Numerical verification for positive solutions of Allen–Cahn equation using sub- and super-solution method

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Abstract. This paper describes a numerical verification method for positive solutions of the Allen–Cahn equation on the basis of the sub- and super-solution method. Our application range extends to global-in-time solutions that converge or sufficiently approach to stable stationary solutions. The proposed verification method has almost the same memory requirements as the computation for obtaining an approximate solution.

Keywords: Allen–Cahn equation, Numerical verification method, Sub- and super-solution method

1. Introduction

Let \( \Omega = (a, b)^N \) \((N \in \{1, 2, 3\})\) with \(a, b \in \mathbb{R}\), and \(Q = \Omega \times (0, \tau)\) given \(\tau \in (0, \infty)\). We are concerned with the parabolic problem of the Allen–Cahn equation

\[
\begin{align*}
\frac{\partial u(x, t)}{\partial t} - \Delta u(x, t) - g(u(x, t)) &= 0, \quad (x, t) \in Q, \quad (1a) \\
u(x, 0) - u_0(x) &= 0, \quad x \in \Omega, \quad (1b) \\
u(x, t) &= 0, \quad x \in \partial \Omega, \quad t \in (0, \tau), \quad (1c)
\end{align*}
\]

where \(g : \mathbb{R} \rightarrow \mathbb{R}\) is given by \(g(s) = \varepsilon^{-2}(s - s^3)\) \((\varepsilon > 0)\), and \(u_0 \in L^2(\Omega) := \{u \in L^2(\Omega) : u(x) \geq 0 \text{ a.e. } x \in \Omega\}\) (the positive cone of \(L^2(\Omega)\)) is a given initial function.

The Allen–Cahn equation was proposed as a simplified model for the phase separation process of a binary alloy at a fixed temperature [1]. This equation also describes many other phase separation processes. It is known that solutions of the Allen–Cahn equation converge to those describing mean curvature flows under suitable conditions [8, 9].
Various numerical verification methods for parabolic partial differential equations have been developed over the last decade. The following two approaches are known to be effective methods. Nakao, Kinoshita, and Kimura succeeded in verifying the existence of solutions to parabolic problems by estimating the norm of an inverse operator related to parabolic operators [12, 13, 14]. Subsequently, Mizuguchi, Takayasu, Kubo, and the third author of this paper proposed another method based on semigroup theories [17, 18, 19]. These two approaches were summarized in detail in a recent survey [15]. However, there is no definitive method for parabolic problems. In particular, in both of these previous approaches, the errors increase and accumulate at every time step, potentially leading to verification failure.

From this background, we study a new approach for the numerical verification of parabolic problems on the basis of the sub- and super-solution method (see, for example, [7]), anticipating a successful application to (1). Although the applicable range of our method is more limited than in the abovementioned two methods (see Subsection 3.3), our approach is characterized as being robust against increasing errors at every time step. Even if the errors increase, the verification itself is achieved as long as the sub- and super-solutions maintain a certain sense of order. Moreover, our verification procedure has almost the same memory requirements as the computation process for obtaining an approximate solution.

The remainder of this paper is organized as follows. In Section 2, some required notation and definitions are introduced. In Section 3, a numerical verification technique based on the sub- and super-solution method is proposed for parabolic problems, and this is then applied to the Allen–Cahn equation (1). In Section 4, we present numerical results that verify the existence of global-in-time solutions of (1) with concrete settings.

### 2. Preliminaries

Let $L^2(B)$ be the space of all second-power Lebesgue integrable functions over domain $B$ and $H^1(B)$ be the first-order $L^2$ Sobolev space. We define $H^1_0(B)$ as the closure of $C^\infty_0(B)$ in $H^1(B)$. Moreover, $H^{-1}(B)$ and $H^{-1}_0(B)$ denote the dual spaces of $H^1(B)$ and $H^1_0(B)$, respectively. The inner products on $L^2(B)$ and $H^1(B)$ are, respectively, defined by

$$(u, v)_{L^2(B)} := \int_B u(x)v(x)dx, \quad (u, v)_{H^1(B)} := (\nabla u, \nabla v)_{L^2(B)} + (u, v)_{L^2(B)}.$$ 

For a Hilbert space $H$ and its dual space $H^*$, the duality pairing for $u \in H$ and $f \in H^*$ is denoted by $\langle f, u \rangle$. We define the Lebesgue space $L^2(0, \tau; H)$ and the inner product therein as follows:

