NUMERICAL RESOLUTION AND SIMULATION OF THE ALLEN-CAHN EQUATION IN THE TWO-DIMENSIONAL CASE

1 Abstract

In this paper, we perform a resolution and simulation of the Allen-Cahn equation inn this article, we solve and simulate the Allen-Cahn equation in the two-dimensional case. This equation has been the basis of many theoretical and numerical studies. It should be noted that several techniques have been used to treat nonlinearity. In our specific case, we linearized this equation by approaching the nonlinear term by a limited Taylor series development in the vicinity of an initial reference solution.

Numerical simulations carried out with the help of MATLAB software have highlighted the efficiency of the Allen-Cahn equation for modeling transition or phase separation phenomena in materials science.

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2 Introduction

The phenomenon of phase separation is present in several industrial processes in materials science. Numerical simulations make it possible to achieve a certain level of knowledge on the course of a physical phenomenon without having to conduct experiments in the laboratory or in industry.
The numerical approach can be seen as an experimental complement that allows to reduce the costs and the number of experiments to be carried out by determining in a preliminary manner the parameters and the characteristics of the components to be used. In the era of more available and powerful computing resources, it is very advantageous to take advantage of these advances to save time, money, resources and risks related to experimentation. These advances also open the door to a new process of experimentation where it is now possible to explore complex physical models. This is the case for the Allen-Cahn equation whose applications in several fields have been studied for phase separation and the growth of structures in materials science.
In this article, we will firstly make a theoretical study on the existence and uniqueness of solution of our model as well as its properties such as the maximum principle and the convergence towards equilibrium states.
We will then perform a numerical resolution of the model using the finite element method in two-dimensional space.
Finally, using MATLAB software, we will carry out numerical simulations highlighting phase separation in materials.

3 Mathematical model and description of the Allen Cahn equation

In general, the Allen-Cahn equation is used to model a phase separation process in which domains form from a homogeneous state. It is a well-known reaction-diffusion equation, fundamentally in materials science [2], which is written :

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,t) - \varepsilon \Delta u(x,t) + f(u(x,t)) = 0; & \text{for } x \in \Omega, t \geq 0 \\ \dfrac{\partial u}{\partial n} = 0; & \text{for } x \in \partial\Omega, t \geqslant 0 \\ u(x,0) = u_0(x); & \text{for } x \in \Omega \end{cases} \tag{3.1}$$

where Ω is an open set of $\mathbb{R}^d$; d = 1; 2; 3, ε is a small strictly positive parameter and f is the derivative of a two-well potential.
Ω is the volume occupied by the material, u is an order parameter which represents for example the ordering of atoms per unit cell in a crystal lattice, and the wells of the potential F correspond to the two phases of the material. Classically, we use the function

$$F(u) = \frac{(u^2-1)^2}{4} \quad with \quad F'(u) = f(u) \tag{3.2}$$

whose two wells, at -1 and +1 , are at the same energy level. For $\varepsilon = 0$, equation (2.1) reduces to an ODE, and $u(x,t)$ then evolves towards +1 or -1 depending on whether $u(x,0) > 0$ or $u(x,0) < 0$

respectively. The term $\varepsilon\Delta u(x,t)$ is a diffusion term that occurs on a slower scale than the reaction $F(u)$. The solution u of (3.1) separates Ω two regions where $u \approx 1$ and $u \approx -1$ respectively.
Equation (3.1) is considered as the gradient flow of the energy functional

$$E(u) = \int_\Omega \left[\frac{\varepsilon}{2}|\nabla u|^2 + F(u)\right] dx \qquad (2.3)$$

for the scalar product $L^2(\Omega)$. The term $F(u)$ represents the energy for a uniform parameter u and the term $\frac{\varepsilon}{2}|\nabla u|^2$ represents the interface energy, introduced by Cahn and Hilliard [1].

4 Theoretical study

4.1 Variational Formulation of the Model

The variational formulation is a theoretical writing of a problem described by a partial differential equation in order to study the existence and uniqueness of the solution of this problem. The principle of the variational approach for the resolution of partial differential equations is to replace the equation by an equivalent formulation, called variational, obtained by integrating the equation multiplied by any function, called test function.
A classical solution (also called a strong solution) of the PDE is a solution $u \in C^2(\Omega) \cap C(\overline{\Omega})$, which implies that the right-hand side f must belong to $C(\Omega)$. This classical formulation unfortunately poses a certain number of problems for demonstrating the existence of a solution. This is why we will replace the classical formulation of problem (3.1) by a formulation, called variational, which is much more advantageous.
An immediate interest of the variational formulation is that it makes sense if the solution u is only a function of $C^1(\overline{\Omega})$, unlike the classical formulation of problem (2.1) which requires that u belongs to $C^2(\Omega)$. We can already sense that it is simpler to solve the variational formulation than problem (3.1) since we are less demanding on the regularity of the solution.
The variational formulation is also sometimes called the weak formulation of the boundary value problem (3.1).
Let us multiply equation (3.1) by a test function $v(x)$ which does not depend on time t and integrate using Green's formula [5].

$$\begin{aligned}
&\int_\Omega \frac{\partial u}{\partial t}(x,t)v(x)dx - \int_\Omega \varepsilon v(x)\Delta u(x,t)dx + \int_\Omega v(x)f(u(x,t))dx = 0 \\
&= \int_\Omega \frac{\partial u}{\partial t}(x,t)v(x))dx - \int_\Omega \varepsilon\Delta u(x,t)v(x)dx + \int_\Omega f(u(x,t))v(x)dx = 0 \\
&= \int_\Omega \frac{\partial u}{\partial t}(x,t)v(x)dx + \varepsilon\int_\Omega \nabla v(x)\nabla u(x,t)dx - \varepsilon\int_{\partial\Omega} \frac{\partial u}{\partial n}(x)v(x)ds + \int_\Omega f(u(x,t))v(x)dx = 0 \\
&= \int_\Omega \frac{\partial u}{\partial t}(x,t)v(x)dx + \varepsilon\int_\Omega \nabla v(x)\nabla u(x,t)dx + \int_\Omega f(u(x,t))v(x)dx = 0 \qquad (3.3)
\end{aligned}$$

More precisely, if we give ourselves a time $T > 0$ (possibly equal to $+\infty$), we consider the functions

$$u :]0,T[\to H^1(\Omega) \qquad t \mapsto u(t)$$

Choosing the test function in the space H^1 and defining elsewhere, for all u and v in $H^1(\Omega)$, the bilinear form

$$a(u,v) = \int_\Omega \nabla u \nabla v dx$$

and m the scalar product L^2 given by

$$m(u,v) = \int_\Omega uv dx$$

we can then put (3.3) in the form of an ordinary differential equation in t. We therefore obtain the following variational formulation [5]
find $u(t)$ from $]0,T[$ with values in $H^1(\Omega)$ such that :

$$\begin{cases} \dfrac{d}{dt}(m(u(t),v) + \varepsilon a(u(t),v) + m(f(u(t)),v) = 0 & \forall v \in H^1(\Omega), 0 < t < T \\ u(t=0) = u_0 \end{cases} \tag{3.4}$$

[5]
At fixed ε, the existence and uniqueness of the solution to this variational formulation can be demonstrated [6].

