Numerical Report

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1 Introduction of the model and method

1.1 Allen-Cahn equation

This report presents the numerical results of the following Allen-Cahn equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \varepsilon \Delta u + \dfrac{1}{\varepsilon} f(u) \\ f(u) = u(1-u^2) \end{cases} \tag{1}$$

The equation describes the evolution of a scalar field u in time t and space x with a diffusion coefficient ε. The function $f(u)$ is a nonlinear term that drives the phase transition of the field u. The equation is solved on a domain Ω with boundary $\partial\Omega$ and initial condition $u(x,0) = u_0(x)$ and periodic boundary conditions.

By the knowledge of calculus of variations, if we define the following energy functional:

$$E(u) = \int_\Omega \left(\frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} F(u) \right) dx,$$

then the equation is the gradient flow of energy functional with respect to u, where $F(u)$ is defined by $F(u) = \frac{1}{4}(1-u^2)^2$.

As it is shown in [1], the equation

$$\begin{cases} \dfrac{\partial u}{\partial t} = \Delta u + \dfrac{1}{\varepsilon^2} f(u) \\ f(u) = u(1-u^2) \end{cases}$$

is an approximation for mean curvature flows. Thus equation 1 is also an approximation to the mean curvature flow in another time scale. If we take u_0 as the smoothed characteristic function of a domain, then the solution of the equation will converge to the mean curvature flow of the domain when ε goes to zero.

1.2 SAV-Scheme

To discretize the equation, we use the SAV scheme. The scheme is based on the semi-implicit Euler method. The time derivative is discretized by the backward Euler method, and the spatial derivative is discretized by the finite element method. First we introduce the following scalar auxiliary variable r:

$$r = \sqrt{E_1(u) + C_0},$$

where $E_1(u) = \int_\Omega F(u)dx$ and C_0 is a constant. Then the equation can be rewritten as:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \varepsilon \Delta u + \dfrac{1}{\varepsilon} \dfrac{r(t)}{\sqrt{E_1(u) + C_0}} f(u), \\ \dfrac{\partial r}{\partial t} = \dfrac{1}{2\sqrt{E_1[u] + C_0}} \displaystyle\int_\Omega F'(u) u_t dx. \end{cases} \tag{2}$$

Thus a BDF2 scheme yields:

$$\begin{cases} \dfrac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = \varepsilon \Delta u^{n+1} + \dfrac{1}{\varepsilon} \dfrac{r^{n+1}}{\sqrt{E_1(u^{n+\frac{1}{2}}) + C_0}} f(u^{n+\frac{1}{2}}), \\ \dfrac{3r^{n+1} - 4r^n + r^{n-1}}{2\Delta t} = \dfrac{1}{2\sqrt{E_1[u^{n+\frac{1}{2}}] + C_0}} \displaystyle\int_\Omega F'(u^{n+\frac{1}{2}}) \dfrac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} dx, \end{cases} \tag{3}$$

where $u^{n+\frac{1}{2}}$ is an explicit $O(\Delta t^2)$ approximation for u^{n+1}. Here we solve

$$\frac{u^{n+\frac{1}{2}} - u^n}{\Delta t} = \varepsilon \Delta u^{n+\frac{1}{2}} + \frac{1}{\varepsilon} f(u^n)$$

to get $u^{n+\frac{1}{2}}$. However, when the time step is large, we use fully implicit Euler method to avoid the stability issue.

By eliminating r^{n+1}, we obtain the following equation:

$$\left(1 - \frac{2\Delta t}{3} \varepsilon \Delta\right) u^{n+1} + \frac{\Delta t}{3\varepsilon} b^n (b^n, u^{n+1}) = g^n, \tag{4}$$

where

$$\begin{aligned} b^n =& \frac{F'(u^{n+\frac{1}{2}})}{\sqrt{E_1(u^{n+\frac{1}{2}}) + C_0}}, \\ g^n =& \frac{4}{3} u^n - \frac{1}{3} u^{n-1} - \frac{2\Delta t}{9\varepsilon} \left(4r^n - r^{n-1} - \frac{1}{2}(b^n, 4u^n - u^{n-1})\right) b^n. \end{aligned}$$

Denoting $A = \left(1 - \frac{2\Delta t}{3} \varepsilon \Delta\right)$, by taking inner product with b^n in (4), we get

$$(b^n, u^{n+1}) = \frac{(b^n, A^{-1} g^n)}{1 + \frac{\Delta t \gamma^n}{3\varepsilon}},$$

where $\gamma^n = (b^n, A^{-1} b^n)$.

