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Gradient stability of high-order BDF methods and some applications

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ABSTRACT

It is well-known that the backward differentiation formulae (BDF) of order 1, 2 and 3 are gradient stable. This means that when such a method is used for the time discretization of a gradient flow, the associated discrete dynamical system exhibit properties similar to the continuous case, such as the existence of a Lyapunov functional. By means of a Lojasiewicz-Simon inequality, we prove convergence to equilibrium for the 3-step BDF scheme applied to the Allen-Cahn equation with an analytic nonlinearity. By introducing a notion of quadratic-stability, we also show that the BDF methods of order 4 and 5 are gradient stable, and that the k -step BDF schemes are not gradient stable for $k \geq 7$. Some numerical simulations illustrate the theoretical results.

KEYWORDS

BDF methods; gradient flow; Allen-Cahn equation; Lojasiewicz-Simon inequality

1. Introduction

We consider k -step backward differentiation formulae (BDF) applied to gradient flows in finite and infinite dimension. We are interested in the asymptotic behaviour, as time goes to infinity, of the sequences generated by these methods. Our model problem in the infinite dimensional case is the Allen-Cahn equation, which was introduced to describe the process of phase transition [3]. It reads

$$u_t - \Delta u + g(u) = 0, \quad t > 0, \quad x \in \Omega, \quad (1)$$

where Ω is a bounded subset of \mathbb{R}^d with smooth boundary and $g \in C^1(\mathbb{R}, \mathbb{R})$ is the derivative of a potential G . A standard choice is the double-well potential $G(s) = (s^2 - 1)^2/4$. The unknown function u represents the order parameter. Throughout the paper, we will consider Dirichlet boundary conditions.

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The Allen-Cahn equation (1) is a gradient flow of the energy

$$E(u) = \int_{\Omega} \frac{1}{2} |\nabla u|^2 + G(u) dx \quad (2)$$

for the $L^2(\Omega)$ scalar product. The theoretical picture for (1) is well-known and there is a huge literature on this equation (for the well-posedness and some asymptotic properties, see e.g. [17, 28]). If g is real analytic, then Simon [26] proved that every bounded solution converges to a steady state as time goes to infinity. It is not known if this result still holds for every choice of nonlinearity $g \in C^\infty(\mathbb{R}, \mathbb{R})$ (see [17, 23] and references therein). The proof of Simon is based on a so-called *Lojasiewicz-Simon inequality*, which is an extension to the infinite dimension of the celebrated Lojasiewicz inequality for real analytic functions [20]. We refer the reader to the recent review by Haraux and Jendoubi [18].

Our aim in this paper is to prove that convergence to equilibrium also holds for the BDF methods of high-order (3, 4 or 5) applied to equation (1) with an analytic nonlinearity.

BDF methods of low order (1 or 2) are widely used for the time discretization of gradient-flows such as (1). A crucial feature is that the discrete-in-time dynamical systems defined by these methods have properties similar to the continuous-in-time problem, such as the existence of a Lyapunov functional [25, 27]. We note that for the BDF method of order 1, the Lyapunov functional is the energy E (2), whereas for higher-order BDF schemes, a pseudo-energy (i.e. a modification of E) has to be used.

The one-step BDF method (BDF1) is simply the backward Euler scheme, also known as the proximal algorithm in the context of optimization. Convergence to equilibrium for this scheme has been shown by means of a Lojasiewicz-like inequality in finite and infinite dimension [5, 10, 21]. The finite dimensional case arises naturally when one considers a space semi-discretization of (1) which preserves the gradient-flow structure. This happens with standard finite element or finite difference methods [9, 11].

Convergence to equilibrium for the two-step BDF scheme (BDF2) was proved in finite dimension in [2], and in infinite dimension in [4] for the Cahn-Hilliard equation, which is a gradient flow of E (2) for the H^{-1} scalar product. We note that a restriction on the time step (independent of the initial data) has to be introduced in order for the gradient stability to hold. For the BDF1 scheme, the restriction on the time step can be removed by considering the proximal algorithm [7]. The analysis of the infinite dimensional case is interesting because it is independent of the choice of a particular space discretization.

Since the gradient stability of the three-step BDF method is known [27], convergence to equilibrium can be obtained in finite dimension by applying general results on descent methods, see e.g. [2, 6, 10]. The infinite dimensional case is more involved, but we work it out here in a way similar to the BDF2 case, with a stability restriction on the time step (Theorem 5.4). In contrast, there exist several second-order schemes which are unconditionally gradient stable, such as the secant scheme, but for which convergence to equilibrium in the infinite dimensional setting remains to investigate (see [11, 12, 14, 24, 30] and references therein). If we consider for instance the secant scheme, which is a gradient-stable Crank-Nicolson like scheme, one issue is to obtain the precompactness of trajectories.

In [27, p. 424], Stuart and Humphries conjectured that the BDF schemes of order 4, 5 and 6 are gradient stable. To the best of our knowledge, this assertion has not yet been proved. In this paper, by introducing a notion of quadratic-stability, we prove that this conjecture is true for the BDF4 and BDF5 schemes. For $k \geq 7$, the k -step BDF schemes are not zero-stable [16], so they are not expected to be gradient stable. We make this clear in Remark 2.6. We note that the gradient-stability of the BDF6 scheme remains to be investigated (Remark 2.10).

The convergence result of Simon has been generalized to a great variety of gradient-like equations, in particular to damped wave equations such as the sine-Gordone equation or the modified Allen-Cahn equation (cf. [18] and references therein). Convergence to equilibrium for the backward Euler equation applied to the modified Allen-Cahn equation has been proved in [15, 22]. We note however that BDF schemes of order greater than one do not seem to preserve the gradient-like structure in this situation, so that other energy stable schemes should be considered.

The paper is organized as follows. In Section 2, we introduce the BDF methods applied to a gradient flow in finite dimension, and we define the notion of quadratic-stability. In Section 3, we prove that the BDF4 and BDF5 methods are gradient stable. Convergence to equilibrium for the BDF3 scheme applied to the Allen-Cahn equation is proved in Sections 4 and 5. In the last section, we perform some numerical simulations for the BDF3 scheme applied to (1). They nicely illustrate the theoretical results.

2. Quadratic-stability of BDF methods

2.1. The continuous problem

We denote $\langle \cdot, \cdot \rangle$ the scalar product in \mathbb{R}^M and $\| \cdot \|$ the euclidean norm. We consider the gradient flow in \mathbb{R}^M

$$U'(t) = -\nabla F(U(t)), \quad t \geq 0, \quad (3)$$

where $U : [0, +\infty) \rightarrow \mathbb{R}^M$ and $F \in C^1(\mathbb{R}^M, \mathbb{R})$. Throughout the paper, we assume that F satisfies the following two conditions,

$$\langle \nabla F(V) - \nabla F(W), V - W \rangle \geq -c_F \|V - W\|^2, \quad \forall V, W \in \mathbb{R}^M, \quad (4)$$

for some constant $c_F \geq 0$, and

$$\lim_{\|V\| \rightarrow \infty} F(V) = +\infty. \quad (5)$$

Condition (4) is known as a one-sided Lipschitz condition [27]. This condition is equivalent to the fact that the functional $V \mapsto \nabla F(V) + c_F V$ is a maximal monotone operator on \mathbb{R}^M , or that the function $V \mapsto F(V) + (c_F/2)\|V\|^2$ is convex. Using the Cauchy-Peano theorem, this guarantees, for every $U_0 \in \mathbb{R}^M$, the existence of a unique solution $U \in C^1([0, +\infty), \mathbb{R}^M)$ of (3) such $U(0) = U_0$ [8].

Condition (5) is called a coercivity condition. On multiplying equation (3) by $U'(t)$, we obtain that

$$\frac{d}{dt} F(U(t)) = -\|U'(t)\|^2. \quad (6)$$

In particular, $F(U(t))$ is nonincreasing, and the coercivity condition (5) implies that the solution U is bounded. Using Lasalle's invariance principle [17], we obtain that the ω -limit set of $U(0)$, defined by

$$\omega(U(0)) := \{U^* \in \mathbb{R}^M : \exists t_n \uparrow +\infty \text{ s. t. } U(t_n) \rightarrow U^*\},$$

is a compact and connected subset of \mathbb{R}^M , which is included in the set of critical points of F ,

$$\mathcal{S} = \{V \in \mathbb{R}^M : \nabla F(V) = 0\}. \quad (7)$$

If the critical points of F are isolated, this implies that $U(t) \rightarrow U^*$ as $t \rightarrow +\infty$. If the critical points of F are not isolated, then convergence to equilibrium may fail if $M \geq 2$, even if F is C^∞ (see e.g. [1]). Lojasiewicz [20] proved that if $F : \mathbb{R}^M \rightarrow \mathbb{R}$ is real analytic, then we always have $U(t) \rightarrow U^*$ as $t \rightarrow +\infty$.

2.2. General k -step BDF methods

Let $\Delta t > 0$ be the time step. The general k -step backward differentiation formula (BDF) for (3) is defined by

$$\sum_{j=1}^k \frac{1}{j} \partial^j U^{n+k} = -\Delta t \nabla F(U^{n+k}), \quad n \geq 0, \quad (8)$$

where, for a sequence $(U^n)_{n \geq 0}$, the (backward) difference operator ∂^j is defined recursively by $\partial^j U^n = \partial^{j-1}(U^n - U^{n-1})$ ($j \geq 2, n \geq j$). When $j = 1$, we have $\partial U^n = U^n - U^{n-1}$.

The one-step BDF method is the backward Euler scheme:

$$U^{n+1} - U^n = -\Delta t \nabla F(U^{n+1}), \quad n \geq 0. \quad (9)$$

The two-step BDF method reads

$$\frac{3}{2}U^{n+2} - 2U^{n+1} + \frac{1}{2}U^n = -\Delta t \nabla F(U^{n+2}), \quad n \geq 0. \quad (10)$$

The k -step BDF method (8) is obtained by Newton's divided difference formula which interpolates U by a polynomial of degree k (see Section 4.2 for the case $k = 3$). It is known to have a consistency error of order k . Moreover, it is zero-stable if and only if $k \in \{1, \dots, 6\}$, so that BDF methods are not used for $k \geq 7$ [16]. This also implies that if $F \in C^{k+2}(\mathbb{R}^M, \mathbb{R})$ ($k \leq 6$) and if the initial conditions are well chosen, the error between the solution U of (3) and its approximation given by the BDF scheme (8) is of order $O(\Delta t^k)$ on finite time intervals [27, Theorem 3.5.7].

