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Highlights

- We present a second-order energy-stable time-integration method for the Swift–Hohenberg equation that suppresses numerical instabilities.
- Based on the generalized- α method, numerical dissipation is controlled via the spectral radius.
- A detailed energy-stability proof and an estimate for the stabilization parameter are provided.
- The proposed stabilization vanishes for sufficiently small time step sizes, recovering the original weak form of the equation.
- Numerical results for a pattern-formation example are used to test the convergence and energy-stability.
- We compare the primal and mixed formulation in terms of wall-clock time and approximation error.

An Energy-Stable Generalized- α Method for the Swift–Hohenberg Equation

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Abstract

We propose a second-order accurate energy-stable time-integration method that controls the evolution of numerical instabilities introducing numerical dissipation in the highest-resolved frequencies. Our algorithm further extends the generalized- α method and provides control over dissipation via the spectral radius. We derive the first and second laws of thermodynamics for the Swift–Hohenberg equation and provide a detailed proof of the unconditional energy stability of our algorithm. Finally, we present numerical results to verify the energy stability and its second-order accuracy in time.

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1. Introduction

The Swift–Hohenberg equation, originally presented in 1977, models instabilities in Rayleigh–Bénard convection phenomena [19]. The model belongs to the phase-field family and is derived using thermodynamic arguments from a given free-energy functional. In this equation, the evolution of the phase field is controlled by a fourth-order nonlinear scalar equation in which the mass is not conserved. Since its introduction, the Swift–Hohenberg equation has been used to model pattern formation [5, 17], fluid instabilities [15], and cell organization [18]. Recently, time discretization algorithms that ensure the satisfaction of the second law of thermodynamics have been developed for conservative [11, 13, 22] and non-conservative phase-field equations [12, 14]. Vignal generalized the ideas of previous algorithms into a second-order energy-stable algorithm for both conservative and non-conservative phase-field models [20]. These energy-stable algorithms avoid the presence of non-physical phenomena in numerical results [25]. However, they do not offer direct control over numerical instabilities, which can appear due to steep interfaces in the phase field. Figure 1 presents a comparison of the evolution of a steep interface in the phase field with and without the introduction of controlled numerical dissipation to arrest high-frequency instabilities. This figure shows that numerical instabilities affect the pattern formed by the phase field. In Figure 1 both results are energy-stable and the ones without dissipation exemplify the previously developed algorithms [11–14, 20, 22].

Figure 1: Evolution of a steep interface in the phase field, ϕ , with energy stable discretizations. The lack of numerical dissipation presents numerical instabilities.

In this work, we develop an energy-stable method that introduces numerical dissipation to suppress these high-frequency numerical instabilities. We start describing the Swift–Hohenberg equation and then derive the first and second laws of thermodynamics for this model. Building on this formulation, we propose an energy-stable time-integration algorithm based on the generalized- α method. Then, we introduce a fully implicit algorithm and provide a detailed proof of the unconditional energy stability. Additionally, we present a semi-implicit linear version of the algorithm that offers advantages from the computational point of view, although its energy stability proof relies on physically based arguments that we detail. Moreover, this algorithm provides control over the numerical dissipation via the spectral radius to prevent the evolution of numerical instabilities.

Finally, we solve a test case on pattern formation with a set of different spatial and temporal discretizations to verify the satisfaction of the entropy production inequality and the second-order accuracy of the method.

2. The Swift–Hohenberg model

The Swift–Hohenberg equation (1) models the evolution of the phase field, ϕ , as the free energy, Ψ , is minimized. The phase field, ϕ , is the dimensionless volume fraction of a mixture and its time rate of change, $\dot{\phi}$, represents the temporal change of the mass of the mixture. Here, the temporal change of the mass is considered proportional to the chemical potential, η , which is the variational derivative of the free energy, Ψ , with respect to the phase field. Thus, the strong form of the equation in a bounded domain, $\Omega \in \mathbb{R}^n$, is to find $\phi : \Omega \times]0, T] \rightarrow \mathbb{R}$, subject to an initial condition, ϕ_0 , as

$$\begin{aligned} \dot{\phi}(t) &= -M\eta && \text{in } \Omega \text{ with } t \in]0, T], \\ \phi(t) &= \phi_0 && \text{in } \Omega \text{ with } t = 0. \end{aligned} \tag{1}$$

Here, we denote material derivatives by $(\dot{\cdot})$, and M represents the mass growth or mobility coefficient. The mobility, M , is usually defined as a positive constant or a nonlinear positive function of the phase field that restricts the mass flux to the material interface [1]. In this study, without loss of generality, we consider a constant mobility, $M = 1$. The works of Vignal [22] and Wu [24] offer a detailed explanation on how to deal with non-constant mobilities.

The free energy functional, Ψ , is defined as a function of the phase field, ϕ , and its spatial derivatives. This energy is comprised by the bulk and interfacial energies. The nonlinear double well function $f(\phi)$, corresponding to the bulk free energy, models the entropic effects and induces the phase separation of the mixture [15]. The interfacial

energy represents the nonlocal effects and is a function of the spatial derivatives of the phase field, in this case, the gradient $\nabla\phi$ and the Hessian $\mathbf{H} = \nabla\nabla\phi$. The total free energy and double well function are defined as

$$\Psi(\phi, \nabla\phi, \mathbf{H}) = \int_{\Omega} \psi \, d\Omega, \quad (2)$$

$$f(\phi) = \frac{\phi^2}{2} \left(\frac{\phi^2}{2} - \lambda \right) + \frac{\phi^2}{2}. \quad (3)$$

Here, the parameter λ determines the stable values of the phase field $\phi_s = \pm\sqrt{\lambda-1}$ for $\lambda > 1$, as the minimums of the double well function. Figure 2 shows the double well function, $f(\phi)$, and the stable values of the phase field, ϕ_s .

Figure 2: Double well function, $f(\phi)$, and the stable values of the phase field, ϕ_s , for $\lambda > 1$.

