计算流体力学

第二次作业

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数理算法原理

题目要求构造差分格式,在均匀网格上,针对一阶导数 $\frac{\partial u}{\partial x}$ 和二阶导数 $\frac{\partial^2 u}{\partial x^2}$,各构造两种不同阶数的差分格式。要求为差分格式的模板不超过 4 个网格点。

本课程讲授了四种差分形式构造方法,分别为: 待定系数法(Taylor 展开方法)、多项式方法、积分方法、有限体积法。题目中没有给出控制方程的具体形式,因此,无法通过积分方法、有限体积法构造差分格式。所以本题在待定系数法、多项式方法中选用待定系数法构造差分格式

待定系数法 (Taylor 展开方法):

选取 u_{i-2} u_{i-1} u_{i+1} u_{i+2} 构造差分:

$$u_{j-2} = u_j - 2\Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (2\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} - \frac{1}{3!} (2\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (2\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4} - \frac{1}{5!} (2\Delta x)^5 \frac{\partial^5 u_j}{\partial x^5}$$

$$u_{j-1} = u_j - \Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} - \frac{1}{3!} (\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4} - \frac{1}{5!} (\Delta x)^5 \frac{\partial^5 u_j}{\partial x^5}$$

$$u_{j+1} = u_j + \Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} + \frac{1}{3!} (\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4} + \frac{1}{5!} (\Delta x)^5 \frac{\partial^5 u_j}{\partial x^5}$$

$$u_{j+2} = u_j + 2\Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (2\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} + \frac{1}{3!} (2\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (2\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4} + \frac{1}{5!} (2\Delta x)^5 \frac{\partial^5 u_j}{\partial x^5}$$
假设

$$\frac{\partial u_j}{\partial x} = Au_{j-2} + Bu_{j-1} + Cu_{j+1} + Du_{j+2}$$

应满足方程

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ -2\Delta x & -1\Delta x & 1\Delta x & 2\Delta x \\ 2(\Delta x)^2 & \frac{1}{2}(\Delta x)^2 & \frac{1}{2}(\Delta x)^2 & 2(\Delta x)^2 \\ -\frac{4}{3}(\Delta x)^3 & -\frac{1}{6}(\Delta x)^3 & \frac{1}{6}(\Delta x)^3 & \frac{4}{3}(\Delta x)^3 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

解得

$$\begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \frac{1}{\Delta x} \begin{bmatrix} \frac{1}{12} \\ \frac{2}{3} \\ \frac{2}{3} \\ -\frac{1}{12} \end{bmatrix} (1)$$

精度:

$$\frac{\partial u_j}{\partial x} - (Au_{j-2} + Bu_{j-1} + Cu_{j+1} + Du_{j+2}) = \frac{1}{90} (\Delta x)^4 \frac{\partial^5 u_j}{\partial x^5}$$

算式为四阶精度

假设

$$\frac{\partial^2 u_j}{\partial x^2} = Eu_{j-2} + Fu_{j-1} + Gu_{j+1} + Hu_{j+2}$$

应满足方程

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ -2\Delta x & -1\Delta x & 1\Delta x & 2\Delta x \\ 2(\Delta x)^2 & \frac{1}{2}(\Delta x)^2 & \frac{1}{2}(\Delta x)^2 & 2(\Delta x)^2 \\ \frac{4}{3}(\Delta x)^3 & -\frac{1}{6}(\Delta x)^3 & \frac{1}{6}(\Delta x)^3 & \frac{4}{3}(\Delta x)^3 \end{bmatrix} \begin{bmatrix} E \\ F \\ G \\ H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

解得

$$\begin{bmatrix} E \\ F \\ G \\ H \end{bmatrix} = \frac{1}{(\Delta x)^2} \begin{bmatrix} \frac{1}{3} \\ -\frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix} (2)$$

精度:

$$\frac{\partial^2 u_j}{\partial x^2} - (Eu_{j-2} + Fu_{j-1} + Gu_{j+1} + Hu_{j+2}) = -\frac{5}{8} (\Delta x)^2 \frac{\partial^4 u_j}{\partial x^4}$$

