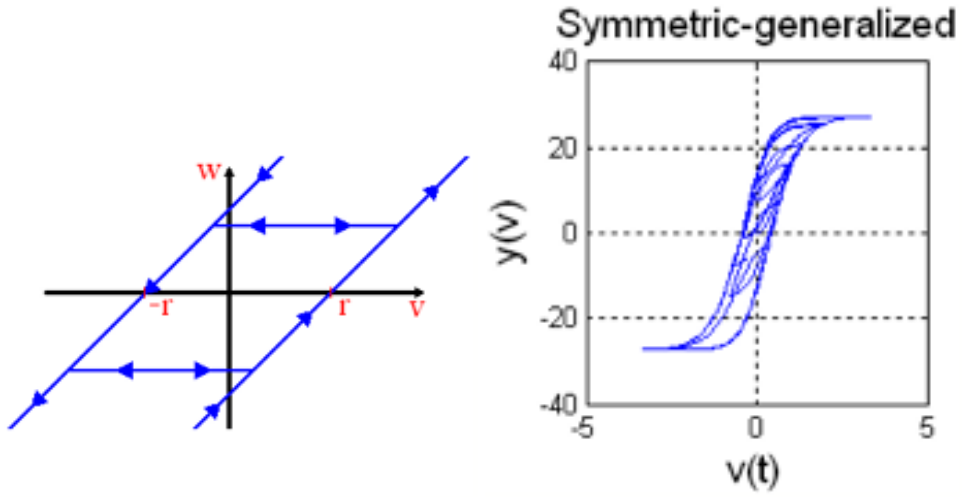



Figure 22: The play operator and symmetric generalized model with input $v$ and output $y$.

**Personal Statement**

This project is my first research project, and I have definitely enjoyed it. I meet one-on-one with a professor regularly and attend the research group meetings. Through my work and these meetings, I have increased my MATLAB skills, increased my knowledge of multifunctional materials, and refreshed my basic mathematics fundamentals.

### 2.3.6 Leslie Watkins

**Summary of Research Activities**

During the 2009 Spring semester, a project was initiated on computational simulation of ultrasonic wave propagation in cardiovascular tissue for ultimate analysis of ultrasound imaging. This project was motivated by a novel imaging technique called Acoustic Radiation Force Impulse (ARFI) that has the potential to non-invasively detect atherosclerotic plaques. Dr. Caterina Gallippi of the joint UNC/NCSU Biomedical Engineering Department is an expert in ARFI imaging techniques and collaborates with Dr. Haider. To initiate the project, in Spring 2009 MATLAB codes were formulated and implemented for simulation of the 1D an 2D wave equations using explicit finite difference schemes. At present (Summer 2009), these models and associated MATLAB codes are being extended by an REU group working with Dr. Haider to simulate wave propagation in elastic and viscoelastic materials with inhomogeneities representing atherosclerotic plaques. Solutions will be applied to inverse analysis of ultrasound data to determine the extent to which material parameter maps can enhance detection of atherosclerosis via non-invasive imaging using ultrasound.

**Personal Statement**

I enjoyed my experience with the RTG program and felt that it was beneficial for developing a career in research. During the program, the focus of my research was numerical methods for modeling waves. Outside of what I learned that was specific to my project, I was able to meet other professors and students that were doing research in the math department. During weekly research training modules (RTMs), I was able to learn what everyone else was doing, which exposed me to a broad array of the research being conducted at NCSU and an opportunity to network with other people involved in mathematics. The most important thing that I got out of this experience, though, was the chance to learn that I do have useful and marketable skills with a math degree.

# 3 Course Development

The NCSU Mathematics Department presently offers approximately 8 undergraduate and 26 graduate courses, discounting special topics courses, in the following areas: model development (4 courses), analysis (6 courses), optimization (4 courses), numerical analysis (7 courses), differential equations (5 courses), control (4 courses) and technical communication (1 course).