In (8), the initial conditions U^0, \dots, U^{k-1} are given in \mathbb{R}^M ; at every step $n \geq 0$, the vector U^{n+k} is computed from $U^n, U^{n+1}, \dots, U^{n+k-1}$ by solving the (generally nonlinear) equation (8). Thanks to the coercivity condition (5), there exists at least one such U^{n+k} . Indeed, (8) reads

$$\Delta t \nabla F(U^{n+k}) + \alpha_k U^{n+k} + L_n = 0, \quad (11)$$

where

$$\alpha_k = \sum_{j=1}^k 1/j > 0 \quad (12)$$

and $L_n \in \mathbb{R}^M$ is a linear combination of the vectors U^n, \dots, U^{n+k-1} . The function

$$V \mapsto \Delta t F(V) + \frac{\alpha_k}{2} \|V\|^2 + \langle L_n, V \rangle$$

is continuous on \mathbb{R}^M and coercive. Thus, it has at least one minimizer U^{n+k} in \mathbb{R}^M , which solves the Euler-Lagrange equation (11).

By using the one-sided Lipschitz condition (4), one can guarantee that the solution U^{n+k} of (11) is unique for Δt small enough (for a given L_n). Indeed, if \tilde{U}^{n+k} is another solution, then the difference $V_n = U^{n+k} - \tilde{U}^{n+k}$ satisfies

$$\Delta t [\nabla F(U^{n+k}) - \nabla F(\tilde{U}^{n+k})] + \alpha_k V_n = 0.$$

On multiplying by V_n and using (4), we see that

$$(\alpha_k - c_F \Delta t) \|V_n\|^2 \leq 0. \quad (13)$$

Thus, if $c_F \Delta t < \alpha_k$, $V_n = 0$ and the sequence $(U^n)_n$ is uniquely defined by its initial values U^0, \dots, U^{n+k-1} and the k -step formula (8).

2.3. Quadratic-stability of BDF methods

In [27], the proof of gradient stability for the BDF methods of order 1, 2 and 3 is essentially based on the following algebraic computations. The authors multiply the left-hand side of (8) by ∂U^{n+k} , and they consider the quantity

$$\Gamma_k = \sum_{j=1}^k \frac{1}{j} \langle \partial^j U^{n+k}, \partial U^{n+k} \rangle. \quad (14)$$

They use that

$$\Gamma_1 = \|\partial U^{n+1}\|^2, \quad (15)$$

$$\Gamma_2 = \|\partial U^{n+2}\|^2 + \frac{1}{4} \|\partial U^{n+2} - \partial U^{n+1}\|^2 + \frac{1}{4} (\|\partial U^{n+2}\|^2 - \|\partial U^{n+1}\|^2), \quad (16)$$

and

$$\begin{aligned} \Gamma_3 &= \frac{5}{6} \|\partial U^{n+3}\|^2 + \frac{1}{4} \|\partial U^{n+3} - \partial U^{n+2}\|^2 \\ &\quad + \frac{1}{6} \|\partial U^{n+3} - \partial U^{n+2} + \partial U^{n+1}\|^2 + \frac{5}{12} (\|\partial U^{n+3}\|^2 - \|\partial U^{n+2}\|^2) \\ &\quad + \frac{1}{6} (\|\partial U^{n+3} - \partial U^{n+2}\|^2 - \|\partial U^{n+2} - \partial U^{n+1}\|^2). \end{aligned} \quad (17)$$

In order to extend similar computations to higher-order schemes, it seems natural to consider Γ_k as a quadratic form depending on the variables $\partial U^{n+k}, \dots, \partial U^{n+1}$.

For this purpose, we consider first the case $M = 1$ (the general case will follow immediately).

We set $x_1 = \partial U^{n+k}, \dots, x_k = \partial U^{n+1}$, and we define the following quadratic form on \mathbb{R}^k :

$$\gamma_k(x_1, \dots, x_k) = \sum_{j=1}^k \frac{1}{j} (\tilde{\partial}^{j-1} x_1) x_j, \quad (18)$$

where $\tilde{\partial}^j$ is the forward difference operator defined recursively by $\tilde{\partial}^j x_1 = \tilde{\partial}^{j-1}(x_1 - x_2)$. We note that

$$\tilde{\partial}^j x_1 = \sum_{i=0}^j (-1)^i \binom{j}{i} x_{1+i},$$

where $\binom{j}{i}$ is the binomial coefficient.

We recall that a quadratic form q on \mathbb{R}^k is uniquely associated to a symmetric matrix $A_q = (a_{ij})_{1 \leq i, j \leq k}$ of size k through

$$q(x_1, \dots, x_k) = \sum_{i=1}^k \sum_{j=1}^k a_{ij} x_i x_j.$$

We will denote $q \sim A_q$ this univoque correspondence. The quadratic form q is positive definite if $q(x_1, \dots, x_k) > 0$ for all $(x_1, \dots, x_k) \in \mathbb{R}^k \setminus \{0\}$, or equivalently, if the matrix A_q is positive definite.

By Sylvester's criterion, a symmetric matrix $A = (a_{ij})_{1 \leq i, j \leq k}$ is positive definite if and only if its leading principal minors are positive, i.e.

$$\forall p \in \{1, \dots, k\}, \quad \Delta_p := \det[(a_{ij})_{1 \leq i, j \leq p}] > 0. \quad (19)$$

Definition 2.1. We say that the k -step BDF method is *quadratic-stable* if

$$\gamma_k(x_1, \dots, x_k) = q_k(x_1, \dots, x_{k-1}) - q_k(x_2, \dots, x_k) + r_k(x_1, \dots, x_k), \quad (20)$$

for all $(x_1, \dots, x_k) \in \mathbb{R}^k$, where q_k is a positive definite quadratic form on \mathbb{R}^{k-1} and r_k is a positive definite quadratic form on \mathbb{R}^k .

Example 2.2. From (16), we see that γ_2 is quadratic-stable with $q_2(x_1) = x_1^2/4$ and $r_2(x_1, x_2) = x_1^2 + (x_1 - x_2)^2/4$. By (17), γ_3 is also quadratic-stable (and by convention, so is γ_1).

Remark 2.3. The quadratic forms q_k and r_k , if they exist, are not unique. Indeed, let $A_{q_k}^\varepsilon$ be a symmetric matrix of size k which is a small perturbation of A_{q_k} in \mathbb{R}^{k^2} , where $q_k \sim A_{q_k}$. Then $A_{r_k}^\varepsilon$, defined through (20) in terms of A_{γ_k} and $A_{q_k}^\varepsilon$, is also a perturbation of A_{r_k} . By Sylvester's criterion (19), if $A_{q_k}^\varepsilon$ is close enough to A_{q_k} , then both $A_{q_k}^\varepsilon$ and $A_{r_k}^\varepsilon$ are positive definite.

We first show that quadratic-stability implies asymptotic stability. For this purpose, we

apply the BDF method to the linear ode

$$y'(t) = -\lambda y(t), \quad t \geq 0, \quad (21)$$

with $\lambda > 0$. Since $y(t) \rightarrow 0$ as $t \rightarrow \infty$, we expect a similar behaviour for the time discrete version, which reads

$$\sum_{j=1}^k \frac{1}{j} \partial^j y^{n+k} = -\lambda \Delta t y^{n+k}, \quad n \geq 0. \quad (22)$$

Proposition 2.4. *If the k -step BDF method is quadratic-stable, then for all $\lambda > 0$ and for any initial conditions y_0, \dots, y_{n+k-1} , the sequence $(y^n)_{n \geq 0}$ generated by (22) tends to 0.*

Proof. We multiply (22) by ∂y^{n+k} , and by definition (18) of γ_k , we obtain

$$\gamma_k(\partial y^{n+k}, \dots, \partial y^{n+1}) = -\lambda \Delta t y^{n+k} (y^{n+k} - y^{n+k-1}), \quad n \geq 0.$$

Using (20) and the well-known identity $a(a-b) = [a^2 - b^2 + (a-b)^2]/2$, we obtain

$$E^{n+k} - E^{n+k-1} + \frac{\lambda}{2} (\partial y^{n+k})^2 + r_k(\partial y^{n+k}, \dots, \partial y^{n+1}) = 0, \quad n \geq 0,$$

where

$$E^{n+k} := \frac{\lambda}{2} (y^{n+k})^2 + q_k(\partial y^{n+k}, \dots, \partial y^{n+2}).$$

By summing on n , we find that

$$\sum_{n=0}^{\infty} r_k(\partial y^{n+k}, \dots, \partial y^{n+1}) \leq E^{k-1} < +\infty.$$

In particular, $r_k(\partial y^{n+k}, \dots, \partial y^{n+1}) \rightarrow 0$ and since r_k is positive definite, this shows that

$$(\partial y^{n+k}, \dots, \partial y^{n+1}) \rightarrow (0, \dots, 0) \text{ in } \mathbb{R}^k.$$

By (22), y^{n+k} is a linear combination of $\partial y^{n+k}, \dots, \partial y^{n+1}$. Thus, $y^{n+k} \rightarrow 0$ and the claim is proved. \square

In the following result, we use that asymptotic stability implies zero-stability.

Corollary 2.5. *If $k \geq 7$, the k -step BDF method is not quadratic-stable.*

Proof. We consider now the BDF method applied to the ode $y'(t) = 0$, that is

$$\sum_{j=1}^k \frac{1}{j} \partial^j y^{n+k} = 0, \quad n \geq 0. \quad (23)$$

This is a linear difference equation of order k . Its characteristic polynomial $\rho(\zeta)$, which is obtained on replacing y^{n+k} by ζ^{n+k} in (23) and dividing by ζ^n , is

$$\rho(\zeta) = \sum_{j=1}^k \frac{1}{j} \sum_{i=0}^j (-1)^i \binom{j}{i} \zeta^{k-i} = \sum_{j=1}^k \frac{1}{j} \zeta^{k-j} (\zeta - 1)^j. \quad (24)$$

By definition, the k -step BDF method is zero-stable if and only if all the roots of ρ lie in the unit disc and the ones on the unit circle are simple. This is true if and only if $k \in \{1, \dots, 6\}$ [16].

