Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0209

Vol. **24**, No. 3, pp. 635-654
September 2018

Stabilized Predictor-Corrector Schemes for Gradient Flows with Strong Anisotropic Free Energy

Jie Shen[1] and Jie Xu[1,*]

[1] *Department of Mathematics, Purdue University, USA.*

Received 30 September 2017; Accepted 19 October 2017

Abstract. Gradient flows with strong anisotropic free energy are difficult to deal with numerically with existing approaches. We propose a stabilized predictor-corrector approach to construct schemes which are second-order accurate, easy to implement, and maintain the stability of first-order stabilized schemes. We apply the new approach to three different type of gradient flows with strong anisotropic free energy: anisotropic diffusion equation, anisotropic Cahn-Hilliard equation, and Cahn-Hilliard equation with degenerate diffusion mobility. Numerical results are presented to show that the stabilized predictor-corrector schemes are second-order accurate, unconditionally stable for the first two equations, and allow larger time step than the first-order stabilized scheme for the last equation. We also prove rigorously that, for the isotropic Cahn-Hilliard equation, the stabilized predictor-corrector scheme is of second-order.

AMS subject classifications: 65M12, 82C24

Key words: Predictor-corrector, anisotropy, Cahn-Hilliard equation, Willmore regularization, degenerate diffusion mobility.

1 Introduction

Many dynamical physical processes can be described by gradient flows of the governing free energy (see for example [1–6]). When dealing with strongly anisotropic systems, the gradient flows are usually characterized by nonlinear couplings of spatial derivatives. We mention some examples here, including concentration-dependent diffusion mobility [7, 8] or elasticity [9], and anisotropic interfacial energy [10–12].

From the computational perspective, it is crucial to construct energy stable numerical schemes. There are several different techniques to construct energy stable schemes, including convex splitting [13, 14], stabilization [15, 16], invariant energy quadratization (IEQ) [9, 17–19] and the newly introduced scalar auxiliary variable (SAV) approach [20].

*Corresponding author. *Email addresses:* shen7@purdue.edu (J. Shen), xu924@purdue.edu (J. Xu)

However, for gradient flows with strong anisotropic free energy, it is difficult to construct robust second-order schemes using these approaches as we explain below. The convex splitting and stabilization approaches usually lead to only first-order schemes, although second-order schemes are available for certain special cases without nonlinear derivative terms. One can formally construct second-order energy stable schemes using IEQ or SAV approach as long as one can split the free energy into two terms, one is a linear quadratic term and the other is bounded from below. But we may not be able to do so with free energies having strong nonlinear derivative terms. Furthermore, the stability of IEQ and SAV is with respect to a modified energy which, in cases of strong nonlinear derivative terms, may not a good approximation of the original energy, could lead to non-physical oscillations [20].

In this work, we construct second-order stabilized predictor-corrector scheme for gradient flows with strongly nonlinear couplings of spatial derivatives. More precisely, we use the first-order stabilized scheme as the predictor, followed by a second-order corrector step. The scheme enjoys the following advantages:

- Simplicity: it only requires solving linear equations with constant coefficients at each time step.
- Stability: we shall show numerically that it is at least as stable as the first-order stabilized scheme.
- Accuracy: we shall show, analytically for a simple case and numerically with extensive examples, that the scheme is second-order accurate.

We shall consider three different types of gradient flows with strong anisotropic free energy, and construct stabilized predictor-corrector schemes for each case. First, we consider in Section 2 an anisotropic diffusion equation, and introduce the stabilized predictor-corrector approach. As a comparison, we also consider the second-order Crank-Nicolson scheme with Adam-Bashforth extrapolation for nonlinear terms. We will show that the stabilized predictor-corrector approach is much more robust than the Crank-Nicolson scheme with Adam-Bashforth extrapolation. We then apply the stabilized predictor-corrector approach to a strongly anisotropic Cahn-Hilliard equation in Section 3 and to the Cahn-Hilliard equation with degenerate diffusion mobility in Section 4. In all cases, our numerical results indicate that the stabilized predictor-corrector schemes are second-order accurate while having good stability. Finally, we carry out a rigorous error analysis in Section 5 to show the second-order convergence for the isotropic Cahn-Hilliard equation.

2 Anisotropic diffusion equation

In order to motivate the stabilized predictor-corrector approach, we consider in this section the following free energy functional,