For convenience, we split the total free energy density, ψ , into the bulk free energy, ψ_b , and the interfacial free energy, ψ_i , defined as

$$\psi_b = \frac{\phi^2}{2} \left(\frac{\phi^2}{2} - \lambda \right), \quad (4)$$

$$\psi_i = \frac{1}{2} \left(\phi^2 - 2(\nabla\phi)^2 + \text{tr}(\mathbf{H})^2 \right), \quad (5)$$

where $\psi = \psi_b + \psi_i$. Equation (5) considers an interfacial energy that depends on the

gradient and the trace of the Hessian of the phase field, $tr(\mathbf{H})$, which corresponds to the Laplacian of the phase field $\Delta\phi$. Thus, the chemical potential, η , is defined as

$$\begin{aligned}\eta = \frac{\delta\Psi}{\delta\phi} &= \frac{\delta\psi_b}{\delta\phi} + \frac{\delta\psi_i}{\delta\phi} = \frac{\partial\psi_b}{\partial\phi} + \frac{\partial\psi_i}{\partial\phi} - \nabla \cdot \left(\frac{\partial\psi_i}{\partial\nabla\phi} \right) + \nabla \cdot \left(\nabla \cdot \left(\frac{\partial\psi_i}{\partial\mathbf{H}} \right) \right), \\ &= \underbrace{\phi(\phi^2 - \lambda)}_{\eta_b = \frac{\delta\psi_b}{\delta\phi}} + \underbrace{\phi + 2\Delta\phi + \Delta\Delta\phi}_{\eta_i = \frac{\delta\psi_i}{\delta\phi}},\end{aligned}\quad (6)$$

where δ denotes the variational derivative and Δ represents the Laplacian operator. The bi-Laplacian operator, $\Delta\Delta$, appearing in the chemical potential renders equation (1) as a nonlinear fourth-order partial differential equation.

3. First and second laws of thermodynamics

We derive the first and second laws of thermodynamics based on the governing (1) and constitutive (6) equations of the model according to [9]. Here, the second law of thermodynamics plays the key role of the energy stability condition. First, the time rate of change of the total free energy density, ψ , is defined as

$$\dot{\psi} = \frac{\partial\psi}{\partial\phi} \dot{\phi} + \frac{\partial\psi}{\partial\nabla\phi} \cdot (\nabla\dot{\phi}) + \frac{\partial\psi}{\partial\mathbf{H}} : (\dot{\mathbf{H}}). \quad (7)$$

Let us multiply the phase-field equation (1) by the chemical potential, η , to recover the temporal derivative of the total free energy, $\dot{\psi}$. Then, using the definition of the variational

derivative of the total free energy, η , and integration by parts yields

$$\begin{aligned}
 \dot{\phi}\eta &= -M\eta^2, \\
 &= \dot{\phi} \left(\frac{\partial \psi}{\partial \phi} - \nabla \cdot \left(\frac{\partial \psi}{\partial \nabla \phi} \right) + \nabla \cdot \left(\nabla \cdot \left(\frac{\partial \psi}{\partial \mathbf{H}} \right) \right) \right), \\
 &= \frac{\partial \psi}{\partial \phi} \dot{\phi} + \frac{\partial \psi}{\partial \nabla \phi} \cdot (\nabla \dot{\phi}) + \frac{\partial \psi}{\partial \mathbf{H}} : (\dot{\mathbf{H}}) \\
 &\quad - \nabla \cdot \left(\dot{\phi} \left(\frac{\partial \psi}{\partial \nabla \phi} - \nabla \cdot \left(\frac{\partial \psi}{\partial \mathbf{H}} \right) \right) + (\nabla \dot{\phi}) \cdot \left(\frac{\partial \psi}{\partial \mathbf{H}} \right) \right). \tag{8}
 \end{aligned}$$

Rearranging equation (8) we identify the temporal derivative of the free energy density, $\dot{\psi}$, and the external rate of work $\dot{w}_{ext}$

$$\dot{\psi} + M\eta^2 = \underbrace{\nabla \cdot \left(\dot{\phi} (-2\Delta\phi - \nabla \cdot \Delta\Delta\phi) + (\nabla \dot{\phi}) \cdot \Delta\Delta\phi \right)}_{\dot{w}_{ext}}. \tag{9}$$

Furthermore, in the absence of heat transfer, the total energy density, e_T , is solely comprised by the internal energy $e_T = e_i$. Thus, the time change of the total energy density is given by the contributions of all external work as $\dot{e}_T = \dot{w}_{ext}$. Substituting the definition of the external work rate from (9), we state the first law of thermodynamics as follows

$$\dot{e}_T = \dot{e}_i = \dot{\psi} + M\eta^2. \tag{10}$$

By definition, the material time derivative of free energy in absence of heat transfer and temperature change is $\dot{\psi} = \dot{e}_i - \theta_0 \dot{s}$, where θ_0 and $\dot{s}$ represent the absolute temperature and the entropy production rate, respectively. Introducing the time rate of change of the internal energy (10) into this definition yields the following expression for the second law

of thermodynamics

$$\theta_0 \dot{s} = M\eta^2 \geq 0, \quad (11)$$

which can be expressed in terms of the free energy density as $\dot{\psi} \leq 0$. The discrete version of the previous expression allows us to verify the energy stability and compute the numerical dissipation, ε , introduced by our discretization as

$$\llbracket \psi \rrbracket \leq 0, \quad (12)$$

$$\varepsilon = \frac{\llbracket \psi \rrbracket}{\tau} + M\llbracket \eta^2 \rrbracket. \quad (13)$$

Here, we denote the discrete time change as $\llbracket \chi \rrbracket = \chi_{n+1} - \chi_n$, with $\chi_n = \chi(t_n)$, and the constant time step size as $\tau = t_{n+1} - t_n$.

