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Convex splitting method for the calculation of transition states of energy functional

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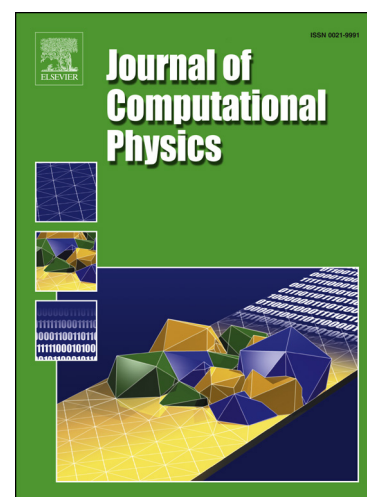
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1 **Convex Splitting Method for the Calculation of**
 2 **Transition States of Energy Functional**

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11 ABSTRACT

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

27
 28 **Keywords:** transition state, saddle point, convex splitting method, iterative
 29 minimization formulation

30 **Mathematics Subject Classification (2010)** Primary 65K05, Secondary
 31 82B05

32 1. INTRODUCTION

33 For an energy functional, both its local minimizers and its unstable saddle points
 34 have important physical meanings for many problems in physics, chemistry, biology
 35 and material sciences. The local minimizers correspond to the stable configurations
 36 in physical models, and they manifest themselves as steady states of the gradient
 37 flow driven by the energy. For the spatially extended systems, these flows appear
 38 mathematically as the time-dependent partial differential equations(PDEs). These
 39 PDEs reflect the true physical dynamics of relaxations and they also serve as a
 40 convenient computational model to calculate the stable steady states. For instance,
 41 as the well-known phase separation and transition models, the Allen-Cahn (AC)
 42 [1] and Cahn-Hillian (CH) [4] equations are the steepest descent dynamics of the

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