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Numerical Methods for PDE's

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# Introduction:

Partial Differential Equations (PDEs) are mathematical tools that describe the temporal and spatial evolution of physical quantities. They facilitate the translation of physical laws into a solvable framework, offering insights into phenomena such as pattern formation, fluid dynamics, and active matter hydrodynamics. One of the simplest examples of a PDE is the diffusion equation, which models how a substance, like ink in water, spreads out over time:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

Here, $c$ represents the concentration of the substance, and $D$ is the diffusion constant. This equation beautifully encapsulates the tendency of systems to move towards uniformity.

In fluid dynamics, the Navier-Stokes equations are essential for describing the motion of liquids and gases. Despite their seemingly simple form, these equations can lead to complex phenomena like turbulence and are crucial in fields such as aerodynamics and climate modeling. However, the equations cannot be solved analytically, and solving them would earn someone the Millennium Prize.

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \mu\nabla^2\mathbf{v} + \mathbf{f} \tag{2}$$

The Cahn-Hilliard equation is a mathematical model used to describe phase separation processes in binary mixtures, such as the separation of oil and water. It captures the dynamics of how different components of a mixture evolve over time and space. The equation is given by:

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

where $\phi$ represents the concentration field, $M$ is the mobility, and $F$ is the free energy functional. This equation is widely used in materials science and fluid dynamics to study pattern formation and interface dynamics.

The Toner-Tu equation describes the collective behavior of active matter, which consists of self-propelled particles such as flocks of birds, schools of fish, or bacterial colonies. These equations extend the Navier-Stokes framework to account for the self-driven nature of active particles. The Toner-Tu equations are given by:

$$\frac{\partial \mathbf{v}}{\partial t} + \lambda(\mathbf{v}\cdot\nabla)\mathbf{v} = \alpha\mathbf{v} - \beta|\mathbf{v}|^2\mathbf{v} - \nabla P + D\nabla^2\mathbf{v} + \mathbf{f}$$

where $\mathbf{v}$ is the velocity field of the active particles, $\lambda$ is a parameter describing the alignment interaction, $\alpha$ and $\beta$ are coefficients related to the speed and density of the particles, $P$ is the pressure, $D$ is the diffusion coefficient, and $\mathbf{f}$ represents external forces. These equations help in understanding the emergent patterns and dynamics in systems of active matter.
This list is far from exhaustive—PDEs form the foundation of countless other models in physics, biology, and engineering, making them indispensable for understanding and predicting complex systems' behavior in nearly every science field.
However, solving these equations analytically is often impossible or extremely challenging, especially for complex systems. This is where computers come to our aid. By employing numerical algorithms, we can approximate solutions to these PDEs. There are also several algorithms to solve PDEs. Among the many methods available, here I discuss two popular approaches: (i) the Euler Finite Time and Central in Space (FTCS) Method, and (ii) the Pseudo Spectral Method.

# Euler Method :

The Euler method is one of the simplest and most widely used numerical methods for solving ordinary differential equations (ODEs) and partial differential equations (PDEs). It is an explicit method that approximates the solution by stepping forward in time, using the current value of the function and its derivative.

$$u(t + \Delta t) = u(t) + \Delta t \cdot f(t, u(x, t)) \tag{3}$$

where, $u(t + \Delta t)$ is the value at time $t + \Delta t$. Here are the spatial derivatives in the central space method.

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} \tag{4}$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{\Delta x^2} + O(\Delta y^2) \tag{5}$$

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} + u_{i-1,j-1} - u_{i+1,j-1} - u_{i-1,j+1}}{4\Delta x \Delta y} + O(\Delta x^2, \Delta y^2) \tag{6}$$

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**Pros:**

- The Euler method is simple and easy to implement.
- It is conditionally stable.

Despite its simplicity, the Euler method has several drawbacks.

**Cons:**

- The Euler method suffers from truncation error.
- Over the course of a long simulation, the error accumulates, potentially leading to numerical instability.
- It is conditionally stable, meaning the timestep $\Delta t$ and spatial resolution must be chosen to satisfy the CFL condition.
- To ensure stability, the timestep $\Delta t$ must be small, which results in longer computational times for extended simulations.
- The method is not suitable for PDEs with nonlinear terms and with higher gradient terms, as it may fail to capture the behavior of such systems accurately.

# Pseudo Spectral Method :

# 1 Introduction

The study of partial differential equations (PDEs) is essential in understanding various phenomena in physics, chemistry, and biology, such as diffusion, phase separation, and pattern formation. The pseudo-spectral method is widely used for problems with periodic boundary conditions due to its high accuracy, especially for smooth solutions.
In this section, we begin by discussing the diffusion equation, a fundamental equation in physics, and then introduce the Cahn-Hilliard equation, which describes phase separation in binary mixtures. We also discuss stiff systems, which arise in nonlinear models like the Cahn-Hilliard equation, and the challenges associated with solving them.