Thus the equation can be solved by the following steps:

1. Compute $u^{n+\frac{1}{2}}$.
2. Compute γ^n.
3. Compute (b^n, u^{n+1}).
4. Compute $Au^{n+1} = g^n - \frac{\Delta t}{3\varepsilon} b^n (b^n, u^{n+1})$.

2 Implementation

In SAV scheme, the key part is to solve different Poisson type equations,

$$\phi - C\Delta\phi = w,$$

where C is some positive constant depending on the equation. We use the finite element method to solve the Poisson equation. The domain is discretized by a triangular mesh. The finite element space V_h is defined by piecewise linear functions with periodic boundary conditions. The FEM problem is to find ϕ_h in V_h such that

$$\int_\Omega \phi_h v dx + C\int_\Omega \nabla\phi_h \cdot \nabla v dx = \int_\Omega w v dx, \qquad \forall v \in V_h.$$

Since the differential operator is positive definite, the PDE and the FEM problem are well-posed. The code is implemented in Python with the help of the FEniCS library. The FEniCS library provides a high-level interface to the finite element method, which makes it easy to implement the numerical scheme. The code is available at `https://github.com/xinqi16/SAV_MAT7620_project2`.

3 Results and analysis of the experiment

3.1 The shrinkage of an ellipse

First we consider the shrinkage of an ellipse. The initial condition is a smoothed characteristic function of an ellipse. The domain is $\Omega = [-1, 1] \times [-1, 1]$. The diffusion coefficient is $\varepsilon = 0.01$. The time step is $\Delta t = 0.1$. The results are shown in Figure 1.

We can see that the ellipse shrinks to a circle as time goes by. The result is consistent with the theoretical prediction that the solution converges to the mean curvature flow of the domain.

3.2 The shrinkage of a circle

Next we consider the shrinkage of a circle. The initial condition is an interpolated characteristic function of a circle with radius 0.5. The domain is $\Omega = [-1, 1] \times [-1, 1]$. The diffusion coefficient is $\varepsilon = 0.01$. The time step is $\Delta t = 0.1$. The results are shown in Figure 2.

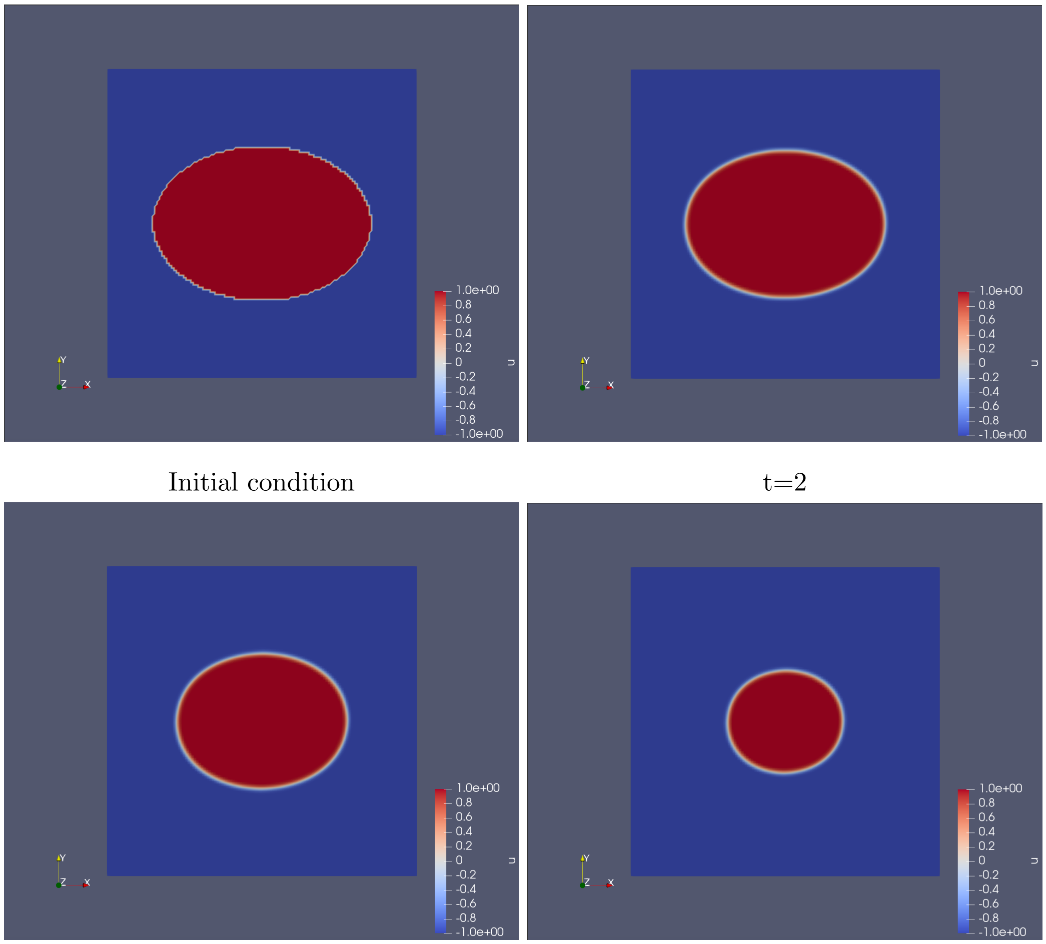
To check the motion of the interface is indeed driven by the mean curvature flow, we approximate the area of the disc by $S \approx \int_\Omega (u + 1)/2dx$. The results are shown in Table 3. According to the mean curvature flow,

