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A Stable Arbitrarily High Order Time-Stepping Method for Thermal Phase Change Problems

Weiwen Wang[1] and Chuanju Xu[1,*]

[1] *School of Mathematical Sciences and Fujian Provincial Key Laboratory of Mathematical Modeling and High Performance Scientific Computing, Xiamen University, Xiamen 361005, P.R. China.*

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Abstract. Thermal phase change problems are widespread in mathematics, nature, and science. They are particularly useful in simulating the phenomena of melting and solidification in materials science. In this paper we propose a novel class of arbitrarily high-order and unconditionally energy stable schemes for a thermal phase change model, which is the coupling of a heat transfer equation and a phase field equation. The unconditional energy stability and consistency error estimates are rigorously proved for the proposed schemes. A detailed implementation demonstrates that the proposed method requires only the solution of a system of linear elliptic equations at each time step, with an efficient scheme of sufficient accuracy to calculate the solution at the first step. It is observed from the comparison with the classical explicit Runge-Kutta method that the new schemes allow to use larger time steps. Adaptive time step size strategies can be applied to further benefit from this unconditional stability. Numerical experiments are presented to verify the theoretical claims and to illustrate the accuracy and effectiveness of our method.

AMS subject classifications: 80A22, 35Q79, 65L06, 65M70

Key words: Thermal phase change problem, gradient flows, unconditional energy stability, auxiliary variable, Runge-Kutta methods, phase field.

1 Introduction

We can model a large class of physical problems with various gradient flows which share the common ground of being a dissipative system. Examples of these dissipative systems include Allen-Cahn equation [3], Cahn-Hilliard equation [12], interface dynamics [4,72], dendritic crystal growth models [40,41,43,44,68,76], thin film models [27,49,60], liquid

*Corresponding author. *Email address:* wangweiwen@stu.xmu.edu.cn (W. Wang), cjxu@xmu.edu.cn (C. Xu)

crystal models [26, 42, 71], etc. These models all agree with the second law of thermodynamics.

In the past few decades, many efficient and accurate energy stable schemes have been proposed for gradient flow models or dissipative systems. Some popular approaches include the fully implicit methods [19, 24, 25], which require that one solves a coupled system of nonlinear equations in each time step. If one chooses the time step for these schemes to be too large, the nonlinear equations have multiple solutions. Moreover, it has been shown in [59] that only a small set of fully implicit schemes are unconditionally energy stable. Eyre [22] applied a new semi-implicit method named convex splitting approach which was first introduced in [21] to resolve the problems associated with both the stiffness and solvability. It splits the nonlinear terms of free energy into the subtraction of two convex functions, and leads to unconditionally energy stable for a large class of gradient flows but requires solving a convex minimization problem at each time step. Another disadvantage is that there does not exist general functional splitting leading to stable schemes of higher order, and it is only possible to design second-order convex-splitting schemes case-by-case [7, 51, 60, 61]. In addition to the convex splitting method, the so-called stabilized linearly implicit approach [54, 65, 78] is widely used, which consists in adding an artificial stabilization term to balance the explicit treatment of the nonlinear term. The advantage of the stabilization method is its efficiency and simplicity, since it only requires solving Poisson systems with constant coefficients at each time step [72]. However, it appears that the unconditionally energy stable stabilized scheme is usually limited to first-order accuracy. An alternative is the exponential time discretization (ETD) method [14, 16, 17, 39, 63], which can lead to unconditionally energy stable schemes by using polynomial interpolations for the nonlinear terms, but we still have yet to obtain theoretical proofs of the energy stability properties of the higher-order ETD schemes.

Recently, the invariant energy quadratization (IEQ), was proposed in a number of papers [28, 67–69, 75–77]. It's a generalization of the method of Lagrange multipliers or of auxiliary variables originally presented in [6, 31]. One can construct linear, second-order, unconditionally energy stable schemes for a class of gradient flows based on the IEQ approach. Chen et al. [13] improved the accuracy and stability of the IEQ method by introducing extra free parameters for phase-field models. As a remedy, Shen et al. [52, 53] extended the IEQ to the so-called scalar auxiliary variable (SAV) approach by introducing scalar auxiliary variables instead of auxiliary function variables. SAV method not only keeps the advantages of the IEQ approach, but also yields more robust schemes with fewer restrictions on the energy functionals. Thanks to the simplicity and efficiency, SAV approach have been used to construct unconditionally energy stable schemes for a large class of nonlinear systems, for instances, Navier-Stokes equations and related systems [45–47, 56, 70], time fractional PDEs [35], nonlinear Schrödinger equation [2, 5, 23], gradient flows [34, 55, 73], etc. Several improved SAV schemes have also been developed, such as the multiple scalar auxiliary variable (MSAV) approach [15] for gradient flows with disparate terms in the free energy, stabilized-scalar auxiliary variable method