4. Proposed algorithm

We propose an unconditionally energy-stable time-integration algorithm that belongs to the generalized- α family in which the dissipation of high-frequencies can be controlled through the spectral radius, ρ_∞ . The generalized- α method was introduced by Chung and Hulbert [2] to solve structural dynamics problems [7, 8]. Subsequently, Jansen, Whiting and Hulbert extended these ideas to the first order in time equations [16]. This method numerically dissipates energy at the highest resolved frequencies while minimizing the dissipation in the lowest frequencies. Moreover, the spectral radius used in the method represents the dissipation of the different frequencies, where for $\rho_\infty = 1$ no dissipation is introduced and $\rho_\infty = 0$ represents the effective damping of the highest frequencies in a single step. The parameters for controlling the amplification α_f , α_m , and γ are based on

the limits of the eigenvalues of the amplification matrix of the method [2], where

$$\alpha_f = \frac{1}{1 + \rho_\infty}, \quad (14)$$

$$\alpha_m = \frac{3 - \rho_\infty}{2(1 + \rho_\infty)}. \quad (15)$$

Accordingly, the method is second-order accurate when the relationship $\gamma = \frac{1}{2} + \alpha_m - \alpha_f$ is satisfied, which yields $\gamma = \alpha_f$. Furthermore, the method is unconditionally stable when $\alpha_m \geq \alpha_f \geq \frac{1}{2}$. Based on the previous definitions, the generalized- α method uses the following evaluation of variables at different time instances

$$\phi_{n+\alpha_f} = \phi_n + \alpha_f \llbracket \phi \rrbracket, \quad (16)$$

$$\phi_{n+1} = \phi_n + \tau((1 - \gamma)v_n + \gamma v_{n+1}), \quad (17)$$

$$v_{n+\alpha_f} = v_n + \alpha_f \llbracket v \rrbracket, \quad (18)$$

$$v_{n+\alpha_m} = v_n + \alpha_m \llbracket v \rrbracket, \quad (19)$$

where $v_{n+\alpha_m}$ represents the temporal derivative of the phase field evaluated at time $t_{n+\alpha_m}$. For simplicity, we write $\alpha_r = (\alpha_m - \alpha_f) = (\alpha_f - \frac{1}{2})$, thus (19) reads

$$v_{n+\alpha_m} = v_{n+\alpha_f} + \alpha_r \llbracket v \rrbracket. \quad (20)$$

Additionally, we denote the jump and average of the phase field as $\llbracket \phi \rrbracket = \phi_{n+1} - \phi_n$ and $\{\phi\} = \frac{1}{2}(\phi_{n+1} + \phi_n)$, respectively. This notation allows us to rewrite the previous defini-

tions in more convenient expressions for the energy stability proof as

$$\begin{aligned}\phi_{n+\alpha_f} &= \phi_n + \left(\alpha_r + \frac{1}{2}\right) \llbracket \phi \rrbracket, \\ &= \{\phi\} + \alpha_r \llbracket \phi \rrbracket,\end{aligned}\tag{21}$$

$$\begin{aligned}\frac{\llbracket \phi \rrbracket}{\tau} &= (1 - \alpha_f) v_n + \alpha_f v_{n+1}, \\ &= v_{n+\alpha_f},\end{aligned}\tag{22}$$

$$v_{n+\alpha_m} = \frac{\llbracket \phi \rrbracket}{\tau} + \alpha_r \llbracket v \rrbracket.\tag{23}$$

With the previous definitions at hand, we propose the following second-order energy-stable algorithm for the time integration of the Swift–Hohenberg model

$$v_{n+\alpha_m} = -M \left((\eta_i)_{n+\alpha_f} + \widehat{(\eta_b)}_{n+\alpha_f} + \beta \phi_{n+\alpha_f} \right),\tag{24}$$

where β is a non-negative stabilization parameter and $\widehat{(\eta_b)}_{n+\alpha_f}$ is an approximation to the nonlinear bulk chemical potential. In order for this method to inherit the second order accuracy of the generalized- α method, the approximation to the bulk chemical potential, $\widehat{(\eta_b)}_{n+\alpha_f}$, needs to be a second order approximation of $(\eta_b)_{n+\alpha_f}$. Therefore, we write the bulk chemical potential as the fully implicit Taylor series expansion

$$(\eta_b)_{n+\alpha_f} = \sum_{a=0}^{\infty} (\eta_b)_{n+1}^{(a)} \frac{(-(1-\alpha_f)\llbracket \phi \rrbracket)^a}{a!},\tag{25}$$

where $(\eta_b)^{(a)}$ denotes the a -th derivative of η_b . Moreover, we select the approximation $\widehat{(\eta_b)}_{n+\alpha_f}$ as

$$\widehat{(\eta_b)}_{n+\alpha_f} \approx (\eta_b)_{n+1} - (\eta_b)'_{n+1} (1-\alpha_f) \llbracket \phi \rrbracket + (\eta_b)''_{n+1} \frac{\llbracket \phi \rrbracket^2}{6},\tag{26}$$

where the superscript ' denotes partial derivatives with respect to the phase field, ϕ . Thus, substituting the derivatives of the bulk chemical potential in the approximation we obtain

$$\widehat{(\eta_b)}_{n+\alpha_f} \approx \phi_{n+1}^3 - \lambda \phi_{n+1} - (3\phi_{n+1}^2 - \lambda) (1 - \alpha_f) \llbracket \phi \rrbracket + \phi_{n+1} \llbracket \phi \rrbracket^2, \quad (27)$$

Following the notation introduced in [20], we denote this approximation implicit as $\widehat{(\eta_b)}_{n+\alpha_f}^i$. This approximation allows our method to inherit the second order accuracy and dissipation control of the generalized- α method. Additionally, it renders a nonlinear, fully implicit time algorithm.