4.1.1 Existence and uniqueness of the solution

Proposition 4.1 :
problem (3.1) admits a unique weak solution belonging to $H^1(\Omega \times [0;+\infty[$

Proof :
This demonstration is divided into 2 steps. In the first step, a sequence of piecewise linear solutions in time is constructed; we will use a semi-discretization in time of the problem (2.12) by constructing a sequence of solutions (u_k) which converges towards the solution u of the problem (3.1).
First step: Semi-discretization of the problem in time and construction of a sequence (u_k) of linear solutions [7].

- **Semi-discretization of the problem in time**
  We will use a classic schemz. Let N be a natural integer, let $\tau = \frac{T}{N}$ and $t_k = k\tau$.
  for $k = 0, ..., N, t \in [0;T]$; we approximate

$$\frac{\partial u(x,t)}{\partial t} \simeq \frac{u(x;t_k) - u(x;t_{k-1})}{t_k - t_{k-1}} \simeq \frac{u(x;t_k) - u(x;t_{k-1})}{\tau} \tag{3.5}$$

- **Semi-discretization in time of the problem(Construction of** $(u_k), k \in \mathbb{N}$)
  We use the approximation (3.4) in formula (3.3) and evaluating the nonlinear term at the previous (time) mesh point, we obtain:

$$\int_\Omega \frac{\partial u}{\partial t}(x,t)v(x)dx + \varepsilon \int_\Omega \nabla v(x) \nabla u(x,t) dx + \int_\Omega f(u(x,t))v(x)dx = 0 \tag{3.3}$$

$$\int_\Omega \frac{u_k(x) - u_{k-1}(x)}{\tau} v(x)dx + \varepsilon \int_\Omega \nabla v(x) \nabla u_k(x) dx + \int_\Omega f(u_{k-1}(x))v(x)dx = 0 \tag{3.6}$$

$$\int_\Omega \frac{u_k(x)}{\tau} v(x)dx + \varepsilon \int_\Omega \nabla v(x)\nabla u_k(x)dx = \int_\Omega \left(\frac{u_{k-1}(x)}{\tau} - f(u_{k-1}(x))\right) v(x)dx$$

$$\frac{1}{\tau}\int_\Omega u_k(x)v(x)dx + \varepsilon \int_\Omega \nabla u_k(x)\nabla v(x)dx = \int_\Omega \left(\frac{u_{k-1}(x)}{\tau} - f(u_{k-1}(x))\right) v(x)dx \qquad (3.7)$$

By posing :

$$a(u_k, v) = \frac{1}{\tau}\int_\Omega u_k(x)v(x)dx + \varepsilon \int_\Omega \nabla u_k(x)\nabla v(x)dx$$

et

$$l(v) = \int_\Omega \left(\frac{u_{k-1}(x)}{\tau} - f(u_{k-1}(x))\right) v(x)dx$$

We obtain the problem:

$$\begin{cases} \text{Find } u_k \in H^1(\Omega) & \text{such that} \\ a(u_k, v) = l(v) \end{cases} \qquad (3.8)$$

Proposition 4.2 :
Problem (3.8) has a unique solution.

Proof :
We will show that in problem (3.8), a is a continuous and coercive bilinear form on $H^1(\Omega) \times H^1(\Omega)$, l is a continuous linear form on $H^1(\Omega)$ and finally use Lax Milgram's theorem to conclude.

- The bilinearity of a and the linearity of l follow trivially from the linearity of the integral.
- Let us show that the bilinear form a is continuous on $H^1(\Omega)$.

$$\begin{aligned}
|a(u_k; v)| &= \left|\frac{1}{\tau}\int_\Omega u_k(x)v(x)dx + \varepsilon \int_\Omega \nabla u_k(x)\nabla v(x)dx\right| \\
|a(u_k; v)| &\leq \frac{1}{\tau}\int_\Omega |u_k(x)v(x)|dx + \varepsilon \int_\Omega |\nabla u_k(x)\nabla v(x)|dx \\
&\leq \frac{1}{\tau}\|u_k\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} + \varepsilon\|\nabla u_k\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} \\
&\leq \frac{1}{\tau}\|u_k\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} + \varepsilon\|u_k\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \\
&\leq \frac{1}{\tau}\|u_k\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} + \varepsilon\|u_k\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \\
&\leq \left(\frac{1}{\tau} + \varepsilon\right)\|u_k\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \\
|a(u_k; v)| &\leq \left(\frac{1}{\tau} + \varepsilon\right)\|u_k\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}
\end{aligned}$$

The bilinear form a is therefore continuous on $H^1(\Omega)$.

– Let us now show that the bilinear form a is coercive on $H^1(\Omega)$.

$$a(u_k;u_k) = \frac{1}{\tau}\int_\Omega (u_k(x))^2 dx + \varepsilon \int_\Omega (\nabla u_k(x))^2 dx$$

$$= \frac{1}{\tau}\|u_k\|^2_{L^2(\Omega)} + \varepsilon \|\nabla u_k\|^2_{L^2(\Omega)}$$

By posing

$$C = min\left(\frac{1}{\tau};\varepsilon\right)$$

We then obtain :

$$a(u_k;u_k) \geq C\left(\|u_k\|^2_{L^2(\Omega)} + \|\nabla u_k\|^2_{L^2(\Omega)}\right)$$

$$\Rightarrow a(u_k;u_k) \geq C\|u_k\|^2_{H^1}$$

Therefore a is coercive on $H^1(\Omega)$

– Let us show that the linear form l is continuous on $H^1(\Omega)$

$$l(v) = \int_\Omega \left(\frac{u_{k-1}(x)}{\tau} - f(u_{k-1}(x))\right) v(x)dx$$

$$\left|l(v)\right| = \left|\int_\Omega \left(\frac{u_{k-1}(x)}{\tau} - f(u_{k-1}(x))\right) v(x)dx\right|$$

$$\left|l(v)\right| \leq \left|\int_\Omega \left(\frac{u_{k-1}(x)}{\tau} v(x)dx\right)\right| + \left|\int_\Omega \left(f(u_{k-1}(x))\right) v(x)dx\right|$$