$L^2(0, \tau; H) := \{ u : (0, \tau) \to H : \|u(\cdot)\|_H \in L^2((0, \tau)) \}$,

$$(u, v)_{L^2(0,\tau;H)} := \int_0^\tau (u(t), v(t))_H dt.$$
The function spaces $X_0$, $W$, and $W_0$ are defined by

$$
X_0 := L^2(0, \tau; H^1_0(\Omega)),
$$
$$
W := \{ u \in L^2(0, \tau; H^1(\Omega)) : \frac{\partial u}{\partial t} \in L^2(0, \tau; H^{-1}(\Omega)) \},
$$
$$
W_0 := \{ u \in L^2(0, \tau; H^1_0(\Omega)) : \frac{\partial u}{\partial t} \in L^2(0, \tau; H^{-1}_0(\Omega)) \}.
$$

The partial ordering and the ordered interval $[\cdot, \cdot]$ in $W \subset L^2(Q)$ are defined by

$$
u \leq v \iff v - u \in L^2(Q), \quad [v, u] := \{ w \in W : v \leq w \leq u \},
$$

where $L^2_+(Q)$ is the positive cone of $L^2(Q)$. The operator $f : W \to L^2(Q)$ is characterized by $f(u(x, t)) = g(u(x, t))$. Under this notation, we look for a weak solution $u \in W_0$ of (1) satisfying

$$
\langle \partial_t u - \Delta u - f(u), \varphi \rangle = 0 \quad \text{for all } \varphi \in X_0 \cap L^2_+(Q),
$$
$$
u(x, 0) = u_0(x), \quad x \in \Omega.
$$

Also, we consider the case in which problem (2) has a global-in time solution in the sense that a solution $u \in W_0$ of (2) exists for an initial function $u_0 \in L^2_+(\Omega)$ for all $\tau > 0$ and satisfies

$$
\text{ess sup}_{\tau \in (0, \infty)} \| u(\cdot, \tau) \|_{H^1(\Omega)} < \infty.
$$

See Subsection 3.2 for a discussion of global-in time solutions.

### 3. Numerical verification using sub- and super-solution method

In this section, we describe a numerical verification method for a weak solution of (1) on the basis of the sub- and super-solution method. Sub- and super-solutions of (1) are defined as follows:

**Definition 1.** A function $\overline{u} \in W$ is called a super-solution of problem (1) if $\overline{u}$ satisfies

$$
\langle \partial_t \overline{u} - \Delta \overline{u} - f(\overline{u}), \varphi \rangle \geq 0 \quad \text{for all } \varphi \in X_0 \cap L^2_+(Q),
$$
$$
\overline{u}(x, 0) \geq u_0(x), \quad x \in \Omega,
$$
$$
\overline{u}(x, t) \geq 0, \quad x \in \partial \Omega, \quad t \in (0, \tau).
$$

**Definition 2.** A function $\underline{u} \in W$ is called a sub-solution of problem (1) if $\underline{u}$ satisfies

$$
\langle \partial_t \underline{u} - \Delta \underline{u} - f(\underline{u}), \varphi \rangle \leq 0 \quad \text{for all } \varphi \in X_0 \cap L^2_+(Q),
$$
$$
\underline{u}(x, 0) \leq u_0(x), \quad x \in \Omega,
$$
$$
\underline{u}(x, t) \leq 0, \quad x \in \partial \Omega, \quad t \in (0, \tau).
$$

Our method is based on the following argument:
Theorem 1 ([7, Theorem 3.37]). Let \( u \in W \) be a sub-solution of (1) and \( \overline{u} \in W \) be a super-solution of (1). Assume that \( u \leq \overline{u} \) and there exists some \( k \in L^2(\Omega) \) such that
\[
|g(s)| \leq k(x, t), \quad \text{for a.e. } (x, t) \in \Omega, \quad \forall s \in [u(x, t), \overline{u}(x, t)].
\] (6)

Problem (1) then has a solution \( u \in W_0 \) within the interval \([u, \overline{u}]\).

Remark 1. Theorem 1 holds for general Carathéodory functions \( g : \mathbb{R} \to \mathbb{R} \), and is not restricted to the Allen–Cahn equation; see [7, Theorem 3.37].