Let now $k \geq 7$. It is shown in [16] that ρ has at least one root $\lambda_k \in \mathbb{C}$ outside the unit disc, i.e. $|\lambda_k| > 1$. For $\varepsilon > 0$, we consider now the polynomial

$$\rho_\varepsilon(\zeta) = \rho(\zeta) + \varepsilon \zeta^k.$$

This is the characteristic polynomial of the linear difference equation (22) with $\varepsilon = \lambda \Delta t$. As $\varepsilon \rightarrow 0^+$, the roots of ρ_ε converge to the roots of ρ , so that for $\varepsilon > 0$ small enough, ρ_ε has at least one root $\lambda_{k,\varepsilon}$ such that $|\lambda_{k,\varepsilon}| > 1$. Therefore, we have a sequence $(\lambda_{k,\varepsilon}^n)_{n \geq 0}$ of complex numbers which complies with (22), and which is unbounded. By Proposition 2.4, this k -step BDF method cannot be quadratic-stable. We note here that the result in Proposition 2.4 is proved for a sequence $(y^n)_n$ of real numbers, but it extends immediately to complex numbers, by considering the real and imaginary parts. \square

Remark 2.6. The proof above shows that for $k \geq 7$, the k -step BDF schemes are *not gradient stable* in the sense of [27, Definition 1.8.9]. Indeed, consider the function $F(y) = \lambda y^2/2$ with $\lambda > 0$, so that (21) is the gradient flow of F . Assume by contradiction that a k -step BDF scheme is gradient stable for some $k \geq 7$. Then every sequence $(y^n)_n$ defined by (22) would be bounded, by [27, Theorem 1.8.10]. But we have seen that for $\Delta t > 0$ small enough, this k -step BDF scheme produces an unbounded sequence.

Proposition 2.7. *The 4-step BDF method is quadratic-stable. Namely,*

$$\gamma_4(x_1, x_2, x_3, x_4) = q_4(x_1, x_2, x_3) - q_4(x_2, x_3, x_4) + r_4(x_1, x_2, x_3, x_4),$$

for all $(x_1, x_2, x_3, x_4) \in \mathbb{R}^4$, where

$$q_4 \sim \frac{1}{144} \begin{pmatrix} 225 & -92 & 39 \\ -92 & 150 & -46 \\ 39 & -46 & 75 \end{pmatrix} \quad \text{and} \quad r_4 \sim \frac{1}{144} \begin{pmatrix} 75 & -46 & 39 & -18 \\ -46 & 75 & -46 & 39 \\ 39 & -46 & 75 & -46 \\ -18 & 39 & -46 & 75 \end{pmatrix}. \quad (25)$$

Proof. We give a constructive proof. We seek A_{q_4} in the form of a symmetric matrix

$$A_{q_4} = \begin{pmatrix} a & d & g \\ d & b & f \\ g & f & c \end{pmatrix}.$$

The quadratic form

$$\tilde{q}_4(x_1, x_2, x_3, x_4) = q_4(x_1, x_2, x_3) - q_4(x_2, x_3, x_4)$$

is given by

$$A_{\tilde{q}_4} = \begin{pmatrix} a & d & g & 0 \\ d & b-a & f-d & -g \\ g & f-d & c-b & -f \\ 0 & -g & -f & -c \end{pmatrix}.$$

We note that the sum of the elements in each diagonal of $A_{\tilde{q}_4}$ amounts to 0. Since $A_{r_4} = A_{\gamma_4} - A_{\tilde{q}_4}$, this shows that the sum of the elements in each diagonal of A_{r_4} and A_{γ_4} are equal. By definition, we have

$$A_{\gamma_4} = \begin{pmatrix} 25/12 & -23/24 & 13/24 & -1/8 \\ -23/24 & 0 & 0 & 0 \\ 13/24 & 0 & 0 & 0 \\ -1/8 & 0 & 0 & 0 \end{pmatrix}$$

An easy way to choose the coefficients of A_{r_4} is to take the elements of a given diagonal all equal. This gives A_{r_4} , and in turn, $A_{\tilde{q}_4}$ and A_{q_4} . Using Sylvester's criterion (19), we easily check that A_{q_4} and A_{r_4} , given by (25), are positive definite. Indeed, the principal minors of A_{q_4} are $225/144$, $25\,286/144^2$ and $1\,522\,296/144^3$, whereas the principal minors of A_{r_4} are

$$75/144, \quad 3\,509/144^2, \quad 155\,448/144^3 \quad \text{and} \quad 6\,460\,912/144^4.$$

□

Proposition 2.8. *The 5-step BDF method is quadratic-stable. Namely,*

$$\gamma_5(x_1, x_2, x_3, x_4, x_5) = q_5(x_1, x_2, x_3, x_4) - q_5(x_2, x_3, x_4, x_5) + r_5(x_1, x_2, x_3, x_4, x_5), \quad (26)$$

for all $(x_1, x_2, x_3, x_4, x_5) \in \mathbb{R}^5$, where

$$q_5 \sim \begin{pmatrix} 1.85 & -1.19 & 0.75 & -0.3 \\ -1.19 & 1.45 & -0.84 & 0.3 \\ 0.75 & -0.84 & 0.9 & -0.37 \\ -0.3 & 0.3 & -0.37 & 0.3 \end{pmatrix} \quad (27)$$

and

$$r_5 \sim \frac{1}{600} \begin{pmatrix} 260 & -101 & 235 & -135 & 60 \\ -101 & 240 & -210 & 270 & -180 \\ 235 & -210 & 330 & -282 & 180 \\ -135 & 270 & -282 & 360 & -222 \\ 60 & -180 & 180 & -222 & 180 \end{pmatrix}. \quad (28)$$

Proof. By definition, we have

$$\gamma_5 \sim \frac{1}{120} \begin{pmatrix} 274 & -163 & 137 & -63 & 12 \\ -163 & 0 & 0 & 0 & 0 \\ 137 & 0 & 0 & 0 & 0 \\ -63 & 0 & 0 & 0 & 0 \\ 12 & 0 & 0 & 0 & 0 \end{pmatrix},$$

so it is easily seen that (26) holds, with q_5 and r_5 as above. Using Sylvester's criterion, we can check numerically that q_5 and r_5 are positive definite (the computation is exact since we work with rational numbers of reasonable size), and the proof is complete (see Remark 2.9 for a constructive approach). \square

Remark 2.9. The argument used in Proposition 2.7 is not sufficient in order to obtain q_5 and r_5 . We have actually obtained q_5 by numerical investigation with a Scilab program. More precisely, let

$$q_5 \sim A_{q_5} = (a_{i,j})_{1 \leq i,j \leq 4},$$

where the ten coefficients $a_{i,j}$ for $1 \leq i \leq j \leq 4$ are unknown (the other coefficients are obtained by symmetry of A_{q_5}). The idea is to check a large number of values of the coefficients $a_{i,j}$ in order to obtain the positivity of q_5 and r_5 . We have used a grid of stepsize 0.15 in \mathbb{R}^{10} for these coefficients. Remark 2.3 shows that for a stepsize small enough, this approach should give a result, if γ_5 is indeed quadratic stable.

In order to reduce the computational time, we used the following simple facts. The diagonal coefficients of A_{r_5} being positive, we deduce from (26) that

$$274/120 > a_{1,1} > a_{2,2} > a_{3,3} > a_{4,4} > 0.$$

For each nondiagonal coefficient $a_{i,j}$, we note that the minor $a_{i,i}a_{j,j} - a_{i,j}^2$ corresponding to q_5 is positive, that is $|a_{i,j}| < \sqrt{a_{i,i}a_{j,j}}$. For every choice of A_{q_5} in our program, we checked whether the matrices A_{q_5} and A_{r_5} were positive definite or not by a numerical calculation of their eigenvalues.

Remark 2.10. We have investigated numerically the quadratic-stability of γ_6 in a manner similar to γ_5 (cf. Remark 2.9). We used a grid of stepsize 0.1 in \mathbb{R}^{15} for the fifteen unknown coefficients of A_{q_6} . We have not been successful. It could be interesting to perform numerical simulations with a smaller stepsize, but we were limited by the computational time.

3. Gradient stability of the BDF4 and BDF5 methods

3.1. From \mathbb{R} to \mathbb{R}^M

Now, we turn back to the general case $M \geq 1$. If

$$q(x_1, \dots, x_k) = \sum_{i=1}^k \sum_{j=1}^k a_{ij} x_i x_j$$

is a quadratic function on \mathbb{R}^k , associated to the symmetric matrix $A_q = (a_{ij})_{1 \leq i, j \leq k}$, we define the following quadratic form on $(\mathbb{R}^M)^k$:

$$Q(V_1, \dots, V_k) = \sum_{i=1}^k \sum_{j=1}^k a_{ij} \langle V_i, V_j \rangle.$$

Then Q inherits the properties of q . In particular, if q is positive definite, then so is Q . Indeed, if A_q is positive definite, there exists a matrix $P \in O(k)$ such that

$$A_q = P^t \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_k \end{pmatrix} P,$$

where $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k$ are the eigenvalues of A_q . This reads, for all $X = (x_1, \dots, x_k)^t \in \mathbb{R}^k$,

$$q(x_1, \dots, x_k) = X^t A_q X = \sum_{i=1}^k \lambda_i \left(\sum_{j=1}^k p_{ij} x_j \right)^2,$$

where $P = (p_{ij})_{1 \leq i, j \leq k}$. Thus, for $(V_1, \dots, V_k) \in (\mathbb{R}^M)^k$, we have

$$\begin{aligned} Q(V_1, \dots, V_k) &= \sum_{i=1}^k \lambda_i \left\| \sum_{j=1}^k p_{ij} V_j \right\|^2 \\ &\geq \lambda_1 \sum_{i=1}^k \left\| \sum_{j=1}^k p_{ij} V_j \right\|^2 \\ &\geq \lambda_1 \sum_{i=1}^k \sum_{j=1}^k \sum_{m=1}^k p_{ij} p_{im} \langle V_j, V_m \rangle. \end{aligned} \tag{29}$$

Since $P^t P = Id_k$, we have $\sum_{i=1}^k p_{ij} p_{im} = \delta_{jm}$, where δ_{jm} is the Kronecker symbol. Thus, (29) reads

$$Q(V_1, \dots, V_k) \geq \lambda_1 \sum_{j=1}^k \|V_j\|^2,$$

and the claim is proved.

