计算流体力学第二次作业

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1 数理算法原理

1.1 对于一阶导数 $rac{\partial u}{\partial x}$ 的差分格式

1.1.1 采用两个网格点的一阶格式

利用泰勒展开式,对于 u_{i+1} ,我们有:

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} + O(\Delta x^2) \tag{1}$$

在等式两侧同时除以 Δx , 我们可以得到:

$$\frac{u_{i+1} - u_i}{\Delta x} = \frac{\partial u}{\partial x} + O(\Delta x) \tag{2}$$

由此可知,差分格式为:

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} \tag{3}$$

将右侧展开后观察阶数:

$$\frac{u_{i+1} - u_i}{\Delta x} = \frac{u_i + \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} + O(\Delta x^3) - u_i}{\Delta x}$$

$$= \frac{\Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} + O(\Delta x^3)}{\Delta x}$$

$$= \frac{\partial u}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u}{\partial x^2} + O(\Delta x^2)$$
(4)

由于截断误差为一阶,所以,该格式为一阶格式。

1.1.2 采用四个网格点的三阶格式

采用待定系数法,我们采用四个网格点来构造差分格式,设这一格式为:

$$\frac{\partial u}{\partial x} = a_1 u_{i-1} + a_2 u_i + a_3 u_{i+1} + a_4 u_{i+2} \tag{5}$$

将 u_{i-1} 、、 u_{i+1} 、 u_{i+2} 分别用泰勒展开式展开,得到:

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$$u_{i+2} = u_i + 2\Delta x \frac{\partial u}{\partial x} + 2(\Delta x)^2 \frac{\partial^2 u}{\partial x^2} + \frac{4(\Delta x)^3}{3} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$
(6)

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带入 (4) 式中, 得到:

$$\frac{\partial u}{\partial x} = a_1 \left(u_i - \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right) + a_2 u_i
+ a_3 \left(u_i + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right)
+ a_4 \left(u_i + 2\Delta x \frac{\partial u}{\partial x} + 2(\Delta x)^2 \frac{\partial^2 u}{\partial x^2} + \frac{4(\Delta x)^3}{3} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right)
= (a_1 + a_2 + a_3 + a_4) u_i + (-a_1 + a_3 + 2a_4) \Delta x \frac{\partial u}{\partial x} + \left(\frac{a_1}{2} + \frac{a_2}{2} + a_3 + 2a_4 \right) (\Delta x)^2 \frac{\partial^2 u}{\partial x^2}
+ \left(-\frac{a_1}{6} + \frac{a_2}{6} + \frac{a_3}{6} + \frac{4a_4}{3} \right) (\Delta x)^3 \frac{\partial^3 u}{\partial x^3} + O(\Delta x^3)$$
(7)

比较两侧系数得到一下方程组:

$$\begin{cases} a_1 + a_2 + a_3 + a_4 &= 0\\ \Delta x (-a_1 + a_3 + 2a_4) &= 1\\ \frac{a_1}{2} + \frac{a_3}{2} + 2a_4 &= 0\\ -\frac{a_1}{6} + \frac{a_3}{6} + \frac{4a_4}{3} &= 0 \end{cases}$$
(8)

解得:

$$\begin{cases} a_1 &= -\frac{1}{3\Delta x} \\ a_2 &= -\frac{1}{2\Delta x} \\ a_3 &= \frac{1}{\Delta x} \\ a_4 &= -\frac{1}{6\Delta x} \end{cases}$$
(9)

因此,最终的四网格点差分格式为:

$$\frac{\partial u}{\partial x} = \frac{-2u_{i-1} - 3u_i + 6u_{i+1} - u_{i+2}}{6\Delta x} \tag{10}$$

为了分析差分格式 $\frac{\partial u}{\partial x} = \frac{-2u_{i-1} - 3u_i + 6u_{i+1} - u_{i+2}}{6\Delta x}$ 的截断误差阶数,我们使用泰勒展开法,将各节点值在 u_i 处展开:

$$\begin{split} u_{i-1} &= u_i - \Delta x \frac{\partial u}{\partial x}\bigg|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2}\bigg|_i - \frac{\Delta x^3}{6} \frac{\partial^3 u}{\partial x^3}\bigg|_i + \frac{\Delta x^4}{24} \frac{\partial^4 u}{\partial x^4}\bigg|_i + O(\Delta x^5), \\ u_{i+1} &= u_i + \Delta x \frac{\partial u}{\partial x}\bigg|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2}\bigg|_i + \frac{\Delta x^3}{6} \frac{\partial^3 u}{\partial x^3}\bigg|_i + \frac{\Delta x^4}{24} \frac{\partial^4 u}{\partial x^4}\bigg|_i + O(\Delta x^5), \\ u_{i+2} &= u_i + 2\Delta x \frac{\partial u}{\partial x}\bigg|_i + 2\Delta x^2 \frac{\partial^2 u}{\partial x^2}\bigg|_i + \frac{4\Delta x^3}{3} \frac{\partial^3 u}{\partial x^3}\bigg|_i + \frac{2\Delta x^4}{3} \frac{\partial^4 u}{\partial x^4}\bigg|_i + O(\Delta x^5). \end{split}$$