$$\frac{dr}{dt} = \frac{\varepsilon}{r},$$

r^2 is linear with time. The result is consistent with the theoretical prediction. Moreover, the analytic slope is $k_a = -2\varepsilon\pi$, and the numerical test yields a slope $k = -0.0726$. Considering the error induced by the width of the interface, this is consistent with the theoretical result.

3.3 The shrinkage of a dungbell

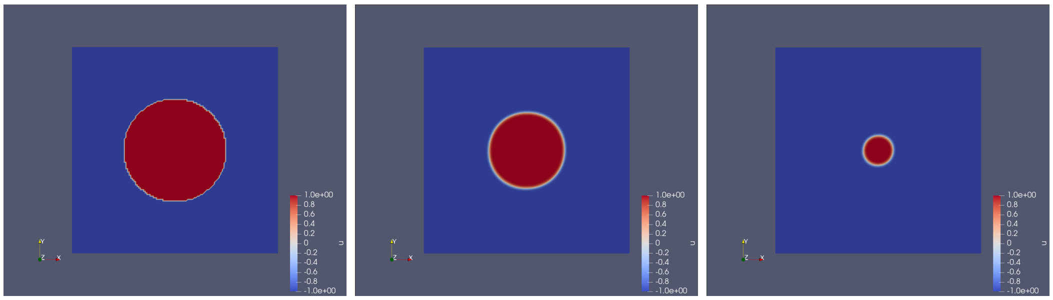
Finally we consider the shrinkage of a dungbell. The dungbell is consisted by two circles with radius $r = 0.25$ centered at $(-0.5, 0)$ and $(0.5, 0)$ respectively, and a rectangular $[-0.5, 0.5] \times [-0.1, 0.1]$