3.2. Gradient stability of the BDF4 method

From Proposition 2.7, we deduce:

Lemma 3.1. *The quadratic forms Γ_4 , Q_4 and R_4 associated to γ_4 , q_4 and r_4 satisfy*

$$\Gamma_4(V_1, V_2, V_3, V_4) = Q_4(V_1, V_2, V_3) - Q_4(V_2, V_3, V_4) + R_4(V_1, V_2, V_3, V_4) \quad (30)$$

for all $(V_1, V_2, V_3, V_4) \in (\mathbb{R}^M)^4$. In particular, Q_4 and R_4 are positive definite. Moreover,

$$R_4(V_1, V_2, V_3, V_4) = \frac{41}{144} \|V_1\|^2 + \tilde{R}_4(V_1, V_2, V_3, V_4), \quad (31)$$

where \tilde{R}_4 is positive definite on $(\mathbb{R}^M)^4$.

Proof. It remains only to prove that \tilde{R}_4 is positive definite. For this purpose, we consider the quadratic form on \mathbb{R}^4 defined by

$$\tilde{r}_4(x_1, x_2, x_3, x_4) = r_4(x_1, x_2, x_3, x_4) - \frac{41}{144} x_1^2.$$

Using Sylvester's criterion, we easily check that $A_{\tilde{r}_4}$ is positive definite. The claim on \tilde{R}_4 follows. We point out that the coefficient $41/144$ was found by numerical investigation and that it is not optimal. \square

For $\hat{V} = (V_0, V_1, V_2, V_3) \in (\mathbb{R}^M)^4$, we define

$$\hat{F}_4(\hat{V}) = F(V_0) + \frac{1}{\Delta t} Q_4(V_1, V_2, V_3),$$

and for a sequence $(U^n)_{n \geq 0}$ in \mathbb{R}^M , we define

$$\hat{U}^{n+4} = (U^{n+4}, \partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}),$$

so that

$$\hat{F}_4(\hat{U}^{n+4}) = F(U^{n+4}) + \frac{1}{\Delta t} Q_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}).$$

Theorem 3.2. *If $c_F \Delta t \leq 41/72$, the 4-step BDF method (8) is gradient-stable, i.e.*

$$\hat{F}_4(\hat{U}^{n+4}) + \frac{1}{\Delta t} \tilde{R}_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \leq \hat{F}_4(\hat{U}^{n+3}), \quad n \geq 0. \quad (32)$$

Proof. We multiply (8) by ∂U^{n+4} in \mathbb{R}^M , and we find

$$\Gamma_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) = -\Delta t \langle \nabla F(U^{n+4}), U^{n+4} - U^{n+3} \rangle,$$

where Γ_4 is defined by (14). Since $V \mapsto F(V) + (c_F/2) \|V\|^2$ is convex, we have

$$F(V) - F(U) + \frac{c_F}{2} \|V - U\|^2 \geq \langle \nabla F(U), V - U \rangle, \quad \forall U, V \in \mathbb{R}^M. \quad (33)$$

We apply this relation with $U = U^{n+4}$ and $V = U^{n+3}$ and we use (30). This yields

$$\hat{F}_4(\hat{U}^{n+4}) + \frac{1}{\Delta t} R_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \leq \hat{F}_4(\hat{U}^{n+3}) + \frac{c_F}{2} \|\partial U^{n+4}\|^2,$$

for all $n \geq 0$. Finally, using (31) and $\frac{1}{\Delta t} \frac{41}{144} - \frac{c_F}{2} \geq 0$, we find (32). \square

Let

$$\omega((U^n)_n) = \{U^* \in \mathbb{R}^M : \exists n_p \rightarrow +\infty \text{ s.t. } U^{n_p} \rightarrow U^*\}$$

denote the ω -limit set of a sequence $(U^n)_n$, and recall that \mathcal{S} denotes the set of critical point of F (cf. (7)).

From the gradient stability of the BDF4 method, we infer:

Corollary 3.3. *Assume that $c_F \Delta t \leq 41/72$, and let (U^n) be a sequence in \mathbb{R}^M defined by the 4-step BDF method. Then $\omega((U^n)_n)$ is a compact and connected subset of \mathbb{R}^M included in \mathcal{S} .*

Proof. Since F is continuous on \mathbb{R}^M and coercive (assumption (5)), F is bounded from below, i.e. there exists a real number m such that

$$F(V) \geq m, \quad \forall V \in \mathbb{R}^M.$$

By (32), the sequence $\hat{F}_4(\hat{U}^{n+3})$ is nonincreasing; it is also bounded from below (by m), so it converges to a value $F^* \in \mathbb{R}$. By induction, we obtain from (32) that for all $N \geq 0$,

$$\hat{F}_4(\hat{U}^{N+4}) + \frac{1}{\Delta t} \sum_{n=0}^N \tilde{R}_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \leq \hat{F}_4(\hat{U}^3).$$

Letting N tend to $+\infty$, we find that

$$\frac{1}{\Delta t} \sum_{n=0}^{+\infty} \tilde{R}_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \leq \hat{F}_4(\hat{U}^3) - m < +\infty.$$

In particular, $\tilde{R}_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \rightarrow 0$. Since \tilde{R}_4 is positive definite, we know that

$$\begin{aligned} & \lambda (\|\partial U^{n+4}\|^2 + \|\partial U^{n+3}\|^2 + \|\partial U^{n+2}\|^2 + \|\partial U^{n+1}\|^2) \\ & \leq \tilde{R}_4(\partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}), \end{aligned}$$

for some constant $\lambda > 0$ independent of n , and so $\partial U^{n+1} \rightarrow 0$. The boundedness of $\hat{F}_4(\hat{U}^{n+3})$ also implies that $(U^n)_n$ is bounded. A standard argument shows then that $\omega((U^n)_n)$ is a compact and connected subset of \mathbb{R}^M . If $U^* = \lim_{p \rightarrow +\infty} U^{n_p+4}$ is an element of $\omega((U^n)_n)$, then the right hand-side of (8) (with $k = 4$) tends to $-\Delta t \nabla F(U^*)$, while the left hand-side tends to 0. Thus $U^* \in \mathcal{S}$, and the proof is complete. \square

Corollary 3.4. *Assume that $c_F \Delta t \leq 41/72$, and let (U^n) be a sequence in \mathbb{R}^M defined by the 4-step BDF method. Assume moreover that either one of the following assumptions hold:*

- i) the space dimension is $M = 1$;
- i) the critical points of F are isolated;
- ii) the function F is real analytic on \mathbb{R}^M .

Then the whole sequence $(U^n)_n$ converges to a single point U^* which is a critical point of F .

Proof. If i) holds, a proof similar to [15, Corollary 2] can be carried out. It uses that \mathbb{R} is an ordered field. Details are left to the reader.

If assumption ii) holds, then the result is a direct consequence of Corollary 3.3.

If assumption iii) holds, the claim follows from general results on descent methods. We refer for instance to [2, Theorem 2.4]. In this case, the crucial point is the Lojasiewicz inequality for real analytic functions: it applies here to the Lyapunov function \hat{F}_4 . \square

3.3. Gradient stability of the BDF5 method

From Proposition 2.8, we deduce:

Lemma 3.5. *The quadratic forms Γ_5 , Q_5 and R_5 associated to γ_5 , q_5 and r_5 satisfy*

$$\Gamma_5(V_1, V_2, V_3, V_4, V_5) = Q_5(V_1, V_2, V_3, V_4) - Q_5(V_2, V_3, V_4, V_5) + R_5(V_1, V_2, V_3, V_4, V_5) \quad (34)$$

for all $(V_1, V_2, V_3, V_4, V_5) \in (\mathbb{R}^M)^5$. In particular, Q_5 and R_5 are positive definite. Moreover,

$$R_5(V_1, V_2, V_3, V_4, V_5) = \frac{1}{20} \|V_1\|^2 + \tilde{R}_5(V_1, V_2, V_3, V_4, V_5), \quad (35)$$

where \tilde{R}_5 is positive definite on $(\mathbb{R}^M)^5$.

Proof. It remains only to prove that \tilde{R}_5 is positive definite. For this purpose, we consider the quadratic form on \mathbb{R}^5 defined by

$$\tilde{r}_5(x_1, x_2, x_3, x_4, x_5) = r_5(x_1, x_2, x_3, x_4, x_5) - \frac{1}{20} x_1^2.$$

Using Sylvester's criterion, we easily check that $A_{\tilde{r}_5}$ is positive definite. The claim on \tilde{R}_5 follows. As previously, the coefficient $1/20$ was found by numerical investigation and it is not optimal. \square

For $\hat{V} = (V_0, V_1, V_2, V_3, V_4) \in (\mathbb{R}^M)^5$, we define

$$\hat{F}_5(\hat{V}) = F(V_0) + \frac{1}{\Delta t} Q_5(V_1, V_2, V_3, V_4),$$

and for a sequence $(U^n)_{n \geq 0}$ in \mathbb{R}^M , we define

$$\hat{U}^{n+5} = (U^{n+5}, \partial U^{n+5}, \partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}),$$

so that

$$\hat{F}_5(\hat{U}^{n+5}) = F(U^{n+5}) + \frac{1}{\Delta t} Q_5(\partial U^{n+5}, \partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}).$$

By arguing as in the proof of Theorem 3.2 and using Lemma 3.5, we find:

Theorem 3.6. *If $c_F \Delta t \leq 1/10$, the 5-step BDF method (8) is gradient-stable, i.e.*

$$\hat{F}_5(\hat{U}^{n+5}) + \frac{1}{\Delta t} \tilde{R}_5(\partial U^{n+5}, \partial U^{n+4}, \partial U^{n+3}, \partial U^{n+2}, \partial U^{n+1}) \leq \hat{F}_5(\hat{U}^{n+4}), \quad n \geq 0. \quad (36)$$

As a consequence of the gradient stability of BDF5 method, Corollaries 3.3 and 3.4 are also valid for a sequence $(U^n)_n$ generated by the BDF5 scheme (assuming the stability condition $c_F \Delta t \leq 1/10$ for the time step).

In Table 1, we sum up the results obtained so far regarding uniqueness and gradient stability of k -step BDF schemes. Uniqueness is ensured if $c_F \Delta t < \alpha_k$ (cf. (12)-(13)) and gradient stability is ensured if $c_F \Delta t < \beta_k$. The values of β_k ($1 \leq k \leq 3$) obtained in [27] have been improved here by a factor two, thanks to (33). For $k = 1$, we can have $\beta_1 = +\infty$ if the BDF1 scheme is the proximal algorithm [5, 21]. For $k = 1, 2$, we have $\alpha_k < \beta_k$: a particular choice of initial values may produce several gradient stable sequences. In contrast, for $3 \leq k \leq 5$, we have $\alpha_k > \beta_k$, so that provably gradient stable sequences are uniquely defined. We note that the values of β_4 and β_5 are not optimal (cf. Lemmas 3.1 and 3.5), and we do not know if β_3 is optimal. If the function F is convex, then $c_F = 0$ and the BDF methods are unconditionnally stable for $1 \leq k \leq 5$.

