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A Novel Lagrange Multiplier Approach with Relaxation for Gradient Flows

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Abstract. In this paper, we propose a novel Lagrange multiplier approach, named zero-factor (ZF) approach to solve a series of gradient flow problems. The numerical schemes based on the new algorithm are unconditionally energy stable with the original energy and do not require any extra assumption conditions. We also prove that the ZF schemes with specific zero factors lead to the popular SAV-type method. To reduce the computation cost and improve the accuracy and consistency, we propose a zero-factor approach with relaxation, which we named the relaxed zero-factor (RZF) method, to design unconditional energy stable schemes for gradient flows. The RZF schemes can be proved to be unconditionally energy stable with respect to a modified energy that is closer to the original energy, and provide a very simple calculation process. The variation of the introduced zero factor is highly consistent with the nonlinear free energy which implies that the introduced ZF method is a very efficient way to capture the sharp dissipation of nonlinear free energy. Several numerical examples are provided to demonstrate the improved efficiency and accuracy of the proposed method.

AMS subject classifications: 65M12, 35K20, 35K35, 35K55, 65Z05

Key words: Lagrange multiplier approach, zero-factor approach, gradient flows, relaxation, energy stable, numerical examples.

1 Introduction

Gradient flows are a kind of important models to simulate many physical problems such as the interface behavior of multi-phase materials, the interface problems of fluid mechanics, environmental science and material mechanics. In general, as the highly complex high-order nonlinear dissipative systems, it is a great challenge to construct effective

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and accurate numerical schemes with physical constraints such as energy dissipation and mass conservation. Many experts and scholars considered some unconditionally energy stable schemes. These numerical schemes preserve the energy dissipation law which does not depend on the time step. Some popular and widely used methods include convex splitting approach [7,14,18], linear stabilized approach [17,24], exponential time differencing approach [5,6,20], invariant energy quadratization approach [8,21,23,24,27], scalar auxiliary variable (SAV) approach [11,15,16], Lagrange multiplier approach [2] and so on.

Gradient flow models are generally derived from the functional variation of free energy. In general, the free energy $E(\phi)$ contains the sum of an integral phase of a nonlinear functional and a quadratic term

$$E(\phi)=\frac{1}{2}(\phi,\mathcal{L}\phi)+E_1(\phi)=\int_\Omega \frac{1}{2}\phi(\mathcal{L}\phi)+F(\phi)d\mathbf{x}, \tag{1.1}$$

where $\mathcal{L}$ is a symmetric non-negative linear operator, and $E_1(\phi)=\int_\Omega F(\phi)d\mathbf{x}$ is nonlinear free energy. $F(\mathbf{x})$ is the energy density function. The gradient flow from the energetic variation of the above energy functional $E(\phi)$ in Eq. (1.1) can be obtained as follows:

$$\frac{\partial\phi}{\partial t}=-\mathcal{G}\mu,\quad \mu=\mathcal{L}\phi+F'(\phi), \tag{1.2}$$

where $\mu=\delta E/\delta\phi$ is the chemical potential. $\mathcal{G}$ is a positive operator. For example, $\mathcal{G}=I$ for the L^2 gradient flow and $\mathcal{G}=-\Delta$ for the H^{-1} gradient flow. It is not difficult to find that the above phase field system satisfies the following energy dissipation law:

$$\frac{d}{dt}E=\left(\frac{\delta E}{\delta\phi},\frac{\partial\phi}{\partial t}\right)=-(\mathcal{G}\mu,\mu)\le 0,$$

which is a very important property for gradient flows in physics and mathematics.

Recently, many SAV-type methods are developed to optimize the traditional SAV method (detailed introduction, please see Section 2.2). For example, in [25], the authors introduced the generalized auxiliary variable method for devising energy stable schemes for general dissipative systems. An exponential SAV approach in [13] is developed to modify the traditional method to construct energy stable schemes by introducing an exponential SAV. In [9], the authors consider a new SAV approach to construct high-order energy stable schemes. In [2], the authors introduce a new Lagrange multiplier approach which is unconditionally energy stable with the original energy. However, the new approach requires solving a nonlinear algebraic equation for the Lagrange multiplier which brings some additional costs and theoretical difficulties for its analysis. Some other related work dealing with Lagrange multiplier approaches in flow problems, please see [1,19]. Recently, Jiang *et al.* [10] present a relaxation technique to construct a relaxed SAV (RSAV) approach to improve the accuracy and consistency noticeably. Some other efficient methods for preserving the original energy dissipation laws, please see [26].