Method of Finite Differences

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1   1-Dimensional Diffusion Equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

1.1   FTCS method

"Forward in time, central in space." Diffusion Equation is written as

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2}$$

Rearranging, we find that

$$C_i^{n+1} = C_i^n + D\Delta t\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2}$$

1.1.1   Forward Euler Time Scheme

Taylor series centered at a:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 \ldots$$

Taylor series centered at time t:

$$f(t + \Delta t) = \underbrace{f(t) + f'(t)\Delta t}_{\text{Forward Euler}} + \underbrace{\frac{f''(t)}{2!}\Delta t^2 + \frac{f'''(t)}{3!}\Delta t^3 \ldots}_{\text{Truncation Error}}$$

For the Forward Euler method, the local truncation error with each timestep is given by

$$\frac{f''(t)}{2!}\Delta t^2 + \frac{f'''(t)}{3!}\Delta t^3 + \frac{f''''(t)}{4!}\Delta t^4 \dots$$

Which scales as $\mathcal{O}(\Delta t^2)$. However, the global error is given by the number of time steps N multiplied by the local error. Since N is given by $(t_f - t_0)/\Delta t$, we can write the global error as

$$\frac{t_f - t_0}{\Delta t}\left(\frac{f''(t)}{2!}\Delta t^2 + \frac{f'''(t)}{3!}\Delta t^3 + \frac{f''''(t)}{4!}\Delta t^4 \dots\right)$$

$$= (t_f - t_0)\left(\frac{f''(t)}{2!}\Delta t + \frac{f'''(t)}{3!}\Delta t^2 + \frac{f''''(t)}{4!}\Delta t^3 \dots\right)$$

From this we can see that the global error scales as $\mathcal{O}(\Delta t)$.

1.1.2 Central Difference

Taylor series centered at x:

$$f(x + \Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \frac{f'''(x)}{3!}\Delta x^3 \dots$$

$$f(x - \Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 - \frac{f'''(x)}{3!}\Delta x^3 \dots$$

Adding together

$$f(x + \Delta x) + f(x - \Delta x) = 2f(x) + \frac{2f''(x)}{2!}\Delta x^2 + \frac{2f''''(x)}{4!}\Delta x^4 \dots$$

Rearranging to solve for $f''(x)$

$$f''(x) = \underbrace{\frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2}}_{\text{Central Difference}} + \underbrace{\frac{f''''(x)}{12}\Delta x^2}_{\text{Truncation Error}} \dots$$

From this we can see that the truncation error for the central difference scheme scales as $\mathcal{O}(\Delta x^2)$.

1.1.3 Von Neumann Stability Analysis

The amplification factor g for an error term ϵ is defined as

$$g = \frac{\epsilon_j^{n+1}}{\epsilon_j^n}$$

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In order for a numerical scheme to be stable, the errors must not grow exponentially in time. This means that a condition for stability is $|g| \leq 1$.

Fourier Transform:

$$\epsilon(x, t) = \sum_{k} \hat{\epsilon}(t) e^{ikx}$$

FTCS method error terms:

$$\frac{\epsilon_j^{n+1} - \epsilon_j^n}{\Delta t} = D \frac{\epsilon_{j+1}^n - 2\epsilon_j^n + \epsilon_{j-1}^n}{\Delta x^2}$$

Replacing ϵ_j^{n+1} with $g\epsilon_j^n$ and plugging in the Fourier mode of the error terms

$$\frac{g\hat{\epsilon}^n e^{ikj\Delta x} - \hat{\epsilon}^n e^{ikj\Delta x}}{\Delta t} = D \frac{\hat{\epsilon}^n e^{ik(j+1)\Delta x} - 2\hat{\epsilon}^n e^{ikj\Delta x} + \hat{\epsilon}^n e^{ik(j-1)\Delta x}}{\Delta x^2}$$

Dividing through by $\hat{\epsilon}^n e^{ikj\Delta x}$ leaves

$$\frac{g - 1}{\Delta t} = D \frac{e^{ik\Delta x} - 2 + e^{-ik\Delta x}}{\Delta x^2}$$