Table 1. Uniqueness and gradient stability conditions for BDF methods

k	1	2	3	4	5	6	≥ 7
α_k	1	3/2	11/6	25/12	137/60	49/20	$\sum_{j=1}^k 1/j$
β_k	2 or ∞	2	5/3	41/72	1/10	?	0 (not g. s.)

4. The BDF3 scheme applied to the Allen-Cahn equation

4.1. Notation and assumptions

Let $H = L^2(\Omega)$ be equipped with the $L^2(\Omega)$ norm $|\cdot|_0$ and product (\cdot, \cdot) . We denote $V = H_0^1(\Omega)$ the standard Sobolev space, and $|\cdot|_1 = |\nabla \cdot|_0$ the associated hilbertian norm. Recall that $-\Delta : V \rightarrow V'$ is an isomorphism associated to the inner product on V through

$$\langle -\Delta u, v \rangle_{V' \times V} = (\nabla u, \nabla v) \quad \forall u, v \in V.$$

We assume that the nonlinearity $g : \mathbb{R} \rightarrow \mathbb{R}$ in (1) is real analytic on \mathbb{R} and if $d \geq 2$, we assume that there exist $c > 0$ and $p \geq 0$ such that

$$(d-2)p < 4 \quad \text{and} \quad |g'(s)| \leq c(1 + |s|^p) \quad \forall s \in \mathbb{R}. \quad (37)$$

No growth assumption is required if $d = 1$. Moreover, there exists a constant $c_g \geq 0$ such that

$$g'(s) \geq -c_g \quad \forall s \in \mathbb{R}. \quad (38)$$

The last assumption is a coercivity condition which yields

$$\liminf_{|s| \rightarrow \infty} \frac{g(s)}{s} > -\lambda_1, \quad (39)$$

where $\lambda_1 > 0$ is the first eigenvalue of $-\Delta$, that is

$$\lambda_1 = \inf_{v \in V \setminus \{0\}} \frac{|v|_1^2}{|v|_0^2}. \quad (40)$$

The Poincaré inequality implies that $\lambda_1 > 0$. We note that H is continuously imbedded in V' and for all $v \in H$, we have

$$\|v\|_{V'} := \sup_{|w|_1 \leq 1} \langle v, w \rangle_{V' \times V} = \sup_{|w|_1 \leq 1} (v, w) \leq \sup_{|w|_1 \leq 1} |v|_0 |w|_0 \leq \frac{1}{\sqrt{\lambda_1}} |v|_0. \quad (41)$$

By the mean value theorem, we have

$$(g(b) - g(a))(a - b) \geq -c_f(a - b)^2, \quad \forall a, b \in \mathbb{R}. \quad (42)$$

Conversely, this relation implies (38), which can therefore be considered as a one-sided Lipschitz condition on g (cf. (4)).

We define G as the functional $G(s) = \int_0^s g(r) dr$. Assumption (38) implies that G is *semi-convex*, i.e. $s \mapsto G(s) + (c_g/2)s^2$ is convex.

We note that the standard choice $g(s) = s^3 - s$ satisfies (37)-(39) in space dimension $1 \leq d \leq 3$.

4.2. Derivation of the BDF3 scheme

Consider a uniform grid on $[0, +\infty)$ with a positive stepsize Δt and times $t_n = n\Delta t$ ($n = 0, 1, \dots$). We shall compute $u(t)$ at these points, and we denote (momentarily) $u^n = u(t^n)$. Consider the third degree polynomial P_u interpolating u^n, u^{n-1}, u^{n-2} and u^{n-3} at times t_n, t_{n-1}, t_{n-2} and t_{n-3} respectively,

$$P_u(t) = \sum_{k=0}^3 \prod_{\substack{j=0 \\ j \neq k}}^3 \frac{t - t_{n-j}}{t_{n-k} - t_{n-j}} u^{n-k}.$$

Since the grid is uniform, this interpolation polynomial P_u can also be written in Newton form (divided differences),

$$P_u(t) = u^n + \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \prod_{j=0}^{k-1} (t - t_{n-j}) \partial^k u^n,$$

where $\partial^k u^n$ is recursively defined by $\partial^k u^n = \partial^{k-1}(\partial u^n) = \partial^{k-1}(u^n - u^{n-1})$, for $k \geq 1$. If the last equation is differentiated with respect to t , one gets

$$\begin{aligned} \frac{d}{dt} P_u(t) &= \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \left(\frac{d}{dt} \prod_{j=0}^{k-1} (t - t_{n-j}) \right) \partial^k u^n \\ &= \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \left(\sum_{p=0}^{k-1} \prod_{\substack{j=0 \\ j \neq p}}^{k-1} (t - t_{n-j}) \right) \partial^k u^n, \end{aligned}$$

that is

$$\frac{d}{dt} P_u(t) = \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \left(\underbrace{\sum_{p=1}^{k-1} \prod_{\substack{j=0 \\ j \neq p}}^{k-1} (t - t_{n-j}) + \prod_{j=1}^{k-1} (t - t_{n-j})}_{P(t)} \right) \partial^k u^n.$$

Since t_n is a root of the polynomial P , by setting $t = t_n$, we obtain

$$\begin{aligned} \frac{d}{dt} P_u(t_n) &= \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \left(\prod_{j=1}^{k-1} (t_n - t_{n-j}) \right) \partial^k u^n \\ &= \sum_{k=1}^3 \frac{1}{\Delta t^k k!} \left(\prod_{j=1}^{k-1} j \Delta t \right) \partial^k u^n. \end{aligned}$$

Thus, we have

$$\frac{d}{dt} P_u(t_n) = \frac{1}{\Delta t} \sum_{k=1}^3 \frac{1}{k} \partial^k u^n. \quad (43)$$

Substituting (43) into (1) yields the 3-step backward differentiation formula applied to the Allen-Cahn equation,

$$\frac{1}{\Delta t} \sum_{k=1}^3 \frac{1}{k} \partial^k u^n - \Delta u^n + g(u^n) = 0, \quad (44)$$

that is,

$$\frac{1}{\Delta t} \left(\frac{11}{6} u^n - 3u_{n-1} + \frac{3}{2} u_{n-2} - \frac{1}{3} u_{n-3} \right) - \Delta u^n + g(u^n) = 0.$$

We note that (44) holds only up to order $(\Delta t)^3$ if $u^n = u(t_n)$, so that the sequence $(u^n)_n$ generated by (44) only defines an approximation of the values $(u(t_n))_n$. The third order

accuracy of the BDF3 scheme is well-known in the finite dimensional case [27]. It could also be carried out in our situation by using standard techniques and by assuming enough regularity on the solution of (1). We refer to [29] for an error analysis of a fully discrete version of (1) based on the BDF1 (i.e. backward Euler) scheme for the time discretization; see also [25] for an error analysis in the case of a second-order scheme.

We shall study the scheme in the following form: let $u^0, u^1, u^2 \in V$, and for $n = 2, 3, \dots$, let $u^{n+1} \in V$ solve

$$u^{n+1} - \frac{18}{11}u^n + \frac{9}{11}u^{n-1} - \frac{2}{11}u^{n-2} - \frac{6}{11}\Delta t \Delta u^{n+1} + \frac{6}{11}\Delta t g(u^{n+1}) = 0 \quad (45)$$

in V' .

4.3. Existence, uniqueness and stability

Proposition 4.1 (Existence). *For any $(u^0, u^1, u^2) \in V^3$, there exists at least one sequence $(u^n)_{n \geq 0}$ in V which complies with (45).*

Proof. Let u^{n-2}, u^{n-1}, u^n be fixed in V . Then u^{n+1} can be obtained as a minimizer of the functional

$$\begin{aligned} \mathcal{G}_n : V &\longrightarrow \mathbb{R} \\ u &\longmapsto \frac{1}{2}|u|_0^2 + \frac{1}{11}(u, -18u^n + 9u^{n-1} - 2u^{n-2}) + \frac{3}{11}\Delta t |u|_1^2 + \frac{6}{11}\Delta t (G(u), 1). \end{aligned}$$

The growth restriction (37) and Sobolev imbeddings imply that the functional $u \mapsto (G(u), 1)$ is well-defined and of class C^1 on V [19]. The coercivity condition (39) implies the existence of constants $k_1 < \lambda_1$ and $k_2 \geq 0$ such that, for all s in \mathbb{R} ,

$$G(s) \geq -\frac{k_1}{2}s^2 - k_2.$$

By integration on Ω ,

$$\begin{aligned} (G(u), 1) &\geq -\frac{k_1}{2}|u|_0^2 - k_2|\Omega| \\ &\geq -\frac{k_1}{2\lambda_1}|u|_1^2 - k_2|\Omega|, \end{aligned} \quad (46)$$

where in the last inequality, we use the Poincaré inequality (40). A direct consequence is that

$$\mathcal{G}_n(u) \geq \frac{1}{4}|u|_0^2 + \left(1 - \frac{k_1}{\lambda_1}\right) \frac{3}{11}\Delta t |u|_1^2 - c_n \quad (47)$$

for some constant $c_n \geq 0$ independent of $u \in V$. In particular, \mathcal{G}_n is bounded from below. Denote then $m = \inf_{v \in V} \mathcal{G}_n(v)$ and consider a minimizing sequence $(v_k)_{k \geq 0} \subset V$. By (47), $(v^k)_k$ is bounded in V and we know by Rellich's theorem that V is compactly imbedded in H . Hence we can extract a subsequence of (v_k) , also denoted (v_k) , such that (v_k) converges weakly in V , strongly in H , and a.e. in Ω to some function $u^* \in V$. Using Fatou's lemma and the lower

semi-continuity of the V -norm, we obtain

$$\mathcal{G}_n(u^*) \leq \liminf_k \mathcal{G}_n(v_k) = m = \inf_{v \in V} \mathcal{G}_n(v).$$

As a consequence, u^* is a minimizer of \mathcal{G}_n : it satisfies the associated Euler-Lagrange equation, i.e. $(\frac{d}{du} \mathcal{G}_n(u^*), w) = 0, \forall w \in V$, which reads

$$(u^*, w) + \frac{1}{11}(-18u^n + 9u^{n-1} - 2u^{n-2}, w) + \frac{6}{11} \Delta t [(\nabla u^*, \nabla w) + (g(u^*), w)] = 0.$$