5. Energy stability

We prove the energy stability of the method by recovering the temporal rate of change of the total free energy, $\llbracket \Psi \rrbracket$, from the weak form of equation (24). First, we substitute the weighting functions in the weak form with the change in the phase field, $\llbracket \phi \rrbracket$, and obtain the following

$$(\llbracket \phi \rrbracket, v_{n+\alpha_m}) = -M \left(\llbracket \phi \rrbracket, \left((\eta_i)_{n+\alpha_f} + \widehat{(\eta_b)}_{n+\alpha_f}^i + \beta \phi_{n+\alpha_f} \right) \right). \quad (28)$$

Here, $(\cdot, \cdot)$ denotes the L_2 inner product in Ω . Then, substituting the definition of the interfacial chemical potential (6) in the first term on the right-hand side and using integration by parts leads to

$$\begin{aligned} (\llbracket \phi \rrbracket, (\eta_i)_{n+\alpha_f}) &= (\llbracket \phi \rrbracket, \phi_{n+\alpha_f} + 2\Delta \phi_{n+\alpha_f} + \Delta \Delta \phi_{n+\alpha_f}), \\ &= (\llbracket \phi \rrbracket, \{\phi\}) - 2(\nabla \llbracket \phi \rrbracket, \nabla \{\phi\}) + (\Delta \llbracket \phi \rrbracket, \Delta \{\phi\}) \\ &\quad + \alpha_r ((\llbracket \phi \rrbracket, \llbracket \phi \rrbracket) - 2(\nabla \llbracket \phi \rrbracket, \nabla \llbracket \phi \rrbracket) + (\Delta \llbracket \phi \rrbracket, \Delta \llbracket \phi \rrbracket)). \end{aligned} \quad (29)$$

Here, we observe that all the terms in the last line are positive, and can be written as $\alpha_r(1 + \Delta)^2 \llbracket \phi \rrbracket$, and since α_r is non-negative, this contribution is always non-negative. Moreover, we can write the rest of the terms as the time rate of change of the interfacial energy

$$(\llbracket \phi \rrbracket, \{\phi\}) - 2(\nabla \llbracket \phi \rrbracket, \nabla \{\phi\}) + (\Delta \llbracket \phi \rrbracket, \Delta \{\phi\}) = \int_{\Omega} \llbracket \psi_i \rrbracket d\Omega. \quad (30)$$

Additionally, we relate the temporal change of interfacial energy, $\llbracket \psi_i \rrbracket$, to the total free energy, Ψ , by evaluating the discrete time change of equation (2)

$$\llbracket \Psi \rrbracket = \int_{\Omega} (\llbracket \psi_b \rrbracket + \llbracket \psi_i \rrbracket) d\Omega. \quad (31)$$

Then, by introducing the latter relation into equation (28) we obtain

$$\begin{aligned} (\llbracket \phi \rrbracket, v_{n+\alpha_m}) = & -M \left(\llbracket \Psi \rrbracket - \int_{\Omega} \llbracket \psi_b \rrbracket d\Omega + \left(\llbracket \phi \rrbracket, \widehat{(\eta_b)}_{n+\alpha_f}^i \right) \right) \\ & - M \int_{\Omega} (\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket + \alpha_r(1 + \Delta)^2 \llbracket \phi \rrbracket) d\Omega. \end{aligned} \quad (32)$$

We rearrange this expression using definition (22) and write the temporal rate of change in total free energy as

$$\begin{aligned} \llbracket \Psi \rrbracket = & -\frac{1}{M} (\tau v_{n+\alpha_f}, v_{n+\alpha_m}) + \int_{\Omega} \llbracket \psi_b \rrbracket d\Omega - \left(\llbracket \phi \rrbracket, \widehat{(\eta_b)}_{n+\alpha_f}^i \right) \\ & - \int_{\Omega} (\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket + \alpha_r(1 + \Delta)^2 \llbracket \phi \rrbracket) d\Omega. \end{aligned} \quad (33)$$

Here, we achieve the unconditional energy stability by proving that all the terms on the right-hand side are non-positive, therefore satisfying the monotonic decrease of the total free energy (12). In this case, the terms in the bottom line of equation (33) are always non-

positive, whereas the terms in the first line must be proven to be non-positive or bounded by the negative terms. We expand the first term on the right-hand side, using definitions (22) and (23), to prove that it is always non-positive as

$$(\tau v_{n+\alpha_f}, v_{n+\alpha_m}) = \int_{\Omega} \tau \left(v_{n+\alpha_f}^2 + \alpha_r \alpha_f \llbracket v \rrbracket^2 \right) d\Omega + \int_{\Omega} \tau \alpha_r v_n \llbracket v \rrbracket d\Omega, \quad (34)$$

where the first term on the right-hand side is always positive. We take the following triangular inequality based on equation (22), and considering that by definition $\alpha_r \leq \frac{\alpha_f}{2}$ we write

$$\frac{\llbracket \phi \rrbracket^2}{2\tau^2} = \frac{v_{n+\alpha_f}^2}{2} \geq \frac{v_n^2 + \alpha_f^2 \llbracket v \rrbracket^2}{2} \geq |\alpha_f v_n \llbracket v \rrbracket| \geq |\alpha_r v_n \llbracket v \rrbracket|. \quad (35)$$

Thus, the last term of equation (34) is bounded by $\frac{1}{2\tau} \llbracket \phi \rrbracket^2$. This proves that the term $-(\tau v_{n+\alpha_f}, v_{n+\alpha_m})$ is always negative and contributes to the stability as a negative variation of the total free energy. Furthermore, we introduce the previous inequality in (33) to write

$$\begin{aligned} \llbracket \Psi \rrbracket \leq & -\frac{1}{M} \int_{\Omega} \left(\frac{\llbracket \phi \rrbracket^2}{2\tau} + \tau \alpha_r \alpha_f \llbracket v \rrbracket^2 \right) d\Omega + \int_{\Omega} \llbracket \psi_b \rrbracket d\Omega - \left(\llbracket \phi \rrbracket, \widehat{(\eta_b)}_{n+\alpha_f}^i \right) \\ & - \int_{\Omega} (\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket + \alpha_r (1 + \Delta)^2 \llbracket \phi \rrbracket) d\Omega. \end{aligned} \quad (36)$$

Hence, we only need to bound the terms corresponding to the bulk free energy.