Initial condition | t=2

t=10 | t=5

Figure 1: Shrinkage of an ellipse



Initial condition t=5 t=10

Figure 2: Shrinkage of a circle

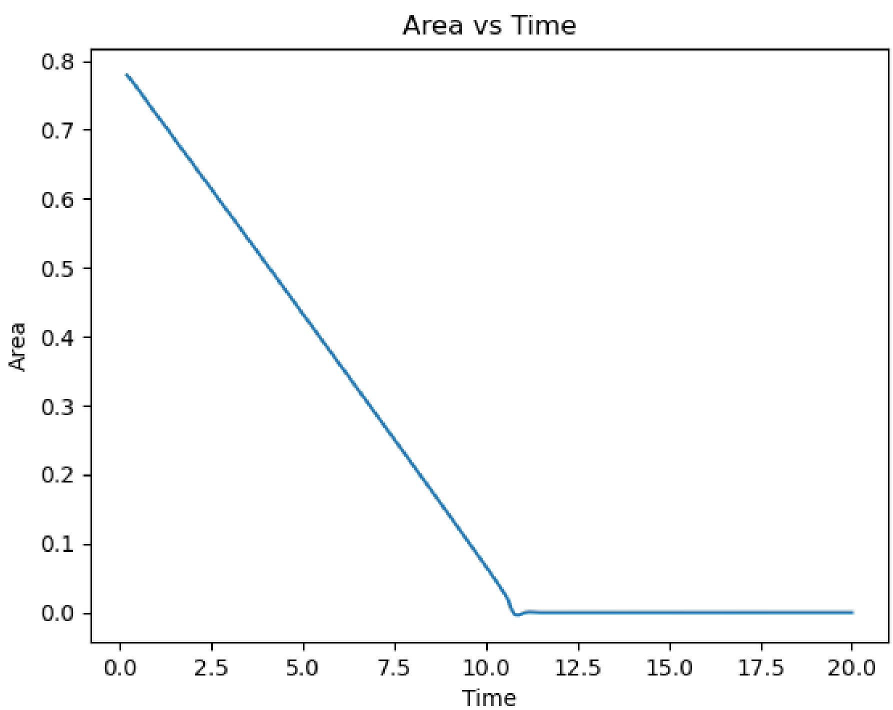
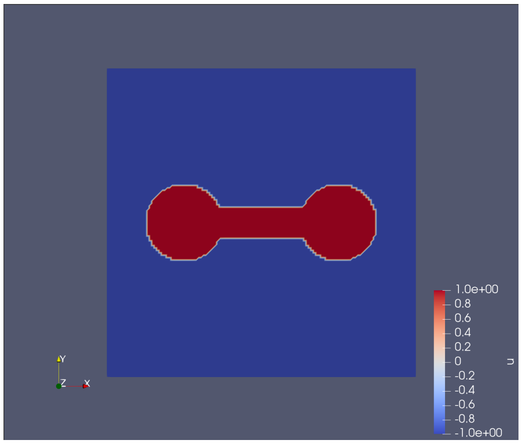
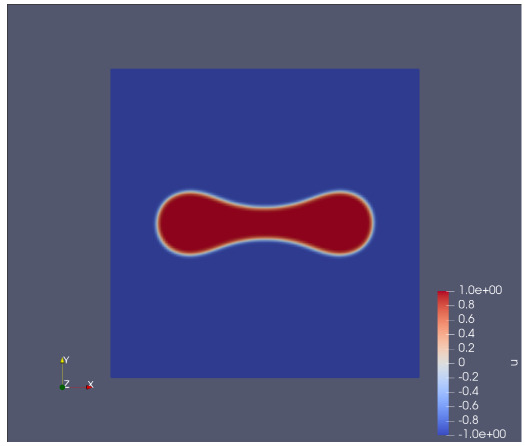


Figure 3: Area of the circle

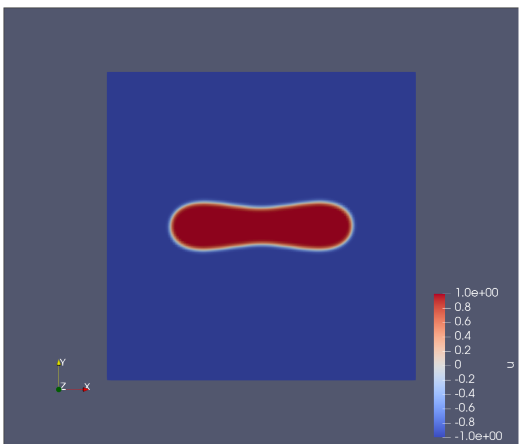
The initial condition is an interpolated characteristic function of a dungbell. The domain is $\Omega = [-1,1] \times [-1,1]$. The diffusion coefficient is $\varepsilon = 0.01$. The time step is $\Delta t = 0.05$. The results are shown in Figure 4.



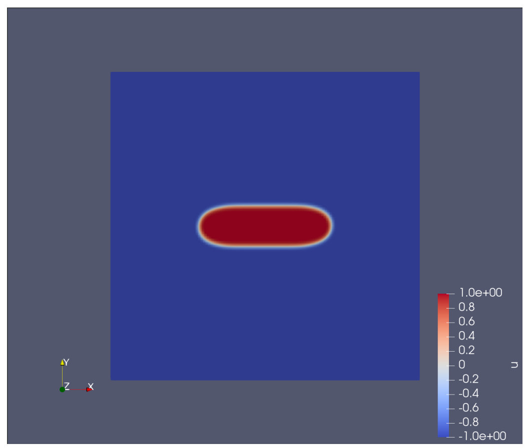
Initial condition



t=1



t=2.5



t=4

Figure 4: Shrinkage of a dungbell

References

[1] Xiaobing Feng and Andreas Prohl. Numerical analysis of the allen-cahn equation and approximation for mean curvature flows. *Numerische Mathematik*, 94:33–65, 2003.