算式为二阶精度

选取 u_{j-1} u_j u_{j+1} 构造差分:

$$u_{j-1} = u_j - \Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} - \frac{1}{3!} (\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4}$$

$$u_j = u_j$$

$$u_{j+1} = u_j + \Delta x \frac{\partial u_j}{\partial x} + \frac{1}{2!} (\Delta x)^2 \frac{\partial^2 u_j}{\partial x^2} + \frac{1}{3!} (\Delta x)^3 \frac{\partial^3 u_j}{\partial x^3} + \frac{1}{4!} (\Delta x)^4 \frac{\partial^4 u_j}{\partial x^4}$$

假设

$$\frac{\partial u_j}{\partial x} = Iu_{j-1} + Ju_j + Ku_{j+1}$$

应满足方程

$$\begin{bmatrix} 1 & 1 & 1 \\ -\Delta x & 0 & \Delta x \\ \frac{1}{2!}(\Delta x)^2 & 0 & \frac{1}{2!}(\Delta x)^2 \end{bmatrix} \begin{bmatrix} I \\ J \\ K \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

解得

$$\begin{bmatrix} I \\ J \\ K \end{bmatrix} = \frac{1}{\Delta x} \begin{bmatrix} -\frac{1}{2} \\ 0 \\ \frac{1}{2} \end{bmatrix} (3)$$

精度

$$\frac{\partial u_j}{\partial x} - (Iu_{j-1} + Ju_j + Ku_{j+1}) = -\frac{1}{3} (\Delta x)^2 \frac{\partial^3 u_j}{\partial x^3}$$

算式为二阶精度 假设

$$\frac{\partial^2 u_j}{\partial x^2} = Lu_{j-1} + Mu_j + Nu_{j+1}$$

应满足方程

$$\begin{bmatrix} 1 & 1 & 1 \\ -\Delta x & 0 & \Delta x \\ \frac{1}{2!} (\Delta x)^2 & 0 & \frac{1}{2!} (\Delta x)^2 \end{bmatrix} \begin{bmatrix} L \\ M \\ N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

解得

$$\begin{bmatrix} L \\ M \\ N \end{bmatrix} = \frac{1}{(\Delta x)^2} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} (4)$$

精度

$$\frac{\partial^2 u_j}{\partial x^2} - (Lu_{j-1} + Mu_j + Nu_{j+1}) = -\frac{1}{12} (\Delta x)^2 \frac{\partial^4 u_j}{\partial x^4}$$

算式为二阶精度。

代码生成与调试

所生成的代码见'homework.py', 'homework-question4.py'文件。

代码调试过程: 请见 gi thub 截图:

Github 网址: https://github.com/firewaterr/cfdHW1.git

到作业提交截止日期后,我会将 Gi tHub 项目改为"公开",助教学长可以检查每次更改的结果。

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数值验证格式的精度:

此处采用事后验证方法验证格式精度。对于一串网格点序列,分别用一倍步长和 q 倍步长计算该网格点出差分格式的结果,得到 u_h 和 u_{ah} ,设真实值为u,则数值格式的格式精度为

$$p = log_q \frac{\|u - u_{qh}\|}{\|u - u_h\|}$$

其中 $\|u\| = \sqrt{\sum_{i=1}^n u_i^2}$,具体求解见代码。运行代码可发现,一阶微分的第一种格式,数值精度为四阶,一阶微分的第二种格式和二阶微分的两种格式,数值精度均为二阶。这些结果和理论计算的结果一致。

结果讨论和物理解释

舍入误差和截断误差的规律:

- (1)对于一次、二次方程,四种格式均无截断误差,舍入误差较小,但可以发现,二阶微分的舍入误差比一阶微分的舍入误差大两个数量级,这是因为作二阶微分时,除数和被除数都更小,所以误差增长较大;
- (2) 到了三次、四次方程,可以看出一阶微分的两种格式精度相差很大,此时截断误差起主要效果;
- (3)减小步长,会增大舍入误差;
- (4)减小步长,会增大截断误差。

单精度和双精度的影响:

NumPy 默认使用双精度浮点值,为了分析单精度和双精度的影响,'homework-question4.py'文件中用'np. float32'语句将所有双精度浮点运算改为单精度浮点运算。对比两份代码中误差的不同,可以看出:

- (1) 单精度浮点运算比双精度误差大很多;
- (2) 双精度占用的内存空间比单精度大很多。