RESEARCH STATEMENT

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My research interests span the areas of numerical methods and analysis for micromagnetics simulations, machine learning method for scientific computing, modeling and simulations for free boundary and interface problems, molecular and spin dynamics modeling. My thesis is focused on the numerical methods and analysis for Landau-Lifshitz equation, which stem from micromagnetics. A series of semi-implicit methods for Landau-Lifshitz equation are proposed, that have been proved to be accurate and efficiency. The optimal convergence rate and unique solvability of these methods are proved in our paper. My visiting research is focused on the machine learning method, instead of using absorbing boundary conditions for Schrödinger equation over unbounded domains, molecular and spin dynamics modeling. My postdoctoral research is focused on the modeling and simulation for free boundary and interface problems, especially developing the machine learning method for topology optimization, modeling and simulations for moving contact line problems.

1 Background

Micromagnetics is a field of physics dealing with the prediction of magnetic behaviors at sub-micrometer length scales. Magnetization in a continuum approximation, is considered to be a continuous vector field as a function of space and time, and represented by a normalized magnetization field. A very common phenomenological model for magnetization dynamics is the Landau-Lifshitz (LL) equation in [1, 2]. This model has been successfully used to interpret various experimental observations. The LL equation is technically quasilinear, nonlocal and has a non-convex constraint, which poses interesting challenges in designing efficient numerical methodologies. Besides, the magnetization reversal process requires numerical methods to resolve different length and temporal scales in the presence of domain walls, vortices and skyrmions, due to their important roles in the switching process. As a result, numerical methods for LL equation with high accuracy and efficiency are highly demanding. I will describe my work below.

2 Numerical methods and analysis for Landau-Lifshitz equation

There exists a rich body of previous work of developing numerical algorithms for LL equation in the past few decades. The spatial derivative is typically approximated by the finite element method and finite difference method. In terms of temporal discretization, explicit schemes, fully implicit schemes and semi-implicit schemes have been extensively explored. One has known that, explicit schemes suffer from severe stability constraints, which can be overcomed by fully implicit schemes, but have to solve a time-consuming (nonsymmetric) nonlinear systems of equations at each time step. One can use the nonlinear multigrid method or fixed point iteration technique to handle this nonlinearity. As a result, we need to design more accurate and efficient numerical methods for LL equation with numerical analysis guarantees.

2.1 Numerical methods for Landau-Lifshitz equation

One of the most popular methods is the Gauss-Seidel projection method (GSPM) developed by Wang, García-Cervera, and E in [3, 4, 5]. This method is based on a combination of a Gauss-Seidel implementation of a fractional step implicit solver for the gyromagnetic term, and the projection step for the heat flow of harmonic maps to overcome the difficulties associated with the stiffness and nonlinearity. It is tested that GSPM is unconditionally stable with first order accuracy in time. Two numerical schemes have been developed, based on GSPM in [6] from the perspective of improving the efficiency of GSPM, which has been proved to be unconditionally stable. The first improved method updates the gyromagnetic term and the damping term simultaneously and follows by a projection step. The second one introduces two sets of approximate solutions, and updates both for the gyromagnetic and damping term for one set of approximate solutions and apply the projection step to the other set of approximate solutions in an alternating manner. Compared to original GSPM [4] which has to solve heat equations seven times at each time step, the improved methods solve heat equations five times and three times,

respectively. Say, the recorded running times suggest that savings of both methods are about 2/7 and 4/7 for the same accuracy requirements, respectively.

To find high order numerical scheme, we explore semi-implicit schemes in [7] that achieve a desired balance between stability and efficiency. The methods are based on the second order backward differentiation formula and the second order interpolation formula using the information at previous two temporal steps. The unconditional unique solvability of both semi-implicit methods is proved with their second-order accuracy verified through numerical examples in both 1D and 3D. Compared to Implicit-Explicit (IMEX) method, in which two linear systems with variable coefficients need to be solved, and GSPM, both semi-implicit methods are shown to be more efficiency and accuracy. Besides, these semi-implicit methods are applied into the first benchmark problem for a ferromagnetic thin film material developed by the micromagnetic modeling activity group from National Institute of Standards and Technology [8]. The numerical methods above are constructed under the small damping case. The second order methods with unconditional stability for LL equation under large damping case have been explored in [12]. Meanwhile, we have analyzed error estimates of such linear numerical schemes with Poisson solver in [13].

