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Noise propagation in hybrid models of nonlinear systems: The Ginzburg–Landau equation

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ABSTRACT

Every physical phenomenon can be described by multiple models with varying degrees of fidelity. The computational cost of higher fidelity models (e.g., molecular dynamics simulations) is invariably higher than that of their lower fidelity counterparts (e.g., a continuum model based on differential equations). While the former might not be suitable for large-scale simulations, the latter are not universally valid. Hybrid algorithms provide a compromise between the computational efficiency of a coarse-scale model and the representational accuracy of a fine-scale description. This is achieved by conducting a fine-scale computation in subdomains where it is absolutely required (e.g., due to a local breakdown of a continuum model) and coupling it with a coarse-scale computation in the rest of a computational domain. We analyze the effects of random fluctuations generated by the fine-scale component of a nonlinear hybrid on the hybrid's overall accuracy and stability. Two variants of the time-dependent Ginzburg–Landau equation (GLE) and their discrete representations provided by a nearest-neighbor Ising model serve as a computational testbed. Our analysis shows that coupling these descriptions in a one-dimensional simulation leads to erroneous results. Adding a random source term to the GLE provides accurate prediction of the mean behavior of the quantity of interest (magnetization). It also allows the two GLE variants to correctly capture the strength of the microscale fluctuations. Our work demonstrates the importance of fine-scale noise in hybrid simulations, and suggests the need for replacing an otherwise deterministic coarse-scale component of the hybrid with its stochastic counterpart.

1. Introduction

Numerical modeling of complex nonlinear systems requires the development of multi-algorithm computational solvers capable of handling a wide range of spatial and/or temporal scales. While coarse-scale models are more computationally efficient than their fine-scale counterparts, they are not universally valid. For instance, continuum-scale finite element models of crack propagation break down near a crack's tip [1], and macroscopic (Darcy-scale) models of flow and transport in porous media break down for localized phenomena with high pore-scale gradients [2–4]. Standard coarse-scale models also fail to capture the effects of spontaneous microscale fluctuations on macroscopic behavior, such as spontaneous formation of ordered spatial concentration patterns in an unstirred chemical medium [5].

Fine-scale algorithms (e.g., molecular dynamics/quantum tight-binding and pore-scale simulations in the first and second examples, respectively) can model such processes, but their high computational cost renders them impractical for modeling large-scale problems. Hybrid algorithms, which are also referred to as algorithm refinement, employ such fine-scale

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models only in subdomains wherein their coarse-scale counterparts break down, potentially yielding a significant reduction in computational cost [6]. With a few exceptions [7,8], coupling of the fine- and coarse-scale components of a hybrid requires multiple iterations to ensure the continuity of state variables and their fluxes at the interface between the two components. Design and computationally efficient implementation of such coupling procedures remain a key challenge in hybrid modeling.

Stochastic fluctuations generated by a hybrid's fine-scale (particle-based) component exacerbate this task [9]. Averaging out this noise (i.e., coupling averaged quantities such as particle density and mass flux to their counterparts computed with a coarse-scale deterministic component) is adequate for computing the mean behavior of linear systems, but artificially reduces the fluctuation variance in the particle region near the particle-continuum interface [10]. In weakly nonlinear systems, such as the train model of viscous transport in gases, the averaging dampens the long-range correlations of velocity fluctuations and "can lead to a greatly altered time-dependent behavior" [11]. A nonlinear hybrid model consisting of asymmetric excluded random walk (the fine-scale component) and a viscous Burgers' equation (the coarse-scale component) revealed that the averaging tends to suppress the drift of shock location [12]. In each case, addition of a Gaussian white noise term to the hybrid's deterministic (coarse-scale) components corrected these shortcomings.