During the first year of the RTG, we initiated 3 new courses on topics relating to program research areas: (i) *Applied Modeling and Analysis Techniques,* (ii) *Mathematical Fluid Mechanics*, and (iii) *Validation, Verification and Uncertainty Quantification.* We have additionally developed the courses (iv) *Numerical Methods for Model Calibration* and (v) *Introduction to Continuum Mechanics of Elastic and Viscoelastic Solids* during the second year of the RTG. Details regarding these courses are provided here.

## 3.1 Numerical Methods for Model Calibration – Fall 2008

**Instructors:** Pierre Gremaud and C.T. Kelley

**Course Webpage:** `http://www.math.ncsu.edu/~gremaud/MA798C/`

**Course Description**

The class covered the following topics

- Review of probability concepts: random variables, probability distribution, law of large numbers, multivariate distribution, covariance matrix, Bayesian inference, examples
- Review of linear least squares: theory, computational methods, implementation, examples
- Kalman filtering: derivation, implementation, examples
- Computing gradients and Jacobians: sensitivities, adjoints, automatic differentiation
- Nonlinear least squares: theory, computational methods, implementation, examples
- Monte Carlo methods: pseudo random numbers, Monte Carlo integration, variance reduction, implementation, examples
- Optimization without derivatives: Nelder-Meade, implicit filtering
- Ensemble Kalman filtering: theory, computational methods, implementation, examples

Several guest lecturers presented applications related to their own research which pertained to model calibration. The models seen in class were used to solved these problems. Arnaud Doucet, the leader of the 2008-09 SAMSI program on Sequential Monte-Carlo methods also presented particle methods to the class. It is expected to run this class on a regular basis, every other year at NCSU.

**Dissemination**

Gremaud and Kelley are also in the process of writing a textbook on the class material (to be submitted to SIAM for publication).

**Enrollment:** 10 students

## 3.2 Introduction to Continuum Mechanics of Elastic and Viscoelastic Solids

**Instructor:** Mansoor Haider

**Course Webpage:** `http://www4.ncsu.edu/%7emahaider/MA591Z_S09.pdf`

### Course Description

Continuum models have been widely employed in describing the mechanics of many solid and solid-like materials. In these models, appropriate kinematic quantities (vectors, tensors etc.) are introduced to quantify deformation in the material relative to an undeformed reference state. For a specific application, constitutive laws are then formulated to relate the kinematic quantities to forces inside the material. Finally, balance laws are employed to enforce conservation of mass, momentum and energy, resulting in a closed system of governing equations for a specified geometry and boundary conditions. This course will introduce the student to continuum mechanics models for elastic, viscoelastic and poroelastic materials. Applications will be included, with an emphasis on continuum modeling in biomechanics.

### Topics

- Mathematical Concepts: Vector fields, tensor analysis, orthogonal curvilinear coordinates.
- Kinematics and Strain: Measures of strain, strain tensors, compatibility.
- Stress and Conservation Laws: The stress tensor, stress-strain relations, linear elasticity, conservation of mass, momentum and energy
- Applied Linear Elasticity: Mathematical solutions for plane stress, plane strain and axisymmetric boundary value problems, energy methods.
- Linear Viscoelasticity: Discrete models (Maxwell, Kelvin, Voigt), hereditary integrals, creep, stress relaxation, dynamic loading, hysteresis.
- Introduction to Poroelasticity: Two-phase (fluid-solid) mixture models, balance laws for mass/momentum/energy, applications to biological tissues.
- Introduction to Nonlinear Elasticity.

**Enrollment:** 13 students

# 4 Research Training Modules (RTM)

An integral training component of the program consists of Research Training Modules (RTM) that have been developed to introduce students and postdocs to research and career topics not typically covered in coursework. As illustrated in Table 5, these included a number of training topics such as introductions to MATLAB, LaTeX and poster design in addition to discussions focused on general topics pertaining to graduate school and subsequent career options.

