INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 15, Number 6, Pages 884–918

A GENERAL STRATEGY FOR NUMERICAL APPROXIMATIONS OF NON-EQUILIBRIUM MODELS–PART I: THERMODYNAMICAL SYSTEMS

JIA ZHAO, XIAOFENG YANG, YUEZHENG GONG, XUEPING ZHAO, XIAOGANG YANG, JUN LI, AND QI WANG

Abstract. We present a general approach to deriving energy stable numerical approximations for thermodynamical consistent models for nonequilibrium phenomena. The central idea behind the systematic numerical approximation is the energy quadratization (EQ) strategy, where the system's free energy is transformed into a quadratic form by introducing new intermediate variables. By applying the EQ strategy, one can develop linear, high order semi-discrete schemes in time that preserve the energy dissipation property of the original thermodynamically consistent model equations. The EQ method is developed for time discretization primarily. When coupled with an appropriate spatial discretization, a fully discrete, high order, linear scheme can be developed to warrant the energy dissipation property of the fully discrete scheme. A host of examples for phase field models are presented to illustrate the effectiveness of the general strategy.

Key words. Energy stable schemes, nonequilibirum models, thermodynamic consistent models, energy quadratization.

1. Introduction

Time-dependent dynamics or transient dynamics in nonequilibrium phenomena is ubiquitous in science and engineering. One objective of scientific and engineering research is to develop mathematical models to describe the complex dynamics for various nonequilibrium systems. For material systems, especially, flowing materials, the development of a viable models to describe nonequilibrium phenomena at a given degree of freedoms is often not governed by a single physical equation unlike the Maxwell equation in the electromagnetic theory or the Schrodinger equation in quantum mechanics. Namely, universally accepted physical laws do not exist in many material systems once the choice of the variables, time and length scales is made. The Onsager principle has been proven to be an effective tool for one to arrive at a reasonable theory for describing near nonequilibrium dynamics [34, 35, 57, 66, 67, 26]. The Onsager principle is consisted of the linear response theory for kinetics and appropriate choices for describing reversible and irreversible dynamics within the regime of the time and length scale selected. It is equivalent to the GENERIC or the Poisson bracket formalism for non-equilibrium phenomena [2, 36], the energetic variational principle coupled with the minimum dissipation principle [13, 46, 25], and the second law of thermodynamics. But, the Onsager principle is easier to use in practice.

In a nutshell, the Onsager principle [34, 35] simply states that for a matter system, after one has identified the generalized coordinate, flux, and forces, there exists a balance between the frictional force and the totality of the other forces. It provides a specific way to calculate the frictional and the other forces. The Onsager principle was proposed for dissipative systems. It can be extended to yield a generalized Onsager principle to include reversible processes corresponding to

Received by the editors December 12, 2017.
2000 *Mathematics Subject Classification.* 65N30.

transport phenomena. A large majority of the thermodynamic and hydrodynamic models, if they are derived correctly, obey the generalized Onsager principle in that the models possess a variational structure and admit energy dissipation laws.

Now that many models can be derived using the generalized Onsager principle, can we develop a systematic approach to fully utilize the variational as well as the dissipative structure in the models? The answer is positive. This paper aims at developing such a systematic approach to obtaining a second order temporal discretization for the thermodynamic model equations. This can form a paradigm for the future development of effective numerical approximations to models that describe non-equilibrium phenomena, enabling one to focus on more fine details or higher order approximations as well as implementation efficiency.

For a given non-equilibrium model consisted of partial differential equations, a high order approximation, computational efficiency as well as property preserving at the discrete level are always the desired properties to attain. For the dissipative system, one of the properties, one would like to preserve firstly, is the positive entropy production rate, or equivalently the second law of thermodynamics. In the isothermal case, it implies energy dissipation, commonly known as the energy law. The type of numerical schemes that retains the energy dissipate property at the discrete level is called the energy stable scheme. When the energy stability property of the scheme is independent of the discrete step size, the scheme is termed unconditionally energy stable. For these schemes, a large step size can be chosen to compute numerical solutions of the model equations.

In the past, two distinct, broadly-used strategies for developing energy stable schemes were proposed, which are the convex splitting approach [17, 53, 39, 52, 24] and the stabilizing approach [32, 69, 73, 31, 42, 45, 44, 70, 74, 54, 7, 68, 43]. The convex-splitting strategy relies on the existence of a pair of convex components that give rise to the free energy as the difference of the two functions. If such a splitting exists, a nonlinear scheme can be devised to render an unconditionally energy stable scheme. The stabilizing approach augments discretized equations by high order terms to turn the scheme into an energy stable scheme. Usually, this is accomplished by adding additional dissipation to the numerical scheme. Both strategies can yield dissipative schemes but do not guarantee to preserve the dissipation rate. Recently, Badia, Guillen-Gonzales, Gutierres-Santacreu and Tierra explored a new idea of transforming the free energy into a quadratic functional to derive energy stable schemes [1, 23]. Recently, it is amplified and systematically applied to many specific thermodynamic models by Yang, Zhao, Shen and Wang [58, 61, 8, 62, 56, 60, 65, 70, 64, 71, 72, 21, 22]. Yang, Zhao and Wang coined the name Invariant Energy Quadratization (IEQ) method for this class of methods. Later, we abbreviated the name to simply Energy Quadratization (EQ) method, which is more appropriate. This strategy bypasses the traditional complicated ones to arrive at semi-discrete, second order or higher order in time linear schemes readily. This strategy is so general that it has little restriction on the specific expression of the free energy.

In this paper, we summarize the works that we have done using the EQ strategy and present a general framework to discretize the thermodynamically consistent models in forms of partial differential equations to arrive at linear, second order, energy stable numerical schemes. Implied by the name of EQ, one introduces new intermediate variables to quadratize the free energy of the model. Then, one reformulates the thermodynamic model in the new variables. In all cases, the second order in time, numerical scheme based on the linearized, implicit Crank-Nicolson method can be applied to the models to arrive at energy stable schemes. The