A proper treatment of noise is even more important in highly nonlinear systems, wherein even small changes in the magnitude of microscopic fluctuations can significantly affect the macroscopic dynamics. In such systems, coupling the averages of fine-scale quantities with their deterministic coarse-scale counterparts can lead to erroneous predictions of the mean system behavior. The Ginzburg–Landau theory [13] provides an ideal setting to study noise propagation in hybrid models, since it establishes a relationship between fine-scale (a nearest-neighbor Ising model with spin-flip dynamics) and coarse-scale (a Ginzburg–Landau partial differential equation) representations of a highly nonlinear system. It can be used, for example, to describe the evolution of (scalar) magnetization of a uniaxial ferromagnet to thermal equilibrium [14–16].

In Section 2 we formulate a nearest-neighbor Ising (NNI) model and two variants of the time-dependent Ginzburg–Landau equations (GLEs). A hybrid algorithm coupling these two levels of description is discussed in Section 3. Simulation results reported in Section 4 reveal that one has to add a random source term to the Ginzburg–Landau component of the hybrid in order to correctly predict the mean and variance of the magnetization for a ferromagnet evolving to thermodynamic equilibrium. This finding facilitates the analysis of noise propagation in the NNI–GLE hybrid by allowing one to replace its NNI component with a stochastic Ginzburg–Landau equation (sGLE). A solution of the latter is presented in terms of moment equations (deterministic equations describing the evolution of the mean and covariance of magnetization). The main conclusions of our analysis are summarized in Section 5.

2. Two modeling scales in the Ginzburg–Landau theory

The dynamics of ferromagnetic systems can be described either microscopically with Ising models [17] or macroscopically with the Ginzburg–Landau theory [15,16,18]. Both levels of description are formulated below in the context of the magnetization of a one-dimensional (1D) ferromagnet.

2.1. Nearest-neighbor Ising models with spin-flip dynamics (NNIs)

Consider a ferromagnet whose atoms are arranged on a 1D lattice with sites $i = 1, \ldots, N$. A microscopic representation of this system is given by an Ising model with nearest-neighbor interactions [17]. It assumes that the spin s_i of the atom at site i can be in one of the two states designated by $s_i = \pm 1$, and interacts only with its two adjacent spins. The N-spin configuration $\mathbf{s} = \{s_1, \ldots, s_N\}$ defines the ferromagnet's state at time t; the joint probability of finding the ferromagnet in state $\mathbf{s}$ at time t is denoted by $P(\mathbf{s}; t)$. Let $\mathbf{s}'$ denote an N-spin configuration that differs from configuration $\mathbf{s}$ by the value of a single spin s_j. The kinetic nearest-neighbor Ising model with spin-flip dynamics [19] (NNI) defines the evolution of $P(\mathbf{s}; t)$ as a solution of the master equation

$$\frac{\mathrm{d}P(\mathbf{s};t)}{\mathrm{d}t} = \sum_{\mathbf{s}'}\left[w(\mathbf{s}'\to\mathbf{s})P(\mathbf{s}';t) - w(\mathbf{s}\to\mathbf{s}')P(\mathbf{s};t)\right] \tag{1}$$

where $w(\mathbf{s}\to\mathbf{s}')$ is the transition rate from state $\mathbf{s}$ to state $\mathbf{s}'$, and the summation is over all possible states $\mathbf{s}'$. Among the plethora of suggested functional forms for the transition rate w we consider two. The first is the Suzuki–Kubo rate

$$w_{\mathrm{SK}}(\mathbf{s}\to\mathbf{s}') = \frac{\lambda}{2}\left[1 - s_j \tanh\left(\beta J \sum_{L_j} s_{L_j}\right)\right], \tag{2a}$$

where λ^{-1} is the time scale of the spin-flip process that can depend both on the system temperature T and the spins other than s_j, $\beta = 1/(k_B T)$ with k_B denoting the Boltzmann constant, J is the spatially uniform exchange coupling energy associated with the interaction between neighboring spins, and L_j indicates summation over the nearest neighbors of s_j.

The second alternative is the heat-bath rate

$$w_{\mathrm{hb}}(\mathbf{s}\to\mathbf{s}') = \kappa\left[1 + \mathrm{e}^{\beta\mathcal{H}(\mathbf{s}')-\beta\mathcal{H}(\mathbf{s})}\right]^{-1}, \tag{2b}$$