A possible value of u^{n+1} is then u^* . □

Proposition 4.2 (Uniqueness). *Assume that $\lambda_1 + \frac{11}{6\Delta t} > c_g$. Then for every choice of $(u^{n-2}, u^{n-1}, u^n) \in V^3$, there exists at most one $u^{n+1} \in V$ which satisfies (45).*

Proof. Let u^{n-2}, u^{n-1} and u^n be fixed in V . Suppose that u^{n+1} and v^{n+1} are two solutions of the scheme. We have

$$\begin{cases} u^{n+1} - \frac{18}{11}u^n + \frac{9}{11}u^{n-1} - \frac{2}{11}u^{n-2} - \frac{6}{11}\Delta t \Delta u^{n+1} + \frac{6}{11}\Delta t g(u^{n+1}) = 0, \\ v^{n+1} - \frac{18}{11}u^n + \frac{9}{11}u^{n-1} - \frac{2}{11}u^{n-2} - \frac{6}{11}\Delta t \Delta v^{n+1} + \frac{6}{11}\Delta t g(v^{n+1}) = 0. \end{cases}$$

Denote $\delta u = u^{n+1} - v^{n+1}$. We have

$$\delta u - \frac{6}{11}\Delta t \Delta(\delta u) + \frac{6}{11}\Delta t (g(u^{n+1}) - g(v^{n+1})) = 0$$

On multiplying by δu in H , we get

$$|\delta u|_0^2 + \frac{6}{11}\Delta t |\delta u|_1^2 + \frac{6}{11}\Delta t (g(u^{n+1}) - g(v^{n+1}), \delta u) = 0$$

Using the one-sided Lipschitz condition (42), we obtain

$$(g(u^{n+1}) - g(v^{n+1}), \delta u) \geq -c_g |\delta u|_0^2.$$

Hence,

$$|\delta u|_0^2 + \frac{6}{11}\Delta t |\delta u|_1^2 \leq \frac{6}{11}\Delta t c_g |\delta u|_0^2,$$

and by the Poincaré inequality (40), we have

$$\left(\lambda_1 + \frac{11}{6\Delta t} - c_g \right) |\delta u|_0^2 \leq 0.$$

The proof is complete. □

Remark 4.3. Notice that if $c_g \Delta t \leq 11/6$, then uniqueness is ensured.

In order to achieve stability, the idea is to exhibit a Lyapunov functional for (45) in a way such that the set of equilibria set associated to the functional is related to the set of equilibria of the Allen-Cahn equation.

First recall the energy functional associated to the Allen-Cahn equation (cf. (2)),

$$\begin{aligned} E : V &\longrightarrow \mathbb{R} \\ u &\longmapsto E(u) = \frac{1}{2} |u|_1^2 + (G(u), 1). \end{aligned}$$

The growth assumption (37) on g and Sobolev imbeddings imply that E is well-defined and of class C^1 on V [19].

The set of critical points of E is defined as

$$\mathcal{S} = \{u \in V, -\Delta u + g(u) = 0 \text{ in } V'\}.$$

The Lyapunov functional $\mathcal{E} : V^3 \longrightarrow \mathbb{R}$ associated to the BDF3 is defined by

$$\mathcal{E}(u, v, w) = E(u) + \frac{5}{12\Delta t} |v|_0^2 + \frac{1}{6\Delta t} |w|_0^2. \quad (48)$$

Remark that the set of critical points of \mathcal{E} is $\mathcal{S} \times \{0\} \times \{0\}$, which, in a sense, is equivalent to \mathcal{S} .

The following proposition shows the nonincreasing property. As a shortcut, we denote $\mathcal{E}^n = \mathcal{E}(u^n, \partial u^n, \partial^2 u^n)$ for all $n \geq 2$.

Proposition 4.4 (Lyapunov stability). *Assume that $\frac{5}{6\Delta t} \geq c_g$ and let $(u^n)_{n \geq 2}$ be a sequence in V generated by (45). Then for all $n \geq 2$,*

$$\begin{aligned} \mathcal{E}^{n+1} + \frac{1}{2} |\partial u^{n+1}|_1^2 + \left(\frac{5}{6\Delta t} - c_g\right) |\partial u^{n+1}|_0^2 + \frac{1}{4\Delta t} |\partial^2 u^{n+1}|_0^2 \\ + \frac{1}{6\Delta t} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \leq \mathcal{E}^n. \end{aligned} \quad (49)$$

Proof. We write the BDF3 scheme (45) in the following form, valid for all $n \geq 2$ (cf. (44)),

$$\frac{1}{\Delta t} \sum_{j=1}^3 \frac{1}{j} \partial^j u^{n+1} - \Delta u^{n+1} + g(u^{n+1}) = 0. \quad (50)$$

On multiplying (50) by ∂u^{n+1} in H , we obtain

$$\underbrace{\frac{1}{\Delta t} \sum_{j=1}^3 \frac{1}{j} (\partial^j u^{n+1}, \partial u^{n+1})}_{\Sigma} + (\nabla u^{n+1}, \nabla(\partial u^{n+1})) + (g(u^{n+1}), \partial u^{n+1}) = 0. \quad (51)$$

By the Taylor-Lagrange theorem and (38), we deduce that

$$\forall a, b \in \mathbb{R} \quad G(b) - G(a) \geq (b - a)g(a) - \frac{c_g}{2}(a - b)^2,$$

and so

$$\frac{1}{\Delta t}\Sigma + (\nabla u^{n+1}, \nabla(\partial u^{n+1})) \leq (G(u^n), 1) - (G(u^{n+1}), 1) + c_g |\partial u^{n+1}|_0^2.$$

Using the well known identity

$$(A, A - B) = \frac{1}{2}(A, A) - \frac{1}{2}(B, B) + \frac{1}{2}(A - B, A - B), \quad (52)$$

we obtain

$$\frac{1}{\Delta t}\Sigma + \frac{1}{2} \left(|u^{n+1}|_1^2 - |u^n|_1^2 \right) + \frac{1}{2} |\partial u^{n+1}|_1^2 \leq (G(u^n), 1) - (G(u^{n+1}), 1) + c_g |\partial u^{n+1}|_0^2.$$

By mimicking identity (17), we check that Σ can be written

$$\begin{aligned} \Sigma &= \frac{5}{6} |\partial u^{n+1}|_0^2 + \frac{1}{4} |\partial^2 u^{n+1}|_0^2 + \frac{1}{6} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \\ &\quad + \frac{5}{12} \left(|\partial u^{n+1}|_0^2 - |\partial u^n|_0^2 \right) + \frac{1}{6} \left(|\partial^2 u^{n+1}|_0^2 - |\partial^2 u^n|_0^2 \right). \end{aligned} \quad (53)$$

This is the key to the Lyapunov stability. Indeed, we find

$$\begin{aligned} \mathcal{E}^{n+1} + \frac{1}{2} |\partial u^{n+1}|_1^2 + \frac{5}{6\Delta t} |\partial u^{n+1}|_0^2 + \frac{1}{4\Delta t} |\partial^2 u^{n+1}|_0^2 \\ + \frac{1}{6\Delta t} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \leq \mathcal{E}^n + c_g |\partial u^{n+1}|_0^2, \end{aligned}$$

and the proposition is proved. \square

5. Convergence to equilibrium for the BDF3 scheme

Let $(u^n)_n$ be a sequence in V . We define its ω -limit set by

$$\omega((u^n)_n) = \{u^* \in V, \exists n_k \longrightarrow \infty \text{ s.t. } u^{n_k} \longrightarrow u^* \text{ in } V\}.$$

Throughout this section, we assume that the stability condition holds, that is $\frac{5}{6\Delta t} \geq c_g$. In particular, the uniqueness condition is also valid.

Proposition 5.1. *Let $(u^n)_{n \geq 2}$ be a sequence in V generated by (45). Then $(u^n)_{n \geq 2}$ is bounded in V , $\partial u^n \longrightarrow 0$ in V , $\partial^j u^n \longrightarrow 0$ in H for $j = 2, 3$ and E is constant on $\omega((u^n)_n)$.*

Proof. We deduce from (46) that

$$\mathcal{E}(u, v, w) \geq \frac{1}{2} \left(1 - \frac{k_1}{\lambda_1} \right) |u|_1^2 + \frac{5}{12\Delta t} |v|_0^2 + \frac{1}{6\Delta t} |w|_0^2 - k_2 |\Omega|, \quad (54)$$

for all $(u, v, w) \in V \times H \times H$. In particular, \mathcal{E}^n is bounded from below. Adding the fact that $(\mathcal{E}^n)_n$ is nonincreasing by the stability inequality (49), we conclude that \mathcal{E}^n converges in \mathbb{R}

to some real number \mathcal{E}^* . From the boundedness of (\mathcal{E}^n) and estimate (54), we deduce that $(u^n)_{n \geq 2}$ is bounded in V . Using now the stability inequality (49), we have

$$\frac{1}{2} |\partial u^{n+1}|_1^2 + \frac{1}{4\Delta t} |\partial^2 u^{n+1}|_0^2 + \frac{1}{6\Delta t} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \leq \mathcal{E}^n - \mathcal{E}^{n+1}, \quad (55)$$

for all $n \geq 2$. By summing on n , we find that

$$\sum_{n=2}^{\infty} \left(|\partial u^{n+1}|_1^2 + |\partial^2 u^{n+1}|_0^2 \right) \leq C \sum_{n=2}^{\infty} (\mathcal{E}^n - \mathcal{E}^{n+1}) < C (\mathcal{E}^2 - \mathcal{E}^*),$$

where $C = (\min\{1/2, 1/4\Delta t\})^{-1}$. Since $\mathcal{E}^2 = \mathcal{E}(u^2, \partial u^2, \partial^2 u^2) < \infty$, this implies that $\partial u^n \rightarrow 0$ in V and $\partial^2 u^n \rightarrow 0$ in H . Thus, $E(u^n)$ tends to the same limit \mathcal{E}^* as \mathcal{E}^n . This implies that E is constant and equal to \mathcal{E}^* on $\omega((u^n)_n)$.

