Research Statement

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My research is in applied mathematics, specifically the sub-disciplines of scientific computation and numerical analysis. In the ever-evolving field of scientific computation, I believe that there are three primary mathematical aims that together allow insight within scientific applications:

(a) the development of robust and accurate numerical methods for solution of mathematical models,

(b) the extension of these methods to enable their use on increasingly-larger computational hardware, and

(c) the incorporation of increased realism into mathematical models of physical systems.

In my own research, I have contributed to each of these challenges through highly-collaborative investigations centered around the accurate, robust and efficient solution of multi-physics models. These problems are typically characterized by time-dependent systems of nonlinear partial differential equations, wherein each component of the system arises from a different physical process. Examples of such problems abound in the physical sciences, including the tightly-coupled interaction between fluid motion and electromagnetism in models of plasma dynamics; the delicate balance between radiation pressure and gravitational forces in stars preceding core-collapse supernovae; and the interplay between dark matter dynamics, gravitational clustering, radiation transport and chemical ionization that formed the universe we know today.

My scientific collaborations have focused on each of the above applications. In these collaborations, my research strives to contribute through exploring three questions:

(1) How can we efficiently solve multi-physics PDE systems that evolve on disparate temporal and spatial scales?

(2) Can we develop optimally efficient and accurate time evolution algorithms to create robust and stable solvers for multi-rate problems?

(3) Is it possible to create and analyze multi-scale modeling algorithms that efficiently incorporate first-principles atomistic information within macroscopic systems of partial differential equations?

In addition to helping answer these questions, I have successfully incorporated student training within my research, and in a short 4 year period I have supervised two Ph.D. students (one in progress, one finished) as well as one undergraduate honors project.

In the following sections, I elaborate on these three questions, introducing the relevant physical applications and models, the role of students, and all publications resulting from each research area.

Scalable, Robust and Efficient Solvers for Multi-Physics Problems

The last 50 years have seen tremendous progress in scientific computing, with a multitude of new methods that can achieve unprecedented accuracy with remarkable speed, and that can effectively utilize tens of thousands of processors on the largest supercomputers ever built. However, a common trait of much of this work has been a focus on specific physical processes or idealized mathematical equations, c.f. Laplace's equation or the Fourier transform. Unfortunately reality is rarely so simple, and although different algorithms may prove optimal for specific processes in isolation, none of those algorithms typically remain optimal for the system formed as a combination of those parts. It is in this "multi-physics" context that my research fits.

Throughout my career, I have worked to develop fully implicit computational approaches for time evolution of multi-physics PDE systems. In my Ph.D. thesis research, I focused on a thermodynamic model for simulating

the dynamics of shape memory alloy (SMA) wires [3, 4, 5, 6, 10, 11, 12, 13, 14, 20],

$$\begin{aligned} \rho_0 \ddot{u} &= \nabla \cdot (\rho_0 \partial_\gamma \Psi + A\dot{\gamma}) + \rho_0 b, \\ \rho_0 c_p \dot{\theta} &= \rho_0 \theta \partial_{\gamma\theta} \Psi \cdot \dot{\gamma} + \mathrm{Tr}\left(\dot{\gamma}^T A \dot{\gamma}\right) + \nabla \cdot (\kappa \det(\gamma) \nabla \theta) + \rho_0 r, \end{aligned} \tag{1}$$

where u is the macroscopic material deformation, θ is the material temperature, $\gamma = \nabla u$, and $\Psi(\gamma, \theta)$ is the material-dependent Helmholtz free energy density.

As a post-doctoral researcher, I added to my set of application areas with collaborations studying visco-resistive magnetohydrodynamics (MHD), arising in studies of astrophysical and fusion plasmas, and radiation hydrodynamics (RHD), used to model core-collapse supernova explosions and cosmological reionization in the early universe. In a DOE-funded collaboration with researchers from Princeton Plasma Physics Laboratory, Lawrence Livermore National Laboratory and KAUST [25, 26, 27, 28, 33], I have studied a visco-resistive MHD model that couples the compressible viscous Euler equations for modeling plasma hydrodynamics,

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ \partial_t (\rho \mathbf{v}) + \nabla \cdot \left(\rho \mathbf{v}\mathbf{v}^T\right) + \nabla p + \mathbf{B} \times \mathbf{J} &= \nabla \cdot \overline{\tau}, \\ \partial_t e + \nabla \cdot \left((e + p - \tfrac{1}{2}\mathbf{B} \cdot \mathbf{B})\mathbf{v}\right) + \nabla \cdot (\mathbf{E} \times \mathbf{B}) &= \nabla \cdot (\overline{\tau}\mathbf{v}) + \nabla \cdot (\kappa \nabla T), \end{aligned} \tag{2}$$

with the low-frequency Maxwell equations that model the evolution of electromagnetic fields,