3.1. Construction of sub- and super-solutions for fixed \( \tau \)

We apply Theorem 1 to the verification of positive solutions of the Allen–Cahn equation (1). The key point of our verification method is how to construct sub- and super-solutions satisfying \( u \leq \overline{u} \). To construct a super-solution \( \overline{u} \) of problem (1), we consider a perturbed problem by adding a positive real \( \delta \) to the right side of (1a), and compute an approximate solution \( \overline{u}' \) of the perturbed problem with an initial super-solution \( \overline{u}_0 \in L^2(\Omega) \), which will be specified later. We employ \( \overline{u}' \) as a candidate of \( \overline{u} \) and verify that \( \overline{u}' \) satisfies the definition of a super-solution. To construct \( u^* \), we first calculate \( \overline{u}'(\cdot, t_i) \in C^2(\Omega) \) numerically for each \( i = 1, 2, \cdots, n+1 \), where \( 0 = t_0 < t_1 < \cdots < t_{n+1} = \tau \) for a specific \( n \in \mathbb{N} \). The function \( \overline{u}' \in C([0, \tau]; C^2(\Omega)) \) is constructed through linear interpolation between \( \overline{u}'(x, t_i) \) and \( \overline{u}'(x, t_{i+1}) \) for each \( i = 0, 1, \cdots, n \). Because \( \overline{u}' \in C^3((t_i, t_{i+1}); C^2(\Omega)) \cap C([t_i, t_{i+1}); C^2(\Omega)) \) for each \( i = 0, 1, \cdots, n \), we need only ensure the inequalities in the strong sense corresponding to (4). Similarly, a candidate \( u^* \) of a sub-solution \( _\perp u \) is constructed by solving (1) with a negative perturbation \( -\delta \) to the right side of (1a).

Because both \( u^* \) and \( \overline{u}' \) are constructed to be bounded, \( g \) always satisfies the required growth condition (6). The sub- and super-solutions are constructed to be highly regular in the process. However, it is worth noting that solutions within \([u^*, \overline{u}]\) do not have to be regular, but need only exist in \( W_0 \). Hereafter, we use the following notation:
\[
C = \left( C([0, \tau]; C^0(\Omega)) \right) \cap \left( \bigcap_{i=0}^{n} C^3((t_i, t_{i+1}); C^0(\Omega)) \right),
\]
\[
\mathcal{A} = \left( C([0, \tau]; C(\Omega)) \right) \cap \left( \bigcap_{i=0}^{n} C^3((t_i, t_{i+1}); C(\Omega)) \right).
\]
The operators \( F_+: C \to \mathcal{A} \) and \( F_- : C \to \mathcal{A} \) are defined by
\[
F_+(u)(\cdot, t) := \partial_{t^+} u(\cdot, t) - \Delta u(\cdot, t) - \varepsilon^{-2}(u(\cdot, t) - u(\cdot, t)^3),
\]
(7)
\[
F_-(u)(\cdot, t) := \partial_{t^-} u(\cdot, t) - \Delta u(\cdot, t) - \varepsilon^{-2}(u(\cdot, t) - u(\cdot, t)^3),
\]
(8)
where \( \partial_{t^+} \) (\( \partial_{t^-} \)) is the right (left) differential operator. Note that \( F_+(u^*)(\cdot, t) \) and \( F_-(u^*)(\cdot, t) \) may differ at the borders \( t_i, t_{i+1} \), but coincide inside each interval \( (t_i, t_{i+1}) \), that is,
\[
F_+(u^*)(\cdot, t) = F_-(u^*)(\cdot, t), \quad t \in (t_i, t_{i+1})
\]
(9)
for all \( i = 0, 1, \cdots, n \). On the basis of the following propositions, we confirm that \( u^* \) and \( \overline{u}' \) satisfy the definitions of sub- and super-solutions, respectively.
Proposition 2. Let $u^* \in C$ be the linear interpolation between $u^+_i(x, t_i)$ and $u^-_i(x, t_{i+1})$ for $i = 0, \cdots, n$. Function $u^*$ is a sub-solution of problem (1) if
\begin{equation}
\tilde{u}^*(x, t_0) \leq u_0(x) \quad \text{for all } x \in \Omega
\end{equation}
and, for each $i = 0, \cdots, n$,
\begin{equation}
u^*_i(x, t_i) \geq 0, \quad \tilde{u}^*(x, t_{i+1}) \geq 0, \quad F_+(u^*)(x, t_i) \leq 0, \quad F_-(u^*)(x, t_{i+1}) \leq 0 \quad \text{for all } x \in \Omega.
\end{equation}
Proof. As $\tilde{u}^*(\cdot, t) \in C^2_0(\Omega)$ and $\tilde{u}^*(x, t_0) \leq u_0(x)$, we are left to show that $u^*$ satisfies
\begin{equation}
\langle \partial u^* - \Delta u^* - f(u^*), \varphi \rangle \leq 0 \quad \text{for all } \varphi \in X_0 \cap L^2_1(Q).
\end{equation}
To this end, we prove that
\begin{equation}
F_+(u^*)(x, t) \leq 0, \quad t \in (t_i, t_{i+1})
\end{equation}
for all $i = 0, 1, \cdots, n$. Let $x \in \Omega$ and $i \in \{0, 1, \cdots, n\}$ be arbitrarily fixed. We denote $a(x) = (u^*(x, t_i) - \tilde{u}^*(x, t_{i+1}))/ (t_i - t_{i+1})$ and $b(x) = u^*(x, t_i) - a(x)t_i$. This readily implies that $u^*(x, t) = a(x)t + b(x)$. Under the given notation, we have
\begin{equation}
\partial_t^2 F_+(u^*)(x, t) = 6e^{-2}a(x)^2(a(x)t + b(x)) = 6e^{-2}a(x)^2u^*(x, t) \geq 0
\end{equation}
for all $t \in (t_i, t_{i+1})$; recall that we assumed $u^*(x, t_i) \geq 0$ and $\tilde{u}^*(x, t_{i+1}) \geq 0$. Inequality (13) follows from (14) and the assumptions that $F_+(u^*)(x, t_i) \leq 0, \quad F_-(u^*)(x, t_{i+1}) \leq 0$. As a result, we have
\begin{equation}
\partial_t^2 F_+(u^*)(x, t) - \Delta u^*(x, t) - f(u^*)(x, t) \leq 0, \quad t \in (t_i, t_{i+1})
\end{equation}
for all $i = 0, 1, \cdots, n$. This ensures that (12) is satisfied.

