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An energy-stable time-integrator for phase-field models

P. Vignal^a, N. Collier^b, L. Dalcin^{c,d}, D.L. Brown^e, V.M. Calo^{f,g}

^a*Materials Science and Engineering (MSE)
King Abdullah University of Science and Technology (KAUST)
Thuwal, Saudi Arabia*

^b*Computer Science and Mathematics Division, Oak Ridge National Laboratory
Tennessee, United States*

^c*Extreme Computing Research Center (ECRC)
King Abdullah University of Science and Technology (KAUST)
Thuwal, Saudi Arabia*

^d*Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET)
Santa Fe, Argentina*

^e*School of Mathematical Sciences
University of Nottingham
Nottingham, United Kingdom*

^f*Applied Geology Department, Western Australian School of Mines,
Faculty of Science and Engineering, Curtin University,
Perth, Western Australia, 6845, Australia*

^g*Mineral Resources, Commonwealth Scientific and Industrial Research Organisation
(CSIRO), Kensington, WA, Australia 6152*

Abstract

We introduce a provably energy-stable time-integration method for general classes of phase-field models **with polynomial potentials**. We demonstrate how Taylor series expansions of the nonlinear terms present in the partial differential equations of these models can lead to expressions that guarantee energy-stability implicitly, which are second-order accurate in time. The spatial discretization relies on a mixed finite element formulation and isogeometric analysis. We also propose an adaptive time-stepping discretization that relies on a first-order backward approximation to give an error-estimator. **This error estimator is accurate, robust, and does not require the computation of extra solutions to estimate the error.** This methodology can be applied to any second-order accurate time-integration scheme. We present numerical examples in two and three spatial dimensions, which confirm the stability and robustness of the method. The implementation of the numerical schemes is done in PetIGA, a high-performance isogeometric analysis framework.

Keywords: Phase-field models, PetIGA, high-order partial differential equation, mixed finite elements, isogeometric analysis, time integration

1. Introduction

The theory behind phase-field models, defined by [Van der Waals](#) [46] over a century ago, has matured and taken off in the last couple of decades. The phase-field framework implicitly describes surfaces and interfaces by continuous scalar fields that take constant values in the bulk phases and vary continuously but steeply across a diffuse front [44]. The phase-field parameter is used within a free energy functional that defines the physical behavior of the system, and here lies one of the key advantages over other methods. The diffuse interface is introduced through an energetic variational procedure that results in a thermodynamically consistent coupling. This consistency gives the method solid mathematical and physical footings, and explains why applications range from spinodal decomposition of immiscible binary mixtures [7, 21, 61], tumor angiogenesis [58, 59], [wetting](#) [14] and [elasto-capillarity](#) [5, 53], image processing [40] to water infiltration in porous media [22]. Another advantage of the phase-field method over sharp interface descriptions comes from the fact that under appropriate assumptions [6], a diffuse-interface description can asymptotically converge to its sharp-interface counterpart by decreasing the interfacial thickness.

Even though phase-field modeling has been qualitatively successful, it is not without its own drawbacks. Phase-field modeling usually involves the solution of high-order partial differential equations (PDEs), and including realistic features comes at the expense of nonlinear terms (such as a nonlinear mobility for the different components involved). Given the nature of the PDEs, using explicit methods is restrictive for stability reasons, and this has motivated research on implicit algorithms [21, 36, 54]. Another issue has to do with the resolution used to describe the interfacial thickness. If the interfacial layer is not well resolved, the solution can have spurious oscillations, particularly in the vicinity of the interface [62]. Irrespective of the discretization method used, these last two points lead to the need for robust and scalable software to solve these types of problems. Last but not least, phase-field models should possess strong energy stability [30]: free energy must decrease in time. The goal of this paper is to devise a time discretization scheme that applies to both conserved and non-conserved phase-field

models **with a polynomial potential**, within a high-performance framework, with the longterm goal of obtaining quantitative results for industrially relevant applications.

Numerical techniques that satisfy thermodynamic relations at the discrete level in phase-field models have been developed for both conserved [23, 25] and non-conserved phase-field models [24, 27]. This work generalizes some of these algorithms, and shows that the nonlinear terms present in the equations can be discretized in time using **a Taylor series expansion** to guarantee both second-order accuracy and strong energy stability. Given the difference in time scales that can exist in these models, we also present an **a-posteriori** error estimator that can be used to adapt the scheme in time.

Regarding the spatial discretization, we use isogeometric analysis (IGA) [13], a generalization of the finite element method, where, for example, Non-Uniform Rational B-spines (NURBS) [43] are used as basis functions. The method has successfully been applied in its Galerkin version to solve the Cahn-Hilliard equation [21, 23], the advective [39] and Navier-Stokes-Cahn-Hilliard equations [19, 56], the Swift-Hohenberg equation [24] and the phase-field crystal equation [25, 54, 57]. IGA possesses some advantages over standard finite element methods, which include being able to easily generate high-order, globally continuous basis functions as well as exact geometrical representations as the finite element space is refined. However, when used to discretize the higher-order partial differential equations, the NURBS-based spaces result in expensive linear systems that need efficient and scalable solvers that mitigate the increased cost (**see [8–10] for a thorough discussion on the issues**). For this reason, we implemented our algorithm in a high-performance isogeometric analysis framework, PetIGA [12, 15]. Recently, isogeometric collocation methods have also been used to discretize phase-field models [26, 49].

The paper is structured as follows: in section 2, we describe the general class of phase-field models dealt with in this work, and present the development of our unconditionally stable time integrator. In section 3, we present our spatial discretization strategy, detail the numerical solution process, and present our novel time-adaptive algorithm. In section 4, we present four different phase-field models, which we proceed to solve in section 5 using different time-stepping schemes. We conclude with section 6.

2. Energy stability of phase-field models

To model interfacial problems, phase-field methods represent the sharp interfaces between the different phases through thin transition regions that distribute the interfacial forces. In these models, the phase-field or order-parameter varies smoothly (i.e., continuously) over **these** thin layers, with a key point being that the energy of these models needs to be dissipated as time progresses. The existence of a Lyapunov functional for these diffuse-interface problems implies strong energy stability [60], a property which can be lost if inadequate algorithms and/or spatio-temporal resolutions are used to solve the partial differential equation [24, 48, 55, 60]. This work addresses the nonlinear stability issue for both conserved and non-conserved phase-field variables, and presents a simple process that relies on Taylor series to handle the nonlinear terms present in the partial differential equation.

2.1. Phase-field modeling

The phase-field framework relies on the minimization of a free energy functional that models **how the system undergoes phase transition**. This functional depends on a phase-field variable ϕ and its derivatives, and tries to capture both the bulk behavior of the components involved as well as their interfacial behavior. The free energy functional $\mathcal{F}$ for many important phase-field models can generally be written as [45]

$$\mathcal{F}[\phi(\mathbf{x})] = \int_{\Omega} (f(\phi, \nabla\phi, \Delta\phi) + \Psi(\phi)) d\Omega, \quad (1)$$

where f is a function of ϕ and its derivatives, such that

$$\begin{aligned} f(\phi, \nabla\phi, \Delta\phi) &= f_1(\phi) + f_2(\nabla\phi) + f_3(\Delta\phi) \\ &= \frac{1}{2} (c_0\phi^2 + c_1|\nabla\phi|^2 + c_2(\Delta\phi)^2), \end{aligned} \quad (2)$$

where c_0 , c_1 , and c_2 are real-valued constants, ∇ and Δ represent the gradient and Laplacian operators, respectively, and Ψ , a Landau-type free energy density [45], is a polynomial function of ϕ given by

$$\Psi(\phi) = \frac{1}{4}a_0 - \frac{1}{2}a_2\phi^2 + \frac{1}{4}a_4\phi^4, \quad (3)$$

where a_0 , a_2 and a_4 are real-valued constants, and a_2 and a_4 are strictly positive. This implies that the fourth derivative of Ψ with respect to ϕ is a positive constant

$$\frac{\partial^4 \Psi(\phi)}{\partial \phi^4} = \Psi^4(\phi) \geq 0.$$

To simplify notation, we write $\mathcal{F}[\phi(\mathbf{x})]$ as $\mathcal{F}(\phi)$, and $f(\phi, \nabla \phi, \Delta \phi)$ as $f(\phi)$. The phase field models considered in this work are those obtained through variational arguments, where the evolution in time of the phase-field variable is related to the variational derivative of the free energy functional defined in equation (1). These particular phase-field models have a gradient-flow structure. The initial boundary value problem with periodic boundary conditions over the spatial domain Ω (see equations (6)-(10) in [25] for the formal boundary conditions that lead to the phase-field crystal equation) and time interval $[0, T]$ of such cases is formulated as: given $\phi_0 : \Omega \rightarrow \mathbb{R}$, find $\phi : \Omega \times [0, T] \rightarrow \mathbb{R}$ such that

$$\begin{cases} \frac{\partial \phi}{\partial t} = (-\nabla)^a \cdot \left(-M \nabla^a \frac{\delta \mathcal{F}(\phi)}{\delta \phi} \right) & \text{on } \Omega \times]0, T], \\ \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}) & \text{on } \bar{\Omega}. \end{cases} \quad (4)$$

where t stands for a time-like variable, and the parameter a takes a value of one if the phase-field represents a conserved quantity or zero otherwise. Here, $M \equiv M(\phi)$ represents mobility and is defined as $M = \bar{M}$, with $\bar{M}$ a positive constant, or through the nonlinear expression

$$\begin{cases} M = \bar{M} \left(\frac{a_2}{a_4} - \phi^2 \right) \geq 0 \quad \forall \quad \phi \in \left[-\sqrt{\frac{a_2}{a_4}}, \sqrt{\frac{a_2}{a_4}} \right], \\ M = 0 \quad \text{otherwise.} \end{cases} \quad (5)$$

The initial condition is given by $\phi_0(\mathbf{x})$, and the variational derivative operator $\frac{\delta}{\delta \phi}$ is defined formally as

$$\frac{\delta}{\delta \phi} = \frac{\partial}{\partial \phi} - \nabla \cdot \frac{\partial}{\partial \nabla \phi} + \Delta \frac{\partial}{\partial \Delta \phi}. \quad (6)$$

for models including up to Laplacians in $\mathcal{F}$. Higher order models can also be considered by extending equation (6). Periodic or no-flux boundary conditions are used in all directions for all the problems considered in this work.

Many phase-field models may be derived from Lyapunov functionals using variational arguments [42], which endows them with nonlinear stability. We satisfy this property for a number of models by guaranteeing strong energy stability [60], defined discretely in time as

$$\mathcal{F}(\phi(t_{n+1})) \leq \mathcal{F}(\phi(t_n)) \quad \forall n = 1, 2, \dots, r. \quad (7)$$

Thermodynamically consistent algorithms (i.e., energy stable) are necessary. If inadequate discretizations are used to solve the partial differential equations involved, unphysical results where free energy increases can follow [24, 54]. Considering equation (7), the jump in free energy $\llbracket \mathcal{F} \rrbracket$ is defined as

$$\begin{aligned} \llbracket \mathcal{F} \rrbracket &= \mathcal{F}(\phi(t_{n+1})) - \mathcal{F}(\phi(t_n)), \\ &= \int_{\Omega} (\llbracket f \rrbracket + \llbracket \Psi \rrbracket) d\Omega \end{aligned} \quad (8)$$

where

$$\begin{aligned} \llbracket f \rrbracket &= f(\phi(t_{n+1})) - f(\phi(t_n)), \\ \llbracket \Psi \rrbracket &= \Psi(\phi(t_{n+1})) - \Psi(\phi(t_n)). \end{aligned}$$

With the goal of proving that our method guarantees

$$\llbracket \mathcal{F} \rrbracket \leq 0,$$

irrespectively of the mesh and time step sizes used, the free energy jump can be obtained using the weak form of equation (4) as shown in section 2.3.

2.2. A stable scheme

We propose a new second-order accurate, unconditionally energy-stable scheme for phase field models, given by

$$\frac{\llbracket \phi \rrbracket}{\Delta t} = (-\nabla)^a \cdot (-M \nabla^a \sigma), \quad (9)$$

$$\sigma = \frac{\partial f_1(\{\phi\})}{\partial \phi} + \tilde{\Psi}' - \nabla \cdot \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} + \Delta \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi}, \quad (10)$$

where

$$\llbracket \phi \rrbracket = \phi_{n+1} - \phi_n; \quad \Delta t = t_{n+1} - t_n; \quad \{\phi\} = 1/2 (\phi_{n+1} + \phi_n).$$

The function $\tilde{\Psi}'$ represents an approximation to Ψ' such that the scheme is energy-stable. The approximation is defined as

$$\tilde{\Psi}' = \Psi'_{n+1} - \Psi''_{n+1} \frac{[\phi]}{2} + \Psi'''_{n+1} \frac{[\phi]^2}{6}, \quad (11)$$

where Ψ'_m is written instead of $\Psi'(\phi_m)$ for the sake of brevity.

