计算物理作业 8

李明钰 22307110156

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1 题目 1：解 Possion 方程

1.1 题目描述

Consider the Poisson equation$^2\phi(x, y) = -\rho/\epsilon_0$from electrostatics on a rectangular geometry with $x \in [0, L_x]$ and $y \in [0, Ly]$ Write a program that solves this equation using the relaxation method. Test your program with:
(a) $\rho(x, y) = 0, \varphi(0, y) = \varphi(L_x, y) = \varphi(x, 0) = 0, \varphi(x, L_y) = 1\text{V},\ L_x = 1\text{m}, \text{and } L_y = 1.5\text{m};$
(b) $\rho(x, y)/\varepsilon_0 = 1\text{V/m}^2, \varphi(0, y) = \varphi(L_x, y) = \varphi(x, 0) = \varphi(x, L_y) = 0, \text{and } L_x = L_y = 1\text{m}.$

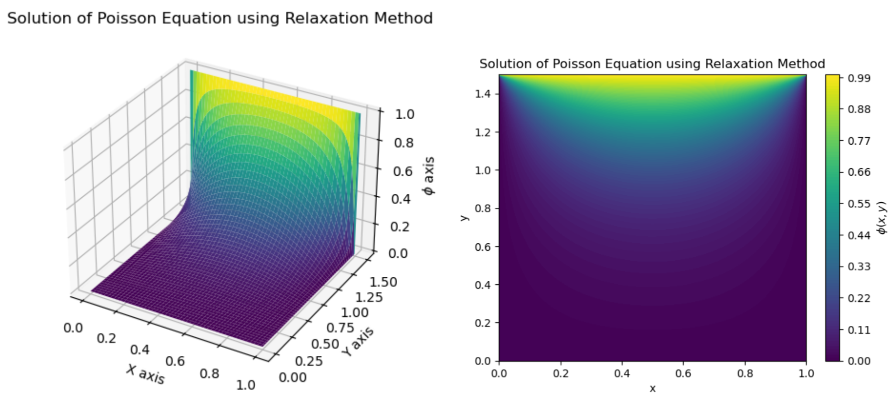
1.2 程序描述

先将泊松方程的右边 ρ/ϵ_0 视作一个整体的 $f(x, y)$, 然后和边界条件一起作为输入输入松弛算法 (算法1) 即可得到两个不同情况下的泊松方程的解。

1.3 伪代码

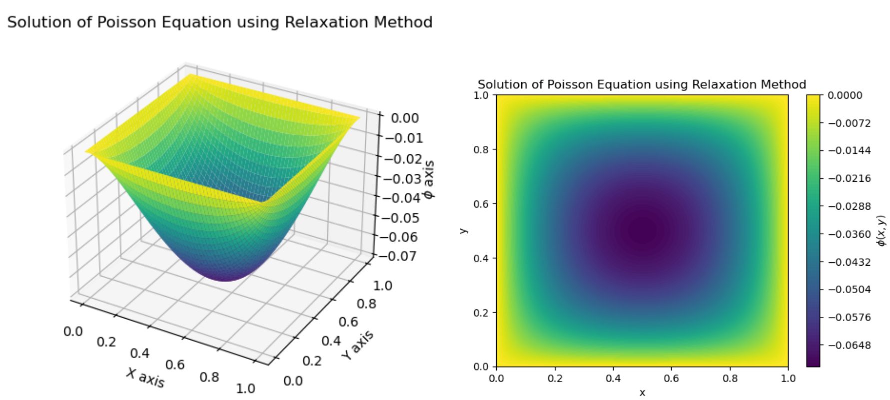
Algorithm 1 Relaxation Method for Poisson Equation

Input: Function f (Poisson equation right-hand side), Grid Z (with boundary conditions)
Output: Solution grid Z
Set n_x = number of columns in Z
Set n_y = number of rows in Z
for inter = 1 **to** max_inter **do**
  $Z_{\text{new}} \leftarrow Z$
  for $i = 1$ **to** $n_y - 1$ **do**
    for $j = 1$ **to** $n_x - 1$ **do**
      $Z_{\text{new}}[i, j] \leftarrow \frac{1}{4}\left(Z[i+1, j] + Z[i-1, j] + Z[i, j+1] + Z[i, j-1] - h^2 f[i, j]\right)$
    end for
  end for
  $err \leftarrow \max\left(|Z_{\text{new}} - Z|\right)$
  $Z \leftarrow Z_{\text{new}}$
end for
Return Z



(a) 三维视图 (b) 二维视图

图 1: 用松弛法解第一问泊松方程



(a) 三维视图 (b) 二维视图

图 2: 用松弛法解第二问泊松方程

1.4 输入输出实例

2 题目 2：解含时薛定谔方程

2.1 题目描述

Solve the time-dependent Schrodinger equation using both the Crank–Nicolson scheme and stable explicit scheme. Consider the one-dimensional case and test it by applying it to the problem of a square well with a Gaussian initial state coming in from the left.