Proposition 3. Let $\tilde{u}^* \in C$ be the linear interpolation between $\tilde{u}^+_i(x, t_i)$ and $\tilde{u}^-_i(x, t_{i+1})$ for $i = 0, \cdots, n$. Function $\tilde{u}^*(x, t) \in C$ is a super-solution of problem (1) if
\begin{equation}
\tilde{u}^*(x, t_0) \geq u_0(x) \quad \text{for all } x \in \Omega
\end{equation}
and, for each $i = 0, \cdots, n$,
\begin{equation}1/2(F_+(\tilde{u}^*)(x, t_i) + F_-(\tilde{u}^*)(x, t_{i+1})) - (t_{i+1} - t_i)^2M(x) \geq 0 \quad \text{for all } x \in \Omega,
\end{equation}
where $M(x) = \max_{t \in (t_i, t_{i+1})} \partial_t^2 F_+(\tilde{u}^*)(x, t)$.
Proof. As $\tilde{u}^*(\cdot, t) \in C^2_0(\Omega)$, $\tilde{u}^*(x, t_0) \geq u_0(x)$, we prove that
\begin{equation}F_+(\tilde{u}^*)(x, t) \geq 0, \quad t \in (t_i, t_{i+1}),
\end{equation}
for all $i = 0, 1, \cdots, n$ as a means of verifying that
\begin{equation}\langle \partial_t \tilde{u}^* - \Delta \tilde{u}^* - f(\tilde{u}^*), \varphi \rangle \geq 0 \quad \text{for all } \varphi \in X_0 \cap L^2_1(Q).
\end{equation}
Let \( x \in \Omega \) and \( i \in \{0, 1, \cdots, n\} \) be arbitrarily fixed. We define the quadratic polynomial \( h \) with respect to \( t \) by \( \partial^2_t h(x, t) = M(x), \ t \in (t_i, t_{i+1}) \) with the boundary conditions

\[
h(x, t_i) = F_+(\bar{u}^r)(x, t_i), \quad h(x, t_{i+1}) = F_-(\bar{u}^r)(x, t_{i+1}).
\]  
(19)

As \( \partial^2_t h(x, t) = M(x) := \max_{i \in \{t_i, t_{i+1}\}} \partial^2_t F_+(\bar{u}^r)(x, t) \), we have

\[
\partial^2_t (h(x, t) - F_+ (\bar{u}^r)(x, t)) \geq 0, \ t \in (t_i, t_{i+1}).
\]  
(20)

It follows from (19) and (20) that

\[
F_+ (\bar{u}^r)(x, t) \geq h(x, t), \ t \in (t_i, t_{i+1}).
\]  
(21)

By calculating the value of the vertex of \( h \), its minimum value is obtained as

\[
\frac{1}{2} (F_+ (\bar{u}^r)(x, t_i) + F_-(\bar{u}^r)(x, t_{i+1})) - (t_{i+1} - t_i)^2 M(x),
\]

which is assumed to be nonnegative. Therefore, we have

\[
\partial_t \bar{u} - \Delta \bar{u} - f(\bar{u}) \geq 0, \ t \in (t_i, t_{i+1})
\]

for all \( i = 0, 1, \cdots, n \). This implies that (18) holds. \( \Box \)

### 3.2. Verification for global-in-time solutions

A method of constructing sub- and super-solutions to problem (1) with fixed \( \tau \in (0, \infty) \) was proposed in Subsection 3.1. We now apply this construction method to the verification process for global-in-time solutions. Recall that \( u \in W_0 \) of (1) is called a global-in-time solution if, for a certain initial function \( u_0 \), \( u \) can be extend to a solution for \( t \in (0, \tau) \) for an arbitrarily large number \( \tau > 0 \) and satisfies (3).

