土木所魏廷儒 r10521601
MATH 7422: Numerical Partial Differential Equations
March 26, 2023

Project 2

We will study the evolution process of a phase-field model in 2D. You can also search for Cahn-Hilliard model and Allan-Cahn model. We shall neglect the fluid part, only concentrate the evolution of the order parameter.

In this project, we analyze the Allen-Cahn equation, which describes the order parameter u for a material with two distinct phases (-1 and 1). The equation is given by:

$$u_t = \Delta u + u - u^3$$

We consider a rectangular domain with Neumann boundary conditions. To discretize the equation, we separate it into two distinct terms: the diffusion term and the reaction term.

1) Diffusion term Δu We first discretize the diffusion term as follows:

$$u_t = \frac{1}{h^2} L\mathbf{u} + \frac{1}{h}\mathbf{b}$$

Here, we assume no flux on the boundary grids, meaning $\frac{\partial u}{\partial x_i} = 0$. The 1D discretization can be written as:

$$\begin{bmatrix} \frac{1}{2}\dot{u}_0 \\ \dot{u}_1 \\ \dots \\ \dot{u}_{N-1} \\ \frac{1}{2}\dot{u}_N \end{bmatrix} = \frac{1}{h^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \dots & \dots & \dots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ u_{N-1} \\ u_N \end{bmatrix} + \frac{1}{h} \begin{bmatrix} \sigma_0 \\ 0 \\ 0 \\ 0 \\ \sigma_1 \end{bmatrix}$$

where σ_1 and σ_1 is equal to zero.

To extend the discretization to 2D, we flatten the 2D grid and renumber the grid points from 0 to $N_x \times N_y$, where N_x is the number of discretization points in the x-direction and N_y is the number of discretization points in the y-direction.

$$L = \frac{1}{\Delta y^2}(K_y \otimes I_{Nx}) + \frac{1}{\Delta x^2}(I_{Ny} \otimes K_x)$$

where $\otimes$ denotes the Kronecker product, K_x and K_y are the tridiagonal matrices for the x and y dimensions respectively, and I_{Nx} and I_{Ny} are the identity matrices of size $N_x \times N_x$ and $N_y \times N_y$ respectively.

The tridiagonal matrices K_x and K_y have the following structure:

$$K_x = K_y = \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{bmatrix}$$

With the 2D Laplacian matrix L, I implemented the implicit scheme to calculate the diffusion term. This can be written as follows:

$$\frac{u_{t+1} - u_t}{\Delta t} = L u_{t+1}$$

where u_t and u_{t+1} represent the solution at time steps t and $t+1$, respectively.

This equation can be written in matrix form as:

$$(I - \Delta t\, L) u_{t+1} = u_t$$

where I is the identity matrix. To solve for u_{t+1} at each time step, I utilize the sparse linear system solver in the `Scipy` package.

2) Reaction term: $u - u^3$

I initially attempted to treat the reaction term using an implicit scheme, which can be written as follows:

$$u_{t+1} - u_t = \Delta t(u_{t+1} - {u_{t+1}}^3)$$

To solve this nonlinear equation, I attempted to use Newton-Raphson and fixed-point methods. However, these approaches led to difficulties with convergence, resulting in impractical computation times.

As a result, I employed an explicit scheme to handle the reaction term:

$$u_{t+1} = u_t + \Delta t(u_t - {u_t}^3)$$

This approach led to a true error of $O(\Delta t)$.

To solve the diffusion and reaction terms, two strategies were considered: the coupled method and the decoupled method. In the coupled method, the two terms are solved simultaneously using a single equation. The discretized form of the equation is given by:

1) coupling

The discretition equation can be written as belows:

$$(I - \Delta t\, L)u_{t+1} = u_t + \Delta t(u_t - {u_t}^3)$$

where L is the Laplacian matrix for both the boundary grids and interior grids. In the implementation, the boundary grids and interior grids are calculated separately due to the different Laplacian matrices.