2.2 程序描述

本程序使用自然单位制度, 使用 rank-Nicolson Scheme(算法2) 和 Explicit Scheme(算法3) 的数值计算方法解出了一维情况下质量 $m = 1$ 的粒子在方势阱：

$$V(x) = \begin{cases} -V_0 = -1 & |x| < 0.5 \\ 0 & other \quad cases \end{cases} \tag{1}$$

下的含时薛定谔方程

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi \tag{2}$$

2.3 伪代码

Algorithm 2 Crank-Nicolson Scheme for Schrödinger Equation

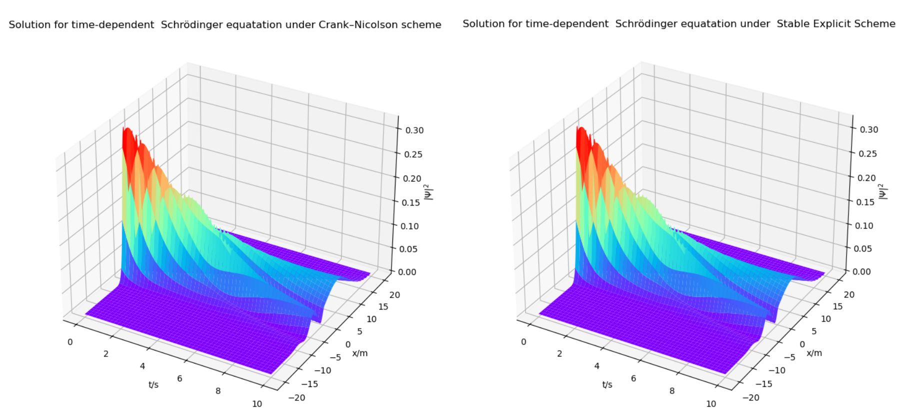
Input: Potential V, Initial wavefunction ψ_0
Output: Time-evolved wavefunction Ψ
Set $\Psi \leftarrow \text{zeros}(Nt, Nx)$
Set $\Psi[0,:] \leftarrow \psi_0$ ▷ Initial wavefunction
Set $\alpha \leftarrow \frac{h_t}{h_x^2}$ ▷ Discretization coefficient for Crank-Nicolson
Set $B \leftarrow \text{zeros}(Nx, Nx)$ ▷ Matrix for discretized equation
for a $= 0$ **to** $Nx - 1$ **do**
  for b $= 0$ **to** $Nx - 1$ **do**
    if $a - b = 0$ **then**
      $B[a,b] \leftarrow -0.5V[a]\frac{h_t}{\hbar} - 0.5\alpha\frac{\hbar}{m}$
    else if $|a - b| = 1$ **then**
      $B[a,b] \leftarrow 0.25\alpha\frac{\hbar}{m}$
    end if
  end for
end for
for $j = 1$ **to** $Nt - 1$ **do**
  $\Psi[j] \leftarrow (i \cdot I_{Nx} + B)^{-1}(i \cdot I_{Nx} - B)\Psi[j-1]$
end for
Return Ψ

Algorithm 3 Explicit Scheme for Schrödinger Equation

Input: Potential V, Initial wavefunction ψ_0
Output: Time-evolved wavefunction Ψ
Set $\alpha \leftarrow \frac{h_t}{h_x^2}$ ▷ Discretization coefficient
Set $\Psi \leftarrow \text{zeros}(Nt, Nx)$
Set $\Psi[0] \leftarrow \psi_0$ ▷ Initial wavefunction
Set $A \leftarrow$ diagonal matrix with entries $\left(-i\frac{\hbar^2}{m}\alpha - ih_tV\right)$ ▷ Matrix A
Set $A \leftarrow A +$ off-diagonal elements $\left(i\frac{\hbar^2}{2m}\alpha\right)$
Set $\Psi[1] \leftarrow \psi_0 + A\psi_0$
for $j = 2$ **to** $Nt - 1$ **do**
    Set $A \leftarrow \text{zeros}(Nx, Nx)$
    for $a = 0$ **to** $Nx - 1$ **do**
        for $b = 0$ **to** $Nx - 1$ **do**
            if $a - b = 0$ **then**
                $A[a, b] \leftarrow -2j\frac{\hbar^2}{m}\alpha - 2jh_tV[a]$
            else if $|a - b| = 1$ **then**
                $A[a, b] \leftarrow i\frac{\hbar^2}{m}\alpha$
            end if
        end for
    end for
    $\Psi[j] \leftarrow \Psi[j-2] + A\Psi[j-1]$ ▷ Explicit step for time evolution
end for
Return Ψ

2.4 输入输出实例

结果如图3所示, 可以发现两种解法得到的解相差很小。



(a) Crank-Nicolson Scheme (b) Explicit Scheme

图 3: 两种不同方法解含时薛定谔方程