The method described below is applicable to a global-in-time solution that converges or sufficiently approaches to a stable stationary solution. To construct global-in-time sub- and super-solutions for arbitrarily large \( \tau > 0 \), we calculate \( \bar{u}^r(\cdot, t) \) and \( u^r(\cdot, t) \) for \( t \in [0, t_n] \) in the same way as described in Subsection 3.1, where \( t_n \) should be taken as sufficiently large so that both \( \bar{u}^r(\cdot, t_n) \) and \( u^r(\cdot, t_n) \) approach to some stationary functions. The functions at \( t = t_n \) are then directly extended to \( t \in [t_n, \tau) \). More precisely, we regard \( \bar{u}^r(\cdot, t) = u^r(\cdot, t_n) \) and \( u^r(\cdot, t) = u^r(\cdot, t_n) \) for all \( t \in [t_n, \tau) \) for an arbitrarily selected \( \tau \in (t_n, \infty) \). Note that \( \bar{u}^r(\cdot, t) \) and \( u^r(\cdot, t) \) are chosen independent of \( \tau \) so that the functions between them are satisfies (3).

It is useful to compute a stationary solution of the perturbed problem with the positive \( \delta \) (negative \( -\delta \)) used in Subsection 3.1 to construct \( \bar{u}^r(u^r) \), and set this to \( \bar{u}^r(\cdot, t_n) (u^r(\cdot, t_n)) \) in the actual computations; see Section 4. Propositions 2 and 3 can be directly used to confirm that \( u^- \) and \( \bar{u}^- \) satisfy the definitions of sub- and super-solutions, respectively.
3.3. Applicable range

We now discuss the applicable range of our verification method. For the sake of simplicity, we employ the backward Euler method to discretize the time space, and assume that \( u(t), \tilde{u}(t) \in C^2(\Omega) \) so that \( \Delta u(t) \) and \( \Delta \tilde{u}(t) \) are understood in the strong sense. We denote \( u_i = u(t_i) \) and \( \tilde{u}_i = \tilde{u}(t_i) \) for \( i = 0, 1, \cdots, n + 1 \). In addition, we assume that the initial sub- and super-solutions \( u_0 \) and \( u_0 \) satisfy \( u_0 - u_0 \geq 0 \). For \( i = 1, 2, \cdots, n + 1 \), \( u_i \) and \( \tilde{u}_i \) are obtained by

\[
\frac{\tilde{u}_i - \tilde{u}_{i-1}}{t_i - t_{i-1}} - \Delta \tilde{u}_i - f(\tilde{u}_i) = \delta, \tag{22}
\]

\[
\frac{u_i - u_{i-1}}{t_i - t_{i-1}} - \Delta u_i - f(u_i) = -\delta, \tag{23}
\]

where \( \delta > 0 \). We then define \( \psi_i := \tilde{u}_i - u_i \). Under the assumption that \( \psi_{i-1} \geq 0 \), we consider a sufficient condition for \( \psi_i \geq 0 \). Subtracting (23) from (22), we have

\[
\frac{\psi_i}{t_i - t_{i-1}} - \Delta \psi_i - f(\psi_i + u_i) + f(u_i) = 2\delta + \frac{\psi_{i-1}}{t_i - t_{i-1}} \geq 0. \tag{24}
\]

The linearized operator \( L \) of \( -\Delta \psi_i - f(\psi_i) \) at \( u_i \) is given by

\[
L(\psi_i) = -\Delta \psi_i - \psi_i f'(u_i),
\]

where \( f'(u_i) \) is the Fréchet derivative of \( f \) at \( u_i \). Inequality (24) coincides with

\[
L(\psi_i) \geq 0 \tag{25}
\]

if an \( O(\psi_i) \) difference is allowed. Therefore, the positivity of \( L \) is an approximately sufficient (and probably almost necessary) condition for \( \psi_i \geq 0 \).

Thus, the class of problems to which our method can be applied is limited, but once (25) is satisfied for \( i = 1, 2, \cdots, n + 1 \) under the condition \( \tilde{u}_0 - u_0 \geq 0 \), our method enables successful verification.