Eulers Formula:
$$e^{ix} = \cos x + i \sin x$$

From Euler's formula, we can say that $e^{ik\Delta x} + e^{-ik\Delta x}$ is equal to $2\cos(k\Delta x)$, and substitute this term into our equation

$$\frac{g - 1}{\Delta t} = D \frac{2\cos(k\Delta x) - 2}{\Delta x^2}$$

Rearranging for g

$$g = 1 - \frac{D\Delta t}{\Delta x^2} (2 - 2\cos(k\Delta x))$$

Using the half angle formula $\sin^2(\theta/2) = (1-\cos(\theta))/2$ we can further simplify to

$$g = 1 - \frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right)$$

The value of the $\sin^2$ term will be between 0 and 1. Based on the condition that $-1 \leq g \leq 1$ for stability, we know that the value of $4D\Delta t/\Delta x^2$ must

be between 0 and 2. This means that in order for the FTCS method to be stable, a Δt and Δx must be chosen such that

$$\Delta t \leq \frac{\Delta x^2}{2D}$$

2   Phase Field Methods

2.1   Sharp Interface Models

Many systems can be described as two or more domains of distinct phases separated by a thin interface. Some examples are phase separation by spinodal decomposition and crystal growth. Modeling these systems is difficult because it requires solving transport equations for a moving boundary, whose location must be explicitly tracked.

2.2   Diffuse Interface Approach

A solution to the problem of sharp interfaces is to describe the phases of the system using fields which are continuous functions of x and t. In these models, the interface is a region of finite width, where a continuous transition from one phase to another takes place. This eliminates the need to explicitly track the location of the interface, and allows its motion in time to be described by a free energy functional $F[\phi]$. ϕ is known as the "order parameter," whose value distinguishes separate phases (i.e. concentration). The interface can be identified by looking at where $\phi(x,t)$ takes on its interfacial value.

2.3   Conserved vs. non-conserved order parameters

An example of a conserved order parameter is concentration. During spinodal decomposition, a homogeneous mixture separates out into two distinct phases (i.e. oil and water) below a certain critical temperature. However, the average overall chemical composition of the system remains the same.

An example of a non-conserved order parameter is average-magnetization. Above the critical temperature, a system of magnetic spins will point in random directions, with an average magnetization of zero. Below the critical temperature, the spins will align themselves, leading to a non-zero average magnetization.

2.4 Cahn-Hilliard Equation

A good resource I found for understanding phase field models was the following textbook available as a pdf online, which I used for my notes in this section. The book itself goes into greater detail on expressions for the free energy, and how to derive models such as the Cahn-Hilliard equation.

Provatas, Nikolas, and Ken Elder. *Phase-Field Methods in Materials Science and Engineering.* Wiley-VCH, 2010.

A homogeneous "disordered" mixture of two phases will undergo phase separation if its temperature is less a critical temperature T_c. Under isothermal conditions, this process are driven by gradients in the chemical potential. The local chemical potential can be derived as a *functional* of the concentration.

$$\mu = \frac{\delta F[\phi]}{\delta c}$$

Note that the right hand side of the above equation represents a variational derivative. Since ϕ represents the difference in concentration, its change in time is given by

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \vec{J}$$

Where the flux $\vec{J}$ is given by

$$-M\nabla \cdot \mu$$

Substituting these equations gives the Cahn-Hilliard Equation

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left(M\nabla \frac{\delta F}{\delta \phi} \right)$$

Applying the calculus of variations (see slides) we can say that

$$\frac{\delta F}{\delta \phi} = \frac{df}{d\phi} - \varepsilon^2 \nabla^2 \phi$$

The free energy density $f(\phi)$ can be modeled in different ways, and typically takes the form of a double well potential. In this case we choose to define it as

$$f(\phi) = \frac{W}{4}\phi^2(1 - \phi^2) \quad \Rightarrow \quad \frac{df}{d\phi} = \frac{W}{2}\phi(1 - \phi)(1 - 2\phi)$$

Which gives us a final equation of

$$\frac{\partial \phi}{\partial t} = M \nabla^2 \left(\frac{df}{d\phi} - \varepsilon^2 \nabla^2 \phi \right)$$

2.4.1   Cahn-Hilliard Equation: Equilibrium Solutions

A steady state solution to the 1-Dimensional Cahn-Hilliard equation in is

$$\phi = \tanh \left(\frac{x - x_0}{2\ell} \right)$$

At equilibrium, $\frac{\partial \phi}{\partial t} = 0$. Imposing this condition on the Cahn-Hilliard equation leads us to say that

$$\frac{df}{d\phi} - \varepsilon^2 \nabla^2 \phi = 0$$

Using the properties of hyperbolic tangent, we can say that at equilibrium

$$\frac{\partial^2 \phi}{\partial x^2} = -\frac{1}{2\ell^2} \left(\phi(1 - \phi^2) \right)$$