From the full implicit Taylor series expansion of the bulk free energy (25), we recover the approximation $\widehat{(\eta_b)}_{n+\alpha_f}^i$ from equation (26) as

$$\begin{aligned} \llbracket \psi_b \rrbracket &= (\eta_b)_{n+1} \llbracket \phi \rrbracket - (\eta_b)'_{n+1} \frac{\llbracket \phi \rrbracket^2}{2} + (\eta_b)''_{n+1} \frac{\llbracket \phi \rrbracket^3}{6} - (\eta_b)'''_{n+1} \frac{\llbracket \phi \rrbracket^4}{24}, \\ &= \widehat{(\eta_b)}_{n+\alpha_f}^i \llbracket \phi \rrbracket - \underbrace{(\eta_b)'_{n+1} \alpha_r \llbracket \phi \rrbracket^2}_{R^i} - (\eta_b)'''_{n+1} \frac{\llbracket \phi \rrbracket^4}{24}. \end{aligned} \quad (37)$$

Then, we substitute the remaining terms $R^i = \int_{\Omega} \llbracket \psi_b \rrbracket d\Omega - \left(\llbracket \phi \rrbracket, \widehat{(\eta_b)}_{n+\alpha_f}^i \right)$ in equation (36) and express the jump in the free energy as

$$\begin{aligned} \llbracket \Psi \rrbracket \leq & -\frac{1}{M} \int_{\Omega} \left(\frac{\llbracket \phi \rrbracket^2}{2\tau} + \tau \alpha_r \alpha_f \llbracket v \rrbracket^2 \right) d\Omega + R^i \\ & - \int_{\Omega} (\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket + \alpha_r (1 + \Delta)^2 \llbracket \phi \rrbracket) d\Omega. \end{aligned} \quad (38)$$

Here, the remaining terms, R^i , are the only ones that need a bound to prove that the total free energy does not increase. To bound these terms, we evaluate the maximum value of their summation and obtain an expression for the necessary stabilization parameter, β . First, let us introduce definition (21) in the stabilization term as

$$\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket = \beta (\{\phi\} + \alpha_r \llbracket \phi \rrbracket) \llbracket \phi \rrbracket, \quad (39)$$

$$= \frac{\beta}{2} (\phi_{n+1}^2 + \phi_n^2) + \beta \alpha_r (\phi_{n+1}^2 - 2\phi_{n+1}\phi_n + \phi_n^2). \quad (40)$$

Furthermore, we use the inequality $(\phi_{n+1}^2 + \phi_n^2) \geq -2\phi_{n+1}\phi_n$, in which we can add $2\{\phi\}\llbracket \phi \rrbracket$ on both sides of the inequality and write $4\{\phi\}\llbracket \phi \rrbracket \geq \llbracket \phi \rrbracket^2$. Thus, we obtain the following expression for the stabilization term

$$\beta \phi_{n+\alpha_f} \llbracket \phi \rrbracket \geq \beta \left(\frac{1}{4} + \alpha_r \right) \llbracket \phi \rrbracket^2. \quad (41)$$

Additionally, we rewrite the remaining terms as follows

$$R^i = \left((\lambda - 3\phi_{n+1}^2) \alpha_r - \frac{\llbracket \phi \rrbracket^2}{4} \right) \llbracket \phi \rrbracket^2 = A^i \llbracket \phi \rrbracket^2. \quad (42)$$

Taking the maximum of A^i with respect to ϕ_n and ϕ_{n+1} , we find that the maximum of R^i

is $\max_{\phi_n, \phi_{n+1}}(R^i) = \max_{\phi_n, \phi_{n+1}}(A^i) \llbracket \phi \rrbracket^2$, where

$$\max_{\phi_n, \phi_{n+1}}(A^i) = \lambda \alpha_r. \quad (43)$$

Appendix A follows this procedure to prove the energy stability of a semi-implicit algorithm that uses a truncated explicit Taylor series expansion to approximate the bulk chemical potential as

$$\widehat{(\eta_b)}_{n+\alpha_f}^e \approx (\eta_b)_n + (\eta_b)'_n \alpha_f \llbracket \phi \rrbracket. \quad (44)$$

However, in the semi-implicit case an additional consideration regarding the phase field bounds is necessary to evaluate the maximum of the remaining terms, R^e . This is necessary because the polynomial double well potential does not bound the phase field as it does with the logarithmic bulk free energy commonly used in the Cahn–Hilliard equation [10–13, 23]. For this reason, we consider the bounds of the phase field to be $-\lambda < \phi < \lambda$ from a physical, rather than a numerical, point of view. Considering that this assumption holds, we have derived the energy stability proof for the semi-implicit algorithm. We also include numerical results of the semi-implicit algorithm that show its energy stability for this specific case and evaluate its computational advantages over the implicit algorithm. In this case, we write the remaining terms as R^e and its maximum as $\max_{\phi_n, \phi_{n+1}}(R^e) = \max_{\phi_n, \phi_{n+1}}(A^e) \llbracket \phi \rrbracket^2$. Thus, we obtain the following expression that needs to be bounded

$$\max_{\phi_n, \phi_{n+1}}(A^e) = \frac{(\lambda + 3\alpha_r + 12\alpha_r^2 + 3\lambda\alpha_r) \lambda}{3 + 12\alpha_r}. \quad (45)$$

Figure 3 shows the behavior of $\max_{\phi_n, \phi_{n+1}}(A)$, with $\lambda = 2$, for the explicit and implicit approx-

imations as a function of α_r and the spectral radius, ρ_∞ .

Figure 3: Behavior of $\max_{\phi_n, \phi_{n+1}}(A)$ for the explicit and implicit approximations with $\lambda=2$.