$$\leq \left|\int_\Omega \frac{u_{k-1}(x)}{\tau} v(x)dx\right| + \sup_{x\in(\Omega)}\left|f(u_{k-1}(x))\right|\left|\int_\Omega v(x)dx\right|$$

$$\leq \left(\int_\Omega (\frac{u_{k-1}(x)}{\tau})^2 dx\right)^{\frac{1}{2}}\left(\int_\Omega (v(x))^2 dx\right)^{\frac{1}{2}} + \sup_{x\in(\Omega)}|f(u_{k-1}(x))|\left(\int_\Omega dx\right)^{\frac{1}{2}}\left(\int_\Omega (v(x))^2 dx\right)^{\frac{1}{2}}$$

$$\leq C\sqrt{mes(\Omega)}\|v\|_{L^2(\Omega)} + \frac{1}{\tau}\|u_{k-1}\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)}$$

$$\leq \lambda\|v\|_{L^2(\Omega)}$$

$$\leq \lambda\|v\|_{H^1(\Omega)}$$

with $C = \sup_{x\in(\Omega)}|f(u_{k-1}(x))|$ et $\lambda = \max\left(C\sqrt{mes(\Omega)}; \frac{1}{\tau}\|u_{k-1}\|_{L^2(\Omega)}\right)$

We deduce that l is a continuous linear form on $H^1(\Omega)$.

Finally, the Lax-Milgram theorem allows us to conclude that the problem (3.8) admits a unique solution in $H^1(\Omega)$

Second step: Convergence of the sequence of solutions (u_k) towards the solution of problem (3.1).

Proposition 4.3 :

the sequence of solutions (u_k) converges to u the unique solution of problem (3.1)

Proof :

Let us make τ tend towards zero in the relation (3.5)

$$\lim_{\tau \longrightarrow 0} \left(\int_\Omega \frac{u_k(x) - u_{k-1}(x)}{\tau} v(x)dx + \varepsilon \int_\Omega \nabla v(x) \nabla u_k(x)dx + \int_\Omega f(u_{k-1}(x))v(x)dx \right) = 0$$

$$\lim_{\tau \longrightarrow 0} \int_\Omega \frac{u_k(x) - u_{k-1}(x)}{\tau} v(x)dx + \varepsilon \int_\Omega \nabla v(x) \nabla u_k(x)dx + \int_\Omega f(u_{k-1}(x))v(x)dx = 0$$

$$\lim_{t_k \longrightarrow t_{k-1}} \int_\Omega \frac{u_k(x) - u_{k-1}(x)}{t_k - t_{k-1}} v(x)dx + \varepsilon \lim_{t_k \longrightarrow t_{k-1}} \int_\Omega \nabla v(x) \nabla u_k(x)dx + \lim_{t_k \longrightarrow t_{k-1}} \int_\Omega f(u_{k-1}(x))v(x)dx = 0$$

$$\int_\Omega \frac{\partial u(x,t_k)}{\partial t} v(x)dx + \varepsilon \int_\Omega \nabla v(x) \nabla u(x,t_k)dx + \int_\Omega f(u(x,t_k))v(x)dx = 0$$

$$\int_\Omega \left(\frac{\partial u(x,t_k)}{\partial t} v(x) - \varepsilon \Delta u(x,t_k)v(x) + f(u(x,t_k)v(x) \right) dx = 0$$

$$\int_\Omega \left(\frac{\partial u(x,t_k)}{\partial t} - \varepsilon \Delta u(x,t_k) + f(u(x,t_k) \right) v(x)dx = 0$$

$$\left(\frac{\partial u(x,t_k)}{\partial t} - \varepsilon \Delta u(x,t_k) + f(u(x,t_k) \right) v(x) = 0$$

From where

$$\left(\frac{\partial u(x,t_k)}{\partial t} - \varepsilon \Delta u(x,t_k) + f(u(x,t_k) \right) = 0$$

Consequently when τ tends towards 0 u_k travels the interval $[0;T]$ which gives us:

$$\frac{\partial u(x,t)}{\partial t} - \varepsilon \Delta u(x,t) + f(u(x,t) = 0$$

4.1.2 Maximum principle

In this subsection, we will show that the solutions of the Allen Cahn equation verify the Maximum Principle.

The maximum principle is a property of the solutions of certain partial differential equations, of elliptic or parabolic type, which states that a solution function of such an equation on a domain reaches its maximum on the boundary of the domain. More precisely, the strong maximum principle says that if the function reaches its maximum inside the domain, it is constant. The weak maximum principle says that the maximum of the function is reached on the boundary of the domain, but can also possibly be reached inside the domain. An even weaker maximum principle simply limits the function by its maximum on the boundary [8]

A very large number of results of regularity, uniqueness or existence of solutions in second-order elliptic problems can be established using the maximum principle. Moreover, the different types of maximum principles (very often we say the maximum principle) are very useful for establishing estimates, a priori, on possible solutions [9].

The maximum principle is an extremely useful result, it allows us to obtain information about the solutions of partial differential equations without any knowledge of the solutions themselves, in particular to obtain a priori upper bounds of solutions of linear or nonlinear second-order equations.

Proposition 4.4 (Weak maximum principle for the Allen Cahn equation) :
Let problem (3.1)

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,t) - \varepsilon \Delta u(x,t) + f(u(x,t)) = 0; & \text{for } x \in \Omega, t \geqslant 0 \\ \\ \frac{\partial u}{\partial n} = 0; & \text{for } x \in \partial\Omega, t \geqslant 0 \\ \\ u(x,0) = u_0(x); & \text{for } x \in \Omega \end{cases} \tag{3.1}$$

Let $u \in H^1(\Omega)$ a solution to the problem (3.1);
If $\max\limits_{x \in \partial\Omega} |u_0(x)| \leq 1$ so $\max\limits_{x \in \Omega} |u(x)| \leq 1$ almost everywhere in (Ω).