$$\begin{aligned} \partial_t \mathbf{B} &= -\nabla \times \mathbf{E}, \\ \mathbf{J} &= \nabla \times \mathbf{B}, \\ \mathbf{E} &= -\mathbf{v} \times \mathbf{B} \; + \; \eta \mathbf{J}, \\ \nabla \cdot \mathbf{B} &= 0, \end{aligned} \tag{3}$$

where here ρ is the density, $\mathbf{v}$ is the velocity, $\mathbf{B}$ is the magnetic induction, $\mathbf{J}$ is the electric current, $\mathbf{E}$ is the electric field, and e is the total energy. Similarly, in a NSF-funded collaboration with scientists from the University of California at San Diego, Columbia University, Stanford University, Michigan State University and others [1, 2, 7, 15, 16, 17, 18, 19, 21, 22, 24, 32], I have focused on models for cosmological radiation hydrodynamics, that couple hydrodynamic motion,

$$\begin{aligned} \partial_t \rho_b + \frac{1}{a}\mathbf{v}_b \cdot \nabla \rho_b &= -\frac{1}{a}\rho_b \nabla \cdot \mathbf{v}_b, \\ \partial_t \mathbf{v}_b + \frac{1}{a}\left(\mathbf{v}_b \cdot \nabla\right)\mathbf{v}_b &= -\frac{\dot{a}}{a}\mathbf{v}_b - \frac{1}{a\rho_b}\nabla p - \frac{1}{a}\nabla \phi, \\ \partial_t e + \frac{1}{a}\mathbf{v}_b \cdot \nabla e &= -\frac{2\dot{a}}{a}e - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla \phi + G - \Lambda, \end{aligned} \tag{4}$$

with models for self-gravity,

$$\nabla^2 \phi = \frac{4\pi g}{a}(\rho_b + \rho_{dm} - \langle \rho \rangle), \tag{5}$$

radiation transfer,

$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) = \nabla \cdot (D \nabla E) - \frac{\dot{a}}{a}E - c\kappa E + \eta, \tag{6}$$

and chemical ionization,

$$\partial_t \mathtt{n}_i + \frac{1}{a}\nabla \cdot (\mathtt{n}_i \mathbf{v}_b) = \alpha_{i,j}\mathtt{n}_e \mathtt{n}_j - \mathtt{n}_i \Gamma_i^{ph}, \qquad i = 1, \ldots, N_s. \tag{7}$$

Here, ρ_b is the comoving baryonic density, $\mathbf{v}_b$ is the proper peculiar baryonic velocity, e is the total gas energy per unit mass, ϕ is the modified gravitational potential, E is the comoving grey radiation energy density, and $\mathtt{n}_i$ is the comoving number density for the i^{th} chemical species. Finally, in a DOE-funded collaboration with

scientists from SUNY Stony Brook and Lawrence Livermore National Laboratory [29, 30], I have studied similar RHD models applied to gravitational radiation hydrodynamics within core-collapse supernovae.

While many details of the above models (1)-(7) have been left out from this discussion, a recurring theme among each of them is that groups of variables can evolve on drastically different time and space scales. As a result, basic explicit and operator-split time integration techniques fail to efficiently and accurately track their dynamics, resulting in inaccurate, unstable, or at least highly inefficient numerical methods. Moreover, to accurately capture the scientifically interesting components of most of these systems would require spatial resolutions that may only be attainable on the world's largest supercomputers. As a result, the proper derivation of solution algorithms for these problems is critical to their success as accurate, efficient and scalable scientific tools. Moreover, the nature of modern scientific research requires that these tools be disseminated to the scientific community. Even the most gifted scientist cannot be expected to be an expert in mathematical algorithms, so these solvers must also be very robust, with clean user interfaces, understandable documentation, and well-chosen default parameters.

My research has therefore focused on the development of accurate, efficient, scalable and robust numerical methods for solving multi-physics problems. With a focus on accuracy and scalability, I have investigated fully implicit approaches for solving these systems. Such approaches follow a standard path [8, 9]: implicit time discretization to reduce the problem to a nonlinear algebraic system of equations, iterative nonlinear solvers that require the repeated solution of large linear systems of equations, and iterative linear solvers that strive to minimize computational work within each solve.

For the SMA problem (1), my algorithmic contributions focused on the nonlinear solver stage. In these applications, the unique "shape memory" properties of such materials result from a non-convex free energy potential Ψ. As a result, their variational PDE formulations do not satisfy weak lower semicontinuity, and therefore preclude the use of standard PDE existence theory and computational solution techniques. For such problems, I developed an efficient and robust solution approach based on *natural parameter continuation*, in which I employed the material viscosity A to regularize the modeling system, thereby allowing convergence of the nonlinear solvers, and producing a simulation code capable of successfully predicting the unique material properties of SMA wires [10, 20].