代入分子表达式并合并同类项:

$$-2u_{i-1} = -2u_i + 2\Delta x \frac{\partial u}{\partial x}\Big|_i - \Delta x^2 \frac{\partial^2 u}{\partial x^2}\Big|_i + \frac{\Delta x^3}{3} \frac{\partial^3 u}{\partial x^3}\Big|_i - \frac{\Delta x^4}{12} \frac{\partial^4 u}{\partial x^4}\Big|_i + \cdots,$$

$$6u_{i+1} = 6u_i + 6\Delta x \frac{\partial u}{\partial x}\Big|_i + 3\Delta x^2 \frac{\partial^2 u}{\partial x^2}\Big|_i + \Delta x^3 \frac{\partial^3 u}{\partial x^3}\Big|_i + \frac{\Delta x^4}{4} \frac{\partial^4 u}{\partial x^4}\Big|_i + \cdots,$$

$$-u_{i+2} = -u_i - 2\Delta x \frac{\partial u}{\partial x}\Big|_i - 2\Delta x^2 \frac{\partial^2 u}{\partial x^2}\Big|_i - \frac{4\Delta x^3}{3} \frac{\partial^3 u}{\partial x^3}\Big|_i - \frac{2\Delta x^4}{3} \frac{\partial^4 u}{\partial x^4}\Big|_i + \cdots.$$

合并后:

分子 =
$$\left(6\Delta x \frac{\partial u}{\partial x}\Big|_{i}\right) + \left(-\frac{1}{2}\Delta x^{4} \frac{\partial^{4} u}{\partial x^{4}}\Big|_{i}\right) + O(\Delta x^{5})$$

除以 $6\Delta x$ 后得到:

$$\left. \frac{\partial u}{\partial x} \right|_{i} - \frac{1}{12} \Delta x^{3} \frac{\partial^{4} u}{\partial x^{4}} \right|_{i} + O(\Delta x^{4})$$

截断误差的主项为 $-\frac{1}{12}\Delta x^3 \frac{\partial^4 u}{\partial x^4}\Big|_i$,故截断误差是三阶的。

1.2 对于二阶导数 $\frac{\partial^2 u}{\partial x^2}$ 的差分格式

1.2.1 采用三个网格点的一阶格式

利用泰勒展开式,对于 u_{i+1} ,我们有:

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} + O(\Delta x^3)$$
(11)

对于 u_{i+2} , 我们有:

$$u_{i+2} = u_i + 2\Delta x \frac{\partial u}{\partial x} + 2(\Delta x)^2 \frac{\partial^2 u}{\partial x^2} + O(\Delta x^3)$$
(12)

利用 (10) 式和 (11) 式,消去 $\frac{\partial u}{\partial x}$,我们可以得到该差分公式:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+2} - 2u_{i+1} + u_i}{(\Delta x)^2}$$
 (13)

将右侧展开后观察阶数:

$$\frac{u_{i+2} - 2u_{i+1} + u_i}{(\Delta x)^2} = \frac{1}{(\Delta x)^2} \cdot \left[(u_i + 2\Delta x \frac{\partial u}{\partial x} + 2(\Delta x)^2 \frac{\partial^2 u}{\partial x^2} + \frac{4(\Delta x)^3}{3} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right)
- 2(u_i + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right]
= \frac{(\Delta x)^2 \frac{\partial^2 u}{\partial x^2} + (\Delta x)^3 \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)}{(\Delta x)^2}
= \frac{\partial^2 u}{\partial x^2} + (\Delta x) \frac{\partial^3 u}{\partial x^3} + O(\Delta x^2)$$
(14)

因此, 该格式为一阶格式。

1.2.2 采用三个网格点的二阶格式

同理,首先设定差分格式为:

$$\frac{\partial^2 u}{\partial x^2} = b_1 u_{i-1} + b_2 u_i + b_3 u_{i+1} \tag{15}$$

对于 u_{i-1} 、 u_{i+1} ,我们有:

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$
(16)