The RTM were led by RTG graduate students, postdocs and faculty and were open and advertised to all RTG participants as well as all Mathematics graduate students and postdocs.

| Date | Topic |
|---|---|
| 9/5/08 | Organizational Meeting |
| 9/12/08 | Introduction to MATLAB |
| 9/19/08 | Fundamentals of LaTeX I |
| 9/26/08 | Fundamentals of LaTeX II |
| 10/24/08 | Creating Figures Using Adobe Illustrator |
| 10/31/08 | Creating Figures Using XFIG |
| 11/7/08 | Fundamentals of PowerPoint |
| 11/14/08 | Job Search Tactics |
| 1/30/09 | Poster Design |
| 2/13/09 | Training Opportunities to Prepare for Grad School |
| 3/13/09 | Group Research Updates I |
| 3/20/09 | Group Research Updates II |
| 3/27/09 | Group Research Updates III |
| 4/3/09 | Group Research Updates IV |
| 4/17/09 | End of Year Meeting |

Table 5: RTM schedule; details can be found at the RTM website.

**RTM Website:** `http://www4.ncsu.edu/~mahaider/NCSU_RTG_Site/RTG_RTMs.html`

This provides a repository for the RTM schedule, presentations, associated software, and graduate school and career resources.

# 5 Student and Postdoc Seminars

All students and postdocs in the research training program were required to participate in the Numerical Analysis or Applied Mathematics seminars that are run weekly in the Department of Mathematics. During these seminars, all presentations are given by the students and postdocs with feedback provided by the other participants and the program faculty. This has proven highly successful in preparing students for seminars, conferences, and interviews.

**Seminar Websites:** `http://www4.ncsu.edu/%7ejmhaugh2/AMGSSf08/`
`http://www4.ncsu.edu/~jmhaugh2/AMGSS/`

# 6 Awards and Honors

**Donovan Shickley**

- *Provost Research Fellowship:* Received a single year $5000 award upon admittance to the NCSU Applied Mathematics doctoral program.

# 7 Papers and Presentations

## 7.1 Papers

**Michael Stuebner**

- N.G. Medhin and M. Stuebner, "An evolutionary algorithm for molecular dynamics simulation," in preparation.
- M. Stuebner, J. Atulasimha and R.C. Smith, "Frequency response of piezoelectric and magnetostrictive materials based hysteretic nonlinear systems," Proceedings of SMASIS08, ASME 2008 Conference on Smart Materials, Ellicott City, MD, October 28-30, 2008.
- M. Stuebner, J. Atulasimha and R.C. Smith, "Quantification of Hysteresis and Nonlinear Effects on the Frequency Response of Ferroelectric and Ferromagnetic Materials," CRSC Technical Report CRSC-TR09-06; *Smart Materials and Structures*, submitted.
- M. Stuebner, R.C. Smith, M. Hays and W.S. Oates, "Modeling the Nonlinear Behavior of Macro-Fiber Composite Actuators," CRSC-TR09-08; Proceedings of the SPIE, Smart Structures and Materials 2009.

**Jeb Collins**

- J. Collins and P. Gremaud, "A simple model for laser drilling," *Mathematics and Computers in Simulation*, submitted.

**Amanda Criner**

- "H.T. Banks, B. Boudreaux, A.K. Criner, K. Foster, C. Uttal, T. Vogel, W.P. Winfree, "Thermal Based Damage Detection in Porous Materials," *Inverse Problems in Science and Engineering*, accepted with revision.

**Lisa Downen**

- L. Downen, T. Glover, L. Hallock, S. King, J. Shor, J. Wallace and R.C. Smith, "Efficient Algorithms for Implementation of Hysteresis Models," Proceedings of the SPIE, Smart Structures and Materials 2009.

**Nick Giffen**

- N. Giffen and M. Shearer, "Shock formation and shock breaking in models of particle size segregation," in preparation.