2.3. Building up $[\mathcal{F}]$ from the weak form

The auxiliary variable σ appearing in equations (9) and (10) is defined as

$$\sigma = \frac{\delta \mathcal{F}(\phi)}{\delta \phi},$$

which in turn modifies the definition of the partial differential equation (4), that now reads

$$\frac{\partial \phi}{\partial t} = (-\nabla)^a \cdot (-M \nabla^a \sigma), \quad (12)$$

$$\sigma = \frac{\delta \mathcal{F}(\phi)}{\delta \phi}. \quad (13)$$

Let us define the functional space $\mathcal{V} \in \mathcal{H}^m$, where $\mathcal{H}^m$ is the Sobolev space of square integrable functions with square integrable derivatives up to order m . Here the value of m can be 1, 2 or 3. For the Cahn–Hilliard equation, $m = 2$, for the phase-field crystal equation we set $m = 3$ and for the Allen–Cahn equation we set $m = 1$ in their respective variational forms. Essentially, m is the natural number of derivatives for the PDE under study. In the following, we derive the weak form of equations (12)–(13), obtained by multiplying them by test functions $w, q \in \mathcal{V}$, respectively, and integrating them by parts. The problem then becomes to find $\phi, \sigma \in \mathcal{V}$, such that for all $w, q \in \mathcal{V}$,

$$\left(w, \frac{\partial \phi}{\partial t} \right)_{\Omega} + (\nabla^a w, M \nabla^a \sigma)_{\Omega} = 0, \quad (14)$$

$$(q, \sigma)_{\Omega} - \left(q, \frac{\delta \mathcal{F}(\phi)}{\delta \phi} \right)_{\Omega} = 0, \quad (15)$$

where the $\mathcal{L}^2$ inner product over the domain is indicated by $(\cdot, \cdot)_\Omega$. Recalling equations (6) and (15), we have that

$$\begin{aligned} (q, \sigma)_\Omega &= \left(q, \frac{\delta \mathcal{F}(\phi)}{\delta \phi} \right)_\Omega \\ &= \left(q, \frac{\partial}{\partial \phi} \left(f_1(\phi) + \Psi(\phi) \right) - \nabla \cdot \frac{\partial f_2(\phi)}{\partial \nabla \phi} + \Delta \frac{\partial f_3(\phi)}{\partial \Delta \phi} \right)_\Omega \\ &= \left(q, \frac{\partial f_1(\phi)}{\partial \phi} \right)_\Omega + \left(\nabla q, \frac{\partial f_2(\phi)}{\partial \nabla \phi} \right)_\Omega + \left(\Delta q, \frac{\partial f_3(\phi)}{\partial \Delta \phi} \right)_\Omega \\ &\quad + \left(q, \frac{\partial \Psi(\phi)}{\partial \phi} \right)_\Omega. \end{aligned} \quad (16)$$

Recalling the time integration scheme proposed, we substitute equation (9) in (14) to obtain

$$\left(w, \frac{[\![\phi]\!]}{\Delta t} \right)_\Omega + (\nabla^a w, M \nabla^a \sigma)_\Omega = 0, \quad (17)$$

and substitute equation (10) in (16) to recover

$$\begin{aligned} (q, \sigma)_\Omega &= \left(q, \frac{\partial f_1(\{\phi\})}{\partial \phi} \right)_\Omega + \left(\nabla q, \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} \right)_\Omega + \left(\Delta q, \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi} \right)_\Omega \\ &\quad + \left(q, \tilde{\Psi}' \right)_\Omega. \end{aligned} \quad (18)$$

Now, by taking the test function q to be equal to $[\![\phi]\!]$, and taking the test function w as equal to σ , equations (17) and (18) become

$$(\sigma, [\![\phi]\!])_\Omega = -\Delta t (\nabla^a \sigma, M \nabla^a \sigma)_\Omega, \quad (19)$$

$$\begin{aligned} ([\![\phi]\!], \sigma)_\Omega &= \left([\![\phi]\!], \frac{\partial f_1(\{\phi\})}{\partial \phi} \right)_\Omega + \left(\nabla [\![\phi]\!], \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} \right)_\Omega + \left(\Delta [\![\phi]\!], \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi} \right)_\Omega \\ &\quad + \left([\![\phi]\!], \tilde{\Psi}' \right)_\Omega. \end{aligned} \quad (20)$$

Substituting (19) in (20), we recover that

$$\begin{aligned} -\Delta t (\nabla^a \sigma, M \nabla^a \sigma)_\Omega &= \left([\![\phi]\!], \frac{\partial f_1(\{\phi\})}{\partial \phi} \right)_\Omega + \left(\nabla [\![\phi]\!], \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} \right)_\Omega \\ &\quad + \left(\Delta [\![\phi]\!], \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi} \right)_\Omega + \left([\![\phi]\!], \tilde{\Psi}' \right)_\Omega. \end{aligned} \quad (21)$$

Using equation (8), it follows that

$$\begin{aligned} \int_{\Omega} \llbracket f \rrbracket d\Omega &= \llbracket \mathcal{F}(\phi) \rrbracket - \int_{\Omega} \llbracket \Psi \rrbracket d\Omega \\ &= \left(\llbracket \phi \rrbracket, \frac{\partial f_1(\{\phi\})}{\partial \phi} \right)_{\Omega} + \left(\nabla \llbracket \phi \rrbracket, \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} \right)_{\Omega} + \left(\Delta \llbracket \phi \rrbracket, \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi} \right)_{\Omega}. \end{aligned}$$

Substituting this result in equation (21), we recover that

$$\begin{aligned} \llbracket \mathcal{F}(\phi) \rrbracket &= -\Delta t (\nabla^a \sigma, M \nabla^a \sigma)_{\Omega} + \int_{\Omega} \llbracket \Psi \rrbracket d\Omega - \left(\llbracket \phi \rrbracket, \tilde{\Psi}' \right)_{\Omega} \\ &= -\Delta t (\nabla^a \sigma, M \nabla^a \sigma)_{\Omega} + \int_{\Omega} \left(\llbracket \Psi \rrbracket - \llbracket \phi \rrbracket \tilde{\Psi}' \right) d\Omega. \end{aligned} \quad (22)$$

Remark 1. Since M is a non-negative quantity (considering equation (5) or its definition as a positive constant), the approximation for Ψ' can be chosen to yield a stable scheme with second order accuracy in time.

Remark 2. Even though the mixed formulation allows to recover the free energy jump in the case of conserved phase-field models, primal formulations can be used in the case of non-conserved phase-field variables.

2.4. Handling nonlinearities: Taylor expansions guarantee energy-stability

Assuming the free energy functionals to be analytic, the nonlinear term involving Ψ in the free energy $\mathcal{F}$ can be expressed at time levels n or $n+1$ as a Taylor series expansion, from $\Psi_{n+1} = \Psi(\phi_{n+1})$ and $\Psi_n = \Psi(\phi_n)$, respectively. This allows us to write:

$$\Psi_{n+1} = \sum_{k=0}^{\infty} \Psi_n^{(k)} \frac{\llbracket \phi \rrbracket^k}{k!} \quad (23)$$

$$\Psi_n = \sum_{k=0}^{\infty} \Psi_{n+1}^{(k)} \frac{(-1)^k \llbracket \phi \rrbracket^k}{k!} \quad (24)$$

where $\Psi_m^{(a)}$ is the k -th derivative of Ψ with ϕ evaluated at t_m , such that

$$\Psi_m^{(k)} = \frac{d^k \Psi(\phi(t_m))}{d\phi^k}.$$

The jump in Ψ can then be equivalently expressed as:

$$[[\Psi]] = \Psi_{n+1} - \Psi_n = \sum_{k=1}^{\infty} \Psi_n^{(k)} \frac{[[\phi]]^k}{k!} \quad (25)$$

$$= \sum_{k=1}^{\infty} \Psi_{n+1}^{(k)} \frac{(-1)^{k+1} [[\phi]]^k}{k!} \quad (26)$$

Depending on how many terms of the expansions given in equations (25) and (26) are kept, different approximations can be obtained. Given the definition of Ψ in equation (3), $[[\Psi]]$ can be expanded from t_{n+1} using equation (26) such that

$$[[\Psi]] = \Psi'_{n+1} [[\phi]] - \Psi''_{n+1} \frac{[[\phi]]^2}{2} + \Psi'''_{n+1} \frac{[[\phi]]^3}{6} - \Psi_{n+\epsilon}^{(4)} \frac{[[\phi]]^4}{24}, \quad (27)$$

where $\Psi_{n+\epsilon}^{(4)}$ represents the exact remainder term [50] of the Taylor series, and is always greater than zero since $a_4 > 0$. Recalling the implicit approximation to the nonlinear function $\tilde{\Psi}'$ given by equation (11), $[[\Psi]]$ can be expressed as

$$[[\Psi]] = \tilde{\Psi}' [[\phi]] - \Psi_{n+\epsilon}^{(4)} \frac{[[\phi]]^4}{24}.$$

Thus, if equation (11) is used to express Ψ' as an approximation to $[[\Psi]]/[[\phi]]$, the jump in free energy of equation (22) becomes

$$[[\mathcal{F}(\phi)]] = -\Delta t (\nabla^a \sigma, M \nabla^a \sigma)_{\Omega} - \int_{\Omega} \Psi_{n+\epsilon}^{(4)} \frac{[[\phi]]^4}{24} d\Omega, \\ \leq 0,$$

and energy stability is proven.

2.5. Order of accuracy

To obtain a bound on the local truncation error, the method can be compared to the Crank–Nicolson scheme. For simplicity of presentation, we suppose that M is constant in this section. When applied to equation (4), the scheme reads

$$\frac{[[\phi]]}{\Delta t} = (-\nabla)^a \cdot \left(-M \nabla^a \frac{\delta \mathcal{F}(\{\phi\})}{\delta \phi} \right), \\ = (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi\})}{\delta \phi} + \frac{\partial \Psi(\{\phi\})}{\partial \phi} \right) \right), \quad (28)$$

where

$$\frac{\delta f(\{\phi\})}{\delta \phi} = \frac{\partial f_1(\{\phi\})}{\partial \phi} - \nabla \cdot \frac{\partial f_2(\{\phi\})}{\partial \nabla \phi} + \Delta \frac{\partial f_3(\{\phi\})}{\partial \Delta \phi}.$$

Substituting the discrete time solution $\{\phi\}$ by the time-continuous solution $\{\phi(t_n)\}$ into the above equation gives rise to the local truncation error. Indeed, we have

$$\begin{aligned} \frac{[\![\phi]\!]}{\Delta t} &= (-\nabla)^a \cdot \left(-M \nabla^a \frac{\delta \mathcal{F}(\{\phi(t_n)\})}{\delta \phi} \right), \\ &= (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi(t_n)\})}{\delta \phi} + \frac{\partial \Psi(\{\phi(t_n)\})}{\partial \phi} \right) \right) + \tau(t_n), \end{aligned} \quad (29)$$

where $\tau(t_n)$ represents the global truncation error. Such a scheme gives a bound $\tau(t_n) \leq C \Delta t^2$ which can be shown using Taylor series.