2.2 Numerical analysis for Landau-Lifshitz equation

Two critical numerical properties would be considered that are unique solvability and optimal convergence rate.

1. *Unique solvability*

   Numerous numerical approaches (e.g. finite elements or finite differences) in the literature basically have first-order or second-order in time and second-order in space. Those second order methods are unconditionally stable, but require a nonlinear solver at each time step which leads to unavailable theoretical justification of the unique solvability. The unique solvability analysis for these nonlinear schemes has been a very challenging issue at the theoretical level, due to the highly complicated form in the nonlinear term. The only relevant analysis was reported in [9], in which the unique solvability was proved under a very restrictive step-size condition that the temporal stepsize be proportional to the square of the spatial gridsize. The unconditionally unique solvability has been done in [10] by usage of monotonicity theorem.

2. *Optimal convergence rate*

   It is noticed that, for all existing works with the established convergence analysis, a nonlinear solver has to be used at each time step, for the sake of numerical stability. As a desired result, these semi-implicit schemes [7, 10] are proposed in some sense, with second-order accuracy in time and linearity of the scheme at each time step, so that the length of magnetization is preserved in the point-wise sense, and an optimal rate error could be established at a theoretical level. It is the first such result to report an optimal convergence analysis (under the step-size condition that the temporal stepsize be proportional to the spatial gridsize) with second-order accuracy in both time and space.

I will describe two research topics during my visiting period below, one is about the machine learning approaches for Schrödinger equation over unbounded domain. The other is focused on the molecular and spin dynamics modeling.

3 Machine learning approaches for Schrödinger equation over unbounded domain

Significant advancements in deep learning, recently, have driven the development of scientific computing, especially in the high dimensional problems. One has focused on solving the high dimensional elliptic and parabolic PDEs using the deep neural networks over bounded domain. To solve the problem over unbounded domain, the time-dependent wave equations in [11] are focused. Given a compactly supported initial condition, the entire-space problem is firstly restricted into finite-region problem. A map from the initial condition parameterized by wave packet width and wave numbers to the PDEs solution is trained using data provided either by the exact solution or numerical solution, instead of using absorbing boundary condition. Such a map surprisingly has

good *interpolative* and *extrapolative* property. On the one hand, the map can generate accurate results in which the specific initial condition is not included in the training sets but can be interpolated using initial conditions in the training sets. On the other hand, by extrapolation, the map can generate satisfactory results when the wave hits the boundary of the finite region although the training is for temporal instances before the wave hits the boundary. This method provides an alternative for finite time simulation of wave propagation. In deed, the solution of the Gross-Pitaevskii equation in Bose-Einstein condensate can be predicted at later times over unbounded domain using this sort of machine learning approaches.

4 Molecular and spin dynamics modeling

Using a classical model that treats translational and spin degrees of freedom on an equal footing, phonon-magnon interactions in BCC iron with combined molecular and spin dynamics methods are studied. The atomic interactions are modeled via an empirical many-body potential while spin dependent interactions are established through a Hamiltonian of the Heisenberg form with a distance dependent magnetic exchange interactions obtained from first principles electronic structure calculations and a Gilbert damping term. The temporal evolution of translational and spin degrees of freedom was determined by numerically solving the coupled equations of motion, using an algorithm based on the second order Suzuki-Trotter decomposition of the exponential operators. This model with Gilbert damping has explored the pressure, temperature (lattice, spin, electron level) effect versus the fluctuation of damping under strong magnetic field. The temperature derived from Schrödinger equation will be explored.

I will describe two research topics during my postdoctroal research period below. My research is focused on the modeling and simulations for the free boundary and interface problems. One is about the machine learning methods for topology optimization. The other is about modeling and simulations for moving contact line problems.