2) splitting method

In the decoupled method, the diffusion and reaction terms are treated separately using a splitting method. The Allan-Cahn equation can be written as:

$$u_t = \Delta u + f(u) \approx \Delta(u - u_0) + f'(u - u_0)$$

Let $v = u - u_0$, then:

$$v_t = \Delta(v) + f'(v)$$

Let $Av = \Delta v$ and $Bv = f(u_0)v$, then:

$$v_t = Av + Bv$$

The solutions to $e^{\Delta t A}$ and $e^{\Delta t B}$ can be calculated separately.

a. $e^{\Delta t A}$:

solve the equation below:

$$e^{\Delta t A} = u_{t+1} = (I - \Delta t\, L)^{-1} u_t$$

b. $e^{\Delta t B}$:

solve the equation below:

$$e^{\Delta t B} = u_{t+1} = u_t + \Delta t(u_t - {u_t}^3)$$

The solutions $e^{\Delta t A}$ and $e^{\Delta t B}$ can be merged by multiplying them together. For example, for $t = \Delta t$ the solution can be computed as:

$$u = e^{t(A+B)} u_0 \approx e^{\Delta t B} e^{\Delta t A} u_0$$

Similarly, for $t = 2\Delta t$ and $t = n\Delta t$ the solution can be computed as:

$$u = e^{t(A+B)}u_0 \approx e^{\Delta tB}e^{\Delta tA}e^{\Delta tB}e^{\Delta tA}u_0$$
$$u = e^{t(A+B)}u_0 \approx e^{\Delta tB}e^{\Delta tA}...e^{\Delta tB}e^{\Delta tA}u_0$$

I also utilize the spectral method to solve this equation. Spectral methods involve representing the solution as a sum of basis functions and determining the coefficients of the basis functions using the given equation. The basis functions are chosen such that they satisfy the boundary conditions of the problem. The solution can be approximated using a truncated series of basis functions.

For the diffusion-reaction equation, the basis functions can be chosen as the Fourier basis functions, which are periodic and satisfy the boundary conditions of the problem. The solution can be expressed as:

$$u(x,y,t) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \hat{u}_{mn}(t)e^{i(mx+ny)}$$

where $\hat{u}_{mn}(t)$ are the Fourier coefficients of $u(x,y,t)$.

The time derivative of $u(x,y,t)$ can be obtained as:

$$\frac{\partial u}{\partial t} = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \frac{d\hat{u}_{mn}}{dt}e^{i(mx+ny)}$$

The Laplacian of $u(x,y,t)$ can be obtained using the Fourier basis functions as:

$$\nabla^2 u(x,y,t) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} (-m^2-n^2)\hat{u}_{mn}(t)e^{i(mx+ny)}$$

Substituting these expressions in the given diffusion-reaction equation, we get:

$$\frac{d\hat{u}_{mn}}{dt} = -(m^2+n^2)\hat{u}_{mn} + \hat{u}_{mn} - \hat{u}_{mn}^3$$
$$\frac{\hat{u}_{mn}^{t+1} - \hat{u}_{mn}^{t}}{\Delta t} = -(m^2+n^2)\hat{u}_{mn}^{t+1} + \hat{u}_{mn}^{t} - \hat{u}_{mn}^{t3}$$
$$\hat{u}_{mn}^{t+1}(I + \Delta t(m^2+n^2)) = \hat{u}_{mn}^{t} + \Delta t(\hat{u}_{mn}^{t} - \hat{u}_{mn}^{t3})$$

$$\Rightarrow \hat{u}_{mn}^{t+1} = \frac{\hat{u}_{mn}^{t} + \Delta t(\hat{u}_{mn}^{t} - \hat{u}_{mn}^{t3})}{(I + \Delta t(m^2+n^2))}$$

Here, m and n are the wavenumbers in FFT. Once the Fourier coefficients are obtained, the solution $u(x,y,t)$ can be reconstructed using the inverse Fourier transform.

This project codes and animation can be found in the repository (`https://github.com/BerryWei/nurmical-PDE/tree/main/project2`).

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