**Janine Haugh and Jeff Olander**

- J.M. Haugh and M.A. Haider, "A reaction-diffusion model for extracellular matrix regeneration in the local environment of a chondrocyte seeded in a hydrogel," in preparation.

- J. Olander, R.F. Arnold, D.F. Marous, A.J. McLamb, K.C. Thompson, W.R. Woodruff, J.M. Haugh and M.A. Haider, "A mathematical model for cartilage growth in a cell-seeded hydrogel scaffold," in preparation.

**Ellen Peterson**

- E. Peterson, M. Shearer, T. Witelski, R. Levy, "Stability of Traveling Waves in Thin Liquid Films Driven by Gravity and Surfactant," Proceedings, 12th International Conference on Hyperbolic Problems: Theory, Numerics, Applications, Hyp 2008, To appear.

## 7.2 Presentations

**Michael Stuebner**

- "Frequency Response of Piezoelectric and Magnetostrictive Hysteretic Nonlinear Systems," ASME Conference on Smart Materials, Adaptive Structures and Intelligent Systems, Ellicott City, MD, October 2008.
- "Modeling the nonlinear behavior of macro fiber composite actuators," SPIE Conference on Smart Structures/Nondestructive Evaluation for Health Monitoring and Diagnostics, San Diego, CA, March 2009.
- "Frequency Response of Ferroelectric and Ferromagnetic Hysteretic Systems," 33rd SIAM Southeastern Atlantic Section Conference, Columbia, SC, April 2009.

**Jeb Collins:**

- "A Simple Model for Laser Drilling," Numerical Analysis Seminar, North Carolina State University, (February 23, 2009).
- "A Simple Model for Laser Drilling," AMS Spring Southeastern Section Meeting, North Carolina State University, Raleigh, NC, (April 5, 2009).

**Amanda Criner**

- "Fundamentals of LaTeX," Research Training Module, North Carolina State University, (September 2008).
- "Thermal Interrogation of Porous Materials," Applied Mathematics Graduate Student Seminar, North Carolina State University, (January 2009).
- "Thermal Interrogation of Porous Materials," Research Training Module, North Carolina State University, (April 2009).

**Nick Giffen**

- "Particle size segregation in granular avalanches: shock formation and shock breaking," Applied Mathematics Graduate Student Seminar, North Carolina State University, (October 2008, April 2009).
- "Particle size segregation in granular avalanches: shock formation and shock breaking," Research Training Module, North Carolina State University, (March 2009).

**Janine Haugh**

- "Your Hips Don't Lie: Modeling Cartilage Regeneration," poster, Department of Mathematics Alumni & Friends Brunch, North Carolina State University, (October 2008).
- "A Reaction-Diffusion Model for Extracellular Matrix Regeneration in a Cell-Seeded Hydrogel," Applied Mathematics Graduate Student Seminar, North Carolina State University (December 2008).
- "Modeling Cartilage Regeneration in the Extracellular Environment of a Cell-Seeded Hydrogel", 2009 Graduate Student Research Symposium, North Carolina State University, (March 2009).
- "Modeling Cartilage Regeneration in the Extracellular Environment of a Cell-Seeded Hydrogel", poster, Mathematics and Statistics Building Dedication, North Carolina State University, (May 2009).

**Ellen Peterson**

- "Thin Fluid Films with Surfactant", Triangle Soft Matter Workshop, North Carolina State University, poster and soundbite, (May 2009).
- "Thin Fluid Films with Surfactant", SAS Hall Dedication, North Carolina State University, poster, (May 2009).
- "An Overview of Thin Fluid Films Research," Research Training Module, North Carolina State University, (March 2009).
- "Thin Fluid Films Under the Influence of Surfactant," Applied Mathematics Graduate Student Seminar, North Carolina State University, (March 2009).
- "Thin Fluid Films with Surfactant," Higher Order Geometric Evolution Equations: Theory and Applications from Microfluidics to Image Understanding, IMA-University of Minnesota, poster, partially funded by RTG (March 2009).
- "Shock Waves: Flow of Thin Liquid Films," North Carolina State Graduate Recruitment Day, (February 2009).
- "Flow of Thin Films with Surfactant: Behavior of Perturbations," Thin Films Day, North Carolina State University, (January 2009).
- "Flow of Thin Films with Surfactant: Behavior of Perturbations," Applied Mathematics Graduate Student Seminar, North Carolina State University, (November 2008).
- "Flow of Thin Films with Surfactant: Beginning Stability Analysis," EDGE Cluster Meeting, North Carolina State University, (October 2008).