Proof :
Let $x \in \Omega$ and let $(u+1)_-$ be the function defined by

$$(u+1)_-(x,t) = \begin{cases} -(u+1) & \text{if } u < -1 \\ 0 & \text{if } u > -1 \end{cases}$$

and let $(u-1)_+$ be the function defined by

$$(u-1)_+(x,t) = \begin{cases} (u-1) & \text{if } u > 1 \\ 0 & \text{if } u < 1 \end{cases}$$

We know that $(u+1)_-$ and $(u-1)_+$ belong to $H_0^1(\Omega)$; it is therefore sufficient to show $(u+1)_- = 0$ and $(u-1)_+ = 0$ to conclude that $|u| \leq 1$ almost everywhere in Ω.
Let us multiply the EDP of the model (3.1) by $(u-1)_+(x,t)$ and integrate over Ω.

$$\int_\Omega (u-1)_+(x,t)\frac{\partial u}{\partial t}(x,t)dx - \varepsilon \int_\Omega (u-1)_+(x,t)\Delta u(x,t)dx + \int_\Omega (u-1)_+(x,t) f(u(x,t))dx = 0$$

$$\int_\Omega (u-1)_+(x,t)\frac{\partial (u-1)_+}{\partial t}(x,t)dx - \varepsilon \int_\Omega (u-1)_+(x,t)\Delta (u-1)_+(x,t)dx + \int_\Omega (u-1)_+(x,t) f(u(x,t))dx = 0$$

$$\frac{1}{2}\frac{d}{dt}\int_\Omega ((u-1)_+(x,t))^2 dx = \varepsilon \int_\Omega (u-1)_+(x,t)\Delta (u-1)_+(x,t)dx - \int_\Omega (u-1)_+(x,t)(u^3(x,t) - u(x,t))dx$$

Using Green's formula and majorizing $f'(u)$, we obtain:

$$\frac{1}{2}\frac{d}{dt}\int_\Omega ((u-1)_+(x,t))^2 dx \leq -\varepsilon \int_\Omega (\nabla (u-1)_+(x,t))^2 dx - \int_\Omega (u-1)_+(x,t)(u^3(x,t) - u(x,t))dx$$

$$\frac{1}{2}\frac{d}{dt}\int_\Omega ((u-1)_+(x,t))^2 dx \leq -\left(\varepsilon \int_\Omega (\nabla (u-1)_+(x,t))^2 dx + \int_\Omega (u-1)_+(x,t)(u^3(x,t) - u(x,t))dx\right)$$

From where $\dfrac{1}{2}\dfrac{d}{dt}\displaystyle\int_\Omega ((u-1)_+(x,t))^2 dx \leq 0$

By setting $G(t) = \displaystyle\int_\Omega ((u-1)_+(x,t))^2 dx$, G is decreasing, so

for $t \geq 0, G(t) \leq G(0) = \int_\Omega ((u-1)_+(x,0))^2 dx = 0$,
Therefore $G(t) \leq 0 \Rightarrow \int_\Omega ((u-1)_+(x,t))^2 dx \leq 0 \Rightarrow (u-1)_+(x,t) = 0$ almost everywhere, therefore $u \leq 1$
We then repeat the same reasoning with $v = (u+1)_-$, we obtain $u \geq -1$
Finally, by combining the two demonstrations we obtain $\|u\|_{L^\infty(\Omega)} \leq 1$.

5 Resolution and numerical simulations of the Allen-Cahn equation in the two-dimensional case

5.1 Semi-discretization in space

This involves discretizing in space only the variational formulation (3.5)
Let $\Omega = [0,1] \times [0,1]$ be a bounded open set of $\mathbb{R}^2$.
Let V_h be the approximation space defined by:

$$V_h = \left\{ v \in H^1(\Omega) \cap C^0(\overline{\Omega}) \quad telque \quad v_{h_{|K}} \in \mathbb{P}_1 \qquad \forall K \in \mathcal{T} \quad \right\} \quad (5.9)$$

where $\mathbb{P}_1$ denotes the set of polynomials of degree 1, $\mathcal{T}$ a mesh of the domain Ω, and K an element of this mesh.
Let $u_{0,h}$ in V_h be an approximation of the initial data u_0, obtained by interpolation on $\mathcal{T}$.
Our semi-discretization in space is given by the following internal variational approximation:
Find $u_h(t)$ function of $[0; +\infty[$ with values in V_h, such that for all $v \in Vh$ and for all $t > 0$,

$$\begin{cases} \dfrac{d}{dt}(m(u_h(t), v) + \varepsilon a(u_h(t), v) + m(f(u_h(t)), v) = 0, \\ u_h(t=0) = u_{0,h} \end{cases} \quad (5.10)$$

The approximate solution is represented by :

$$u_h(x,t) = \sum_{i=1}^{N} u_i(t)\phi_i(x),$$

where u_i are the coefficients to be determined, and ϕ_i are the basis functions associated with the mesh nodes.

Since the nonlinear term is difficult to implement, we will linearize the nonlinear term and then move on to time discretization.

5.2 Linearization of the double well potential

Numerical linearization of the Allen-Cahn model is a method used to approximately solve nonlinear differential equations by transforming them into a linear problem, which can simplify the analysis and solution.
The linearization of the nonlinear function $f(u_h) = u_h^3 - u_h$ is achieved by an approximation around a

solution or a reference state. For a first-order approximation, one can use the Taylor series expansion :

$$f(u_h) \approx f(u_{0,h}) + f'(u_{0,h})(u_h - u_{0,h}), \qquad (5.11)$$

where $u_{0,h}$ is a reference value for u_h and $f'(u_{0,h})$ is the derivative of $f(u_h)$ evaluated at $u_{0,h}$.
Once $f(u_h)$ is linearized, we will introduce the approximation (5.11) into the variational formulation (5.10), we then obtain:
Find $u_h(t)$ function of $[0; +\infty[$ with values in V_h, such that for all $v_h \in V_h$ and for all $t > 0$,

$$\begin{cases} \dfrac{d}{dt}(m(u_h(t), v_h) + \varepsilon a(u_h(t), v_h) + m(f(u_{0,h}) + f'(u_{0,h})(u - u_{0,h}), v_h) = 0, \\ \\ u_h(t=0) = u_{0,h} \end{cases} \qquad (5.12)$$

By rearranging we obtain :
Find $u_h(t)$ function of $[0; +\infty[$ with values in V_h, such that for all $v_h \in V_h$ and for all $t > 0$,

$$\begin{cases} \dfrac{d}{dt}(m(u_h(t), v_h) + \varepsilon a(u_h(t), v_h) + m(f'(u_{0,h})u_h(t), v_h) + m(f(u_{0,h} - f'(u_{0,h})u_{0,h}), v_h) = 0, \\ \\ u_h(t=0) = u_{0,h} \end{cases} \qquad (5.13)$$

This equation is now linear in u. Numerical linearization of the Allen-Cahn model simplifies the nonlinear equation to a linear equation by approximating the nonlinear terms by linear expressions around a solution or reference state. This approach facilitates the application of numerical methods for solving differential equations.

