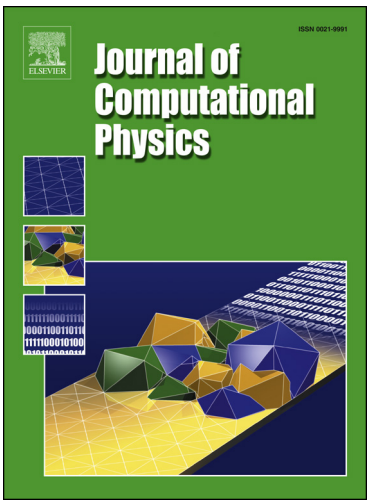

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PII: S0021-9991(17)30281-4
DOI: http://dx.doi.org/10.1016/j.jcp.2017.04.010
Reference: YJCPH 7276

To appear in: *Journal of Computational Physics*

Received date: 21 January 2017
Revised date: 1 April 2017
Accepted date: 3 April 2017

Please cite this article in press as: Q. Cheng et al., Efficient and accurate numerical schemes for a hydro-dynamically coupled phase field diblock copolymer model, *J. Comput. Phys.* (2017), http://dx.doi.org/10.1016/j.jcp.2017.04.010

EFFICIENT AND ACCURATE NUMERICAL SCHEMES FOR A HYDRO-DYNAMICALLY COUPLED PHASE FIELD DIBLOCK COPOLYMER MODEL

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Abstract. In this paper, we consider numerical approximations of a hydro-dynamically coupled phase field diblock copolymer model, in which the free energy contains a kinetic potential, a gradient entropy, a Ginzburg-Landau double well potential, and a long range nonlocal type potential. We develop a set of second order time marching schemes for this system using the "Invariant Energy Quadratization" approach for the double well potential, the projection method for the Navier-Stokes equation, and a subtle implicit-explicit treatment for the stress and convective term. The resulting schemes are linear and lead to symmetric positive definite systems at each time step, thus they can be efficiently solved. We further prove that these schemes are unconditionally energy stable. Various numerical experiments are performed to validate the accuracy and energy stability of the proposed schemes.

1. Introduction

Block copolymer is a linear-chain molecule composed of two or more subchains linked together to create a polymer chain. When the subchain is made of two (or three) distinct monomer blocks, it is called diblock (or triblock) copolymer. Due to the incompatibility between the blocks, block copolymers undergo a micro-phase separation to form a periodic morphology in nanoscale, which provides an efficient technique to produce nano-structured materials and nano-devices (cf. [12, 20, 21, 31, 33, 48]).

Modeling and numerical simulation are effective means to investigate the phase separation behaviors of block copolymers. In this paper, we consider the phase field based model for diblock copolymer (PF-BCP) model (cf. [4, 7, 8, 16, 26, 32, 48, 50]) known as the dynamic mean field theory, where an order parameter is used to denote the difference between the local volume fractions of two monomers. The evolution of the PF-BCP system is derived from the energetic variation of the action function of the total free energy in the H^{-1} Sobolev space, i.e., the Cahn-Hilliard (CH) type equation. The total free energy for the system is the nonlocal Ohta-Kawasaki functional, that is the standard Cahn-Hilliard free energy supplemented with a nonlocal term, reflecting the first order effects of the connectivity of the monomer chains (cf. [7, 32]). Due to its complexity, particularly the inclusion of a nonlocal potential, it is challenging to develop accurate, stable and efficient numerical schemes for this model. Previous works [34, 45] used only first-order, non energy stable schemes which lack in accuracy and stability.

Key words and phrases. Phase-field, Diblock copolymer, Navier-Stokes, Invariant Energy Quadratization, Energy Stability.

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