**Donovan Shickley**

- "Passive Metamaterial Structures, Applied Mathematics Graduate Student Seminar, North Carolina State University, (April 20, 2009).

**Rachael Gordon-Wright**

- "Free Granular Surfaces," Math Undergraduate Research Presentations, North Carolina State University, April 22.

**Allison McAlister**

- Progress report at lab meeting, (May 2009).

**Jeff Olander**

- 'ODE Modeling of Cartilage Regeneration in a Cell-Seeded Scaffold," 2009 Spring Math Undergraduate Research Presentations, North Carolina State University, (April 2009).

# 8 Program Diversity

Throughout the first two years of the program, we have been very sensitive to diversity. Of the 20 supported students and postdocs, 10 were female, 1 was Hispanic, and 1 was physically disabled (wheelchair bound since birth due to spinal muscular atrophy). We will continue to maintain and improve upon these demographics in the future.

# 9 Trainees and Faculty during Years 1 and 2

**Postdoc, Graduate Student and Undergraduate Trainees:**

| **Postdoc** | **Graduate Students** | **Undergraduate Students** |
|---|---|---|
| Michael Stuebner (Years 1-2) | Brandy Benedict (Year 1) | Michael Dearman (Year 2) |
| | Jeb Collins (Years 1-2) | Rachael Gordon-Wright (Year 2) |
| | Amanda Criner (Year 2) | Kristopher Kleiner (Year 1) |
| | Lisa Downen (Years 1-2) | Nicole Kroeger (Year 1) |
| | Nicholas Giffen (Years 1-2) | Allison McAlister (Year 2) |
| | Janine Haugh (Year 2) | Travis McCaw (Year 1) |
| | Sarah Olson (Year 1) | Jeff Olander (Years 1-2) |
| | Ellen Peterson (Years 1-2) | David Pate (Year 2) |
| | Donovan Shickley (Year 2) | Roberto Rodriguez (Year 1) |
| | Ryan Siskind (Year 1) | Leslie Watkins (Year 2) |

**Trainees Leaving Group:**

*Graduate Students:*

- Brandy Benedict: PhD in 2008 – Faculty member at Merrimack College
- Sarah Olson: PhD in 2008 – VIGRE Postdoc at Tulane University
- Ryan Siskind: PhD in 2008 – Employed at Advertising.com

*Undergraduate Students:*

- Kristopher Kleiner: Completed ABM degree at NCSU. Will attend graduate school at Duke in Fall 2009.
- Nicole Kroeger: Awarded Goldwater Scholarship to support her senior year and participated in the MASS Program at Penn State in the Fall of 2008. Will start mathematics PhD program at Notre Dame in Fall 2009 through support from a Notre Dame Presidential Fellowship.
- Travis McCaw: Completed his BS in Math and BS in Physics at NCSU. Will start PhD program at Wisconsin in Medical Physics in Fall 2009.
- Jeff Olander: Completed his BS in Math and BS in Physics at NCSU. Will start PhD program at UNC in Physics in Fall 2009.
- Roberto Rodriguez: Graduated in May 2008 and has a math career-track job in the private sector.

**Senior Faculty:**

- Ralph Smith: Mentored Michael Stuebner, Ryan Siskind, Lisa Downen, Kristopher Kleiner and David Pate; developed and taught the new course *Validation, Verification and Uncertainty Quantification*.
- Pierre Gremaud: Mentored Jeb Collins, Rachael Gordon-Wright and Roberto Rodriguez. Developed and co-taught the new course *Numerical Methods for Model Calibration*.