We can bound the maximum of the term R in equation (38) by the stabilization term, $\beta \left(\frac{1}{4} + \alpha_r \right) \llbracket \phi \rrbracket^2$, and write the jump of the free energy as

$$\llbracket \Psi \rrbracket \leq - \int_{\Omega} \left(\frac{\tau \alpha_r \alpha_f}{M} \llbracket v \rrbracket^2 + \left(\frac{1}{2M\tau} + \beta \left(\frac{1}{4} + \alpha_r \right) - \max_{\phi_n, \phi_{n+1}}(A) \right) \llbracket \phi \rrbracket^2 + \alpha_r (1 + \Delta)^2 \llbracket \phi \rrbracket \right) d\Omega, \quad (46)$$

where we define the stabilization constant, β , as

$$\beta = \max \left(0, \frac{\left(\max_{\phi_n, \phi_{n+1}}(A) - \frac{1}{2M\tau} \right)}{\left(\frac{1}{4} + \alpha_r \right)} \right). \quad (47)$$

Therefore, we prove the energy stability of the method. This stabilization parameter depends on the physical constants M and λ , and the numerical parameters α_r and τ . The stabilization term becomes smaller as the time step size decreases, and disappears for sufficiently small time steps, which recovers the original equation without requiring any

additional stabilization.

6. Primal and mixed weak forms

Mixed formulations for phase-field equations are common [6, 21], given that they allow the use of discretization spaces with lower polynomial order and reduced continuity. This leads to cheaper solution schemes [3, 4]. Accordingly, mixed formulations introduce an auxiliary variable and equation. Here, we compare the results computed with the following primal weak form

$$\begin{aligned} (w, v_{n+\alpha_m}) = & -M \left(w, (\widehat{\eta_b})_{n+\alpha_f} + \beta \phi_{n+\alpha_f} \right) \\ & - M \left((w, \phi_{n+\alpha_f}) - 2(\nabla w, \nabla \phi_{n+\alpha_f}) + (\Delta w, \Delta \phi_{n+\alpha_f}) \right), \end{aligned} \quad (48)$$

and the following mixed weak form

$$\begin{aligned} (w, v_{n+\alpha_m}) = & -M \left(w, (\widehat{\eta_b})_{n+\alpha_f} + \beta \phi_{n+\alpha_f} \right) - M \left((w, \sigma) - (\nabla w, \nabla \sigma) \right) \\ (q, \sigma) = & (q, \phi_{n+\alpha_f}) - (\nabla q, \nabla \phi_{n+\alpha_f}). \end{aligned} \quad (49)$$

Where the auxiliary variable, σ , corresponds to the interfacial chemical potential terms, and w and q represent the weighing functions for the phase-field and auxiliary equations, respectively. The primal formulation involves up to second derivatives of the phase field, requiring a discretization with at least globally C^1 spaces. The mixed formulation involves only first derivatives of the phase field, ϕ , and the auxiliary variable, σ . This allows discretizations using C^0 spaces particularly for lowest-order methods, such as bilinear or trilinear discretizations. In the next section, we present a comparison of the computational times and errors of the primal and mixed formulations.

7. Numerical results

We present numerical results for a two-dimensional pattern formation case. We analyze the energy stability, dissipation, convergence, and computational time tests on our algorithm using different spatial and temporal discretizations to solve the example case. The test case presents an initial condition built with two sinusoidal functions in a square domain, $\Omega = [0, 40] \otimes [0, 40] \in \mathbb{R}^2$, given by

$$\phi = \tanh \left(\left(y - \sin \left(\frac{\pi x}{5} \right) - 18 \right) \frac{48}{5} \right) - \tanh \left(\left(y - \sin \left(\frac{\pi x}{4} \right) - 22 \right) \frac{48}{5} \right) - 1. \quad (50)$$

Figure 4 illustrates the initial condition of the phase field and domain dimensions. This initial condition is unstable which drives the evolution of the system, where the red region grows forming a pattern that fills the entire domain. The spatial variation of the initial condition is steep around the interface which induces instabilities in the evolution of the phase field. In this test case, we consider a parameter $\lambda = 2$ to define the bulk free energy, a constant mobility, $M = 1$, and periodic boundary conditions on both axes. Figure 5 presents the evolution of the phase field in the reference solution from time $t = 0$ to the final time $t = 200$, depicting how the pattern grows until it fills the whole domain.

Figure 4: Domain description and initial condition for the phase field, ϕ .

Figure 5: Evolution of the phase field in the reference solution.

For a thorough test of our algorithm, we consider different spatial and temporal discretizations, the primal and mixed weak forms, and the implicit and explicit approximations of the nonlinear terms. We evaluate grids with 128^2 , 256^2 , and 512^2 elements and polynomial order $p = 2$ and interelemental continuity $\varsigma = 1$ for the primal formulation, and $p = 1$ and $\varsigma = 0$, for both ϕ and σ , for the mixed formulation. For the temporal discretization, we use three different constant time-step sizes of $\tau = 0.01$, 0.1 and 1 . Additionally, we use three spectral radii with $\rho_\infty = 0.5$, 0.9 , and 1 for each spatial and temporal discretization.

Figure 6: Isocontours of the stabilization parameter β and τ_{max} for $M = 1$ and $\lambda = 2$.

We define the minimum stabilization parameter, β , according to equation (47) for our simulations. Figure 6 shows the isocontours of the stabilization parameter for our test cases, using $M = 1$ and $\lambda = 2$, as a function of the spectral radius and the time-step size. Here, the isocontours labeled as τ_{max} correspond to the threshold where the stabilization vanishes according to equation (47). The shaded areas in Figure 6 represent the regions where no stabilization is required. We do not need to add any stabilization for the implicit approximation with $\rho_\infty = 1$, regardless of the size of the time step. Moreover, among the cases we consider, the ones using the explicit approximation with a time step size $\tau = 1$ are the only ones that require stabilization. Whereas the cases using the implicit approximation do not require stabilization for any of the time step sizes considered. Table 1 presents the stabilization parameter used for the explicit approximation in the case of a time-step size $\tau = 1$, for the different spectral radii.

Table 1: Stabilization parameter β for the explicit approximation using a mobility $M = 1$, $\varphi = 2$, and a time step size $\tau = 1$.