带入得到:

$$\frac{\partial^2 u}{\partial x^2} = b_1 \left(u_i - \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right)
+ b_2 u_i + b_3 \left(u_i + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4) \right)
= (b_1 + b_2 + b_3) u_i + (-b_1 + b_3) \Delta x \frac{\partial u}{\partial x} + (\frac{b_1}{2} + \frac{b_3}{2}) (\Delta x)^2 \frac{\partial^2 u}{\partial x^2}
+ (-\frac{b_1}{6} + \frac{b_3}{6}) (\Delta x)^3 \frac{\partial^3 u}{\partial x^3} + O(\Delta x^2)$$
(17)

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比较两侧系数得到以下方程组:

$$\begin{cases} b_1 + b_2 + b_3 &= 0\\ -b_1 + b_3 &= 0\\ (\Delta x)^2 (\frac{b_1}{2} + \frac{b_3}{2}) &= 1\\ -\frac{b_1}{6} + \frac{b_3}{6} &= 0 \end{cases}$$
(18)

解得:

$$\begin{cases} b_1 &= \frac{1}{\Delta x^2} \\ b_2 &= -2\frac{1}{\Delta x^2} \\ b_3 &= \frac{1}{\Delta x^2} \end{cases}$$
 (19)

因此,最终的三网格点差分格式为:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} \tag{20}$$

同理,将右侧展开后观察阶数可以得知该格式为二阶格式。

2 代码生成与调试

计算误差 error 的思路为:

- 定义一个已知解析解的函数,程序中采用的是三次函数 $f_3(x) = x^3 2x^2 + 3x + 1$ 和三角函数 $g(x) = \sin(kx)$
- 通过数值方法计算出该函数的一阶导数和二阶导数
- 通过解析解计算出该函数的一阶导数和二阶导数
- 计算数值解与解析解的误差

验证精度的思路为:

- 通过不同的网格步长, 计算出数值解
- 计算出不同网格下的误差
- 根据步长与误差的关系,

$$error = C \cdot \Delta x^p + O(\Delta x^{p+1}) + e \tag{21}$$

其中,C 为常数,p 为阶数,e 为舍入误差将步长与误差同时取对数,如果舍入误差可以忽略,则可以

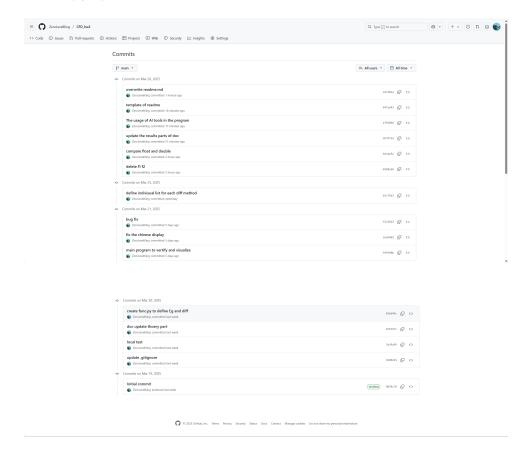
$$\log(error) = \log(C) + p \cdot \log(\Delta x) \tag{22}$$

通过线性拟合函数 y = kx + b,可以得到拟合函数的斜率 k,与理论阶数 p 相比较,可以通过斜率来验证精度

与此同时,还修改了数据的存储精度,比较了单精度和双精度的计算结果。具体的生成与调试参见 github 仓库:

https://github.com/ZeroLevelKing/CFD_hw2.git

git 的 commit 记录如下:



3 结果讨论和物理解释

对于三次函数 $f_3(x)=x^3-2x^2+3x+1$ 和三角函数 $g(x)=\sin(kx)$ (k=0.1),对于 x=1 处的导数和二阶导数,按照上述方法得到的数值解与解析解的误差以及拟合结果如下:

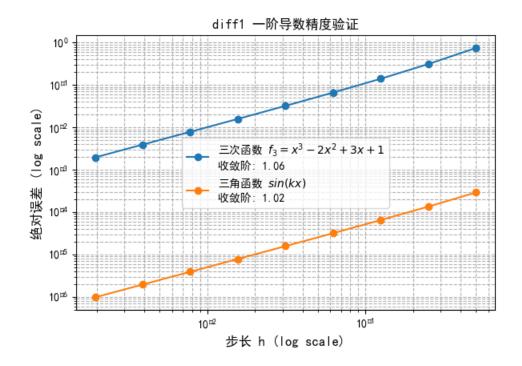


图 1: 差分格式 $\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x}$ 的误差与拟合结果

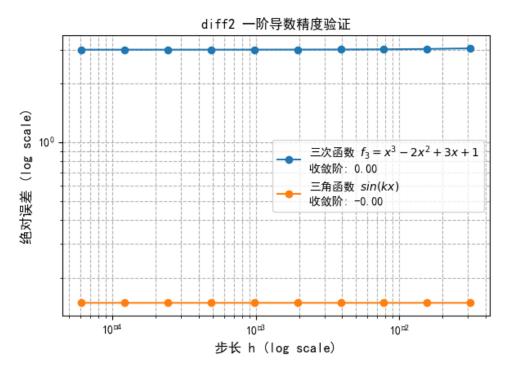


图 2: 差分格式 $\frac{\partial u}{\partial x}=\frac{-2u_{i-1}-3u_i+6u_{i+1}-u_{i+2}}{6\Delta x}$ 的误差与拟合结果