Finally using the spatial discretization where $u_h(x,t) = \sum_{j=1}^{N} u_j(t)\phi_j(x)$, then $v = \phi_i$ we can reformulate the variational equation in terms of the coefficients u_j, we have:

$$\begin{cases} \dfrac{d}{dt} m(u_h, v_h) + \varepsilon a(u_h(t), v_h) \quad + \\ m(f'(u_{0,h})u_h(t), v_h) + m(f(u_{0,h} - f'(u_{0,h})u_{0,h}), v_h) = 0, \\ \\ u_h(t=0) = u_{0,h} \end{cases} \qquad (5.14)$$

$$\begin{cases} \displaystyle\int_{V_h} \frac{\partial u_h}{\partial t} v dr = -\varepsilon \sum_{j=1}^{N} u_j \int_{V_h} \nabla\phi_j(x)\nabla\phi_i(x) dr \quad - \sum_{j=1}^{N} u_j \int_{V_h} f'(u_{0,h})\phi_j(x)\phi_i(x) dr \quad - \\ \displaystyle\int_{V_h} \left[f(u_{0,h} - f'(u_{0,h})u_{0,h}\right] \phi_i(x) dr, \\ \\ u_h(x, t=0) = u_{0,h}(x) = u_0 \end{cases} \qquad (5.15)$$

$$\begin{cases} \displaystyle\int_{V_h} \frac{\partial u_h}{\partial t} v dr = -\varepsilon \sum_{j=1}^{N} u_j \int_{V_h} \nabla\phi_j(x)\nabla\phi_i(x) dr \quad - \sum_{j=1}^{N} u_j \int_{V_h} f'(u_{0,h})\phi_j(x)\phi_i(x) dr \quad + \\ \displaystyle\int_{V_h} \left(2(u_0)^3\right) \phi_i(x) dr, \\ \\ u_h(x, t=0) = u_{0,h}(x) = u_0 \end{cases} \qquad (5.16)$$

We then obtain:

$$\begin{cases} \mathcal{M}U_h'(t) = -\varepsilon\mathcal{R}U_h + \mathcal{D} \\ U_h(0) = U_0 \end{cases} \qquad (5.17)$$

where

$$\mathcal{M}_{i,j} = \int_{V_h} \phi_j(x)\phi_i(x)dr; \quad \mathcal{R}_{i,j} = \int_{V_h} \nabla\phi_j(x)\nabla\phi_i(x)dr + \int_{V_h} f'(u_0)\phi_j(x)\phi_i(x)dr$$

et

$$\mathcal{D}_i = \int_{V_h} 2(u_0)^3\phi_i(x)dr$$

Let K be an element of the mesh $\mathcal{T}$ we have :

$$\phi_{i_{|K}}(x;y) = \lambda_i^K(x;y)$$

and therefore :

$$\mathcal{M}_{i,j} = \sum_k \int_K \lambda_j^K\lambda_i^K dr$$

$$\mathcal{R}_{i,j} = \sum_k \int_K \nabla\lambda_j^K\nabla\lambda_i^K dr + \sum_k \int_K f'(u_{0,h})\lambda_j^K\lambda_i^K dr$$

$$\mathcal{D}_i = \sum_k \int_K 2(u_0)^3\lambda_i^K dr.$$

5.3 Calculations of matrices associated with the problem

Let us recall the formulas for exact integrations on a triangle K of the mesh :

$$\int_K \lambda_i^K dr = \frac{|K|}{3}$$

$$\int_K \left[\lambda_i^K\right]^2 dr = \frac{|K|}{6}$$

$$\int_K \lambda_i^K\lambda_j^K dr = \frac{|K|}{12}$$

$$\int_K \left(\lambda_i^K\right)^{\alpha_1}\left(\lambda_j^K\right)^{\alpha_2}\left(\lambda_l^K\right)^{\alpha_3} dr = \frac{\alpha_1!\alpha_2!\alpha_3!}{2+\alpha_1+\alpha_2+\alpha_3}$$

We then deduce :

- For the matrix $\mathcal{M}_{i,j}^K$

$$\mathcal{M}^K = \frac{|K|}{12}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} \qquad (5.18)$$

- Determination of the matrix $\mathcal{R}_{i,j}^K$

$$\mathcal{R}_{i,j}^K = \int_K \nabla\lambda_j^K \nabla\lambda_i^K dr + \int_K f'(u_{0,h})\lambda_j^K \lambda_i^K dr$$

Let's ask:

$$\mathcal{R}_{i,j}^K = \mathcal{N}_{i,j}^K + \mathcal{A}_{i,j}^K$$

with

$$\mathcal{N}_{i,j}^K = \int_K \nabla\lambda_j^K \nabla\lambda_i^K dr \quad et \quad \mathcal{A}_{i,j}^K = \int_K f'(u_0)\lambda_j^K \lambda_i^K dr$$

We deduce the formulas for barycentric coordinates on a triangle K.

$$\nabla\lambda_1^K = \frac{1}{2|K|}\begin{pmatrix} y_2 - y_3 \\ x_3 - x_2 \end{pmatrix}; \quad \nabla\lambda_2^K = \frac{1}{2|K|}\begin{pmatrix} y_3 - y_1 \\ x_1 - x_3 \end{pmatrix}; \quad \nabla\lambda_3^K = \frac{1}{2|K|}\begin{pmatrix} y_1 - y_2 \\ x_2 - x_1 \end{pmatrix}$$

$$\mathcal{N}^K = \begin{pmatrix} \frac{(y_2-y_3)^2+(x_3-x_2)^2}{4|K|^2} & \frac{(y_2-y_3)(y_3-y_1)+(x_3-x_2)(x_1-x_3)}{4|K|^2} & \frac{(y_2-y_3)(y_3-y_1)+(x_3-x_2)(x_2-x_1)}{4|K|^2} \\ \frac{(y_2-y_3)(y_3-y_1)+(x_3-x_2)(x_1-x_3)}{4|K|^2} & \frac{(y_3-y_1)^2+(x_1-x_3)^2}{4|K|^2} & \frac{(y_3-y_1)(y_1-y_2)+(x_1-x_3)(x_2-x_1)}{4|K|^2} \\ \frac{(y_2-y_3)(y_3-y_1)+(x_3-x_2)(x_2-x_1)}{4|K|^2} & \frac{(y_3-y_1)(y_1-y_2)+(x_1-x_3)(x_2-x_1)}{4|K|^2} & \frac{(y_1-y_2)^2+(x_2-x_1)^2}{4|K|^2} \end{pmatrix}$$