Approximation	Spectral radius		
	$\rho_\infty = 0.5$	$\rho_\infty = 0.9$	$\rho_\infty = 1.0$
Explicit $(\widehat{\eta_b})_{n+\alpha_f}^e$	$\beta = 2.48$	$\beta = 3.0914$	$\beta = 3.3333$

In the next subsections, we present a comparison of the numerical instabilities, energy stability, convergence, and error versus computational cost. First, we illustrate the effect of the spatial discretization in the numerical instabilities, compare our results to state-of-the-art algorithms, and show how the numerical instabilities affect the pattern formed. Then, we introduce the energy stability and convergence results of our algorithm. Finally, we display the error versus computational time when comparing the primal and mixed formulations. Due to the non-linear nature of the equation, no analytical solution is available to verify the quality of our solution. For this reason, we opt to compare our results against a reference solution using an overkill spatial and temporal discretization with a time step size $\tau = 10^{-5}$ and a mesh of 512^2 elements with $p = 4$, $\varsigma = 3$ spaces using the primal formulation.

7.1. Numerical instabilities

We start comparing the evolution of the high-frequency instabilities for the different spatial discretizations, for both the implicit and explicit approximations. Figure 7 shows the numerical instabilities in the solutions of the primal formulation at the final time of the simulation $t = 200$, when using a time-step size $\tau = 1$ and the spectral radius $\rho_\infty = 1.0$. This figure also presents the reference solution for comparison. Here, it is evident that all the considered spatial discretizations present instabilities that resemble the initial condition. Additionally, the intensity of these instabilities grows when the spatial discretization

becomes more refined. The spectral radius $\rho_\infty = 1.0$ used in the temporal discretization introduces no numerical dissipation, therefore it offers no dampening of the instabilities. The pattern created by the explicit approximation differs from that of the reference solution due to the numerical instabilities. Moreover, the temporal evolution of the phase field in the explicit case is delayed due to the addition of the stabilization. However, this delay is only present when the time step size is larger than the threshold τ_{max} .

Figure 7: Instabilities in the solutions of the primal formulation at the final time $t=200$ for a time step $\tau=1$ and spectral radius $\rho_\infty=1.0$. Instabilities are more significant in the more refined spatial discretizations.

Figure 8: Comparison of numerical instabilities in the primal formulation at the final time $t = 200$ for two time step sizes of $\tau = 0.1$ and 1 and $N = 512^2$ elements.

Figure 8 presents a comparison of the numerical instabilities when numerical dissipation is introduced in the primal formulation with the implicit approximation and spectral radii $\rho_\infty = 0.5$ and 1 . Additionally, we present the results of two alternative energy stable algorithms by Gomez and Nogueira [12] and Vignal et al. [21]. We use a mesh of 512^2 elements where the numerical instabilities are most notorious. Moreover, we compare two time-step sizes $\tau = 0.1$ and 1 . The cases without numerical dissipation show instabilities once the time step size is large enough. While the cases with added numerical dissipa-

tion are free from numerical instabilities for the two time-step sizes shown here. These energy stable algorithms are not exempt from numerical instabilities when no numerical dissipation is introduced.

7.2. Energy stability

Figure 9 shows the temporal evolution of the free energy, Ψ , for the explicit and implicit approximations in the cases using a mesh of $N = 512^2$ elements. This figure illustrates the constant decay of the free energy and numerically validates the energy stability of our method. Furthermore, the energy stability condition is satisfied by all the discretizations considered. Additionally, we see a better approximation to the free energy evolution of the reference solution when the time-step size is reduced. The addition of numerical dissipation ($\rho_\infty = 0.9$) improves the approximation to the free energy of the reference solution, over the cases with no dissipation, irrespective of the time-step size and approximation of the nonlinear terms.

Figure 9: Time evolution of the free energy, Ψ . The reference solution is shown in black for comparison.

Figure 10 presents the time evolution of the L^2 error norm of the free energy when comparing the coarser temporal discretizations with the reference solution. Here, we show results for the explicit and implicit approximations with a spatial discretization using $N=512^2$ elements. This figure shows the improvement in the approximation of the free energy when numerical dissipation is introduced. We observe improvements of at least an order of magnitude in the error when using a spectral radius lower than one. An even bigger difference is evidenced during the first instants of the simulation due to the dissipation of the instabilities present in the initial condition.

Figure 10: Time evolution of the L^2 error norm of the free energy, Ψ , for the explicit and implicit approximations.

7.3. Convergence

Figures 11 and 12 show the convergence of the L^2 error of the phase field, ϕ , for the $N=128^2$ and $N=256^2$ spatial discretizations using the primal formulation, respectively. We compute the L^2 errors of the phase field at the final time, $t=200$, as the size of the

time step is reduced. Moreover, these figures show the convergence of the implicit and explicit approximations and all the spectral radii considered. Both approximations to the nonlinear terms inherit the second-order accuracy in time of the generalized- α method. However, the L^2 errors of the explicit approximation are usually higher than those of the implicit approximation.

Figure 11: Convergence in time of the L^2 error norm of ϕ for the primal formulation with a spatial discretization using $N = 128^2$ elements.

Figure 12: Convergence in time of the L^2 error norm of ϕ for the primal formulation with a spatial discretization using $N = 256^2$ elements.

7.4. Wall-clock versus approximation error

We compare the average wall-clock time and the errors of the primal and mixed formulations to evaluate which of this formulations is a better discretization option. Figures 13 and 14 present the comparison of the average wall-clock time per time step for the explicit and implicit algorithms, respectively. Each figure shows the results of the primal ($p = 2$, $\varsigma = 1$) and mixed ($p = 1$, $\varsigma = 0$) formulations. Here, the average wall-clock time was computed using the first 200 time steps of the simulation running on a single core of a workstation (2 Hex-core Xeon X5650, 48 Gb RAM). The mixed formulation presents an average speedup between three and seven times over the primal formulation for the explicit and implicit algorithms, respectively. When comparing the explicit and implicit formulations, we see that the explicit algorithm has an average speedup of six and two times for the primal and mixed forms, respectively. One of the downsides of introducing dissipation in the high frequencies of the problem is that the wall-clock time increased in average 26% with respect to the solutions without dissipation due to an increased number of linear iterations.