To prove second order accuracy in time for our scheme, we compute the next time-step approximation via the scheme applied to the exact solution and compare the result to Taylor expansions. A similar procedure was performed in [61] in the context of the Cahn-Hilliard equation and in [54] in the context of the phase-field crystal equation. Using equations (9)-(10), and reorganizing the splitting into one equation, we have that

$$\begin{aligned} \phi_{n+1} &= \phi(t_n) + \Delta t (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi(t)\})}{\delta \phi} \right. \right. \\ &\quad \left. \left. + \Psi'(\phi(t_{n+1})) - \Psi''(\phi(t_{n+1})) \frac{[\![\phi(t)]\!]}{2} + \Psi'''(\phi(t_{n+1})) \frac{[\![\phi(t)]\!]}{6} \right) \right), \end{aligned} \quad (30)$$

when the first three terms of approximation (11) are used, and $\{\phi(t)\}$ defines the Crank-Nicolson approximation, known to have error that is second-order in time ($\mathcal{O}(\Delta t^2)$). If at least two terms are used in the approximation of $\tilde{\Psi}'$, the rest of the terms are at least of order (Δt^2) , such that equation (30) can be written as

$$\begin{aligned} \phi_{n+1} &= \phi(t_n) + \Delta t (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi(t)\})}{\delta \phi} \right. \right. \\ &\quad \left. \left. + \Psi'(\phi(t_{n+1})) - \Psi''(\phi(t_{n+1})) \frac{[\![\phi(t)]\!]}{2} + \mathcal{O}(\Delta t^2) \right) \right), \end{aligned} \quad (31)$$

We expand $\Psi'(\phi(t_{n+1}))$ such that

$$\begin{aligned}\Psi'(\phi(t_{n+1})) &= \Psi'(\{\phi(t)\}) - \Psi''(\phi(t_{n+1}))(\{\phi(t)\} - \phi(t_{n+1})) + \mathcal{O}(\Delta t^2) \\ &= \Psi'(\{\phi(t)\}) + \Psi''(\phi(t_{n+1})) \frac{\llbracket \phi(t) \rrbracket}{2} + \mathcal{O}(\Delta t^2).\end{aligned}$$

Thus,

$$\Psi'(\{\phi(t)\}) = \Psi'(\phi(t_{n+1})) - \Psi''(\phi(t_{n+1})) \frac{\llbracket \phi(t) \rrbracket}{2} + \mathcal{O}(\Delta t^2). \quad (32)$$

Using equation (32), and substituting it into (31), we obtain

$$\begin{aligned}\phi_{n+1} &= \phi(t_n) \\ &\quad + \Delta t (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi(t)\})}{\delta \phi} + \Psi'(\{\phi(t)\}) + \mathcal{O}(\Delta t^2) \right) \right), \quad (33)\end{aligned}$$

Alternatively, by Taylor expansion of the solution we have

$$\begin{aligned}\{\phi(t)\} &= \phi(t_{n+1}) - \Psi'(\{\phi(t)\}) \left(\frac{\Delta t}{2} \right) - \Psi''(\{\phi(t)\}) \frac{1}{2} \left(\frac{\Delta t}{2} \right) + \mathcal{O}(\Delta t^3), \\ \{\phi(t)\} &= \phi(t_n) + \Psi'(\{\phi(t)\}) \left(\frac{\Delta t}{2} \right) - \Psi''(\{\phi(t)\}) \frac{1}{2} \left(\frac{\Delta t}{2} \right) + \mathcal{O}(\Delta t^3).\end{aligned}$$

Taking the difference of the above two equations and using equation (4) yields

$$\begin{aligned}\phi(t_{n+1}) - \phi(t_n) &= \Delta t \frac{\partial \{\phi(t)\}}{\partial t} + \mathcal{O}(\Delta t^3) \\ &= \Delta t (-\nabla)^a \cdot \left(-M \nabla^a \left(\frac{\delta f(\{\phi(t)\})}{\delta \phi} + \Psi'(\{\phi(t)\}) + \mathcal{O}(\Delta t^3) \right) \right),\end{aligned}$$

Finally, taking the difference of the above expression with equation (33), we obtain the local truncation error

$$\phi(t_{n+1}) - \phi_{n+1} = \mathcal{O}(\Delta t^3). \quad (34)$$

As the global truncation error $\tau(t_n)$ loses an order of accuracy of Δt , the scheme is second-order accurate in time.

2.6. Conserving mass when $a = 1$

Mass conservation is verified for the case in which $a = 1$ by taking the time-discrete version of equation (14) and letting the test function w be equal to one while having test function q equal to zero, such that

$$0 = \left(1, \frac{[\phi]}{\Delta t}\right)_{\Omega} + (0, M \nabla^a \sigma)_{\Omega} = \int_{\Omega} \frac{[\phi]}{\Delta t} d\Omega,$$

which implies that mass is conserved at the discrete time levels, that is

$$\int_{\Omega} \phi_{n+1} d\Omega = \int_{\Omega} \phi_n d\Omega.$$

3. Numerical discretization and time-adaptivity

In this section, we discuss the spatial discretization used to solve equations (17)-(18). We also introduce an adaptive algorithm in time that can be applied together with the stable time-marching scheme proposed. This coupling decreases the computational time needed to reach steady state solutions, and guarantees free energy stability during the simulation.

3.1. Spatial discretization: semi-discrete formulation

Given the weak form presented in equations (17)-(18), H^2 -conforming spaces are needed if the equation is solved with the Galerkin method. This requirement can be fulfilled by using $\mathcal{C}^1$ finite elements. These finite elements are accessible through isogeometric analysis [13]. Even though the equations addressed in this work are not required to go above $m = 2$, it is possible to generate discrete spaces with a higher degree of continuity [57]. As $m = 2$ allows us to tackle all the problems dealt with in this work, we let $\mathcal{V}_2^h \subset \mathcal{V}_2$ denote the finite dimensional functional space in two or three dimensions, where $\mathcal{V}_2$ is the Sobolev space of square integrable functions with square integrable first and second derivatives. The problem can be stated as follows: find $\phi^h, \sigma^h \in \mathcal{V}_2^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$0 = \left(w^h, \frac{\partial \phi^h}{\partial t}\right)_{\Omega} + (\nabla^a w, M(\phi^h) \nabla^a \sigma^h)_{\Omega} \quad (35)$$

$$0 = (q^h, \sigma^h - \Psi'(\phi^h))_{\Omega} - \left(q^h, \frac{\partial f_1(\phi^h)}{\partial \phi^h}\right)_{\Omega} - \left(\nabla q^h, \frac{\partial f_2(\phi^h)}{\partial \nabla \phi^h}\right)_{\Omega} - \left(\Delta q^h, \frac{\partial f_3(\phi^h)}{\partial \Delta \phi^h}\right)_{\Omega} \quad (36)$$

where the weighting functions w^h and q^h , trial solutions ϕ^h and σ^h are defined as the linear combinations

$$w^h = \sum_A W_A N_A(\mathbf{x}), \quad \sigma^h = \sum_A \Sigma_A N_A(\mathbf{x}), \quad (37)$$

$$q^h = \sum_A Q_A N_A(\mathbf{x}), \quad \phi^h = \sum_A \Phi_A N_A(\mathbf{x}), \quad (38)$$

where N_A are the multidimensional basis functions and W_A , Q_A , Σ_A and Φ_A are the control variables.

Remark 3. *Linear finite elements can be used in phase-field equations where the Laplacian term is absent from the free energy functional (i.e., $c_2 = 0$ in equation (2)). Furthermore, the choice to use $\mathcal{C}^1$ finite elements simplifies the presentation of the method, but alternative mixed formulations that only require $\mathcal{C}^0$ finite elements exist [54].*

3.2. Fully-discrete scheme

The **fully-discrete** version of the general phase-field problem presented in equations (12)-(13) may be described as follows: Let the time interval $\mathcal{T} =]0, T[$ be divided into r subintervals $\mathcal{T}_n = (t_n, t_{n+1})$ for $n = 0, \dots, r-1$. The fully discrete solutions are defined as ϕ_n^h and σ_n^h . The problem can now be defined as follows: given ϕ_{n-1}^h , ϕ_n^h and σ_n^h , find ϕ_{n+1}^h and σ_{n+1}^h such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$0 = \left(w^h, \frac{[\![\phi]\!]}{\Delta t} \right)_\Omega + (\nabla^a w^h, M(\phi^h) \nabla^a \sigma_{n+1}^h)_\Omega, \quad (39)$$

$$0 = \left(q^h, \sigma_{n+1}^h - \tilde{\Psi}'(\phi^h) \right)_\Omega - \left(q^h, \frac{\partial f_1(\{\phi^h\})}{\partial \phi^h} \right)_\Omega - \left(\nabla q, \frac{\partial f_2(\{\phi^h\})}{\partial \nabla \phi^h} \right)_\Omega - \left(\Delta q^h, \frac{\partial f_3(\{\phi^h\})}{\partial \Delta \phi^h} \right)_\Omega, \quad (40)$$

where $\tilde{\Psi}'(\phi^h)$ represents the spatially-discrete version of equation (11).

3.3. Numerical implementation

With regards to the numerical implementation, we let the global vectors of degrees of freedom associated to ϕ_n^h and σ_n^h be Φ_n^h and Σ_n^h , respectively.

The residual vectors for this formulation are then given by

$$\begin{aligned} \mathbf{R}_\phi(\Phi_{n-1}, \Phi_n, \Phi_{n+1}, \Sigma_{n+1}); \quad \mathbf{R}_\phi = \{R_A^\phi\}; \quad A = 1, \dots, n_b, \\ \mathbf{R}_\sigma(\Phi_{n-1}, \Phi_n, \Phi_{n+1}, \Sigma_{n+1}); \quad \mathbf{R}_\sigma = \{R_A^\sigma\}; \quad A = 1, \dots, n_b, \end{aligned}$$

where

$$\begin{aligned} R_A^\phi &= \left(N_A, \frac{[\phi]}{\Delta t} \right)_\Omega + (\nabla^a N_A, M(\phi^h) \nabla^a \sigma^h)_\Omega, \\ R_A^\sigma &= \left(N_A, \sigma^h - \tilde{\Psi}'(\phi^h) \right)_\Omega \\ &\quad - \left(N_A, \frac{\partial f_1(\{\phi^h\})}{\partial \phi^h} \right)_\Omega - \left(\nabla N_A, \frac{\partial f_2(\{\phi^h\})}{\partial \nabla \phi^h} \right)_\Omega - \left(\Delta N_A, \frac{\partial f_3(\{\phi^h\})}{\partial \Delta \phi^h} \right)_\Omega. \end{aligned}$$

The resulting system of nonlinear equations for Φ_{n+1} and Σ_{n+1} is solved using Newton's method, where $\Phi_{n+1}^{(i)}$ and $\Sigma_{n+1}^{(i)}$ correspond to the i -th iteration of Newton's algorithm. We solve the linear systems at each step with GMRES [47], to a specified relative tolerance (10^{-5} in this work) with a restart criterion of 100. To start the time integration, we set $\phi_{-1} = \phi_0$.

The codes use PetIGA, a high-performance isogeometric analysis framework [15]. The codes are in the demo section of the repository¹ and free to download.

3.4. Time adaptivity

Many processes modeled with phase-field models are controlled by different time scales as they evolve, and each regime may be orders of magnitude different from the other. Therefore, efficient numerical solutions for these problems usually involve adaptive time stepping schemes. Different strategies have already been proposed, such as the ones found in [21, 27] for the Allen–Cahn and Cahn–Hilliard equations and in [63] for the phase-field crystal equation. Even though the methods presented therein successfully decrease the computational time taken to reach steady state solutions, they still have room for considerable computational savings. In [21], a solution computed with the generalized- α method is compared against a solution obtained with the backward-Euler method. The difference between the two solutions is used as an error estimator to modify the time step size. Even

¹<https://bitbucket.org/dalcin/petiga>

though shown to be robust and used since in other works [23, 35, 39], this strategy is inefficient given that the solution must be computed twice at each time step. In [27, 63], no recovery strategies are proposed when the numerical solver fails. This implies a period of trial and error is necessary to tune the solver parameters for the specific equation being solved. In the following, we propose an adaptive time-stepping strategy for any second-order accurate time-integration scheme. In particular, our stable method. This time adaptive scheme addresses these issues and is based on the generalized- α method. The method is presented in algorithm 1.

Rather than computing the solution twice as done in [21], the solutions at t_n and t_{n-1} can be stored and used to estimate **a-posteriori** the local truncation error of a lower-order method once the solution at t_{n+1} is obtained with the second-order accurate generalized- α method (see Appendix 7.1). The estimation of the local truncation error is done through variable step-size backward differentiation. Borrowing techniques from embedded Runge-Kutta methods [28], we consider the second-order accurate generalized- α method as a high-order scheme, and the first-order backward-Euler method as a lower-order scheme. Our time-adaptive scheme is based on controlling the local truncation error for the lower-order method, i.e., the backward-Euler method. By using Taylor series expansions, it can be shown [37] that the local truncation error of the backward-Euler method is

$$\tau^{BE}(t_{n+1}) = -\frac{\Delta t^2}{2}\mathbf{U}''(t_{n+1}) + \mathcal{O}(\Delta t^3). \quad (41)$$

Given the approximate solutions $\mathbf{U}_{n+1}$, $\mathbf{U}_n$ and $\mathbf{U}_{n-1}$, at times t_{n+1} , t_n and t_{n-1} , respectively, we can express the scaled second derivative $1/2\Delta t^2\mathbf{U}''(t_{n+1})$ using the second order backward difference formula

$$\frac{\Delta t^2}{2}\mathbf{U}''(t_{n+1}) = \frac{1}{\eta}\mathbf{U}_{n+1} - \frac{1}{\eta-1}\mathbf{U}_n + \frac{1}{\eta(\eta-1)}\mathbf{U}_{n-1} + \mathcal{O}(\Delta t^3), \quad (42)$$

where $\eta = (\Delta t + \Delta t_p)/\Delta t = 1 + \Delta t_p/\Delta t$, $\Delta t = t_{n+1} - t_n$ and $\Delta t_p = t_n - t_{n-1}$.

