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Stable large-scale solver for Ginzburg–Landau equations for superconductors

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ABSTRACT

Understanding the interaction of vortices with inclusions in type-II superconductors is a major outstanding challenge both for fundamental science and energy applications. At application-relevant scales, the long-range interactions between a dense configuration of vortices and the dependence of their behavior on external parameters, such as temperature and an applied magnetic field, are all important to the net response of the superconductor. Capturing these features, in general, precludes analytical description of vortex dynamics and has also made numerical simulation prohibitively expensive. Here we report on a highly optimized iterative implicit solver for the time-dependent Ginzburg–Landau equations suitable for investigations of type-II superconductors on massively parallel architectures. Its main purpose is to study vortex dynamics in disordered or geometrically confined mesoscopic systems. In this work, we present the discretization and time integration scheme in detail for two types of boundary conditions. We describe the necessary conditions for a stable and physically accurate integration of the equations of motion. Using an inclusion pattern generator, we can simulate complex pinning landscapes and the effect of geometric confinement. We show that our algorithm, implemented on a GPU, can provide static and dynamic solutions of the Ginzburg–Landau equations for mesoscopically large systems over thousands of time steps in a matter of hours. Using our formulation, studying scientifically-relevant problems is a computationally reasonable task.

1. Introduction

The time-dependent Ginzburg–Landau (TDGL) equations [1,2] are a powerful computational tool for describing the time-dependent dynamics of an order parameter near a phase transition that determine the macroscopic behavior of many system, most importantly type-II superconductors. They are an especially useful tool for addressing the important problem of designing superconducting materials that can support larger critical currents. As the energy dissipation in superconductors arises from the motion of vortices driven by the current-induced Lorentz force, this design problem requires developing a fundamental understanding of vortex dynamics. In contrast with computational models that treat the vortices as elastic strings moving in a viscous medium [3–6], only the TDGL formulation can capture the correct interactions between

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pairs of vortices, vortices and inclusions, and allows vortices to cut and reconnect. The TDGL model provides a reasonable compromise between an approximate phenomenological and an exact microscopic descriptions of the vortex matter.

The strength of the TDGL formalism is that it describes the superconductor as a continuously distributed order parameter, given by a complex-valued scalar field. The amplitude of the order parameter is related to the local superconducting density in the system, which is suppressed by an array of singularities representing the vortices that arise spontaneously in the presence of a magnetic field. Pinning defects of arbitrary shape and size can be treated as either modulations of superconductor's critical temperature or by adding internal boundary conditions. The equations describing the evolution of the order parameter implicitly model the flexibility of the vortex lines, the long-range mutual vortex repulsion, vortex cutting and reconnecting, and even the interruption of current paths due to insulating pinning defects in the media. Although TDGL-based numerical simulations have been used many times to study properties of the vortex state [7–14], a meaningful exploration of the phase space for realistic 3D superconductors has not been possible due to the computationally intensive nature of solving the equations at physically-relevant scales.

Here we address this challenge in two ways. First, we rewrite the TDGL equation in such a way that potential numerical instabilities are minimized and different boundary conditions can be implemented in a relatively simple way. In particular, the Poisson equation governing the scalar potential must be formulated in a stable and solvable way. Second, we implement an implicit iterative solver based on the Jacobi method. The result is a formulation of a solver for the TDGL equations where the value of the order parameter at each grid point of a mesh can be solved in a numerically stable manner using only information from the grid point's nearest neighbors. This type of formulation is critical for implementing a solver in a massively parallel computational environment. In contrast with other published work on solvers for the complex GL equations in massively parallel environments [15,16], we discuss all the aspects necessary to create a scientifically-relevant simulation, (e.g. magnetic fields, boundary condition, and current), each of which add non-trivial numerical complications to a system of equations. The increasing availability of massively parallel computational environments, especially in the form of hardware affordable to any researcher, (e.g. programmable general-purpose GPU devices) means that investigations of large-scale systems using the TDGL equations should no longer be computationally limited.

While here we formulate our problem in the context of modeling a type-II superconductor, the TDGL equations are used to model a variety of problems, ranging from granular materials, self-propelled swimmers [17], fluid and fracture dynamics [18], and cold atoms [19] to solidification from a melt or solution [20]. Many aspects of the numerical formulation would also be relevant for solvers created for these problems as well. In particular, the presented methods are directly applicable to cold atom simulations that use complex coefficients in the Ginzburg–Landau (GL) equation, see e.g. Refs. [19,21].

This paper is organized as follows. In Section 2 we review the TDGL equations and derive the formulation of the equations that we will use in subsequent sections. We simplify the equations by applying an x-axis aligned external current and assuming the large-λ limit, which makes the magnetic field constant everywhere. In Section 3 we introduce a discretization of the coupled partial differential equations and show they can be formulated as a set of linear equations that can be iteratively solved at each time step. In Sections 3.1 and 3.2 we present an implicit discretization schemes of the GL equations and the Poisson equation for the scalar potential, respectively. In Section 3.3 we show how to implement periodic or open boundary conditions with respect to our discretization scheme. In Section 3.4 we discuss how inclusions and different geometries can be modeled. In Section 4 we discuss a computational implementation of this algorithm on a GPU in Section 4.1 and provide several physically relevant examples of systems that can be investigated in Section 4.2. In Section 5 we make concluding remarks.

2. Derivation of equations

2.1. Ginzburg–Landau formalism

The Ginzburg–Landau (GL) equations describe spatial variations of the superconducting order parameter ψ in presence of electromagnetic vector potential $\mathbf{A}$. While a phenomenological theory, the GL theory can be rigorously connected to the microscopic Bardeen–Cooper–Schrieffer theory in the vicinity of the critical temperature T_C of the superconducting phase transition [22]. Far from T_C, the GL equations do not correctly reproduce the physics in the vortex core, but still describe the interaction between vortices correctly, see e.g. Ref. [2]. Equilibrium states of superconductors are found from the GL equations by the minimization of the GL free energy, $\mathcal{F}_{GL}$: $\delta\mathcal{F}_{GL}/\delta\psi^* = 0$ and $\delta\mathcal{F}_{GL}/\delta\mathbf{A} = 0$.

The TDGL equations are the dynamic generalization of the GL equations. For $\psi = \psi(\mathbf{r}, t)$ they can be written as

$$\Gamma\left(\partial_t + \imath\frac{2e}{\hbar}\mu\right)\psi = a_0\epsilon(\mathbf{r})\psi - b|\psi|^2\psi + \frac{1}{4m}\left(\hbar\nabla + \frac{2e}{\imath c}\mathbf{A}\right)^2\psi + \zeta(\mathbf{r}, t), \tag{1}$$

$$\nabla\times(\nabla\times\mathbf{A}) = \frac{4\pi}{c}\left[\mathbf{J}_N + \mathbf{J}_S + \mathcal{I}(\mathbf{r}, t)\right], \tag{2}$$

where $-e$ and m are the electron's charge and mass, c is the speed of light, μ and $\mathbf{A}$ are the scalar and vector potentials, Γ, a_0, b are phenomenological constants that can be derived from the microscopic theory, and $\imath$ is the imaginary unit. The Langevin terms $\zeta(\mathbf{r}, t)$ and $\mathcal{I}(\mathbf{r}, t)$ describing thermal noise have the correlators