In a similar way, we obtain from (55) that

$$\sum_{n=2}^{\infty} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \leq 6\Delta t (\mathcal{E}^2 - \mathcal{E}^*) < +\infty.$$

Thus, $\partial u^{n+1} - \partial u^n + \partial u^{n-1} \rightarrow 0$ in H and since

$$\begin{aligned} \partial^3 u^{n+1} &= \partial u^{n+1} - 2\partial u^n + \partial u^{n-1} \\ &= (\partial u^{n+1} - \partial u^n + \partial u^{n-1}) - \partial u^n, \end{aligned}$$

we see that $\partial^3 u^{n+1} \rightarrow 0$ in H . The proof is achieved. \square

Proposition 5.2. *Let $(u^n)_{n \geq 2}$ be a sequence in V generated by (45). Then the set $\omega((u^n)_n)$ is a nonempty compact and connected subset of V included in \mathcal{S} .*

Proof. We first claim that the set $\{u^n : n \in \mathbb{N}\}$ is precompact in V . The idea is to use elliptic regularity in order to find a constant $q > 1$ such that (u^{n+1}) is bounded in $\mathbb{W}^{2,q}(\Omega)$ with $\mathbb{W}^{2,q}(\Omega)$ compactly imbedded in V . Here, $\mathbb{W}^{2,q}(\Omega)$ is the standard Sobolev space based on the $L^q(\Omega)$ space. It is well-known [13] that $\mathbb{W}^{2,q}(\Omega)$ is compactly imbedded in V if

$$2 - \frac{d}{q} > 1 - \frac{d}{2} \iff q > \frac{2d}{2+d}. \quad (56)$$

From the BDF3 scheme (45), we have

$$\Delta u^{n+1} = l(u^{n+1}, u^n, u^{n-1}, u^{n-2}) + g(u^{n+1}), \quad (57)$$

where the functional l depends linearly on its variable. Thus, $l(u^{n+1}, u^n, u^{n-1}, u^{n-2})$ is bounded in $L^2(\Omega)$ (and also in $L^q(\Omega)$, for any $1 < q \leq 2$). By Proposition 5.1, $(u^n)_n$ is bounded in V . This implies that $(g(u^{n+1}))_n$ is bounded in $L^q(\Omega)$ for an appropriate choice of q . Now we discuss according to d .

First assume that $d \geq 3$. For any $q \in (1, 2]$, we have, using the growth condition (37),

$$\|g(u^{n+1})\|_{L^q(\Omega)} \leq C (1 + \|u^{n+1}\|_{L^{(p+1)q}(\Omega)}),$$

for some constant C independent of n . By Sobolev imbeddings, (u^{n+1}) is bounded in $L^{2^*}(\Omega)$ where $2^* = \frac{2d}{d-2}$. Since $p(d-2) < 4$, we have $p+1 < \frac{d+2}{d-2}$, and by choosing $q = \min\{\frac{2^*}{p+1}, 2\} \in (1, 2]$, relation (56) is satisfied and $g(u^{n+1})$ is bounded in $L^q(\Omega)$. By elliptic regularity [13], from (57) we deduce that (u^{n+1}) is bounded in $\mathbb{W}^{2,q}(\Omega)$ and this concludes the case $d \geq 3$.

If $d = 1$ or $d = 2$, we obtain from Sobolev embeddings that $(g(u^{n+1}))_n$ is bounded in any $L^r(\Omega)$, $r < \infty$, so we may choose $q = 2$ in (57) and we conclude as previously. This proves the claim concerning precompactness of the set $\omega((u^n)_n)$.

It is well known that $\omega((u^n)_n)$ is closed in V , so it is a nonempty compact subset of V . Using that $|\partial u^{n+1}|_1 = |u^{n+1} - u^n|_1$ converges to 0 (cf. Proposition 5.1), a standard argument shows that $\omega((u^n)_n)$ is also connected in V .

Let now $u^* \in \omega((u^n)_n)$. There exists $n_k \rightarrow \infty$ such that $u^{n_k} \rightarrow u^*$ strongly in V and (u^{n_k}) complies with (50). By Proposition 5.1, $\partial^j u^{n_k}$ converges to 0 for $j = 1, 2$ and 3. Hence, $-\Delta u^* + g(u^*) = 0$, so u^* belongs to \mathcal{S} as claimed. \square

The results obtained so far are valid if $g \in C^1(\mathbb{R}, \mathbb{R})$ only. The following lemma, which is the Łojasiewicz-Simon inequality, uses that g is real analytic.

Lemma 5.3. *Let $u^* \in \mathcal{S}$. Then there exist constants $\theta \in (0, \frac{1}{2})$ and $\delta > 0$ depending on u^* such that for any $u \in V$ satisfying $|u - u^*|_1 < \delta$, we have*

$$|E(u) - E(u^*)|^{1-\theta} \leq \| -\Delta u + g(u) \|_{V'}. \quad (58)$$

Proof. The inequality has been proved in [18, Proposition 11.4.1]. \square

Theorem 5.4. *Let $(u^n)_{n \geq 2}$ be a sequence in V generated by (45). Then the whole sequence converges to a steady state u^∞ in V , with $u^\infty \in \mathcal{S}$.*

Proof. The union of balls $\{\mathcal{B}_\delta(u^*), u^* \in \omega((u^n)_n)\}$ forms an open covering of $\omega((u^n)_n)$. Due to the compactness of $\omega((u^n)_n)$ in V , we can extract a finite subcovering $\{\mathcal{B}_{\delta_i}(u_i^*)\}_{i=1, \dots, m}$ in a way that the constants θ_i and δ_i corresponding to u_i^* in Lemma 5.3 are indexed by i .

From the definition of $\omega((u^n)_n)$, we can always find a sufficiently large n_0 such that $u^n \in \bigcup_{i=1}^m \mathcal{B}_{\delta_i}(u_i^*)$ for all $n \geq n_0$. Consider $\theta = \min_{i=1, \dots, m} \{\theta_i\}$, then by Lemma 5.3 and Proposition 5.1, we have for all $n \geq n_0$,

$$|E(u) - \mathcal{E}^*|^{1-\theta} \leq \| -\Delta u + g(u) \|_{V'},$$

where \mathcal{E}^* is the constant value of E on $\omega((u^n)_n)$. We will also choose n_0 large enough so that $|\partial^j u^{n+1}|_0 \leq 1$ for $j = 1, 2$ and for all $n \geq n_0$. Denote $\phi^n = \mathcal{E}^n - \mathcal{E}^*$ so that $(\phi^n)_n$ is nonincreasing and bounded from below by 0.

Let $n \geq n_0$. Using the well-known inequality $(a+b)^{1-\theta} \leq a^{1-\theta} + b^{1-\theta}$ satisfied by all nonnegative numbers a and b , we find that

$$\begin{aligned} (\phi^{n+1})^{1-\theta} &\leq |E(u^{n+1}) - E^\infty|^{1-\theta} + \left(\frac{5}{12\Delta t} |\partial u^{n+1}|_0^2 + \frac{1}{6\Delta t} |\partial^2 u^{n+1}|_0^2 \right)^{1-\theta} \\ &\leq \| -\Delta u^{n+1} + g(u^{n+1}) \|_{V'} + \left(\frac{5}{12\Delta t} |\partial u^{n+1}|_0^2 + \frac{1}{6\Delta t} |\partial^2 u^{n+1}|_0^2 \right)^{1-\theta} \\ &\leq \left\| \frac{1}{\Delta t} \sum_{j=1}^3 \frac{\partial^j u^{n+1}}{j} \right\|_{V'} + \left(\frac{5}{12\Delta t} |\partial u^{n+1}|_0^2 + \frac{1}{6\Delta t} |\partial^2 u^{n+1}|_0^2 \right)^{1-\theta}. \end{aligned}$$

The last inequality is obtained by the version (50) of the BDF3 scheme. Next, we note that

$$\begin{aligned}
\sum_{j=1}^3 \frac{\partial^j u^{n+1}}{j} &= \partial u^{n+1} + \frac{1}{2} (\partial u^{n+1} - \partial u^n) + \frac{1}{3} (\partial u^{n+1} - 2\partial u^n + \partial u^{n-1}) \\
&= \frac{3}{2} \partial u^{n+1} - \frac{5}{6} \partial u^n + \frac{1}{3} (\partial u^{n+1} - \partial u^n + \partial u^{n-1}) \\
&= \frac{2}{3} \partial u^{n+1} + \frac{5}{6} (\partial u^{n+1} - \partial u^n) + \frac{1}{3} (\partial u^{n+1} - \partial u^n + \partial u^{n-1}) \\
&= \frac{2}{3} \partial u^{n+1} + \frac{5}{6} \partial^2 u^{n+1} + \frac{1}{3} (\partial u^{n+1} - \partial u^n + \partial u^{n-1}).
\end{aligned}$$

Since H is continuously imbedded into V' (cf. (41)), this yields

$$\begin{aligned}
(\phi^{n+1})^{1-\theta} &\leq \frac{2\lambda_1^{-1/2}}{3\Delta t} |\partial u^{n+1}|_0 + \frac{5\lambda_1^{-1/2}}{6\Delta t} |\partial^2 u^{n+1}|_0 + \frac{\lambda_1^{-1/2}}{3\Delta t} |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0 \\
&\quad + \left(\frac{5}{12\Delta t}\right)^{1-\theta} |\partial u^{n+1}|_0^{2(1-\theta)} + \left(\frac{1}{6\Delta t}\right)^{1-\theta} |\partial^2 u^{n+1}|_0^{2(1-\theta)} \\
&\leq c \left(|\partial u^{n+1}|_1^2 + |\partial^2 u^{n+1}|_0^2 + |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \right)^{\frac{1}{2}}, \tag{59}
\end{aligned}$$

where c is a constant independent of n .