From equations (41)-(42) the truncation error can be conveniently estimated as

$$\mathbf{E}_{n+1} = -\frac{1}{\eta}\mathbf{U}_{n+1} + \frac{1}{\eta-1}\mathbf{U}_n - \frac{1}{\eta(\eta-1)}\mathbf{U}_{n-1} \approx \tau^{BE}(t_{n+1}).$$

Then, we can calculate a weighted local truncation error (WLTE) [28, equation 4.11] as

$$\text{WLTE} = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{E_i}{\tau_i^{\text{abs}} + \tau_i^{\text{rel}} \max(|U_i|, |U_i + E_i|)} \right)^2}, \quad (43)$$

where $E_i = (\mathbf{E}_{n+1})_i$, $U_i = (\mathbf{U}_{n+1})_i$, τ_i^{abs} and τ_i^{rel} define tunable absolute and relative tolerances, respectively. The WLTE can be used to control the error at each time step. **By definition, values of WLTE smaller or equal to one mean that the local truncation error is within the user-prescribed tolerances; the step just taken can thus be accepted and the time integration can move forward with either the same or a larger time step size. On the contrary, values of WLTE larger than one imply unacceptable errors; the step taken should be rejected and retaken with a smaller time step size. No matter the outcome, either step acceptance or rejection, the updating procedure of the time step size is the same and given by**

$$\Delta t_{\text{next}} = \rho \text{WLTE}^{-1/2} \Delta t,$$

with ρ a safety factor. The default values for the safety factor ρ , the absolute and relative tolerances τ_i^{abs} and τ_i^{rel} are set to 0.9, 10^{-4} and 10^{-4} , respectively.

An initial time derivative $\mathbf{V}_0$ needs to be provided given the non-self-starting nature of the algorithm. By using a finite difference strategy, a reasonable initial time derivative can be estimated (i.e., $\mathcal{O}(\Delta t^2)$). To do this, the backward-Euler method on the system $\frac{d\mathbf{U}}{dt} = F(t, \mathbf{U})$ is used to estimate the value $\mathbf{U}_{1/2}^*$ at time $t_{1/2} = t_0 + 1/2\Delta t$

$$\frac{\mathbf{U}_{1/2}^* - \mathbf{U}_0}{\Delta t/2} = F(\Delta t/2, \mathbf{U}_{1/2}^*).$$

Using the approximation to $\mathbf{U}_{1/2}^*$, a second backward-Euler solve is done to get the value $\mathbf{U}_1^*$ at time $t_1 = t_0 + \Delta t$

$$\frac{\mathbf{U}_1^* - \mathbf{U}_{1/2}^*}{\Delta t/2} = F(\Delta t, \mathbf{U}_1^*).$$

Given $\mathbf{U}_0$, $\mathbf{U}_{1/2}^*$, $\mathbf{U}_1^*$, the initial time derivative can be approximated as

$$\mathbf{V}_0 = \frac{1}{\Delta t} (-3\mathbf{U}_0 + 4\mathbf{U}_{1/2}^* - \mathbf{U}_1^*). \quad (44)$$

Now, given a solution $\mathbf{U}_0$ at time t_0 , it is possible to compute a solution $\mathbf{U}_1^\alpha$ at $t_1 = t_0 + \Delta t$ using the standard generalized- α method [34] for first-order systems.

Algorithm 1 Pseudocode for adaptive time-stepping.

$k_{\max} = 10$, $k_{\min} = 0.1$, $\rho = 0.9$.

```

1: Compute solution  $\mathbf{U}_{n+1}^\alpha$  using  $\Delta t$  and the generalized- $\alpha$  method
2: if nonlinear solve failed to converge then
3:    $k = 0.25$ , update time step size  $\Delta t \leftarrow k\Delta t$ 
4:   goto 1
5: end if
6: Calculate local truncation error  $\mathbf{E}_{n+1}$  using equation (41)
7: Calculate WLTE using equation (43)
8: Compute  $k_{lte} = \rho \text{WLTE}^{-1/2}$ 
9: Set  $k = \max(k_{\min}, \min(k_{lte}, k_{\max}))$ 
10: if WLTE > 1 then
11:   Reject step, update time step size  $\Delta t \leftarrow k\Delta t$ 
12:   goto 1
13: end if
14: Accept step, update time step size  $\Delta t \leftarrow k\Delta t$ 

```

The same strategy developed here for the generalized- α method can be applied to any second-order accurate scheme, and, in particular, the method we propose in section 2.2.

4. Phase-field models

In this section, we focus on four phase-field models that have had considerable success in modeling different phenomena [17, 18, 45]. These are the Allen–Cahn [2], the Cahn–Hilliard [7], the Swift–Hohenberg [51] and the phase-field crystal [16] equations. The Allen–Cahn and Cahn–Hilliard equations, two of the most successful phase-field models to date, are derived as gradient flows of the same free energy functional [27]. The same statement can be made regarding the Swift–Hohenberg and the phase-field crystal equation, which are also derived from the same free energy functional.

These equations were selected because their stable time integration has garnered considerable interest in recent years [23, 24, 52, 54], and this work generalizes some of the numerical schemes that have been put forth in the

context of the Cahn-Hilliard [27, 36] and phase-field crystal equations [54]. Additionally, the discretization in space is done using isogeometric analysis [13], which allows to easily generate high-order and globally continuous basis functions. Given the higher-order nature of the equations and the complicated geometries that can arise in phase-field problems [20], a finite element discretization with improved geometrical properties [31] which allows for a straightforward discretization of the high-order differential operators, seems to be a flexible and robust choice among the myriad of methods available.

4.1. The Allen-Cahn equation

The Allen-Cahn equation governs the behavior of the Ising ferromagnet [44], where the competition between energy and entropy gives way to a phase transition below some critical temperature [2]. The free energy functional for the system is given by

$$\mathcal{F}_{AC} = \int_{\Omega} \left(\Psi_{AC} + \frac{1}{2} |\nabla \phi|^2 \right) d\Omega,$$

where $\Psi_{AC} = \frac{1}{4\epsilon^2} (\phi^2 - 1)^2$ and ϵ is a parameter related to interface thickness. The phase-field parameter is related to the ordering of the phase, which translates to it being a non-conserved quantity. The partial differential equation that describes this order-disorder transition is given by

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -\sigma, \\ \sigma &= \Psi'_{AC}(\phi) - \Delta \phi, \end{aligned}$$

where a constant mobility of value one is considered. The weak formulation, following equations (17)-(18), is given by

$$0 = \left(w, \frac{\partial \phi}{\partial t} + \sigma \right)_{\Omega}, \quad (45)$$

$$0 = (q, \sigma - \Psi'_{AC}(\phi))_{\Omega} - (\nabla w, \nabla \phi)_{\Omega}. \quad (46)$$

The time discretization, using the stable scheme proposed in section 2.2, becomes

$$\begin{aligned} 0 &= \left(w, \frac{\partial \phi}{\partial t} + \sigma \right)_{\Omega}, \\ 0 &= (q, \sigma - \tilde{\Psi}'_{AC}(\phi))_{\Omega} - (\nabla w, \nabla \{\phi\})_{\Omega}. \end{aligned}$$

4.2. The Cahn–Hilliard equation

The Cahn–Hilliard equation governs the evolution of an immiscible binary mixture undergoing phase separation [7]. This is the equation that popularized the use of the phase-field method [45]. In this equation, the phase field represents the concentration of one of the components of the mixture. The dimensionless free energy functional is given by

$$\begin{aligned}\mathcal{F}_{CH} &= \mathcal{F}_{AC} \\ &= \int_{\Omega} \left(\Psi_{CH} + \frac{1}{2} |\nabla \phi|^2 \right) d\Omega\end{aligned}\quad (47)$$

where $\Psi_{CH} = \frac{1}{4\epsilon^2} (\phi^2 - 1)^2$. The parameter ϵ is related to the thickness of the interface. The partial differential equation, given that the phase-field is in this case a conserved quantity, is given by

$$\begin{aligned}\frac{\partial \phi}{\partial t} &= \nabla \cdot (M_{CH} \nabla \sigma), \\ \sigma &= \Psi'_{CH}(\phi) - \Delta \phi,\end{aligned}$$

with $M_{CH} = \bar{M} (1 - \phi^2)$. The variational formulation is then given by

$$0 = \left(w, \frac{\partial \phi}{\partial t} \right)_{\Omega} + (\nabla w, M_{CH} \nabla \sigma)_{\Omega}, \quad (48)$$

$$0 = (q, \sigma - \Psi'_{CH}(\phi))_{\Omega} - (\nabla w, \nabla \phi)_{\Omega}. \quad (49)$$

The time discretization, using the stable scheme proposed, becomes

$$\begin{aligned}0 &= \left(w, \frac{\partial \phi}{\partial t} \right)_{\Omega} + (\nabla w, M_{CH} \nabla \sigma)_{\Omega}, \\ 0 &= (q, \sigma - \tilde{\Psi}'_{CH}(\phi))_{\Omega} - (\nabla w, \nabla \{\phi\})_{\Omega},\end{aligned}$$

where the nonlinear mobility M_{CH} is defined using equation (5).

Remark 4. *The discretization can introduce numerical error that makes the phase-field take values outside of a physically relevant range for the Cahn–Hilliard equation [11], i.e., $\phi \in \left[-\sqrt{a_2/a_4}, \sqrt{a_2/a_4} \right]$. This issue is simply addressed by setting the mobility to zero as done through equation 5.*

4.3. The Swift–Hohenberg equation

The Swift–Hohenberg equation is derived from a phenomenon known as Rayleigh–Bénard convection, in which a fluid is trapped between a hot and a cold plate. The equation describes a convective instability, which occurs when the difference in temperature between the plates becomes large enough. The Swift–Hohenberg equation, a fourth order, nonlinear partial differential equation, is derived as a gradient flow of the dimensionless free energy functional $\mathcal{F}_{SH}$ defined by [24, 51]

$$\mathcal{F}_{SH} = \int_{\Omega} \left[\frac{1}{2} (\phi^2 - 2|\nabla\phi|^2 + (\Delta\phi)^2) + \Psi_{SH}(\phi) \right] d\Omega, \quad (50)$$

where $\Psi_{SH}(\phi) = -\frac{\epsilon}{2}\phi^2 + \frac{1}{4}\phi^4$. Using equations (4), (12), (13) along with the definition of free energy given by equation (50) defines the evolution in time of ϕ

$$\frac{\partial\phi}{\partial t} = -\sigma, \quad (51)$$

$$\sigma = (1 + \Delta)^2 \phi + \Psi'_{SH}(\phi), \quad (52)$$

where $M_{SH} = \bar{M}_{SH} = 1$, $(1 + \Delta)^2 = 1 + 2\Delta + \Delta\Delta$, Ψ'_{SH} is defined as $\Psi'_{SH}(\phi) = \frac{\partial\Psi(\phi)}{\partial\phi} = \phi^3 - \epsilon\phi$, as well as the fact that the order parameter ϕ is not a conserved quantity in the case of this equation such that $a = 0$. The corresponding weak form, following equations (17)-(18), is given by

$$0 = \left(w, \frac{\partial\phi}{\partial t} + \sigma \right)_{\Omega}, \quad (53)$$

$$0 = (q, \sigma - \phi - \Psi'_{SH}(\phi))_{\Omega} + 2(\nabla w, \nabla\phi)_{\Omega} - (\Delta w, \Delta\phi)_{\Omega}. \quad (54)$$

The time discretization, following section 2.2, is given by

$$0 = \left(w, \frac{[\phi]}{\Delta t} + \sigma \right)_{\Omega},$$

$$0 = (q, \sigma - \{\phi\} - \tilde{\Psi}'_{SH})_{\Omega} + 2(\nabla q, \nabla\{\phi\})_{\Omega} - (\Delta q, \Delta\{\phi\})_{\Omega}.$$

where $\tilde{\Psi}'_{SH}$ represents an approximation to $\Psi'_{SH}(\phi)$, as defined in equation (11).

4.4. The phase-field crystal equation

The phase-field crystal equation is used to model the evolution of microstructures at atomistic length scales and diffusive time scales. It is a sixth-order, nonlinear partial differential equation. It can be derived by considering a conservative description of the Rayleigh–Bénard convection problem [16, 45]. It uses the same dimensionless free energy functional as the Swift–Hohenberg equation, such that

$$\begin{aligned}\mathcal{F}_{PFC} &= \mathcal{F}_{SH} \\ &= \int_{\Omega} \left[\frac{1}{2} (\phi^2 - 2|\nabla\phi|^2 + (\Delta\phi)^2) + \Psi_{PFC}(\phi) \right] d\Omega,\end{aligned}$$

with $\Psi_{PFC}(\phi) = -\frac{\epsilon}{2}\phi^2 + \frac{1}{4}\phi^4$. The evolution equation of the phase field ϕ , which now represents an atomistic density field that is a conserved quantity, is given by

$$\begin{aligned}\frac{\partial\phi}{\partial t} &= \Delta\sigma, \\ \sigma &= (1 + \Delta)^2 \phi + \Psi'_{PFC}(\phi),\end{aligned}$$

where the mobility $M = 1$. This leads to the variational formulation

$$0 = \left(w, \frac{\partial\phi}{\partial t} \right)_{\Omega} + (\nabla w, \nabla\sigma)_{\Omega}, \quad (55)$$

$$0 = (q, \sigma - \phi - \Psi'_{PFC}(\phi))_{\Omega} + 2(\nabla q, \nabla\phi)_{\Omega} - (\Delta q, \Delta\phi)_{\Omega}. \quad (56)$$

with a time discretization given by

$$\begin{aligned}0 &= \left(w, \frac{[\phi]}{\Delta t} \right)_{\Omega} + (\nabla w, \nabla\sigma)_{\Omega}, \\ 0 &= (q, \sigma - \{\phi\} - \tilde{\Psi}'_{PFC})_{\Omega} + 2(\nabla q, \nabla\{\phi\})_{\Omega} - (\Delta q, \Delta\{\phi\})_{\Omega}.\end{aligned}$$

5. Numerical examples

In this section, we study the temporal approximation properties of the algorithms resulting from the implicit expansion of Ψ' presented in section 2.2. We compare it with state-of-the-art algorithms developed by Gomez et al. for

Table 1: Summary of section 4 phase-field models within the context of equations (9) and (10).

