Computational Physics Lab

Homework 4

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1 Writing Assignments

1.1 Finite difference method for solving 2D Poisson equation

The 3×3 grids with grid space h and the source term $\rho(x, y)$ can be described as:

$$u_{xx} + u_{yy} = \rho(x, y)$$

where the subscripts mean second partial derivatives of the u with x and y, respectively. Besides, we annotate (x, y) with (i, j) where i and j are from $0 \sim (3 + 1)$ (including boundaries, which are (i, j) = (i, 0), (i, 4), (0, j), and (4, j)), and implement the Euler method for derivative; then we can get:

$$\frac{\partial}{\partial x} \left(\frac{u_{i,j} - u_{i-1,j}}{h} \right) + \frac{\partial}{\partial y} \left(\frac{u_{i,j} - u_{i,j-1}}{h} \right) = \rho(x, y)
\Rightarrow \frac{1}{h} \left(\frac{u_{i+1,j} - u_{i,j}}{h} - \frac{u_{i,j} - u_{i-1,j}}{h} \right) + \frac{1}{h} \left(\frac{u_{i,j+1} - u_{i,j}}{h} - \frac{u_{i,j} - u_{i,j-1}}{h} \right) = \rho(x, y)
\Rightarrow (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = \rho(x, y)h^{2}
\Rightarrow 4_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1} = \rho(x, y)h^{2}$$
(I)

In the wake of knowing the general form of the solution, we apply the boundary conditions; here boundaries are all zeros (i.e., $u_{0,j}$, $u_{i,0}$, $u_{4,j}$, and $u_{i,4} = 0$). Exploiting all i and j, we can get LHS of eq.(I) in the matrix form **A** and RHS in the vector form **b** with source term g_{ij} which represents the splitting of the source function $\rho(x, y)$:

$$\mathbf{A} = \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$
$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}$$

and

$$\mathbf{b} = -h^{2} \begin{bmatrix} g_{11} \\ g_{12} \\ g_{13} \end{bmatrix}$$

$$g_{21} \\ g_{22} \\ g_{23} \\ g_{31} \\ g_{32} \\ g_{33} \end{bmatrix}$$

2 Programming Assignments

- 2.1 (2) Leapfrog method
- 2.2 (3) Energy comparison
- 3 Codes

All the codes are transferred from jupyterlab or python codes; hence, if you want to re-run them, please see the source code in the attached files or my GitHub repository:

<https://github.com/gary20000915/Comphyslab-HW4.git>

3.1 particles.py