- Mansoor Haider: Mentored Michael Stuebner, Brandy Benedict, Janine Haugh, Sarah Olson, Jeff Olander and Leslie Watkins; developed and taught the new course *Applied Modeling and Analysis Techniques*.
- Negash Medhin: Mentored Michael Stuebner, Michael Dearman and Travis McCaw.
- Michael Shearer: Mentored Nicholas Giffen, Ellen Peterson, Nicole Kroeger and Allison McAlister; developed and taught the new course *Mathematical Fluid Mechanics*.
- H.T. Banks: Mentored Amanda Criner.
- Kazi Ito: Will mentor future trainees.
- C.T. Kelley: Developed and co-taught the new course *Numerical Methods for Model Calibration*; will mentor future trainees.

# 10 Trainee and Quantitative Data

## Trainee Data:

**(a) PhD Recipients for Group in Last 5 Years** – Total of 26

| Name | Cit. | BA/BS Institution | Time | Post-PhD Employment | Advisor |
|---|---|---|---|---|---|
| Brian Adams | US | St. Michaels Col. | 5 yrs | Sandia National Labs | Banks |
| Jemina Davis | US | Clemson Univ. | 5 yrs | EPA | Banks |
| Stacey Ernstberger | US | Murray State | 5 yrs | LaGrange College | Banks |
| Nathan Gibson | US | WPI;MS at Tenn. | 4 yrs | NASA/NIA Postdoc | Banks |
| Sarah Grove | US | Youngstown State | 4 yrs | AF Res. Lab, Rome, NY | Banks |
| Jeff Hood | US | BS/MS at Texas Tech | 4 yrs | Midwestern State Univ. | Banks-Medhin |
| Nicholas Luke | US | NC A&T | 5 yrs | EPA Postdoc | Banks |
| John Samuels, Jr., | US | Florida Atlantic Univ. | 5 yrs | Soneticome | Banks |
| Kristen DeVault | US | Maryland | 5 yrs | Epic System Corp. | Gremaud |
| Chris Kuster | US | Knox College | 4 yrs | NCSU Postdoc | Gremaud |
| Brandy Benedict | US | Occidental College | 6 yrs | Merrimack College | Haider |
| Sarah Olson | US | Prov. Coll./MS URI | 5 yrs | Tulane Math Postdoc | Haider |
| Richard Schugart | US | SUNY-Geneseo | 6 yrs | MBI-OSU Postdoc | Haider |
| Greg Hicks | US | Morehead State Univ. | 4 yrs | Kirt. AFB | Ito |
| Yaw Kyei | Ghana | Univ. of Ghana | 7 yrs | NCATT | Ito |
| Karen Dillard | US | RPI/MS UMass-Lowell | 5 yrs | AFIT | Kelley |
| Dan Finkel | US | NCSU | 5 yrs | MIT Lincoln Labs | Kelley |
| Katie Fowler | US | SUNY Plattsburgh | 5 yrs | Clarkson University | Kelley |
| Matthew Lasater | US | NCSU | 4 yrs | MIT Lincoln Labs | Kelley |
| Jill Reese | US | Clarion Univ | 4 yrs | Florida State Postdoc | Kelley |
| Chung-Chien Hong | Taiwan | Nat. Cheng-Kung U. | 5 yrs | New Mex St Postdoc | Medhin |
| Gloria Potter | US | Alabama State | 5 yrs | AFPC/DPAPA USAF | Medhin |
| Wei Wan | China | U. Sci & Tech | 4 yrs | Claflin Univ. | Medhin |
| Rachel Levy | US | Oberlin | 4 yrs | Duke/Harvey Mudd | Shearer |
| Brian Ball | US | WPI | 5 yrs | General Electric | Smith |
| Thomas Braun | US | Ashbury College | 3 yrs | NGA | Smith |
| Jon Ernstberger | US | Murray State | 7 yrs | LaGrange College | Smith |
| Andrew Hatch | US | NCSU | 7 yrs | CNA Corp. | Smith |
| Ryan Siskind | US | | | Advertising.com | Smith |