Eq.	M	$\Psi = \frac{1}{4}a_0 - \frac{1}{2}a_2\phi^2 + \frac{1}{4}a_4\phi^4$	ϵ	f	Mass conservation
AC	1	$a_0 = a_2 = a_4 = \frac{1}{\epsilon^2}$	0.01	$\frac{1}{2} \nabla\phi ^2$	No ($a = 0$)
CH	$\frac{1}{2}(1-\phi^2)$	$a_0 = a_2 = a_4 = \frac{1}{\epsilon^2}$	0.03	$\frac{1}{2} \nabla\phi ^2$	Yes ($a = 1$)
SH	1	$a_0 = 0, a_2 = \epsilon, a_4 = 1$	2	$\frac{1}{2}(\phi^2 - 2 \nabla\phi ^2 + (\Delta\phi)^2)$	No ($a = 0$)
PFC	1	$a_0 = 0, a_2 = \epsilon, a_4 = 1$	0.325	$\frac{1}{2}(\phi^2 - 2 \nabla\phi ^2 + (\Delta\phi)^2)$	Yes ($a = 1$)

the equations presented in section 4, as well as the backward-Euler scheme and the generalized- α method [34] (using a spectral radius $\rho_\infty = 0.5$). As previously mentioned, the spatial discretization is done using isogeometric analysis, which generates the non-standard basis functions needed in the case of the Swift–Hohenberg and phase-field crystal equations. The parameters for the equations that are solved are summarized in table 1.

To focus on temporal error only, we use a uniform mesh with $[512]^2\mathcal{C}^1$ quadratic elements. This is an overkill spatial resolution for the examples solved in this work [23, 24, 38, 54]. An exception is made with regards to the Cahn–Hilliard equation, which uses $[64]^2\mathcal{C}^1$ -quadratic elements, as the degenerate mobility increases the non-linearity of the system considerably. The nonlinear system within each time step requires a time step size on the order of $\Delta t = \mathcal{O}(10^{-10})$ to converge with the fine mesh (i.e., $[512]^2\mathcal{C}^1$ quadratic elements).

The initial conditions specified in the following are only defined for ϕ , not for the auxiliary variable σ presented through equation (13). To correctly initialize σ , a nonlinear L_2 projection is performed to solve equation (35), the semidiscrete version of equation (13).

5.1. Allen–Cahn equation

We simulate the evolution of a star-shaped interface in a curvature-driven flow [38]. The initial condition is given by

$$\phi_{\text{star}}(\mathbf{x}) = \tanh\left(\frac{1/4 + 0.1\cos(7\theta) - \sqrt{(x-0.5)^2 + (y-0.5)^2}}{(3/4)\sqrt{2}}\right), \quad (57)$$

where x and y represent Cartesian coordinates, θ is defined as

$$\theta = \begin{cases} \tan^{-1} \left(\frac{y - 0.5}{x - 0.5} \right) & \text{if } x > 0.5, \\ \pi + \tan^{-1} \left(\frac{y - 0.5}{x - 0.5} \right) & \text{otherwise,} \end{cases}$$

The computational domain is the unit square $\bar{\Omega} = [0, 1]^2$, and no-flux boundary conditions are imposed. For the spatial discretization, we use a uniform mesh of $[512]^2$ - $\mathcal{C}^1$ -quadratic elements. The initial condition is shown in figure 1, along with snapshots of the solution calculated with an overkill temporal resolution ($\Delta t = 10^{-7}$). The tips of the star move inward, while the gaps between the tips move outward. Once the surface becomes circular, the radius of the circle shrinks with increasing speed due to the increasing curvature.

To evaluate the performance of the scheme developed in this work, we compare the provably-stable implicit (Implicit) expansion against the backward-Euler method (BE), the generalized- α method (Generalized- α) and a second-order, provably-stable, state-of-the-art algorithm of Gomez et al. adapted from [24] to solve the Allen–Cahn equation. The temporal integration scheme is applied to the variational formulation presented in equations (45)-(46). The fully discrete formulation for the provably-stable method can be defined as: given ϕ_n^h, σ_n^h , find $\phi_{n+1}^h, \sigma_{n+1}^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$0 = \left(w^h, \frac{[\![\phi]\!]}{\Delta t} \right)_{\Omega} + \left(w^h, \sigma_{n+1}^h \right)_{\Omega}, \quad (58)$$

$$0 = \left(q^h, \sigma_{n+1}^h - \tilde{\Psi}' \right)_{\Omega} - \left(\nabla q^h, \nabla \{\phi\} \right)_{\Omega}, \quad (59)$$

where

- the implicit expansion scheme is recovered with

$$\tilde{\Psi}' = \Psi'_{n+1} - \Psi''_{n+1} \frac{[\![\phi]\!]}{2} + \Psi'''_{n+1} \frac{[\![\phi]\!]^2}{6},$$

- the scheme by Gomez et al. [24] is recovered with

$$\tilde{\Psi}' = \frac{1}{2} (\Psi'_n + \Psi'_{n+1}) - \Psi'''_n \frac{[\![\phi]\!]^2}{12}.$$

Figure 1: Evolution of a star-shaped interface in a curvature-driven flow using the Allen-Cahn equation. The initial condition prescribed by equation (57) is shown, as well as the solution evolution calculated with our implicit algorithm. The simulation is run in a unit square domain $\Omega = [0, 1]^2$ using a computational mesh composed of 512×512 C^1 -quadratic elements, with a time step size $\Delta t = 10^{-7}$. We consider this our reference solution.

The function Ψ is defined in equation (3) with the coefficients given in row AC of table 1. The solution evolution is shown in figure 2 with time step size $\Delta t = 10^{-4}$. In the figure, rows correspond to a particular method (indicated in the leftmost column) while columns indicate the moment in time at which the solution snapshots are taken. Free energy evolutions are plotted in figures 3a-3c. The only discernible difference between the simulations is observed with the backward-Euler method, which seems to reach the circular state faster. Even though counter intuitive, as the scheme is first order accurate in nature, this behavior can be explained by the inherent numerical dissipation introduced by the method. Simulations were also run for $\Delta t = 10^{-5}$ and $\Delta t = 10^{-6}$, but the snapshots are not shown: this example converges by $\Delta t = 10^{-5}$, confirmed by the free energy evolution seen in figure 3b. The computed solutions respect the energy stability property of the Allen–Cahn equation, namely,

$$\mathcal{F}_{AC} \leq 0.$$

All the second-order accurate methods follow the same behavior for the time step sizes studied, seemingly making the stable methods the better options given that they guarantee the monotonic decrease of free energy.

Figure 2: Evolution of a star-shaped interface in a curvature-driven flow. The simulation is run in a unit square domain $\bar{\Omega} = [0, 1]$ using a computational mesh composed of 512×512 $\mathcal{C}^1$ -quadratic elements, with a time step size $\Delta t = 10^{-4}$.

(a) $\Delta t = 10^{-6}$

(b) $\Delta t = 10^{-5}$

(c) $\Delta t = 10^{-4}$

Figure 3: Free energy evolution comparison for the different methods analyzed to solve the Allen-Cahn equation.

5.2. Cahn–Hilliard equation

The phase-separation process we simulate with the Cahn–Hilliard equation starts from the initial condition

$$\phi(\mathbf{x}) = \bar{\phi} + r,$$

where $\bar{\phi} = 0.5$ and r is a random variable with uniform distribution in $[-0.01, 0.01]$. Periodic boundary conditions are considered in both directions, in a unit square domain $\bar{\Omega} = [0, 1]^2$. The uniform mesh uses $[64]^2$ - $\mathcal{C}^1$ -quadratic elements. The initial condition is shown in figure 4a, and represents a mixture which is unstable under those conditions [21]. The reference evolution of the phase is shown in figures 4b through 4d. The mixture goes through an initial spinodal decomposition, which results in two coexisting phases being formed, and is followed by coarsening in later stages, whereby the two distinct phases grow with time to decrease the total interfacial area. The final state is reached when the phase separation is complete: a single bubble remains immersed within the other phase (4d). This solution minimizes the interfacial area for the average concentration proposed, a requirement stemming from the free energy functional $\mathcal{F}_{CH}$ (see equation (47)).

The performance of our provably-stable time-stepping algorithms is once again compared with (BE) and (Generalized- α), as well as the second-order, provably-stable, state-of-the-art algorithm presented in [23] by Gomez et al.. The temporal integration schemes are applied to the variational formulation presented in equations (48)–(49). The state-of-the-art algorithm we compare against [23] can be reinterpreted as a stabilized scheme. **That is, this method can be stated as, given ϕ_n^h, σ_n^h , find $\phi_{n+1}^h, \sigma_{n+1}^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$**

$$\begin{aligned} 0 &= \left(w^h, \frac{[\![\phi]\!]}{\Delta t} \right)_{\Omega} + \left(\nabla w^h, M(\phi_{n+\alpha}^h) \nabla \sigma_{n+1}^h \right)_{\Omega}, \\ 0 &= \left(q^h, \sigma_{n+1}^h - \frac{1}{2} (\Psi'_n + \Psi'_{n+1}) + \Psi''_n \frac{[\![\phi]\!]^2}{12} \right)_{\Omega} - \left(\nabla q^h, \nabla \phi_{n+\alpha}^h \right)_{\Omega}. \end{aligned}$$

where

$$\phi_{n+\alpha}^h = \phi_n^h + \alpha [\![\phi]\!], \quad (60)$$

$$\alpha = \frac{1}{2} + \frac{1}{2} \tanh \left(\frac{\Delta t}{C \epsilon^2} \right), \quad (61)$$

$$C = 10^3. \quad (62)$$

Figure 4: Spinodal decomposition using the Cahn-Hilliard equation. System evolves from a randomly perturbed initial condition that results in a single bubble at steady state. This solution minimizes the surface area of the interface. The unit square domain considered, $\bar{\Omega} = [0, 1]^2$, is meshed using $[64]^2 \mathcal{C}^1$ -quadratic elements. The solution evolution is calculated with our implicit algorithm, with a time step size $\Delta t = 10^{-7}$. We consider this our reference solution.

Substituting equations (61) and (62) in equation (60), we have that

$$\begin{aligned}\phi_{n+\alpha}^h &= \phi_n^h + \alpha \llbracket \phi \rrbracket, \\ &= \{\phi\} + \frac{1}{2} \tanh\left(\frac{\Delta t}{10^3 \epsilon^2}\right) \llbracket \phi \rrbracket.\end{aligned}\quad (63)$$

Using equation (63), the fully discrete formulations for the provably-stable methods to solve the Cahn–Hilliard equation can now be expressed as: given ϕ_n^h, σ_n^h , find $\phi_{n+1}^h, \sigma_{n+1}^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$\begin{aligned}0 &= \left(w^h, \frac{\llbracket \phi \rrbracket}{\Delta t}\right)_\Omega + \left(\nabla w^h, M_{CH} \nabla \sigma_{n+1}^h\right)_\Omega, \\ 0 &= \left(q^h, \sigma_{n+1}^h - \tilde{\Psi}'\right)_\Omega - \left(\nabla q^h, \nabla \{\phi\}\right)_\Omega - \alpha_{CH} \left(\nabla q^h, \nabla \llbracket \phi \rrbracket\right)_\Omega,\end{aligned}$$

where

- the implicit expansion scheme is recovered with

$$M_{CH} = M(\{\phi\}), \quad \tilde{\Psi}' = \Psi'_{n+1} - \Psi''_{n+1} \frac{\llbracket \phi \rrbracket}{2} + \Psi'''_{n+1} \frac{\llbracket \phi \rrbracket^2}{6}, \quad \alpha_{CH} = 0,$$

- the scheme by Gomez et al. [23] is recovered with

$$\begin{aligned}M_{CH} &= M\left(\{\phi\} + \frac{1}{2} \tanh\left(\frac{\Delta t}{C \epsilon^2}\right)\right), \quad C = 1000, \\ \tilde{\Psi}' &= \frac{1}{2} (\Psi'_n + \Psi'_{n+1}) - \Psi'''_n \frac{\llbracket \phi \rrbracket^2}{12}, \quad \alpha_{CH} = \frac{1}{2} \tanh\left(\frac{\Delta t}{C \epsilon^2}\right).\end{aligned}\quad (64)$$

The value of the constant C can be tuned to either increase the accuracy or the robustness of the method [23]. The function Ψ is defined in equation (3) with the coefficients given in row CH of table 1.