To determine the matrices $\mathcal{A}_{i,j}^K$ and $\mathcal{D}_i^K$ we choose to do a numerical integration by Gaussian points (of order 1) [10], using approximate quadrature formulas (midpoint formula), we approximate the integral of a function $m(x,y)$ on any triangle K by a quadrature formula of degree 1; we have:

$$\int_K f'(u_0(x,y))\lambda_j^K(x,y)\lambda_i^K(x,y)dxdy \simeq \frac{1}{2}f'(u_0(x_G,y_G))\lambda_j^K(x_G,y_G)\lambda_i^K(x_G,y_G) \quad (5.19)$$

with

$$x_G = \frac{x_1^K + x_2^K + x_3^K}{3} \quad et \quad y_G = \frac{y_1^K + y_2^K + y_3^K}{3}$$

$$\mathcal{A}_{i,j}^K \simeq \frac{1}{2}\left(3\left[u_0\left(x_G;y_G\right)\right]^2 - 1\right)\lambda_j\left(x_G;y_G\right)\lambda_i\left(x_G;y_G\right)$$

$$\mathcal{A}^K \simeq \frac{1}{2}\left(3\left[u_0\left(x_G;y_G\right)\right]^2 - 1\right)\begin{pmatrix} \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \end{pmatrix}$$

$$\mathcal{A}^K \simeq \frac{1}{18}\left(3\left[u_0\left(x_G;y_G\right)\right]^2 - 1\right)\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \quad (5.20)$$

.

- Determination of the matrix $\mathcal{D}_i^K$

$$\mathcal{D}_i = \int_{V_h} 2(u_0)^3 \phi_i(x) dr$$

$$\mathcal{D}_i^K = \int_K 2\left[u_0\left(x;y\right)\right]^3 \lambda_i\left(x;y\right) dxdy$$

$$\mathcal{D}_i^K \simeq \frac{1}{2} u_0\left(x_G;y_G\right) \lambda_i^K\left(x_G;y_G\right)$$

$$\mathcal{D}^K \simeq \left[u_0\left(x_G;y_G\right)\right]^3 \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}$$

$$\mathcal{D}^K \simeq \frac{1}{3}\left[u_0\left(x_G;y_G\right)\right]^3 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad (5.21)$$

5.4 Total discretization in space-time

Let $\Delta t > 0$ et $t_n = n\Delta t \quad 0 \leqslant n \leqslant N, \quad \Delta t = \frac{T}{N}$.

For a time discretization, let us apply the implicit Euler scheme $\dfrac{\partial U_h}{\partial t} = \dfrac{U_h^{n+1} - U_h^n}{\Delta t}$ to relation (5.17); we obtain

$$\mathcal{M}\frac{U_h^{n+1} - U_h^n}{\Delta t} = -\varepsilon \mathcal{R} U_h^{n+1} + \mathcal{D} \qquad (5.22)$$

Finally, the total discretization of the model gives:

$$(\mathcal{M} + \varepsilon \Delta t \mathcal{R}) U_h^{n+1} = \mathcal{M} U_h^n + \Delta t \mathcal{D} \qquad (5.23)$$

6 Numerical simulations

In this section, we will use MATLAB software to perform a series of simulations of the Allen-Cahn equation. For this, we used an initial distribution u_0 defined by:

$$u_0(x,y) = tanh\left(\frac{\sqrt{(x-0.5)^2 + (y-0.5)^2} - R}{\varepsilon\sqrt{2}}\right)$$

where R is the radius of the initial interface and ε a small positive parameter.
In all simulations, we take $R = 0.6$ and $\varepsilon = 0.9$.
First, we perform simulations on the domain $\Omega = [0,1] \times [0,1]$ subdivided into 162 triangles formed by 100 nodes; we observed the following figures for different time intervals.

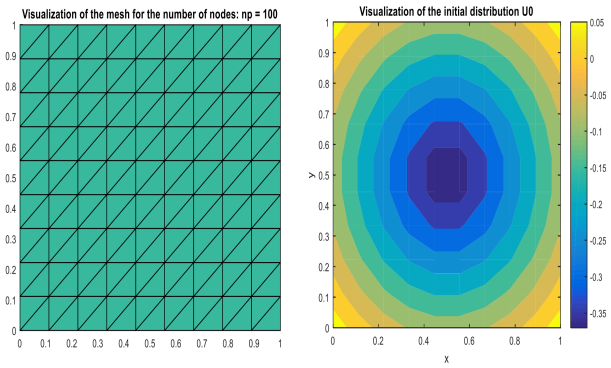

Figure 1: Mesh and initial solution for 100 nodes

Here is the evolution of the solution u at the respective times $t = 0.1$; $t = 0.2$; $t = 1$; $t = 2.5$; $t = 5$; $t = 10s$.
We then present the simulations of the evolution of the solution u for a mesh of the domain $\Omega = [0, 1] \times [0, 1]$ subdivided into 4802 triangles formed of 2500 nodes:

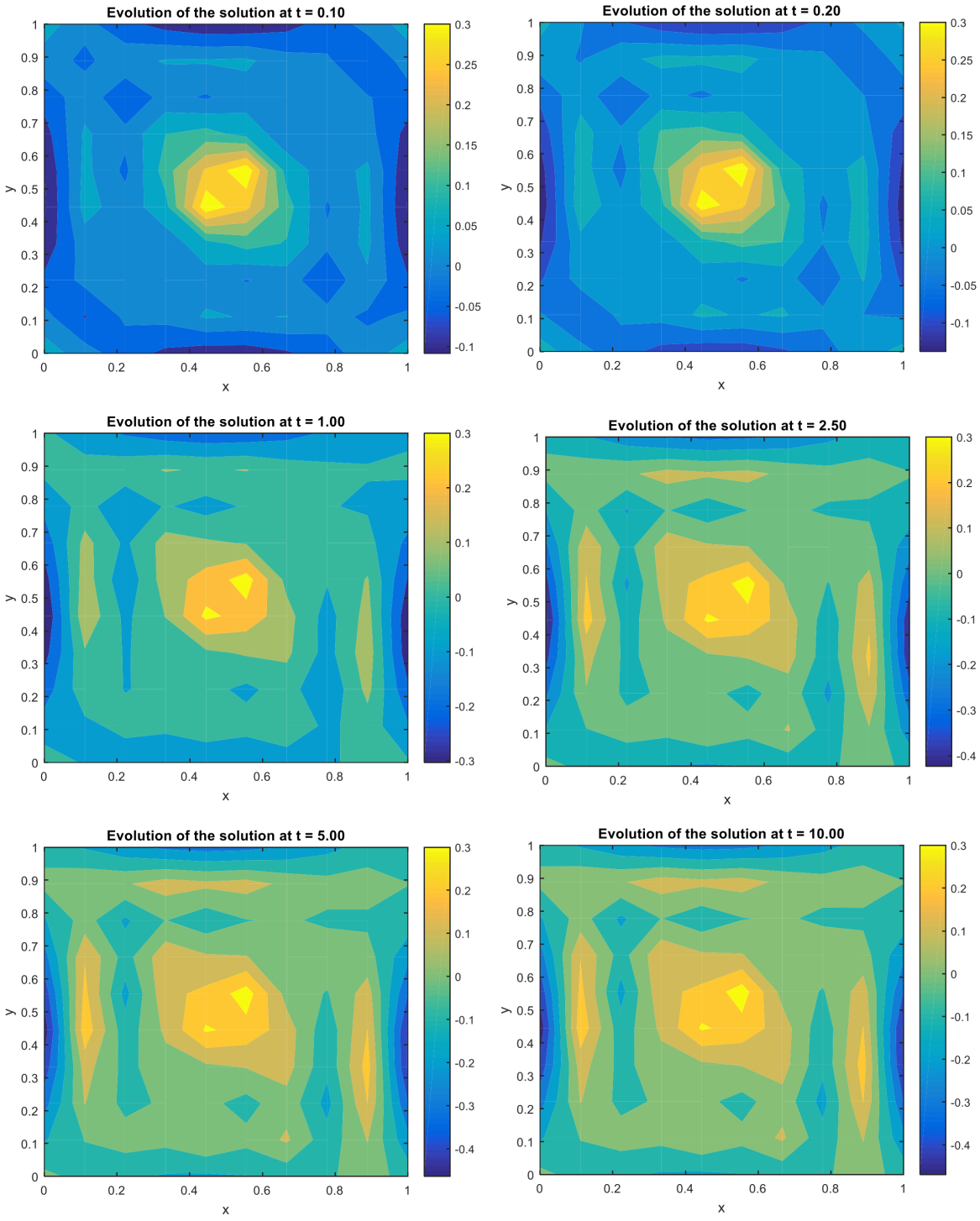

Figure 2: Evolution of the solution u for 100 nodes

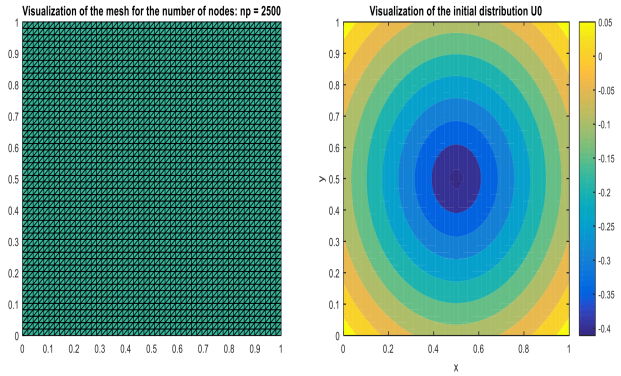

Figure 3: Mesh and initial solution for 2500 nodes

Here is the evolution of the solution u at the respective times $t = 0.1s$; $t = 0.2s$; $t = 1s$; $t = 2.5s$; $t = 5s$; $t = 10s$.

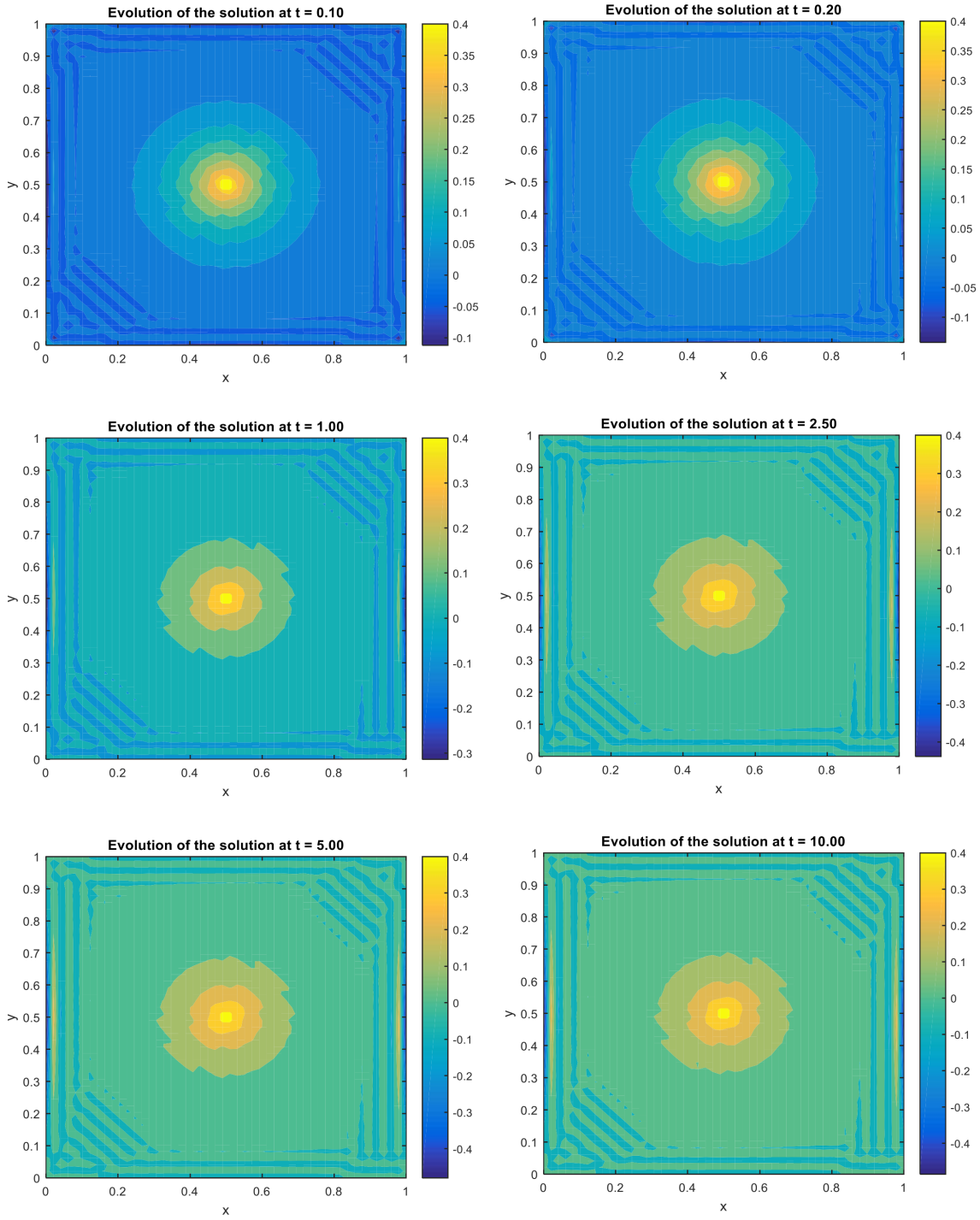

Figure 4: Evolution of the solution u for 2500 nodes

Finally, we present the simulations of the evolution of the solution u for a mesh of the domain $\Omega = [0,1] \times [0,1]$ subdivided into 19602 triangles formed of 10000 nodes:

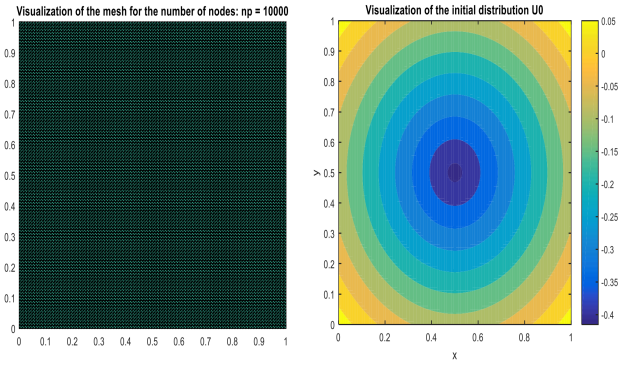

Figure 5: Mesh and initial solution for 10000 nodes

Here is the evolution of the solution u at the respective times $t = 0.1s$; $t = 0.2s$; $t = 1s$; $t = 2.5s$; $t = 5s$; $t = 10s$.

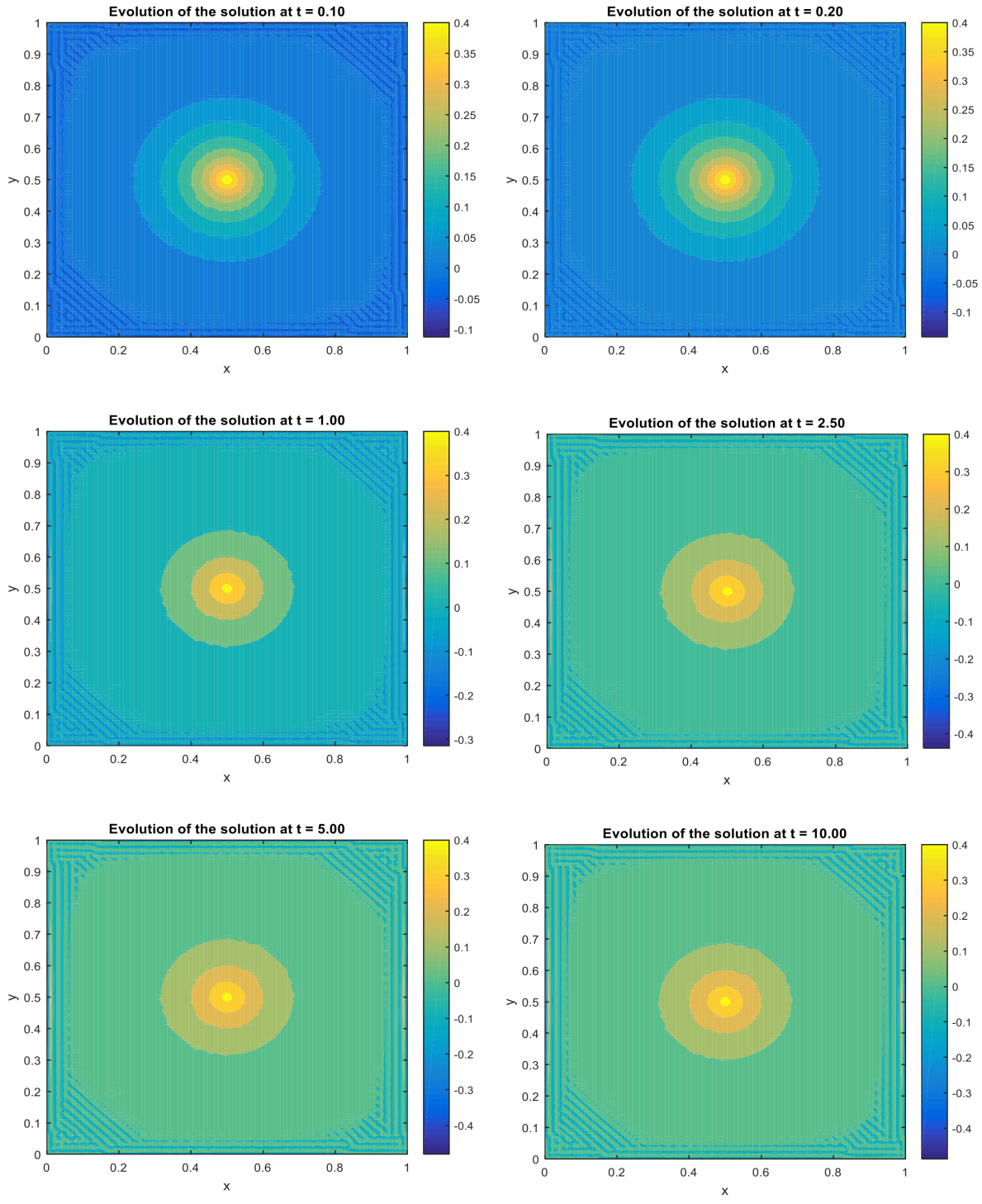

Figure 6: Evolution of the solution u for 10000 nodes

Interpretation of simulation results

- In figure (2) we observe a diffuse phase transition that stabilizes from t = 2.5 s thus establishing a phase separation where the two stable energy levels are represented in the figures by $u = -0.4$ and $u = 0.3$.

- In figure (4) with a slightly more refined mesh than the previous one, we also observe the same diffuse phase transition phenomenon which stabilizes from t = 2.5 s, dedicating a phase separation where the two stable states are reached for $u = -0.4$ and $u = 0.4$.

- Finally in figure (6) where the mesh is extremely refined, we observe the same phenomenon as in figure (4).

- Since the radius of the initial interface that we considered is R = 0.6, we see that in accordance with the theoretical study, the two stable states are the two extrema of the double well potential $F(u)$.

- We also note that, $|u| \leq 1$, for all simulations performed; which is consistent with the maximum principle.

7 Conclusion

The study of the Allen-Cahn equation has provided us with a rich and varied perspective on phase separation processes and interface dynamics in materials. Through a theoretical study we have shown that the Allen-Cahn equation with homogeneous Neumann boundary conditions is a well-posed problem.

Numerical simulations carried out with MATLAB software have allowed us to highlight the effectiveness of the equation for modeling phase transition and separation phenomena in different systems.

The use of the finite element method, particularly with homogeneous Neumann boundary conditions, allowed us to solve the equations and obtain results that are consistent with the theory.

Numerical results showed that the Allen-Cahn equation can capture complex phase transition behaviors in materials, thus demonstrating its efficiency for practical applications in materials science and engineering..

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