**(b) Postdoctoral Associates for Group in Last 5 Years** – Total of 20

| Name | PhD Institution | Mentor | Employment |
|---|---|---|---|
| Vrushali Bokil | Univ. Houston | Banks | Oregon State University |
| Ariel Cintron-Arias | ASU | Banks | East Tennessee State Univ. |
| Sava Dediu | RPI | Banks | Campbell & Co. |
| Nathan Gibson | NCSU | Banks/Winfree | Oregon State University |
| Shuhua Hu | Univ. of Louisiana-Lafayette | Banks | Current |
| Hee-Dae Kwon | Iowa State University | Banks | Inha University, South Korea |
| Yanyun Ma | MIT | Banks | Texas A&M University |
| Hoan Nguyen | VA Tech | Banks | Center for Naval Analysis |
| Karyn Sutton | ASU | Banks | Current |
| Jari Toivanen | Univ. Jyvaskyla | Banks/Ito | Visiting Res., Stanford |
| Chris Kuster | NCSU | Gremaud/Ito | Carroll College |
| Zhonghua Qiao | Hong Kong Baptist Univ. | Ito | Hong Kong Baptist Univ. |
| Tomoya Takeuchi | Univ. of Tokyo | Ito | Current |
| Kai Fan | UNCC | Kelley | |
| Chris Kees | UNC | Kelley | US Army Engr. R&D Center |
| Greg Recine | Stevens Institute | Kelley | Current |
| Peiji Zhao | Stevens Institute | Kelley | ECE Dept., NCSU |
| Jayasimha Atulasimha | Maryland | Smith | Virginia Commonwealth Univ. |
| Emily Lada | NCSU | Smith | SAS Institute Inc. |
| William Oates | GA Tech | Smith | Florida State University |
| Michael Stuebner | LSU | RTG | Current |

**(c) Total Federal Funding for the Group in the Last 5 Years (Including RTG):** Direct Costs

| | 2004-05 | 2005-06 | 2006-07 | 2007-08 | 2008-09 |
|---|---|---|---|---|---|
| REUs* | | $16,000 | $16,000 | $58,000 | $58,000 |
| Graduate Students | $293,000 | $298,000 | $356,000 | $510,000 | $541,960 |
| Postdocs | $219,500 | $219,500 | $207,000 | $355,000 | $261,275 |

* The Mathematics Department has an NSF/NSA funded REU that includes RTG faculty as mentors.

**Quantitative Data:** Totals for the Group (Including RTG Students and Postdocs in 2007-09)

| | 2004-05 | 2005-06 | 2006-07 | 2007-08 | 2008-09 |
|---|---|---|---|---|---|
| Math Grad Students (Total) | 26 | 26 | 24 | 33 | 33 |
| Female Grad Students | 10 | 14 | 14 | 21 | 19 |
| Minority Grad Students | 1 | 2 | 2 | 3 | 2 |
| US Citizen Grad Students | 25 | 22 | 18 | 29 | 28 |
| Math PhDs Granted (Total) | 5 | 4 | 3 | 8 | 5 |
| Female Math PhDs | 0 | 1 | 1 | 5 | 4 |
| Minority Math PhDs | 0 | 1 | 0 | 1 | 0 |
| US Citizen Math PhDs | 5 | 4 | 2 | 7 | 3 |
| Math Postdocs (Total) | 8 | 10 | 6 | 8 | 8 |
| Female Postdocs | 3 | 4 | 2 | 2 | 2 |
| Minority Postdocs | 0 | 0 | 1 | 1 | 1 |
| US Citizen Postdocs | 4 | 5 | 2 | 3 | 2 |

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## References for Research Group Reports in Section 1


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