The solution evolution with the different methods considered is shown in figure 5 with time step size $\Delta t = 10^{-5}$. Free energy evolutions are shown in figure 6. All methods seem to be converged at $\Delta t = 5 \times 10^{-6}$. None of the methods present free energy increases.

Figure 5: Evolution of the concentration ϕ from a randomly perturbed initial condition. The simulation is run in a unit square domain $\bar{\Omega} = [0, 1]^2$ using a computational mesh comprised of 64×64 C^1 -quadratic elements, with a time step size $\Delta t = 10^{-5}$.

(a) $\Delta t = 10^{-6}$

(b) $\Delta t = 5 \times 10^{-6}$

(c) $\Delta t = 10^{-5}$

Figure 6: Free energy evolution comparison for the different methods analyzed to solve the Cahn–Hilliard equation.

5.3. Swift–Hohenberg equation

For this example, we modify an initial condition found in [24] that can be used to study pattern formation. Initially, a curvy horizontal stripe is embedded into a constant state. A square domain $\bar{\Omega} = [0, 40]^2$ is used, and we mesh it uniformly with $[512]^2$ - $\mathcal{C}^1$ -quadratic elements. The stripes are created using two sinusoidal waves defined by

$$\begin{aligned} C_1(\mathbf{x}) &= \sin\left(\frac{2\pi}{40}4x + 19\right), \\ C_2(\mathbf{x}) &= -\sin\left(\frac{2\pi}{40}5x + 21\right). \end{aligned}$$

The phase field variable initially takes a value equal to one within the space created by the two stripes, and a value of minus one outside of it. To create a smooth interface between these two values, a rescaled Gaussian function is used, which leads to the initial condition

$$\phi_0 = \begin{cases} 1 & \text{if } C_1 < y < C_2, \\ 2 \exp\left(-\frac{(y - C_1)^2}{2\nu}\right) - 1 & \text{if } y < C_1, \\ 2 \exp\left(-\frac{(y - C_2)^2}{2\nu}\right) - 1 & \text{if } y > C_2, \end{cases}$$

with $\nu = 4$. To avoid oscillations generated by the projection of ϕ and ensure the monotonic behavior of the phase field, we use a mass lumping technique [64]. This procedure also avoids spurious oscillations generated by the temporal integration schemes encountered in [24] for large time step sizes. The initial condition is shown in 7a, and snapshots of the phase field ϕ at three instances in time can be seen in figures 7b, 7c and 7d. The pattern evolves developing vertical fingers that can bifurcate.

The performance of our provably-stable time-stepping algorithm is once again compared against (BE) and (Generalized- α), as well as the second-order, provably-stable, state-of-the-art algorithm presented by Gomez et al. in [24]. The temporal integration schemes are applied to the variational formulation presented in equations (53)-(54). The fully discrete formulations for the provably-stable methods to solve the Swift–Hohenberg equation can

Figure 7: Pattern formation using the Swift-Hohenberg equation. System evolves from a curvy stripe embedded into a constant state. The pattern develops vertical fingers that can bifurcate throughout the evolution. The square domain considered, $\bar{\Omega} = [0, 40]^2$, is uniformly meshed using $[512]^2 \mathcal{C}^1$ -quadratic elements. The boundary conditions are periodic. The solution evolution is calculated with our implicit algorithm, with a time step size $\Delta t = 10^{-2}$. We consider this our reference solution.

be defined as: given ϕ_n^h, σ_n^h , find $\phi_{n+1}^h, \sigma_{n+1}^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$\begin{aligned} 0 &= \left(w^h, \frac{[\![\phi]\!]}{\Delta t} \right)_{\Omega} + \left(w^h, \sigma_{n+1}^h \right)_{\Omega}, \\ 0 &= \left(q^h, \sigma_{n+1}^h - \tilde{\Psi}' \right)_{\Omega} - 2 \left(\nabla q^h, \nabla \{\phi\} \right)_{\Omega} + \left(\Delta q^h, \Delta \{\phi\} \right)_{\Omega}, \end{aligned}$$

- the implicit expansion scheme is recovered with

$$\tilde{\Psi}' = \Psi'_{n+1} - \Psi''_{n+1} \frac{[\![\phi]\!]}{2} + \Psi'''_{n+1} \frac{[\![\phi]\!]^2}{6},$$

- the scheme by Gomez et al. [24] is recovered with

$$\tilde{\Psi}' = \frac{1}{2} (\Psi'_n + \Psi'_{n+1}) - \Psi'''_n \frac{[\![\phi]\!]^2}{12}.$$

The function Ψ is defined in equation (3) with the coefficients given in row SH of table 1. Snapshots of the phase field ϕ calculated with the different methods and time step sizes $\Delta t = 0.1, 1$, are shown in figures 8 and 9, respectively. The free energy evolutions for $\Delta t = 0.1, 0.5$ and 1, respectively, are plotted in figures 10a, 10b and 10c. **The overestimation of the dissipation rate** is observed in the case of the backward-Euler method, which shows more dissipation of the free energy **as Δt increases**. The solver breaks-down for the case of backward-Euler with $\Delta t = 1$.

Figure 8: Pattern formation using the Swift-Hohenberg equation. The simulation is run in a square domain $\bar{\Omega} = [0, 40]^2$ using a computational mesh comprised of 512×512 C^1 -quadratic elements, periodic boundary conditions along both directions, with a time step size $\Delta t = 0.1$.

Figure 9: Pattern formation using the Swift-Hohenberg equation. The simulation is run in a square domain $\Omega = [0, 40]^2$ using a computational mesh comprised of 512×512 C^1 -quadratic elements, periodic boundary conditions along both directions, with a time step size $\Delta t = 1$.

(a) $\Delta t = 0.1$

(b) $\Delta t = 0.5$

(c) $\Delta t = 1$

Figure 10: Free energy evolution comparison for the different methods analyzed to solve the Swift–Hohenberg equation. The case for backward-Euler with $\Delta t = 1$ is not shown as the solver broke down.

5.4. Phase-field crystal equation

We simulate the two-dimensional growth of a crystal in a supercooled liquid, using a one-mode approximation for the density profile of the crystalline structure [54]. We use a triangular configuration, defined by

$$\phi_S(\mathbf{x}) = \cos\left(\frac{q}{\sqrt{3}}y\right) \cos(qx) - \frac{1}{2}\cos\left(\frac{2q}{\sqrt{3}}y\right), \quad (65)$$

where q represents a wavelength related to the lattice constant [45], and x and y represent the Cartesian coordinates. A solid crystallite is initially placed in the center of a liquid domain, which is assigned an average density $\bar{\phi}$. The initial condition becomes

$$\phi_0(\mathbf{x}) = \bar{\phi} + \omega(\mathbf{x})(A\phi_S(\mathbf{x})), \quad (66)$$

where A represents an amplitude of the fluctuations in density, and the scaling function $\omega(\mathbf{x})$ is defined as

$$\omega(\mathbf{x}) = \begin{cases} \left(1 - \left(\frac{\|\mathbf{x} - \mathbf{x}_0\|}{d_0}\right)^2\right)^2 & \text{if } \|\mathbf{x} - \mathbf{x}_0\| \leq d_0, \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathbf{x}_0$ is the coordinate of the center of the domain, and d_0 is $1/6$ of the domain length in the x -direction. In order to avoid mismatches on the boundaries when the grain boundaries meet, the computational domain $\bar{\Omega}$ is dimensioned in such a way as to make it periodic along both directions. To do this while keeping the problem within a reasonable size, we use the frequency present in equation (65) to define the domain $\bar{\Omega}$ as

$$\bar{\Omega} = \left[0, \frac{2\pi}{q}a\right] \times \left[0, \frac{\sqrt{3}\pi}{q}b\right],$$

where a and b are assigned values of 10 and 12, respectively. These numbers make the domain almost square. The number of elements in the y -direction, N_y , is then defined as

$$N_y = \left\lfloor \frac{b\sqrt{3}}{2a}N_x + \frac{1}{2} \right\rfloor,$$

where N_x represents the number of elements in the x -direction. This adjustment is made to account for the difference in length between both directions, and to have the element size h in both directions be approximately equal. The variables q and A are assigned their corresponding equilibrium values, obtained by minimizing the free energy presented in table 1, with respect to both A and q , while using the approximation of equation (65) to define the atomistic density. For the results presented in this example, the values used are

$$\epsilon = 0.325, \quad \bar{\phi} = \frac{\sqrt{\epsilon}}{2}, \quad A = \frac{4}{5} \left(\bar{\phi} + \frac{\sqrt{15\epsilon - 36\bar{\phi}^2}}{3} \right), \quad q = \frac{\sqrt{3}}{2}.$$

The parameter ϵ is chosen such that the triangular structure is stable [33, 45]. The initial crystallite placed in the center of the domain grows at the expense of the supercooled liquid. This is enforced by the degree of undercooling ϵ .

The performance of our provably-stable time-stepping algorithms is once again compared against (BE) and (Generalized- α), as well as the second-order, provably-stable, state-of-the-art algorithm presented by Gomez et al. in [25]. The temporal integration schemes are applied to the variational formulation presented in equations (55)-(56). The fully discrete formulations for the provably-stable methods to solve the phase-field crystal equation can be defined as: given ϕ_n^h, σ_n^h , find $\phi_{n+1}^h, \sigma_{n+1}^h$ such that for all $w^h, q^h \in \mathcal{V}_2^h$

$$\begin{aligned} 0 &= \left(w, \frac{\partial \phi}{\partial t} \right)_{\Omega} + (\nabla w, \nabla \sigma)_{\Omega}, \\ 0 &= (q, \sigma - \phi - \tilde{\Psi}')_{\Omega} + 2(\nabla q^h, \nabla \phi)_{\Omega} - (\Delta q^h, \Delta \phi)_{\Omega}. \end{aligned}$$

- the implicit expansion scheme is recovered with

$$\tilde{\Psi}' = \Psi'_{n+1} - \Psi''_{n+1} \frac{[\phi]}{2} + \Psi'''_{n+1} \frac{[\phi]^2}{6},$$

- the scheme by Gomez et al. [25] is recovered with

$$\tilde{\Psi}' = \frac{1}{2} (\Psi'_n + \Psi'_{n+1}) - \Psi'''_n \frac{[\phi]^2}{12},$$

The function Ψ is defined in equation (3) with the coefficients given in row PFC of table 1. The simulations with the different temporal schemes are

shown in figures 12 and 13, for time step sizes $\Delta t = 0.1$ and 1, respectively. Free energy evolutions are shown in figure 14. This example follows the same trend as the one shown for the Swift–Hohenberg equation, with the backward-Euler method dissipating more free energy with the increase in time step size than the other schemes.

5.5. Methods: comparison and performance

The cases studied show similar features. The backward-Euler method is the first to break down in every case with the increase in time step size. Another feature that is worthwhile pointing out involves the striking resemblance between the implicit method and the state-of-the-art methods developed in [23–25]. This can be explained by analyzing the structure of the approximation proposed for Ψ' in equation (64). Recalling equation (24) and using the Lagrange remainder, the terms Ψ'_n and Ψ'''_n can be rewritten as

$$\Psi'_n = \Psi'_{n+1} - \Psi''_{n+1} \llbracket \phi \rrbracket + \Psi'''_{n+1} \frac{\llbracket \phi \rrbracket^2}{2} - \Psi_{n+\epsilon_3}^{(4)} \frac{\llbracket \phi \rrbracket^3}{6}, \quad (67)$$

$$\Psi'''_n = \Psi'''_{n+1} - \Psi_{n+\epsilon_4}^{(4)} \llbracket \phi \rrbracket, \quad (68)$$

where $\epsilon_3, \epsilon_4 \in [0, 1]$. Realizing that $\Psi_{n+\epsilon_3}^{(4)} = \Psi_{n+\epsilon_4}^{(4)} = \Psi_{n+1}^{(4)} = \Psi^{(4)}$, and substituting equations (67)–(68) in (64) results in

$$\begin{aligned} \tilde{\Psi}' &= \Psi'_{n+1} + \left(-\Psi''_{n+1} \frac{\llbracket \phi \rrbracket}{2} + \Psi'''_{n+1} \frac{\llbracket \phi \rrbracket^2}{4} - \Psi^{(4)} \frac{\llbracket \phi \rrbracket^3}{12} \right) \\ &\quad - \left(\Psi'''_{n+1} \frac{\llbracket \phi \rrbracket^2}{12} - \Psi^{(4)} \frac{\llbracket \phi \rrbracket^3}{12} \right), \\ &= \Psi'_{n+1} - \Psi''_{n+1} \frac{\llbracket \phi \rrbracket}{2} + \Psi'''_{n+1} \frac{\llbracket \phi \rrbracket^2}{6}. \end{aligned}$$

Thus, the approximations proposed in [24, 25] and in equation (11) for $\tilde{\Psi}'$ are equivalent. This expansion, to the best of our knowledge, was initially proposed in the context of the Navier–Stokes–Cahn–Hilliard equation [36] but the connection between the two had yet to be made. A linear expansion as previously proposed in the context of the Allen–Cahn and Cahn–Hilliard equations [27] and the Navier–Stokes–Cahn–Hilliard equation [1] can be obtained using expansion (24), rather than (23). With regards to the scheme

Figure 11: Crystal growth using the phase-field crystal equation. A small crystallite with a stable triangular structure is placed in the center of the domain. Given the undercooling enforced by ϵ , the crystallite grows and replicates the initial pattern throughout the domain. The rectangular domain considered, $\bar{\Omega} = [0, 40\pi/\sqrt{3}] \times [0, 24\pi]$, is uniformly meshed using $[512] \times [532]$ C^1 -quadratic elements. Periodic boundary conditions are considered along both directions. The solution evolution is calculated with our implicit algorithm, with a time step size $\Delta t = 10^{-2}$. We consider this our reference solution.