Assume first that $\phi^{n+1} > \phi^n/2$. Then we have

$$\begin{aligned}
(\phi^n)^\theta - (\phi^{n+1})^\theta &= \int_{\phi^{n+1}}^{\phi^n} \theta x^{\theta-1} dx \\
&\geq \theta (\phi^n)^{\theta-1} (\phi^n - \phi^{n+1}) \\
&\geq \theta 2^{\theta-1} (\phi^{n+1})^{\theta-1} (\phi^n - \phi^{n+1}).
\end{aligned}$$

From Proposition 4.4 and 59, we obtain

$$(\phi^n)^\theta - (\phi^{n+1})^\theta \geq C \left(|\partial u^{n+1}|_1^2 + |\partial^2 u^{n+1}|_0^2 + |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \right)^{\frac{1}{2}}. \tag{60}$$

If $\phi^{n+1} \leq \phi^n/2$, by using Proposition 4.4 again, we find that for all $n \geq 2$,

$$\begin{aligned}
(\phi^n)^{\frac{1}{2}} - (\phi^{n+1})^{\frac{1}{2}} &\geq \frac{\sqrt{2}-1}{\sqrt{2}} (\phi^n)^{\frac{1}{2}} \\
&\geq \frac{\sqrt{2}-1}{\sqrt{2}} (\phi^n - \phi^{n+1})^{\frac{1}{2}} \\
&\geq C' \left(|\partial u^{n+1}|_1^2 + |\partial^2 u^{n+1}|_0^2 + |\partial u^{n+1} - \partial u^n + \partial u^{n-1}|_0^2 \right)^{\frac{1}{2}}. \tag{61}
\end{aligned}$$

In both cases, inequalities (60) and (61) imply that for all $n \geq n_0$,

$$|\partial u^{n+1}|_1 \leq \frac{1}{C} \left((\phi^n)^\theta - (\phi^{n+1})^\theta \right) + \frac{1}{C'} \left((\phi^n)^{\frac{1}{2}} - (\phi^{n+1})^{\frac{1}{2}} \right).$$

By summing on n , we find that

$$\sum_{n=n_0}^{\infty} |u^{n+1} - u^n|_1 \leq \frac{1}{C}(\phi^{n_0})^\theta + \frac{1}{C'}(\phi^{n_0})^{\frac{1}{2}} < \infty.$$

This implies that $(u^n)_n$ converges to some u^∞ in V . By Proposition 5.2, u^∞ belongs to \mathcal{S} . \square

Remark 5.5. By using the gradient stability proved in Section 3 and by arguing as for the BDF3 scheme, we could obtain a result similar to Theorem 5.4 for the BDF4 and BDF5 methods.

6. Numerical simulations

We present some numerical simulations to illustrate the theoretical results. We consider the 1d Allen-Cahn equation endowed with homogeneous Dirichlet boundary conditions,

$$\begin{cases} u_t - \Delta u + g(u) = 0, & (x, t) \in (0, L) \times (0, T], \\ u(0, t) = u(L, t) = 0, & t \in (0, T], \\ u(x, 0) = u_0(x), & x \in (0, L), \end{cases} \quad (62)$$

where $g(s) = s^3 - s$. Note that $c_g = 1$ (cf. (38)).

For the space discretization, we use P^1 continuous finite elements on a regular subdivision of $[0, L]$ with mesh size $h = 1/(M+1)$. Due to the Dirichlet boundary conditions, the dimension of the finite element space V_h is M . By using an appropriate basis (namely, an orthonormal basis of V_h for the $L^2(0, L)$ scalar product), it is easily seen that this space discrete version of (62) is a gradient flow in \mathbb{R}^M of the form (3), for a function F which satisfies (4)-(5) (see e.g. [2]). Moreover, F is a polynomial of M variables (and therefore real analytic), so that convergence to equilibrium holds for this gradient flow.

For the time discretization, we use the BDF3 scheme. By gradient stability [2, 27], convergence to equilibrium also holds for this fully discrete version of (62).

Regarding the numerical resolution, we use the standard nodal basis of V_h (“hat functions”), and in the following, we identify V_h to \mathbb{R}^M through this basis. We obtain the scheme

$$B_h \frac{11 U^{n+3} - 18 U^{n+2} + 9 U^{n+1} - 2 U^n}{6\Delta t} + A_h U^{n+3} + G_h(U^{n+3}) = 0, \quad (63)$$

where A_h and B_h are $M \times M$ symmetric positive-definite matrix, $G_h : \mathbb{R}^M \rightarrow \mathbb{R}^M$ corresponds to the nonlinearity g , and $U^n \in \mathbb{R}^M$ is the unknown vector (see e.g. [11]). The matrix A_h is a discretization of $-\Delta$ and B_h is the mass matrix.

This scheme is fully implicit. When U^n , U^{n+1} and U^{n+2} are known, U^{n+3} can be obtained as a solution of the nonlinear problem,

$$H_n(V) = 0, \quad (64)$$

where $H_n : \mathbb{R}^M \rightarrow \mathbb{R}^M$ is the function,

$$H_n(V) = B_h \frac{11V - 18U^{n+2} + 9U^{n+1} - 2U^n}{6\Delta t} + A_h V + G_h(V).$$

For the numerical resolution of (64), one possibility is to use a Newton method. This reads: let $V^0 = U^{n+2}$ and for $k = 0, 1, 2, \dots$, until convergence, let V^k solve the linearized equation

$$H_n(V^k) + dH_n(V^k)(V^{k+1} - V^k) = 0, \quad (65)$$

where $dH_n(V) = B_h/\Delta t + A_h + dG_h(V)$ is a $M \times M$ symmetric matrix. Yet, the computation of $dG(V^k)$ is costly, so we actually use an approximate Newton method, i.e. an approximation of $dG(V^k)$.

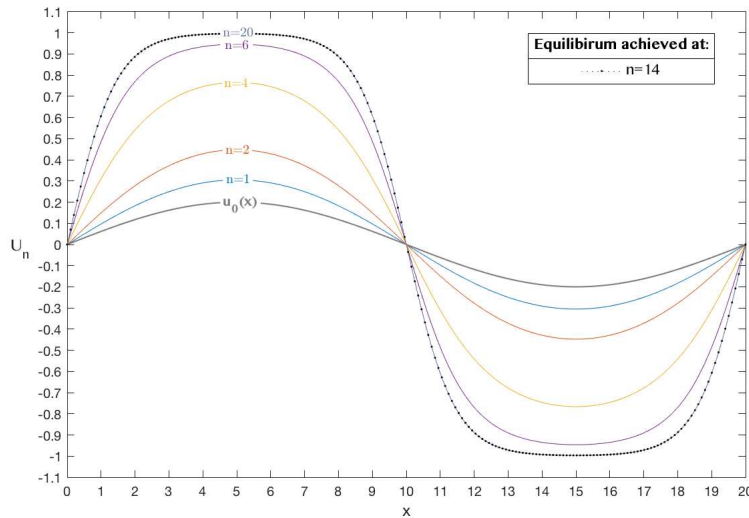


Figure 1. Evolution of U_n to equilibrium from a regular initial condition.

Figure 1 represents the evolution of the sequence (U_n) generated by (63) from a regular initial datum $u_0(x) = \frac{1}{5} \sin(\frac{2\pi x}{L})$. The spatial discretization was chosen small enough to ensure good accuracy of the finite elements method by setting $L = 20$, $\Delta x = 0.0995$ corresponding to $M = 200$ space nodes. The total time of the simulation is $T = 10$ with a time stepsize of $\Delta t = 0.5 \leq \frac{5}{6} c_g$ corresponding to $n = 20$ iterations. The first two iterations U^1 and U^2 are approximated using the Crank-Nicolson scheme, i.e for $n = 0, 1$

$$B(U^{n+1} - U^n)/\Delta t + A(U^{n+1} + U^n)/2 + [G(U^{n+1}) + G(U^n)]/2 = 0.$$

The choice of this second order scheme for U^1 and U^2 guarantees the third order accuracy of the BDF3 scheme [27].

We see that the discrete solution rapidly converges to a steady state, with values close to ± 1 , except for three transition layers (one in the middle, and two near the boundaries 0 and L). The equilibrium is reached graphically after only 14 iterations (i.e. with an accuracy of order 0.01 in the max norm of U^n).

Another simulation that shows the rapidity of convergence to equilibrium is given in Figure 2. It is a plot of the pseudo-energies \mathcal{E}_k^n versus time iteration for the BDF methods of order $k = 1, 2$ and 3. The pseudo-energy here is the Lyapunov function associated to the scheme [27]. In particular, \mathcal{E}_3^n is given by $\mathcal{E}(u_h^n)$ where $u_h^n \in V_h$ corresponds to U^n .

Since Δt is small enough, the pseudo-energies are decreasing, as expected. We note that they all converge to the same value, which is the energy level of the discrete steady state.

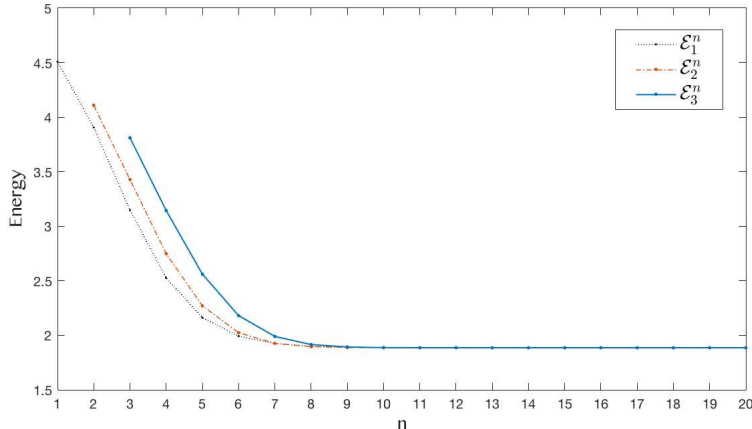


Figure 2. Pseudo-energy vs time iteration for BDF1, BDF2 and BDF3.

Table 2. Convergence error of the BDF3 scheme

N	Δt	$err_{\Delta t}$	ratio
16	1/8	1.8483e-03	—
32	1/16	2.4165e-04	7.6487
64	1/32	3.0741e-05	7.861
128	1/64	3.8251e-06	8.0367
256	1/256	4.2679e-07	8.9624

In order to check numerically the third order accuracy of the BDF3 scheme, we have computed in Table 2 the error for the time discretization,

$$err_{\Delta t} = \max_{0 \leq n \leq N} \left\| u_h^{\Delta t}(t_n) - u_h^{\Delta t_{sol}}(t_n) \right\|_{L^2(0,L)}.$$

The maximum is evaluated on the coarse grid $t_n = n\Delta t$, $n = 0, 1, \dots, N$, with $\Delta t = T/N$. The notation $u_h^{\Delta t}(t_n)$ represents the function in V_h corresponding to U^n at time t_n . Since the exact solution is not known, we used instead the discrete solution $u_h^{\Delta t_{sol}}$ on a fine grid with total time solution $T = 2$ and time stepsize $\Delta t_{sol} = 1/512$ corresponding to 1024 iterations. The values of $M = 200$ and u_0 were chosen as above. We see that the ratio $err_{\Delta t}/err_{\frac{\Delta t}{2}}$ of consecutive errors is close to $8 = 2^3$, and this is consistent with the third order accuracy of the BDF3 scheme.

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