## 1.1 Diffusion Equation in 1D and 2D

The diffusion equation is a classical PDE that describes the distribution of a scalar quantity (such as concentration) over space and time. It is given by:

$$\frac{\partial c}{\partial t} = D\nabla^2 c$$

where $c(x,t)$ is the concentration at position $x$ and time $t$, and $D$ is the diffusion coefficient. In one dimension (1D), the equation simplifies to:

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

In two dimensions (2D), the diffusion equation becomes:

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

The solution to the diffusion equation can be found using various numerical techniques, and it serves as a basis for more complex equations, such as the Cahn-Hilliard equation.

## 1.2 The Cahn-Hilliard Equation

The Cahn-Hilliard equation is a nonlinear PDE that describes the phase separation in binary mixtures. It models the evolution of the concentration field $\phi(x,t)$ of one component of the mixture. The equation is written as:

$$\frac{\partial \phi}{\partial t} = \mu\nabla^2\left(\frac{\delta F}{\delta \phi}\right)$$

Where $\mu$ is the mobility, the free energy $F$ is typically a functional of the concentration field $\phi$ and can include terms that account for interfacial tension, bulk energy, and entropy. The free energy functional is given by, $F[\phi] = \int \left[\frac{\kappa}{2}\nabla^2\phi + v\phi^2(1-\phi)^2\right]$.

So , the equation is given by, $\frac{\partial \phi}{\partial t} = \mu\left[2v\phi(1-\phi)(1-2\phi) - \kappa\nabla^2\phi\right]$

In the Cahn-Hilliard equation, phase separation occurs when regions of different concentrations evolve to minimize the free energy, leading to the formation of domains or droplets. The equation includes both linear diffusion and nonlinear terms that make the system more complex compared to simple diffusion.

## 1.3 Stiff Systems

A stiff system arises when there are widely varying timescales for different components of the system, making it challenging to numerically solve. In the case of PDEs, stiffness often occurs when certain terms (such as diffusion or reaction rates) change very rapidly, while others evolve slowly. Stiffness is particularly common in nonlinear equations, like the Cahn-Hilliard equation, where the free energy function ( $v\phi^2(1-\phi)^2$) may cause fast changes in some regions of the domain while others evolve more slowly.

Stiffness requires careful treatment in numerical methods, as the solution's stability can be highly sensitive to the choice of timestep. If the timestep is too large, the solution may become unstable, causing numerical blow-up. In contrast, very small timesteps are needed to accurately resolve the fast modes of the system, leading to significant computational costs.

## 1.4 Pseudo-Spectral Method

The pseudo-spectral method is a powerful technique often used to solve PDEs with periodic boundary conditions. Instead of solving the equation in physical space, the solution is represented in Fourier space as a sum of complex exponentials:

$$\phi(x,t) = \sum_k \hat{\phi}_k(t)e^{ikx}$$

where $\hat{\phi}_k(t)$ are the Fourier coefficients and $k$ is the wave number associated with each mode. For a domain of length $L$, the allowed values of $k$ are given by:

$$k = \frac{2\pi n}{L}, \quad n = 0, \pm 1, \pm 2, \ldots$$

The Fourier transform allows for the conversion of derivatives in physical space into simple multiplications in Fourier space. The second spatial derivative, for instance, becomes:

$$\frac{\partial^2 \phi}{\partial x^2} = -k^2\hat{\phi}_k(t)$$

This simplification is particularly useful for solving stiff systems, as it allows for efficient computation and high-order accuracy. The Fast Fourier Transform (FFT) is typically used to compute the Fourier coefficients $\hat{\phi}_k$.

## 1.5 IMEX Method for the Cahn-Hilliard Equation

In this method, We evolve the non-linear parts in an explicit way and the linear parts in an implicit way; mathematically, if the PDE is given by,

$$\frac{\partial \phi}{\partial t} = \mathcal{L}\phi + \mathcal{N}(f(\phi)) \tag{7}$$

$$\frac{\phi_k^{(t+1)} - \phi_k^t}{\Delta t} = (-ik)^\alpha \hat{\phi_k}^{(t+1)} + \mathcal{F}(\mathcal{N}(f(\hat{\phi_k}^t))) \tag{8}$$

$$\frac{\partial \phi}{\partial t} = \mathcal{L}\phi + \mathcal{N}(f(\phi)) \tag{9}$$

$$\phi_k^{(t+1)}\left(1 - \Delta t(-ik)^\alpha\right) = \hat{\phi_k}^t + \Delta t\mathcal{F}(\mathcal{N}(f(\hat{\phi_k}^t))) \tag{10}$$

$$\phi_k^{(t+1)} = \frac{\hat{\phi_k}^t + \Delta t\mathcal{F}(\mathcal{N}(f(\hat{\phi_k}^t)))}{\left(1 - \Delta t(-ik)^\alpha\right)} \tag{11}$$

Where $\mathcal{L}$ denotes the linear part and $\mathcal{N}$ denotes the non-linear part. $\mathcal{F}$ denotes the Fourier transformation of variables. $(-ik)^\alpha$ comes from the Fourier transformed of Linear part.(e.g. $\nabla^2 \rightarrow (-ik)^2$)