Figure 12: Snapshots of the approximate dimensionless atomistic density field showing its evolution throughout the simulation, which was run using a computational mesh composed of 512×532 C^1 -quadratic elements, with a time step size $\Delta t = 0.1$.

Figure 13: Snapshots of the approximate dimensionless atomistic density field showing its evolution throughout the simulation, which was run using a computational mesh composed of 512×532 C^1 -quadratic elements, with a time step size $\Delta t = 1$.

(a) $\Delta t = 0.1$

(b) $\Delta t = 0.5$

(c) $\Delta t = 1$

Figure 14: Free energy evolution comparison for the different methods analyzed to solve the phase-field crystal equation.

proposed in [23] for the Cahn–Hilliard equation, recalling equation (63), considering $\frac{\Delta t}{10^3 \epsilon^2} \geq 0$ and $\frac{1}{2} \tanh(x) \leq \frac{x}{2}$, we have the inequality

$$0 \leq \frac{1}{2} \tanh\left(\frac{\Delta t}{10^3 \epsilon^2}\right) \leq \frac{\Delta t}{2 \times 10^3 \epsilon^2}.$$

Thus, the scheme proposed in [23] can be reinterpreted as a stabilized scheme that uses the implicit approximation of equation (11). The stabilization value can be equal to 0 for the polynomial version of the double well potential when the implicit expansion is used. In the case of the logarithmic version of the potential considered for Ψ in [23], it must have a value greater than 0 to guarantee free energy stability.

Regarding computational performance, results are shown in table 2. The equivalence of the implicit method and the methods developed by Gomez et al. is also confirmed numerically, given that the number of nonlinear iterations is the same for all cases studied.

Table 2: Computational performance of the different methods. We show the computational time of the different methods with respect to the methods of Gomez et al. in each one of the different cases, as well as the number of nonlinear iterations. The table entries “nonlinear iterations” and “linear iterations” represent the total number of Newton iterations, the total number of GMRES iterations during the simulation, respectively. The number of nonlinear iterations for the implicit and the methods developed in [23–25] by Gomez et al., which numerically confirms the result of the other methods are equivalent.

		AC			CH			SH			
	Simulation time T	0.02			0.02			70			
	Δt	10^{-6}	10^{-5}	10^{-4}	10^{-6}	5×10^{-6}	10^{-5}	0.1	0.5	1	0.1
BE	Ref. comp. time	0.81	0.84	0.9	0.88	0.93	0.78	1.26	1.95	-	1.49
	Nonlinear iterations	40002	4068	617	40872	9352	5096	2114	566	-	4502
	Linear iterations	314378	32594	9362	289936	106169	71627	736547	414644	-	266852
G- α	Ref. comp. time	0.88	0.84	0.83	0.91	0.85	0.65	0.99	1.47	1.13	1.26
	Nonlinear iterations	40002	4036	608	40623	8652	4748	2103	561	286	4499
	Linear iterations	343589	30661	7684	251562	80766	54966	582343	312996	216314	223000
Implicit	Ref. comp. time	0.96	0.95	0.97	0.92	0.94	0.94	1	1.01	1.01	1
	Nonlinear iterations	40002	4034	608	40987	9098	6028	2101	441	282	3752
	Linear iterations	342864	30415	7675	246534	82039	68429	565271	207023	198043	169523
Gomez et al.	Ref. comp. time	1	1	1	1	1	1	1	1	1	1
	Nonlinear iterations	40002	4034	608	40987	9098	6028	2101	441	282	3752
	Linear iterations	342864	30415	7675	246531	82119	68451	565269	206931	198048	169523

Table 3: Computational gains using the adaptive-implicit algorithm to solve the phase-field problems of sections 5.1-5.4. By using the adaptive-implicit strategy, the number of iterations taken to reach a high-quality solution is drastically reduced, and on the order of the coarser simulations presented in table 2 for each one of the four cases studied.

	AC	CH	SH	PFC
Simulation time T	0.02	0.02	70	150
Total number of steps	309	609	476	178
Nonlinear iterations	820	1944	1425	530
Linear iterations	7991	22956	418464	406882
Rejected steps	0	40	0	0
Maximum Δt	1.59×10^{-4}	1.18×10^{-2}	2.59×10^{-1}	4.70
Minimum Δt	10^{-8}	10^{-11}	10^{-5}	10^{-6}

5.6. Performance of the time-adaptive scheme and three-dimensional simulation of the Cahn–Hilliard equation

The two-dimensional examples presented in sections 5.1-5.4 are solved using the implicit scheme within the context of algorithm 1, with the results shown in terms of the free energy evolution in figure 15. The adaptive-implicit solutions compare well with the overkill solutions for each one of the cases, and can be computed with fewer iterations than the ones used for the highly refined cases, as seen in table 3. The number of iterations for the Swift–Hohenberg and phase-field crystal equations can be reduced further by splitting the equation through the use of another auxiliary variable, resulting in a similar weak form to the one presented in [54]. We plan to study both of these issues in future work.

Finally, to showcase the robustness of the adaptive-implicit method, the three-dimensional counterpart of the example solved in two dimensions for the Cahn–Hilliard equation in section 5.2 is presented in figure 17. Periodic boundary conditions are considered in all directions, in a unit cube domain $\bar{\Omega} = [0, 1]^3$. The uniform mesh uses $[64]^3\text{-}\mathcal{C}^1$ cubic elements. Similarly to what happens in the two-dimensional case, the mixture initially undergoes a fast spinodal decomposition, which results in the formation of two coexisting phases. Once completed, this physical phenomenon is followed by a coarsening stage, that ends when the interfacial area is minimized. For the initial condition considered, the steady state is achieved when a single bubble remains, as seen in figure 17d. The free energy evolution of the solution is shown in figure 18a, and the evolution of the time step size is shown in 18b.

Figure 15: Evaluating the adaptive-implicit time stepping scheme: free energy evolution. The evolution of the free energy is accurately represented for the four phase-field models studied.

Figure 16: Evaluating the adaptive-implicit time stepping scheme: time-adaptivity.

Table 4: Computational performance of the three-dimensional Cahn–Hilliard simulation. Close to 20% of the steps are rejected, while the time-step size changes nine orders of magnitude during the simulation.

Simulation time T	0.02
Total number of steps	928
Nonlinear iterations	9777
Linear iterations	778245
Rejected steps	188
Maximum Δt	5.84×10^{-4}
Minimum Δt	10^{-13}

Close to 20% of the steps are rejected, while the time-step size changes nine orders of magnitude during the simulation, as seen in table 4. These results can be considerably improved by limiting the number of nonlinear iterations taken before a step is rejected.

Figure 17: Three-dimensional simulation of the Cahn–Hilliard equation. System evolves from a randomly perturbed initial condition that results in a single bubble at steady state. This solution minimizes the surface area of the interface. The unit cube domain considered, $\bar{\Omega} = [0, 1]^3$, is meshed using $[64]^2\mathcal{C}^1$ -cubic elements. The solution evolution is calculated with our adaptive-implicit algorithm.

(a) Free energy evolution

(b) Evolution of the time step size

Figure 18: Three-dimensional simulation of the Cahn–Hilliard equation. The equation is solved using the linear-adaptive algorithm. The free energy is decreasing monotonically as seen in figure 18a. The evolution of the time step size Δt is shown in figure 18b, and seems reasonable: the fast changes in free energy match the times at which the time step size decreases considerably. The mesh is comprised of $[64]^3\text{-}\mathcal{C}^1$ cubic elements.

6. Conclusion

We introduce a **provably energy-stable**, second-order time accurate, mixed variational method for general classes of phase-field models **with polynomial potentials**. The numerical strategy relies on a mixed finite element formulation for the space discretization and on a second-order accurate algorithm based on Taylor expansions for the time discretization. This time-integration algorithm preserves mass by construction if needed, and guarantees strong energy stability. The class of time integrators we introduce is implicit by nature. Additionally, an adaptive time-stepping strategy that can be combined with our method is proposed, which overcomes some of the problems of adaptive time-stepping schemes used in the literature. The time step size is controlled by approximating a local truncation error **a-posteriori** through a backward differentiation procedure. Several two-dimensional numerical examples are shown, for both uniform and adaptive time-step sizes, that deal with some of the more popular phase-field models available, such as the Allen–Cahn, Cahn–Hilliard, Swift–Hohenberg, and phase-field crystal equations. A three dimensional example involving the Cahn–Hilliard equation is also presented. The examples support our theoretical findings, and show the efficiency, stability and robustness of the new method, which is able to solve several high-order, nonlinear partial using the same setting. The implementation uses PetIGA, a high-performance isogeometric analysis framework, and the codes are freely available to download.

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7. Appendix

7.1. Generalized- α method for first order systems

The generalized- α method for first-order differential equations in time [34]

$$\mathbf{R}(\mathbf{U}, \dot{\mathbf{U}}) = 0,$$

is defined as: given $\dot{\mathbf{U}}_n, \mathbf{U}_n$, find $\dot{\mathbf{U}}_{n+1}, \mathbf{U}_{n+1}$ such that

$$\begin{aligned} \mathbf{R}(\dot{\mathbf{U}}_{n+\alpha_m}, \mathbf{U}_{n+\alpha_f}) &= 0 \\ \dot{\mathbf{U}}_{n+\alpha_m} &= \dot{\mathbf{U}}_n + \alpha_m (\dot{\mathbf{U}}_{n+1} - \dot{\mathbf{U}}_n) \\ \mathbf{U}_{n+\alpha_f} &= \mathbf{U}_n + \alpha_f (\mathbf{U}_{n+1} - \mathbf{U}_n) \\ \mathbf{U}_{n+1} &= \mathbf{U}_n + \Delta t (\gamma \dot{\mathbf{U}}_{n+1} + (1 - \gamma) \dot{\mathbf{U}}_n) \end{aligned}$$

where $\Delta t = t_{n+1} - t_n$ is the time-step, and α_f, α_m and γ are parameters which control numerical dissipation and define the method. These parameters can be chosen using the spectral radius $\rho_\infty \in [0, 1]$

$$\begin{aligned} \alpha_m &= \frac{1}{2} \left(\frac{3 - \rho_\infty}{1 + \rho_\infty} \right), \\ \alpha_f &= \frac{1}{1 + \rho_\infty}, \\ \gamma &= \frac{1}{2} + \alpha_m - \alpha_f, \end{aligned}$$

to obtain a second-order accurate, unconditionally stable method.

8. References

- [1] S. ALAND, *Time integration for diffuse interface models for two-phase flow*, Journal of Computational Physics, 262 (2014), pp. 58–71.
- [2] S. ALLEN AND J. CAHN, *A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening*, Acta Metallurgica, 27 (1979), pp. 1085–1095.

- [3] S. BALAY, S. ABHYANKAR, M. ADAMS, J. BROWN, P. BRUNE, K. BUSCHELMAN, L. DALCIN, V. EIJKHOUT, W. GROPP, D. KAUSHIK, M. KNEPLEY, L. C. MCINNES, K. RUPP, B. SMITH, S. ZAMPINI, AND H. ZHANG, *PETSc users manual*, Tech. Rep. ANL-95/11 - Revision 3.6, Argonne National Laboratory, 2015.
- [4] —, *PETSc Web page*. <http://www.mcs.anl.gov/petsc>, 2015.
- [5] J. BUENO, C. BONA-CASAS, Y. BAZILEVS, AND H. GOMEZ, *Interaction of complex fluids and solids: theory, algorithms and application to phase-change-driven implosion*, Computational Mechanics, 55 (2014), pp. 1105–1118.
- [6] G. CAGINALP AND X. CHEN, *Convergence of the phase field model to its sharp interface limits*, European Journal of Applied Mathematics, null (1998), pp. 417–445.
- [7] J. CAHN AND J. HILLIARD, *Free energy of a nonuniform system. i. interfacial free energy*, J. Chem. Phys, 28 (1958).
- [8] N. COLLIER, L. DALCIN, AND V. CALO, *On the computational efficiency of isogeometric methods for smooth elliptic problems using direct solvers*, International Journal for Numerical Methods in Engineering, 100 (2014), pp. 620–632.
- [9] N. COLLIER, L. DALCIN, D. PARDO, AND V. M. CALO, *The cost of continuity: performance of iterative solvers on isogeometric finite elements*, SIAM Journal on Scientific Computing, 35 (2013), pp. A767–A784.
- [10] N. COLLIER, D. PARDO, L. DALCIN, M. PASZYNSKI, AND V. CALO, *The cost of continuity: A study of the performance of isogeometric finite elements using direct solvers*, Computer Methods in Applied Mechanics and Engineering, 213-216 (2012), pp. 353 – 361.
- [11] M. COPETTI AND C. ELLIOTT, *Numerical analysis of the Cahn–Hilliard equation with a logarithmic free energy*, Numerische Mathematik, 63 (1992), pp. 39–65.