For the MHD (2)-(3) and core-collapse supernova problems, I have continued my research into nonlinear solver algorithms. In such problems, spatial semi-discretization is often handled through the use of non-differentiable *flux-limiters*, introduced in the context of explicit shock-capturing methods. Unfortunately, implicit solvers based on Newton-like methods require differentiability of the nonlinear system with respect to the solution variables, which no longer holds when these limiters are used. We therefore developed solution techniques that approximated these limiters with differentiable versions for use within the nonlinear solver, allowing absolutely stable solvers for these hyperbolically-dominated multi-physics systems [9, 27, 29, 30].

For the MHD problem I have also focused on the iterative linear solvers at the heart of its solution. Our approach toward solving these linear systems relies on the use of preconditioned Krylov iterative methods (e.g. CG, GMRES, BiCGStab, TFQMR) [9], that build a solution to the linear system $Ax = b$ through construction of a basis for the Krylov subspace of dimension l,

$$K_l(A, b) = \text{span}\{r, Ar, A^2r, \ldots, A^{l-1}r\}, \tag{8}$$

where $r = b - Ax_0$ and x_0 is an initial guess at the solution to the linear system. The convergence of such methods is related to spectrum of the matrix A, with a more tightly-clustered spectrum resulting in faster convergence. The key ingredient in designing robust, efficient and scalable Krylov solvers is the use of a nonsingular *preconditioner*, P. This linear operator is used to transform $Ax = b$ into either the equivalent system $PAx = Pb$ or $APP^{-1}x = b$, with the Krylov method applied to one of $(PA)x = c$ or $(AP)y = b$. Through appropriate selection of P, often chosen such that $P \approx A^{-1}$, the requisite number of Krylov iterations for convergence can be minimized. I have therefore focused on the construction of scalable and robust preconditioning techniques for the resistive MHD system, exploring physics-based approaches that decompose A into fast and slow modes and only precondition the fastest of these [28], as well as domain-decomposition techniques that employ robust one-level and multi-level solvers, and are most applicable when studying challenging geometries and/or incorporating additional physical components [25, 26]. It is

in support of these efforts that I have advised two students: one Ph.D. student focusing on a multi-level Schur complement domain decomposition method for two-dimensional multi-physics applications [34], and one honors undergraduate student working on asynchronous parallel algorithms for scalable smoothers within multi-level solvers posed on large-scale structured grids [31].

Similarly, I have focused on iterative linear solution methods for the cosmology problem (4)-(7). Here, prior to use of Krylov methods I have introduced an operator decomposition based on the Schur complement, to transform a coupled implicit system comprised of equations (6)-(7) and an equation for thermal gas energy feedback, into a scalar-valued diffusion equation, to which I then applied a geometric multigrid preconditioned conjugate gradient method for solution [15, 16, 17, 24]. I am continuing my research in this area to problems posed on block-structured adaptive meshes [23], and to problems involving multiple radiation frequencies. Moreover, I have released all of this work as open-source software to the general scientific community, enabling broader impact of my research than through journal publications alone [1, 2, 21, 22].

Open-Source Solvers for Multi-Rate Systems

In nearly all of the above work, my research has focused on the construction of solver algorithms based on an assumption that the PDE system must be discretized using a fully implicit approach. This fully implicit requirement is indeed valid for a large variety of problems, and solvers designed for fully implicit multi-physics systems have tremendous applicability to systems comprised of simpler processes. Moreover, for stiff problems in which high accuracy and parallel scalability are desired, implicit time discretizations are a necessity. However, many multi-rate problems are not stiff, and in many applications the most difficult component for a nonlinear solver evolves on a slow time scale, e.g. flux limiters acting on hyperbolic components in an advection-diffusion-reaction problem. For these problems, neither fully explicit nor fully implicit methods may be optimal. In fact, both the cosmology and supernova applications exhibit such characteristics, and hence computational physicists have typically tackled them with simple operator-split time discretization approaches, wherein each physical component is evolved separately and inter-physics coordination is only performed through initial conditions on each single-physics solve. Unfortunately, such splittings have been shown to exhibit undesirable numerical properties including poor accuracy and unpredictable stability.

My recent research has therefore turned toward the problem of multi-rate time discretization algorithms. Within my cosmology work, I have developed multi-rate integrators that employ semi-analytical solvers for only the fastest chemical reactions, and I have further explored subcycled operator-split approaches for separately tracking the dynamics of stiff radiation and chemistry processes that themselves operate at different rates [17, 22].