Substituting our expressions for ϕ and $\frac{df}{d\phi}$ into our equation and simplifying using the above property of hyperbolic tangent, we end up with the following cubic equation.

$$\left(W - \frac{\varepsilon^2}{2\ell^2} \right) \phi^3 + \left(\frac{-3W}{2} \right) \phi^2 + \left(\frac{W}{2} + \frac{\varepsilon^2}{2\ell^2} \right) \phi = 0$$

Which has the solutions

$$\phi = 1 \qquad \phi = 0 \qquad \phi = \frac{-\varepsilon^2 - \ell^2 W}{\varepsilon^2 - 2\ell^2 W}$$

If we say that at steady state the two phases must be completely separated, then the value of ϕ must be either 0 or 1. Applying this condition to our third root

$$\frac{-\varepsilon^2 - \ell^2 W}{\varepsilon^2 - 2\ell^2 W} = 1 \text{ or } 0$$

This allows us to derive an expression relating ℓ, ε and W. If we set the above expression equal to 0, we will end up with a complex answer when solving for ℓ, so we will instead set it equal to 1. Solving for ℓ, we find that

$$\ell = \frac{\varepsilon}{\sqrt{W/2}}$$

This gives us a way to relate the parameter ℓ which defines the width of our "diffuse" interface to the gradient energy coefficient ε^2 and the shape of our double well potential, which is influenced by W. ℓ must be much larger than any microscopic length scale in our system, such as the lattice spacing. In addition, our model will be limited to describing structures or patterns on a length scale much larger than ℓ.

2.4.2 Free Energy and Spinodal Decomposition
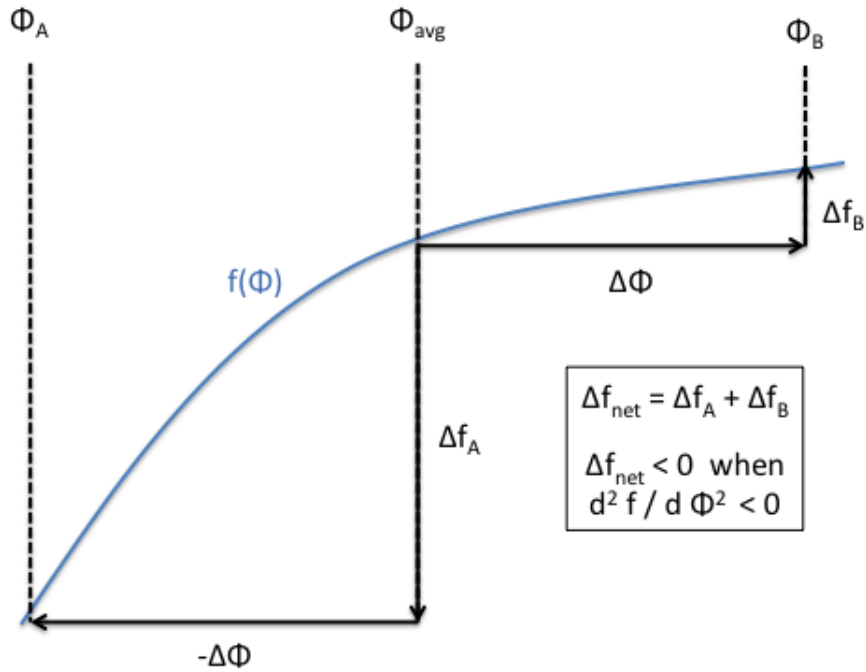
Spinodal decomposition will only occur when it is thermodynamically favorable—that is, when it results in a reduction in the free energy density of the system. As illustrated by the figure above, this will only occur when $f''(\phi) < 0$. There are different functions for the free energy density $f(\phi)$, but if we use the expression from our earlier example where

$$f(\phi) = \frac{W}{4}\phi^2\left(1 - \phi\right)^2$$

Then we can find the range of average initial concentrations ϕ_{avg} for which spinodal decomposition occurs by setting $f''(\phi)$ equal to 0.

$$\frac{\partial^2 f}{\partial \phi^2} = \frac{W}{2}(6\phi^2 - 6\phi + 1) = 0$$

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if we say that W = 1, then this has the solutions

$$\phi \approx 0.21 \qquad \phi \approx 0.79$$

This means that spinodal decomposition will occur when the average concentration in our system ϕ_{avg} is between 0.21 and 0.79.