- [12] A. CÔRTES, P. VIGNAL, A. SARMIENTO, D. GARCÍA, N. COLLIER, L. DALCIN, AND V. CALO, *Solving nonlinear, high-order partial differential equations using a high-performance isogeometric analysis framework*, in High Performance Computing, G. Hernández, C. Barrios Hernández, G. Daz, C. Garca Garino, S. Nesmachnow, T. Prez-Acle, M. Storti, and M. Vzquez, eds., vol. 485 of Communications in Computer and Information Science, Springer Berlin Heidelberg, 2014, pp. 236–247.
- [13] J. A. COTTRELL, T. J. R. HUGHES, AND Y. BAZILEVS, *Isogeometric Analysis: Toward Unification of CAD and FEA*, John Wiley and Sons, 2009.
- [14] L. CUETO-FELGUEROSO AND R. JUANES, *Macroscopic phase-field model of partial wetting: Bubbles in a capillary tube*, Phys. Rev. Lett., 108 (2012), p. 144502.
- [15] L. DALCIN, N. COLLIER, P. VIGNAL, A. CÔRTES, AND V. CALO, *PetIGA: A Framework for High-Performance Isogeometric Analysis*, arxiv, (2015). <http://arxiv.org/abs/1305.4452>.
- [16] K. ELDER, M. KATAKOWSKI, M. HAATAJA, AND M. GRANT, *Modeling elasticity in crystal growth*, Phys. Rev. Lett., 88 (2002), p. 245705.
- [17] H. EMMERICH, *The Diffuse Interface Approach in Materials Science: Thermodynamic Concepts and Applications of Phase-Field Models*, vol. 73, Springer Berlin Heidelberg, 2003.
- [18] H. EMMERICH, H. LÖWEN, R. WITTKOWSKI, T. GRUHN, G. I. TÓTH, G. TEGZE, AND L. GRÁNÁSY, *Phase-field-crystal models for condensed matter dynamics on atomic length and diffusive time scales: an overview*, Advances in Physics, 61 (2012), pp. 665–743.
- [19] L. F. R. ESPATH, A. SARMIENTO, P. VIGNAL, B. VARGA, A. M. A. CORTES, L. DALCIN, AND V. M. CALO, *Energy Exchange Analysis in Droplet Dynamics via the Navier–Stokes–Cahn–Hilliard Model*, Journal of Fluid Mechanics, (2015). Submitted.
- [20] F. H. FENTON, E. M. CHERRY, A. KARMA, AND W.-J. RAPPEL, *Modeling wave propagation in realistic heart geometries using the phase-field method*, Chaos, 15 (2005), p. 013502.

- [21] H. GOMEZ, V. M. CALO, Y. BAZILEVS, AND T. J. HUGHES, *Isogeometric analysis of the Cahn-Hilliard phase-field model*, Computer Methods in Applied Mechanics and Engineering, 197 (2008), pp. 4333–4352.
- [22] H. GOMEZ, L. CUETO-FELGUEROSO, AND R. JUANES, *Three-dimensional simulation of unstable gravity-driven infiltration of water into a porous medium*, Journal of Computational Physics, 238 (2013), pp. 217 – 239.
- [23] H. GOMEZ AND T. J. HUGHES, *Provably unconditionally stable, second-order time-accurate, mixed variational methods for phase-field models*, Journal of Computational Physics, 230 (2011), pp. 5310–5327.
- [24] H. GOMEZ AND X. NOGUEIRA, *A new spacetime discretization for the Swift-Hohenberg equation that strictly respects the Lyapunov functional*, Communications in Nonlinear Science and Numerical Simulation, 17 (2012), pp. 4930–4946.
- [25] —, *An unconditionally energy-stable method for the phase field crystal equation*, Computer Methods in Applied Mechanics and Engineering, 249–252 (2012), pp. 52–61.
- [26] H. GOMEZ, A. REALI, AND G. SANGALLI, *Accurate, efficient, and (iso)geometrically flexible collocation methods for phase-field models*, Journal of Computational Physics, 262 (2014), pp. 153 – 171.
- [27] F. GUILLÉN-GONZÁLEZ AND G. TIERRA, *Second order schemes and time-step adaptivity for Allen–Cahn and Cahn–Hilliard models*, Computers & Mathematics with Applications, 68 (2014), pp. 821–846.
- [28] E. HAIRER, S. NORSETT, AND G. WANNER, *Solving Ordinary Differential Equations: Nonstiff problems. 1*, Solving ordinary differential equations, Springer London, Limited, 1987.
- [29] A. HENDERSON, *Paraview guide, a parallel visualization application*, Tech. Rep. Revision 4.1, Kitware Inc., 2014.
- [30] Z. HU, S. WISE, C. WANG, AND J. LOWENGRUB, *Stable and efficient finite-difference nonlinear-multigrid schemes for the phase field crystal equation*, Journal of Computational Physics, 228 (2009), pp. 5323 – 5339.

- [31] T. HUGHES, J. COTTRELL, AND Y. BAZILEVS, *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*, Computer Methods in Applied Mechanics and Engineering, 194 (2005), pp. 4135–4195.
- [32] J. D. HUNTER, *Matplotlib: A 2D graphics environment*, Computing In Science & Engineering, 9 (2007), pp. 90–95.
- [33] A. JAATINEN, C. V. ACHIM, K. R. ELDER, AND T. ALA-NISSILA, *Thermodynamics of bcc metals in phase-field-crystal models*, Phys. Rev. E, 80 (2009), p. 031602.
- [34] K. E. JANSEN, C. H. WHITING, AND G. M. HULBERT, *A generalized- α method for integrating the filtered Navier-Stokes equations with a stabilized finite element method*, Computer Methods in Applied Mechanics and Engineering, 190 (2000), pp. 305 – 319.
- [35] M. KÄSTNER, P. METSCH, AND R. DE BORST, *Isogeometric analysis of the Cahn–Hilliard equation - a convergence study*, Journal of Computational Physics, (2015), pp. –.
- [36] J. KIM, K. KANG, AND J. LOWENGRUB, *Conservative multigrid methods for Cahn–Hilliard fluids*, Journal of Computational Physics, 193 (2004), pp. 511–543.
- [37] R. LEVEQUE, *Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems (Classics in Applied Mathematics Classics in Applied Mathemat)*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2007.
- [38] Y. LI, H. G. LEE, D. JEONG, AND J. KIM, *An unconditionally stable hybrid numerical method for solving the Allen–Cahn equation*, Computers & Mathematics with Applications, 60 (2010), pp. 1591–1606.
- [39] J. LIU, L. DEDÈ, J. A. EVANS, M. J. BORDEN, AND T. J. HUGHES, *Isogeometric analysis of the advective Cahn–Hilliard equation: Spinodal decomposition under shear flow*, Journal of Computational Physics, 242 (2013), pp. 321 – 350.

- [40] E. MERKURJEV, T. KOSTI, AND A. BERTOZZI, *An mbo scheme on graphs for classification and image processing*, SIAM Journal on Imaging Sciences, 6 (2013), pp. 1903–1930.
- [41] T. E. OLIPHANT, *Python for scientific computing*, Computing in Science & Engineering, 9 (2007), pp. 10–20.
- [42] M. PELETIER, *Energies, gradient flows, and large deviations: a modelling point of view*. 2012.
- [43] L. PIEGL AND W. TILLER, *The NURBS Book*, Monographs in Visual Communication, Springer, New York, 1995.
- [44] M. PLAPP, *Phase-field models*, in Multiphase Microfluidics: The Diffuse Interface Model, R. Mauri, ed., vol. 538 of CISM Courses and Lectures, Springer Vienna, 2012, pp. 129–175.
- [45] N. PROVATAS AND K. ELDER, *Phase-Field Methods in Materials Science and Engineering*, Wiley-VCH, 1st ed., 2010.
- [46] J. ROWLINSON, *Translation of j.d. van der Waals’ “the thermodynamik theory of capillarity under the hypothesis of a continuous variation of density”*, Journal of Statistical Physics, 20 (1979), pp. 197–200.
- [47] Y. SAAD AND M. H. SCHULTZ, *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 7 (1986), pp. 856–869.
- [48] A. SARMIENTO, P. VIGNAL, L. DALCIN, AND V. M. CALO, *Generalized- α method for the Swift–Hohenberg equation*, (2016). In preparation.
- [49] D. SCHILLINGER, M. BORDEN, AND H. STOLARSKI, *Isogeometric collocation for phase-field fracture models*, Computer Methods in Applied Mechanics and Engineering, 284 (2015), pp. 583 – 610. Isogeometric Analysis Special Issue.
- [50] J. STEWART, *Additional topics: Formulas for the Remainder Term in Taylor series*, in Calculus: Early Transcendentals, Brooks Cole, 8 ed., 2015.

- [51] J. SWIFT AND P. C. HOHENBERG, *Hydrodynamic fluctuations at the convective instability*, Phys. Rev. A, 15 (1977), pp. 319–328.
- [52] G. TIERRA AND F. GUILLÉN-GONZÁLEZ, *Numerical Methods for Solving the Cahn–Hilliard Equation and Its Applicability to Related Energy-Based Models*, Archives of Computational Methods in Engineering, 22 (2015), pp. 269–289.
- [53] E. H. VAN BRUMMELEN, M. SHOKRPOUR-ROUDBARI, AND G. J. VAN ZWIETEN, *Elasto-capillarity Simulations based on the Navier–Stokes–Cahn–Hilliard Equations*, ArXiv e-prints, (2015).
- [54] P. VIGNAL, L. DALCIN, D. BROWN, N. COLLIER, AND V. CALO, *An energy-stable convex splitting for the phase-field crystal equation*, Computers & Structures, 158 (2015), pp. 355–368.
- [55] P. VIGNAL, L. DALCIN, D. L. BROWN, N. O. COLLIER, AND V. M. CALO, *Energy-stable time discretizations for the phase-field crystal equation*, in preparation, (2014).
- [56] P. VIGNAL, A. SARMIENTO, A. CÔRTES, L. DALCIN, AND V. M. CALO, *Coupling Navier–Stokes and Cahn–Hilliard equations in a two-dimensional annular flow configuration*, Procedia Computer Science, 51 (2015), pp. 934–943.
- [57] P. A. VIGNAL, N. O. COLLIER, AND V. M. CALO, *Phase field modeling using PetIGA*, Procedia Computer Science, 18 (2013), pp. 1614–1623.
- [58] G. VILANOVA, I. COLOMINAS, AND H. GOMEZ, *Capillary networks in tumor angiogenesis: From discrete endothelial cells to phase-field averaged descriptions via isogeometric analysis*, International Journal for Numerical Methods in Biomedical Engineering, 29 (2013), pp. 1015–1037.
- [59] —, *Coupling of discrete random walks and continuous modeling for three-dimensional tumor-induced angiogenesis*, Computational Mechanics, 53 (2014), pp. 449–464.

- [60] S. WISE, C. WANG, AND J. LOWENGRUB, *An Energy-Stable and Convergent Finite-Difference Scheme for the Phase Field Crystal Equation*, SIAM Journal on Numerical Analysis, 47 (2009), pp. 2269–2288.
- [61] X. WU, G. VAN ZWIETEN, AND K. VAN DER ZEE, *Stabilized second-order convex splitting schemes for Cahn-Hilliard models with application to diffuse-interface tumor-growth models*, Int. J. Numer. Meth. Biomed. Engng., 30 (2014), pp. 180–203.
- [62] P. YUE, J. J. FENG, C. LIE, AND J. SHEN, *A diffuse-interface method for simulating two-phase flows of complex fluids*, Journal of Fluid Mechanics, 515 (2004), pp. 293–317.
- [63] Z. ZHANG, Y. MA, AND Z. QIAO, *An adaptive time-stepping strategy for solving the phase field crystal model*, Journal of Computational Physics, 249 (2013), pp. 204–215.
- [64] O. ZIENKIEWICZ, R. TAYLOR, AND J. ZHU, *Chapter 12 - the time dimension: Semi-discretization of field and dynamic problems*, in The Finite Element Method: its Basis and Fundamentals (Seventh Edition), O. Zienkiewicz, R. Taylor, and J. Zhu, eds., Butterworth-Heinemann, Oxford, seventh edition ed., 2013, pp. 379–405.