Building off of these investigations, under a new DOE grant I have begun implementation of an open-source library for robust, efficient and adaptive multi-rate integrators based on the additive Runge-Kutta family of methods, named *ARKode*. As part of a SciDAC project entitled *Frameworks, Algorithms and Scalable Technologies for Mathematics* (FASTMath), I am implementing this library as a component within the SUNDIALS suite of nonlinear solvers and ODE/DAE integration codes. My primary aim for this library is to enable a highly efficient and customizable solver infrastructure for explicit Runge-Kutta (ERK), diagonally-implicit Runge-Kutta (DIRK), and additive Runge-Kutta (ARK) methods, to allow high-order accurate and stable time integration of multi-rate systems, both in serial and parallel. Such an infrastructure naturally builds off of my previous research into efficient and scalable iterative solvers for nonlinearly implicit PDE systems, and I believe promises to have tremendous impact for researchers focusing on multi-rate systems, as well as for non-multi-rate problems posed on spatially-adaptive grids since it will naturally provide both explicit and implicit, high-order-accurate, adaptive one-step integration methods.

Multi-scale Mathematical Modeling and Simulation

A final research topic that I am currently pursuing focuses on the development of new mathematical models themselves. Historically models have focused on a single scale, be it the macroscopic (via systems of

PDEs) or the microscopic (via first-principles, atomistic equations). However, the connection between first-principles atomistic properties and continuum-level PDE models has remained in the realm of asymptotic analysis, through the construction of closures that relate intrinsic material properties, such as stress-strain and pressure-temperature relationships. Unfortunately, the assumptions required to form these asymptotic approximations often limit the validity of the resulting macroscopic models to specific operating regimes. With the ever-expanding power of modern computational hardware and scalable numerical methods, the frontiers of science now often lie just beyond these limited regimes of model validity.

In my Ph.D. thesis research, in addition to the numerical methods research described above, I also developed a new first-principles-based mathematical model, (1), for simulating multi-scale thermodynamic phase transformation processes in shape memory alloys. Such alloys are already at the forefront of research in materials science and engineering, as they may be used in the production of microscopic devices with the ability to perform work without the use of moving parts. Such behaviors are made possible by the understanding and control of phase transformation processes that occur at the atomistic scale of these materials, in which an ensemble of crystalline transformations coordinate to cause macroscopic nonlinear thermodynamic actions. My thesis research focused on continuum-level PDE models, but required the encoding of a multitude of atomistic material properties within their Helmoltz free energy density functionals, Ψ. In the context of simplified one-dimensional models, we developed stochastic computational processes for computing steady-state averaged crystalline properties [3, 4, 5, 6], and I derived physically accurate free energy functionals for NiTi SMA wires [10, 20]. Finally, once the modeling and simulation framework was completed, I then used the resulting code to design techniques for damping vibrational energy based on thermal actuation [12, 13, 14], resulting in a patent [11].

While these advances have proven fruitful in the modeling of one-dimensional wires, there remains significant work to extend such continuum-level descriptions to realistic models for plates and solids, as these two and three-dimensional systems would require construction of much more complex multi-dimensional free-energy potentials. Instead of following this deterministic modeling approach, I am therefore currently investigating novel *heterogeneous multiscale methods* (HMM) that directly couple macroscopic- and atomistic-scale numerical models to directly supply these constitutive laws numerically.

In addition to investigating HMM approaches for materials modeling, with my current Ph.D. student I am investigating their use in plasma models (2)-(3). For such problems, standard models typically differ in their approximation of Ohm's law, with *ideal MHD* using the form $\mathbf{E} = -\mathbf{v} \times \mathbf{B}$, *resistive MHD* using the form $\mathbf{E} = -\mathbf{v} \times \mathbf{B} + \eta \mathbf{J}$, and so-called *extended MHD* adding new terms in an attempt to account for the separate motion of electrons and ions in plasmas. Unfortunately, none of these existing models have been able to accurately capture the full range of reconnection rates in fusion and solar plasmas, opening the door for multiscale models that directly simulate the electron/ion motion at the atomistic scale to inform the macroscale model of the appropriate relationships between the electric and magnetic fields.

Our multiscale research is therefore two-fold. First, we are working on the numerical analysis and computational implementation of these techniques in order to guarantee a desired level of accuracy with minimal computational work. Second, we are working to develop appropriate pairs of microscale/macroscale models to use in the multiscale modeling of both the SMA and plasma systems.

Summary

My research has contributed to all of the primary aims of scientific computation: the development of robust and accurate numerical methods, the extension of these methods to large-scale computing hardware, and the improvement of mathematical models to capture increased physical realism. However, while my research interests are multi-faceted they share a set of common themes: a focus on multi-physics modeling and a belief in the power of interdisciplinary science. I find these themes to be incredibly exciting, and I have found that they similarly motivate students to appreciate the power of applied mathematics. What's more, although my research requires expertise in applied mathematics, proficiency in computer programming and fluency in the language of science, this inter-disciplinarity allows students to approach my research from a variety of complementary directions. I look forward to continuing this work for years to come, and to helping

guide upcoming generations of students in the process.

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