4. Numerical experiments

In this section, we present the results of numerical experiments in which our method was applied to (1) with concrete settings. All computations were implemented using a single-core processor on a computer with 2.20 GHz Intel(R) Xeon(R) E7-4830 v2 CPU, 2 TB RAM, and CentOS Linux 7.3.1611 using GCC version 4.8.5. All rounding errors were strictly estimated using the kv library (version 0.4.47) [21] and VCP library (version alpha 0.0.6) [22] toolboxes. Therefore, the accuracy of all results was mathematically guaranteed. All numerical values were stored and computed in double-double precision using type “dd” or the “interval< dd >” equipped in the kv library [21].
4.1. One space dimension

We first applied our method to a global-in-time solution of (1) with $\varepsilon = 0.109375$ and $\Omega = (0, 1)$. Sub- and super-solutions were constructed with the polynomials given by

$$\phi_i(x) = \frac{(-1)^{i-1}}{i!} x(1-x) \left( \frac{d}{dx} \right)^i (1-x)^{i-1}, \quad i = 2, 3, \cdots,$$

(26)

where $\{\phi_i\}_{i=2}^\infty$ is a complete orthogonal system in $H^1_0((0, 1))$ [20]. The initial function was set to $u_0(x) = 3\phi_2(x)$, which is symmetric with respect to the center $x = 0.5$. Therefore, we searched for symmetric solutions of (1).

The initial super-solution $\overline{u}_0$ was chosen as $\overline{u}_0 = u_0$. The initial sub-solution $\underline{u}_0$ was constructed by the following process to satisfy the conditions imposed in Proposition 2. First, we constructed an auxiliary function $w$ from the polynomials as

$$w(x) = \sum_{j=1}^M b_j \phi_{2j}(x), \quad b_j \in \mathbb{R},$$

where $M$ is a positive integer. The coefficients $b_j$ were calculated by solving

$$\left( \frac{w - u_0}{t_1 - t_0}, \phi_{2k} \right)_{L^2(\Omega)} + (\nabla w, \nabla \phi_{2k})_{L^2(\Omega)} = (f(w) - \delta, \phi_{2k})_{L^2(\Omega)}, \quad k = 1, 2, \cdots, M. \quad (27)$$

Then, we set

$$\underline{u}_0 = pw, \quad (28)$$

where $p \in (0, 1)$ is a real number close to 1. For each $i = 0, 1, 2, \cdots, n+1$, $\underline{u}_i(x) := u^*(x, t_i)$ and $\overline{u}_i(x) := u^*(x, t_i)$ were constructed as

$$\underline{u}^*_i(x) = \sum_{j=1}^M \overline{a}_j(t_i) \phi_{2j}(x), \quad \overline{u}^*_i(x) = \sum_{j=1}^M \underline{a}_j(t_i) \phi_{2j}(x), \quad \overline{a}_j(t_i), \underline{a}_j(t_i) \in \mathbb{R},$$

where $M$ is the same integer. Each super-solution $\overline{u}^*_i(x)$ was computed using Newton’s method at each time step, that is, the coefficients $\overline{a}_j(t_{i+1})$ were calculated from the previous $\overline{a}_j(t_i)$ by solving

$$\left( \frac{\overline{u}^*_{i+1} - \overline{u}^*_i}{t_{i+1} - t_i}, \phi_{2k} \right)_{L^2(\Omega)} + (\nabla \overline{u}^*_{i+1}, \nabla \phi_{2k})_{L^2(\Omega)} = (f(\overline{u}^*_{i+1}) + \delta, \phi_{2k})_{L^2(\Omega)}, \quad k = 1, 2, \cdots, M. \quad (29)$$

Each $u^*_i(x)$ was obtained by replacing $\overline{u}^*_{i+1}$, $\overline{u}^*_i$, and $\delta$ with $\underline{u}^*_{i+1}$, $\underline{u}^*_i$, and $-\delta$, respectively. The super-solution $\overline{u}^*_n$ (and also $\overline{u}^*_{n+1} = \overline{u}^*(\cdot, \tau)$ for arbitrary $\tau \in (t_n, \infty)$) corresponding to a stationary solution was computed by solving the stationary problem

$$(\nabla \overline{u}^*_n, \nabla \phi_{2k})_{L^2(\Omega)} = (f(\overline{u}^*_n) + \delta, \phi_{2k})_{L^2(\Omega)}, \quad k = 1, 2, \cdots, M. \quad (30)$$

The sub-solution $\underline{u}^*_n(x)$ (also $\underline{u}^*_{n+1} = u^*(\cdot, \tau)$) was calculated in a similar way, replacing $\overline{u}^*_n$ and $\delta$ with $\underline{u}^*_n$ and $-\delta$, respectively. For the candidate sub- and super-solutions $u^*$ and $\overline{u}^*$...
constructed above, we confirmed the required inequalities in Propositions 2 and 3, and the order $\mu' \leq \tilde{\mu}'$, by dividing $\Omega$ into smaller intervals and implementing interval arithmetic.