Figure 13: Average wall-clock time per time step of the explicit approximation run on a single core for the primal and mixed formulations.

Figure 14: Average wall-clock time per time step of the implicit approximation run on a single core for the primal and mixed formulations.

We perform an error comparison to support the time comparison and verify that both algorithms and formulations have similar error ranges. Figure 15 shows the comparison of the L^2 error of the phase field. This figure includes the errors of the primal and mixed forms when the time discretization error is sufficiently small ($\tau = 10^{-2}$). Here, we compute the L^2 errors at the final time $t = 200$ between the coarser spatial discretizations ($N = 128^2, 256^2$) and the reference solution. Figure 15 shows that the error ranges of the primal and mixed discretizations are comparable with the different discretizations considered in this study. A thorough analysis of the discretization error is required to draw a general conclusion about the error orders on more refined spatial discretizations.

Figure 15: Comparison of the L^2 error norm of the phase field, ϕ , at time $t = 200$ between the primal and mixed formulations for the explicit and implicit algorithms.

8. Conclusions

We analyze the Swift–Hohenberg equation and derive the first and second law of thermodynamics for the model as guidelines for the development of discrete energy-stable methods. Then, we introduce a new unconditionally energy-stable, second-order in time algorithm based on the generalized- α method, which provided control over the addition of the numerical dissipation introduced by the time discretization. We present a detailed proof of the unconditional energy stability and derive an estimation of the stabilization parameter. Furthermore, we proved that the stabilization parameter vanishes with a sufficiently small time step, recovering the original weak form of the equation.

We solve a numerical test case that highlights the advantages of our algorithm, corresponding to an initial condition that induces numerical instabilities. Here, we compare several different discretizations in space and time to evaluate the dissipation of numerical instabilities, energy stability, energy approximation, time accuracy of our method, and computational cost. The energy decay is satisfied by all the discretizations considered,

providing numerical evidence of the energy stability of our method. However, satisfying the energy decay is not sufficient to approximate the reference solution. For this reason, we evaluate the approximation of the free energy and show that adding numerical dissipation to the high frequencies of the discrete solution improves the approximation substantially. Additionally, we study the numerical convergence in time of our method and verify that it is second-order accurate in time. Finally, we compare the computational time and error between the primal and mixed formulations, showing that the mixed formulation is faster while obtaining comparable errors to those of the primal formulation.

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Appendix A. Explicit construction of the free energy jump in time

The semi-implicit algorithm is based on an explicit Taylor series expansion of the bulk chemical potential

$$(\eta_b)_{n+\alpha_f}^e = \sum_{a=0}^{\infty} (\eta_b)_n^{(a)} \frac{(\alpha_f \llbracket \phi \rrbracket)^a}{a!}. \quad (\text{A.1})$$

Here we use the following truncated Taylor series expansion as an approximation of $(\eta_b)_{n+\alpha_f}^e$

$$\widehat{(\eta_b)}_{n+\alpha_f}^e \approx (\eta_b)_n + (\eta_b)_n' \alpha_f \llbracket \phi \rrbracket, \quad (\text{A.2})$$

which can be recovered from the jump in the bulk free energy as

$$\begin{aligned} \llbracket \psi_b \rrbracket &= (\eta_b)_n \llbracket \phi \rrbracket + (\eta_b)_n' \frac{\llbracket \phi \rrbracket^2}{2} + (\eta_b)_n'' \frac{\llbracket \phi \rrbracket^3}{6} + (\eta_b)_n''' \frac{\llbracket \phi \rrbracket^4}{24}, \\ &= \widehat{(\eta_b)}_{n+\alpha_f}^e \llbracket \phi \rrbracket - (\eta_b)_n' \alpha_r \llbracket \phi \rrbracket^2 + (\eta_b)_n'' \frac{\llbracket \phi \rrbracket^3}{6} + (\eta_b)_n''' \frac{\llbracket \phi \rrbracket^4}{24}. \end{aligned} \quad (\text{A.3})$$

The remaining terms of the approximation $R^e = \int_{\Omega} \llbracket \psi_b \rrbracket d\Omega - \left(\llbracket \phi \rrbracket, \widehat{(\eta_b)}_{n+\alpha_f}^e \right)$ in equation (36) become

$$R^e = -(\eta_b)_n' \alpha_r \llbracket \phi \rrbracket^2 + (\eta_b)_n'' \frac{\llbracket \phi \rrbracket^3}{6} + (\eta_b)_n''' \frac{\llbracket \phi \rrbracket^4}{24}. \quad (\text{A.4})$$

We rewrite the remaining terms as follows

$$R^e = \left((\lambda - 3\phi_n^2) \alpha_r + \phi_n \llbracket \phi \rrbracket + \frac{\llbracket \phi \rrbracket^2}{4} \right) \llbracket \phi \rrbracket^2 = A^e \llbracket \phi \rrbracket^2, \quad (\text{A.5})$$

and then we take the maximum of A^e with respect to ϕ_n and ϕ_{n+1} . Assuming that the physical bounds of the phase field are $-\lambda < \phi < \lambda$, we write the maximum of the remaining terms, R^e , as $\max_{\phi_n, \phi_{n+1}}(R^e) = \max_{\phi_n, \phi_{n+1}}(A^e) \llbracket \phi \rrbracket^2$, where

$$\max_{\phi_n, \phi_{n+1}}(A^e) = \frac{(\lambda + 3\alpha_r + 12\alpha_r^2 + 3\lambda\alpha_r) \lambda}{3 + 12\alpha_r}. \quad (\text{A.6})$$

In the same way as for the implicit algorithm, we bound $\max_{\phi_n, \phi_{n+1}}(A^e)$ by the stabilization term $(\frac{1}{2M\tau} + \beta(\frac{1}{4} + \alpha_r))$, proving that the explicit algorithm is energy-stable when the phase field is bounded by $-\lambda < \phi < \lambda$.