5 Machine learning methods for topology optimization

In the area of machine learning for scientific computing, one can solve very high dimensional PDEs using machine learning and optimized methods. Machine learning model and method has applied in many engineering applications, especially in large language model and image science. The topology optimization is a workflow for solving the forward problem involving a PDE and inverse problem involving a optimization problem. This can be imagined as a PDE constraint optimization problem. The topology optimized structure data can be collected as the training datasets. More test conditions can be predicted as an application of data-driven methods, see [23]. What I interested is solving PDE using DeepRitz or other machine learning models for several iterations, then we solve the inverse problem by SIMP (penalty method) by ADMM strategy. On the other hand, we can get a better initialization using Deep modeling, and kick start the inverse solver. However, the issue of machine learning methods for scientific computing, esp. low dimensional PDE, is that low efficiency, low accuracy. Thus, machine learning methods is not extensively applicable in low dimensional problems, compared to the classical numerical methods.

6 Modeling and simulations for moving contact line problems

For the multi-phase flow or solid problem, the most interesting aspect is how to model and propose a suitable interface boundary conditions. From past experiments and numerical simulations, it appears that the no-slip boundary condition is unreasonable. In our study, we are particularly interested in modeling and simulating Navier-slip boundary conditions. From the view of numerical methods, mainly two kinds: interface-tracking method and interface-capturing method. As an interface-tracking method, the font-tracking method can be applied into the moving contact line problems, see [14] and [15]. A level-set approach (interface-capturing) method or a phase field method is used to detect the interface. In the simulation, the numerical methods with unconditional energy stability are highly focused. From the modeling, mainly two: the diffuse interface model and sharp interface model. One can also study the sharp interface limit of the diffuse interface model. In the

area of such interface problem of multi-phase and multi-physics modeling, the property of substrate is highly interested. For rigid solid, there are many many works, see [16], [18] and [19]. Recently, the elastic substrate is highly interested. The droplet on the elastic membrane with moving contact line has been studied in [24]. The elastic sheet and elastic bulk material have been reported in the experiments. Mathematically, less work is published. One can also control the droplet dynamics by the external fields. Electrowetting on this dielectric-coated (EWOD) surface has also been studied mathematically and experimentally on the rigid solid substrate. To investigate the anisotropy surface, the moving contact line problem on the rough surface has been studied, see [17] and [20]. To accelerate the droplet motion, one can use the model with the surfactants effect, see [21] and [22].

7 Future perspectives

In the near future, I am still interested in and focus on the areas below:

- Numerical methods and analysis for micromagnetics simulations;
- Molecular and spin dynamics modeling;
- Modeling and simulation for free boundary and interface problems;
- Machine learning methods and applications to scientific computing;

In these aspects, I will devote to develop efficient, accurate and structure preserving numerical methods for different models from material science. In my mind, the modeling is an exciting area. In short, I will focus on two: One is numerical method and its analysis, and applications. The other is the modeling and simulations. Also, I am interested in the applications of Schrödinger equation, quantum control of many body (open) quantum systems, the modeling of multi-physics (magnetoelasticity, magnetoelectricity and magnetohydrodynamics), so on and so forth. Simultaneously, I intend to understand physical model and physical laws, which use a specific machine learning model can be architected. My conjecture is many building blocks from neural nets that learn different parts should be explored. One can take learning PDEs as an example, some parameters to learn the initial and boundary conditions, some of them to learn the physical constraints, all of parameters are formulated by an easy-to-learn optimization problems. I attempt to build a systematic framework to bridge the physical laws and machine learning model. As a matter of fact, the performance using machine learning technique to resolve the Schrödinger equation has not been extremely successful. AI for Science is still not very satisfactory, especially in solving differential equations. Meanwhile, I want to explore how to construct a structure-preserving (symplectity-preserving, volume-preserving, energy-preserving, momentum-preserving) neural networks to the physical dynamics, etc. Besides, the data-driven methods of dynamical system with some controls is also an interesting topic that I hope to devote it. I am excited at the prospect of learning, contributing, giving shape and making an impact in this upcoming and challenging field.

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