We implemented the verification for problem (1) with $\varepsilon = 0.109375$ and $\Omega = (0, 1)$, where we set $\delta = 2$, $M = 6$, $p = 0.9$ (the floating point number nearest to 0.9), and $t_i - t_{i-1} = 2^{-9}$ for $i = 0, 1, \cdots, n$ (= 27). Figure 1 displays the sub- and super-solutions at certain time steps. Figure 2 illustrates the upper bounds for $\|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$ for $t \in [0, t_{27}]$. Table 1 summarizes the verification results, including $\sup_{t \in [0, t_{27}]} \|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$, the memory usage, and the computation time. Here, we estimated $\sup_{t \in [t_n, \tau]} \|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$ independent of $\tau \in (t_n, \infty)$ on the basis of the discussion in Subsection 3.2; therefore, this bound is regarded as a global upper bound for $\sup_{t \in (t_n, \infty)} \|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$.

![Figure 1](image1.png)  
**Figure 1:** Sub- and super-solutions enclosing an exact solution of (1).

![Figure 2](image2.png)  
**Figure 2:** Upper bounds for $\|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$ ($t \in [0, t_{27}]$).

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Table 1: Verification result for (1) with $\varepsilon = 0.109375$ and $\Omega = (0, 1)$, where $\rho(t) := \|u(\cdot, t) - \bar{u}(\cdot, t)\|_{H^1(\Omega)}$. Rows “Approximate” and “Verified” represent the corresponding items in the usual approximate computations with $\delta = 0$ and our verification, respectively. “Memory” and “Time” are given in units of MB and s, respectively.

| $M$ | $t_n$ | $\sup_{t \in [0, t_n]} \rho(t)$ | $\sup_{t \in (t_n, \infty)} \rho(t)$ | Approximate | Verified | Memory | Time | Memory | Time |
|-----|-------|-------------------------------|-------------------------------|------------|---------|--------|------|--------|------|
| 5   | Failed| Failed                        | Failed                        | 8.61       | 1.06e-1 | Failed | Failed|
| 6   | $27 \times 2^{-9}$ | 5.1999e-2                 | 3.4717e-2                      | 8.61       | 1.15e-1 | 8.94   | 5.69 |
| 7   | $27 \times 2^{-9}$ | 5.2002e-2                 | 3.4720e-2                      | 8.88       | 1.23e-1 | 8.93   | 8.20 |

4.2. Two space dimensions

We then applied our method to a global-in-time solution of (1) with $\varepsilon = 0.109375$ and $\Omega = (0, 1)^2$. Sub- and super-solutions were again constructed with the polynomials $\phi_1^{i_1}, \phi_2$ given by (26). The initial function was set to $u_0(x, y) = 6\phi_2(x)\phi_2(y)$. As this is symmetric with respect to the lines $x = 0.5$ and $y = 0.5$, we searched for solutions that were symmetric in this sense.

The initial super-solution $\bar{u}_0$ was set to $\bar{u}_0 = u_0$. The initial sub-solution $\underline{u}_0^s$ was constructed in a similar way to that described in Subsection 4.1 to satisfy the conditions required in Proposition 2. First, we constructed an auxiliary function $w$ with the polynomials as

$$w(x, y) = \sum_{k=1}^{M} \sum_{j=1}^{M} b_{jk}\phi_2(x)\phi_2(y), \quad b_{jk} \in \mathbb{R},$$

where $M$ is a positive integer. The coefficients $b_{jk}$ were calculated by solving

$$\left(\frac{w - u_0}{t_1 - t_0}, \phi_2, \phi_2\right)_{L^2(\Omega)} + (\nabla w, \nabla (\phi_2, \phi_2))_{L^2(\Omega)} = (f(w) - \delta, \phi_2, \phi_2)_{L^2(\Omega)}, \quad j, k = 1, 2, \cdots, M.$$  

(31)

Then, we set

$$\underline{u}_0^s = pw,$$  

(32)

where $p \in (0, 1)$ is a real number close to 1. For each $i = 0, 1, \cdots, n + 1$, $\underline{u}_i(x) := u_i^s(x, t_i)$ and $\bar{u}_i^s(x) := \bar{u}_i^s(x, t_i)$ were constructed as

$$\underline{u}_i^s(x, y) = \sum_{k=1}^{M} \sum_{j=1}^{M} a_{jk}(t_i)\phi_2(x)\phi_2(y), \quad a_{jk}(t_i) \in \mathbb{R},$$

$$\bar{u}_i^s(x, y) = \sum_{k=1}^{M} \sum_{j=1}^{M} \bar{a}_{jk}(t_i)\phi_2(x)\phi_2(y), \quad \bar{a}_{jk}(t_i) \in \mathbb{R},$$

