Analysis and Computation of Coupled Spatially Discrete Phase Transition Equations

In models of phase transitions of polymers in chemical engineering and of alloys in metallurgical engineering (see [5, 6]) one often obtains models that are similar in form to Allen-Cahn equations (where mass is not preserved) and/or Cahn-Hilliard equations (where mass is typically preserved). In multicomponent problems (see [1, 5, 7, 8]) the models often result in coupled Allen-Cahn and Cahn-Hilliard equations (see [6, 10]) which is known as model C in the terminology of Hohenberg and Halperin (see [10]). The purpose of this project is to study microscopic versions of model C that are discrete in space and continuous in time.

The Model

We consider general nonlinear gradient systems on a spatially discrete mesh $\Omega \subset \mathbb{Z}^n$, $n \geq 1$. The gradient is defined in terms of an inner product space H. We are interested in several inner product spaces, in particular in the case $m = 2$ when $H = l^2 \times h^{-1}$, and the case $m = 3$ when $H = l^2 \times h^{-1} \times h^{-1}$. In both of these cases taking the gradient with respect to l^2 will result in an Allen-Cahn type component, while h^{-1} will result in a Cahn-Hilliard type component.

Existence and Stability of Equilibrium and Travelling Wave Solution

Since the differential equations we are considering are gradient it is important to determine the equilibrium solutions since these represent the potential asymptotic solution states. In addition, we will also consider solutions that are of the form of a travelling wave in the first component and an equilibrium in the remaining components.

We will consider the existence and stability of so-called mosaic equilibrium solutions (see [3]). By a mosaic equilibrium solution we mean an equilibrium solution with $u_i(\eta) \in \{-1, 0, +1\}$ for all $\eta \in \Omega$ and $i = 1, ..., m$. We will also consider the stability of such equilibrium solutions in the Lyapunov sense (see [3, 11]), but note the difficulty in determining stability for the components of the problem that are of Cahn-Hilliard type because of the lack of a maximum principle.

We will look for solutions that are a travelling wave solution in the Allen-Cahn component and an equilibrium solution in the Cahn-Hilliard components. By a travelling wave solution in the u_1 component, we mean a solution of the form

$$u_1(\eta, t) = \varphi(\sigma \cdot \eta - ct), \tag{1}$$

where $\varphi : \mathbb{R} \to \mathbb{R}$ and c is the (unknown) wave speed, and with the unit vector $\sigma \in \mathbb{R}^n$, $|\sigma| = 1$, representing the direction of motion, given beforehand. Substitution of the travelling wave Ansatz (1) gives

$$-c\varphi'(\xi) = L_\sigma \varphi(\xi) - \frac{\partial F}{\partial u_1}(\varphi(\xi), u_2, ..., u_m), \qquad \xi \in \mathbb{R}, \tag{2}$$

where L_σ is a difference operator that is associated with the difference operator of the original differential equation.

Numerical Solution

Good numerical solutions to the nonlinear gradient system are vital to motivate analytical results. We intend to obtain good qualitative and quantitative results by using numerical methods which preserve the gradient structure of the flow. The variable time-stepping strategy used in the numerical integration requires careful attention. The asymptotic behaviour of gradient systems is governed by the stable and unstable manifolds of the equilibrium solutions, but standard strategies perform poorly in the neighbourhood of equilibrium solutions (see [9]). We will compare fixed and standard variable time-stepping strategies with new strategies such which preserve the gradient structure, and will seek to develop both the theory and the practical implementation of these new methods.

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