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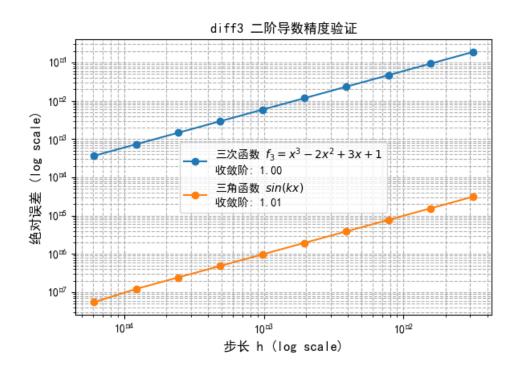


图 3: 差分格式 $\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+2}-2u_{i+1}+u_i}{(\Delta x)^2}$ 的误差与拟合结果

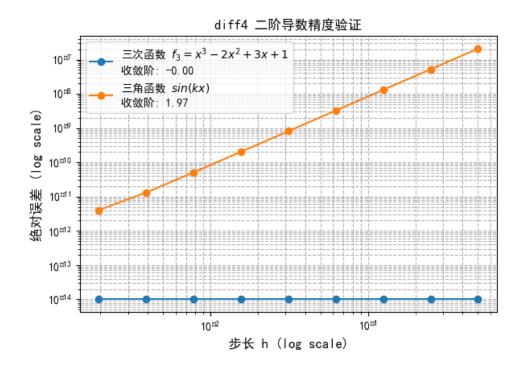


图 4: 差分格式 $\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1}-2u_i+u_{i+1}}{\Delta x^2}$ 的误差与拟合结果

- 通过上述结果可以发现,对于第一种差分格式,可以很明显地观察到其误差与步长的一阶关系,
- 而对于第二种差分格式,理论上应该是三阶关系:对于三次函数,其没有截断误差,只有舍入误差,所以误差不随步长变化;对于三角函数,由于机器精度的限制,舍入误差占据主要因素,

3 结果讨论和物理解释

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在步长较短时,几乎不随步长变化,导致斜率接近于0。

- 由图可知,第三种差分格式的收敛阶是1,与理论吻合很好
- 第四种差分格下: 三次函数无截断误差,舍入误差占据主要因素,导致斜率接近于 0; 三角函数的收敛阶是 2,与理论吻合很好

对于单精度和双精度对于结果的影响探究如下:

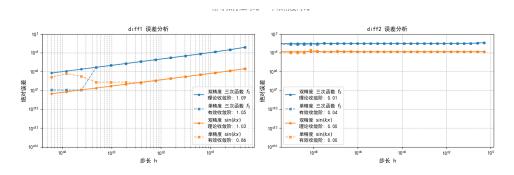


图 5: 单精度和双精度对于一阶导数差分格式的影响

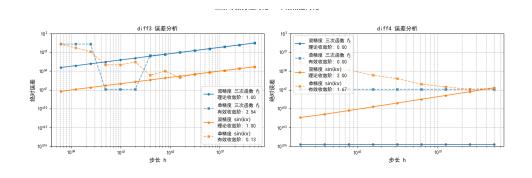


图 6: 单精度和双精度对于二阶导数差分格式的影响

- 可以看出,单精度和双精度的区别主要在步长较小时,舍入误差占据主要因素,单精度由于舍入误差更大,会导致结果偏离理论值。
- 而在步长较大时,单精度和双精度的结果几乎没有区别,说明此时的误差主要影响因素是截断误差。

A AI 工具使用声明表

使用内容	工具名称	使用目的
hw2.tex 1-9 行、图片插入	Github Copilot	调整 pdf 格式,调用宏包,省略插入图片的重复性工作
main.py 6-15 行	DeepSeek	修正 matplotlib 中文显示问题
ReadMe.md 框架	DeepSeek	在 DeepSeek 的帮助下生成一个框架,在此基础上增加而来
.gitignore	Github Copilot	针对于 python 和 latex 的.gitignore 文件,完全由 Copilot 生成