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where \( M \) is the same integer. The coefficients \( \bar{a}_{j,k}(t_i) \) were calculated from the previous \( \bar{a}_{j,k}(t_i) \) by solving

\[
\begin{align*}
\left( \frac{\bar{u}_{i+1} - \bar{u}_i}{t_{i+1} - t_i} , \phi_{2j}\phi_{2k} \right)_{L^2(\Omega)} + (\nabla \bar{u}_{i+1}, \nabla (\phi_{2j}\phi_{2k}))_{L^2(\Omega)} &= (f(\bar{u}_{i+1}) + \delta, \phi_{2j}\phi_{2k})_{L^2(\Omega)}, \\
j, k &= 1, 2, \ldots, M.
\end{align*}
\] (33)

Each \( u_i^\tau(x) \) was obtained by replacing \( \bar{u}_{i+1}, \bar{u}_i, \) and \( \delta \) with \( u_{i+1}^\tau, \ u_i^\tau, \) and \( -\delta, \) respectively. The super-solution \( \bar{u}_n \) (and also \( \bar{u}_{n+1} = \bar{u}(\cdot, \tau) \)) corresponding to a stationary solution was computed by solving the stationary problem

\[
\begin{align*}
(\nabla \bar{u}_n, \nabla (\phi_{2j}\phi_{2k}))_{L^2(\Omega)} &= (f(\bar{u}_{n+1}) + \delta, \phi_{2j}\phi_{2k})_{L^2(\Omega)}, \\
j, k &= 1, 2, \ldots, M.
\end{align*}
\] (34)

The sub-solution \( u_n^\tau(x) \) (also \( u_{n+1}^\tau = u^\tau(\cdot, \tau) \) for arbitrary \( \tau \in (t_n, \infty) \)) was calculated in a similar way, replacing \( u_n^\tau \) and \( \delta \) with \( u_n^\tau \) and \( -\delta, \) respectively. For \( u^\tau \) and \( \bar{u}^\tau \) constructed above, we confirmed the required inequalities in Propositions 2 and 3, and the order \( u^\tau \leq \bar{u}^\tau, \) by dividing \( \Omega \) into smaller squares and implementing interval arithmetic.

We implemented the verification for (1) with the setting \( \delta = 2, \ M = 6, \ p = 0.85 \) (the floating point number nearest to 0.85), and \( t_i - t_{i-1} = 2^{-9} \) for \( i = 0, 1, \ldots, n \) (\( n = 31 \)). Figure 3 displays the sub- and super-solutions and their difference \( u(x, t) - \bar{u}(x, t) \) for \( t = t_0, t = t_1, t = t_6, \) and \( t \geq t_{31} \).

Figure 3: Super-solutions \( \bar{u}(x, t) \) (first row), sub-solutions \( u(x, t) \) (second row), and the difference \( \bar{u}(x, t) - u(x, t) \) (third row) for \( t = t_0, t = t_1, t = t_6, \) and \( t \geq t_{31} \).
### 4.3. Discussion

According to Fig. 2 and Fig. 5, the estimated upper bounds for $\|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)}$ exhibit the same trend—first rising and then decreasing. This seems to be because the solutions rapidly advance toward the corresponding stationary solutions for a while, before the changes stabilize. In the one-dimensional case, as seen in Fig. 2, the upper bound for...
\[ \|u(\cdot, t) - \overline{u}(\cdot, t)\|_{H^1(\Omega)} \text{ decreases slightly in the first interval } t \in [t_0, t_1]. \] This is because the difference between the initial sub- and super-solutions at \( t = t_0 \) (namely \( p \) in (28)) is too large for the target problem; recall that \( p \) was set to the floating point number nearest to 0.9 in this case. Tables 1 and 2 indicate that our verification method consumes almost the same amount of memory as an approximate computation.

5. Conclusion

We have proposed a method for numerically enclosing weak solutions of parabolic problem (1) of the Allen–Cahn equation based on the sub- and super-solution method. Although the applicable range of our method is limited, as mentioned in Subsection 3.3, it was applied to global-in-time solutions that converge or sufficiently approach to stable stationary solutions in both one- and two-dimensional cases. The memory requirements of our verification process are similar to those of the computation for obtaining an approximate solution.

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