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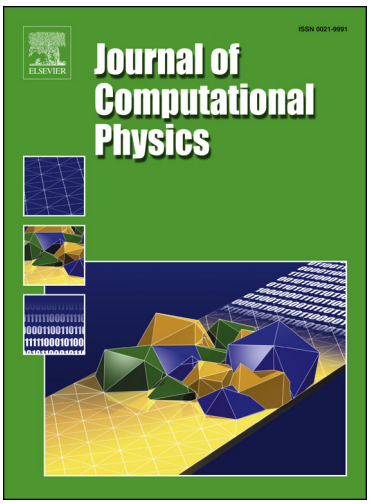

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Convex Splitting Method for the Calculation of Transition States of Energy Functional

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ABSTRACT

Among numerical methods for partial differential equations arising from steepest descent dynamics of energy functionals (e.g., Allen-Cahn and Cahn-Hilliard equations), the convex splitting method is well-known to maintain unconditional energy stability for a large time step size. In this work, we show how to use the convex splitting idea to find transition states, i.e., index-1 saddle points of the same energy functionals. Based on the iterative minimization formulation (IMF) for saddle points (SIAM J. Numer. Anal., vol. 53, p1786, 2015), we introduce the convex splitting method to minimize the auxiliary functional at each cycle of the IMF. We present a general principle of constructing convex splitting forms for these auxiliary functionals and show how to avoid solving nonlinear equations. The new numerical scheme based on the convex splitting method allows for large time step sizes. The new methods are tested for the one dimensional Ginzburg-Landau energy functional in the search of the Allen-Cahn or Cahn-Hilliard types of transition states. We provide the numerical results of transition states for the two dimensional Landau-Brazovskii energy functional for diblock copolymers.

Keywords: transition state, saddle point, convex splitting method, iterative minimization formulation

Mathematics Subject Classification (2010) Primary 65K05, Secondary 82B05

1. Introduction

For an energy functional, both its local minimizers and its unstable saddle points have important physical meanings for many problems in physics, chemistry, biology and material sciences. The local minimizers correspond to the stable configurations in physical models, and they manifest themselves as steady states of the gradient flow driven by the energy. For the spatially extended systems, these flows appear mathematically as the time-dependent partial differential equations(PDEs). These PDEs reflect the true physical dynamics of relaxations and they also serve as a convenient computational model to calculate the stable steady states. For instance, as the well-known phase separation and transition models, the Allen-Cahn (AC) [1] and Cahn-Hillian (CH) [4] equations are the steepest descent dynamics of the

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