计算物理作业 5

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喜闻徐夫子体恤民情!

1 题目 1：五点公式

1.1 题目描述

Derive the five-point formula for the second-order derivative.

1.2 解答

利用函数 f 在点 $i \pm k$ 处的泰勒展开，得到以下差分表达式：

$$
\begin{aligned}
f_{i+2} &= f_i + 2hf_i' + 2h^2 f_i'' + \frac{4h^3}{3} f_i''' + \frac{2h^4}{3} f_i^{(4)} + \frac{8h^5}{15} f_i^{(5)} + \mathcal{O}(h^6), \\
f_{i+1} &= f_i + hf_i' + \frac{h^2}{2} f_i'' + \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{(4)} + \frac{h^5}{120} f_i^{(5)} + \mathcal{O}(h^6), \\
f_{i-1} &= f_i - hf_i' + \frac{h^2}{2} f_i'' - \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{(4)} - \frac{h^5}{120} f_i^{(5)} + \mathcal{O}(h^6), \\
f_{i-2} &= f_i - 2hf_i' + 2h^2 f_i'' - \frac{4h^3}{3} f_i''' + \frac{2h^4}{3} f_i^{(4)} - \frac{8h^5}{15} f_i^{(5)} + \mathcal{O}(h^6).
\end{aligned}
$$

目标是构造一个线性组合以消除一阶导数 f_i'、三阶导数 f_i''' 及五阶导数 $f_i^{(5)}$，不妨设：

$$
Af_{i+2} + Bf_{i+1} + Cf_i + Df_{i-1} + Ef_{i-2} = Kf_i'' + \mathcal{O}(h^6),
$$

通过匹配各阶 h 的系数，可以构建方程组，观察各系数，不妨设 $K = 12$ 并约分，改写为增广矩阵形式，并使用我们在 `Assignment_3/Problem_2` 中实现的高斯消元法解得（不出意外是行满秩的，有重复约束条件）

$$
\left(\begin{array}{ccccc|c}
1 & 1 & 1 & 1 & 1 & 0 \\
2 & 1 & 0 & -1 & -2 & 0 \\
4 & 1 & 0 & 1 & 4 & 24 \\
8 & 1 & 0 & -1 & -8 & 0 \\
16 & 1 & 0 & 1 & 16 & 0 \\
64 & 1 & 0 & -1 & -64 & 0
\end{array}\right)
\rightarrow
\begin{pmatrix} A \\ B \\ C \\ D \\ E \end{pmatrix}
=
\begin{pmatrix} -1 \\ 16 \\ -30 \\ 16 \\ -1 \end{pmatrix}
$$

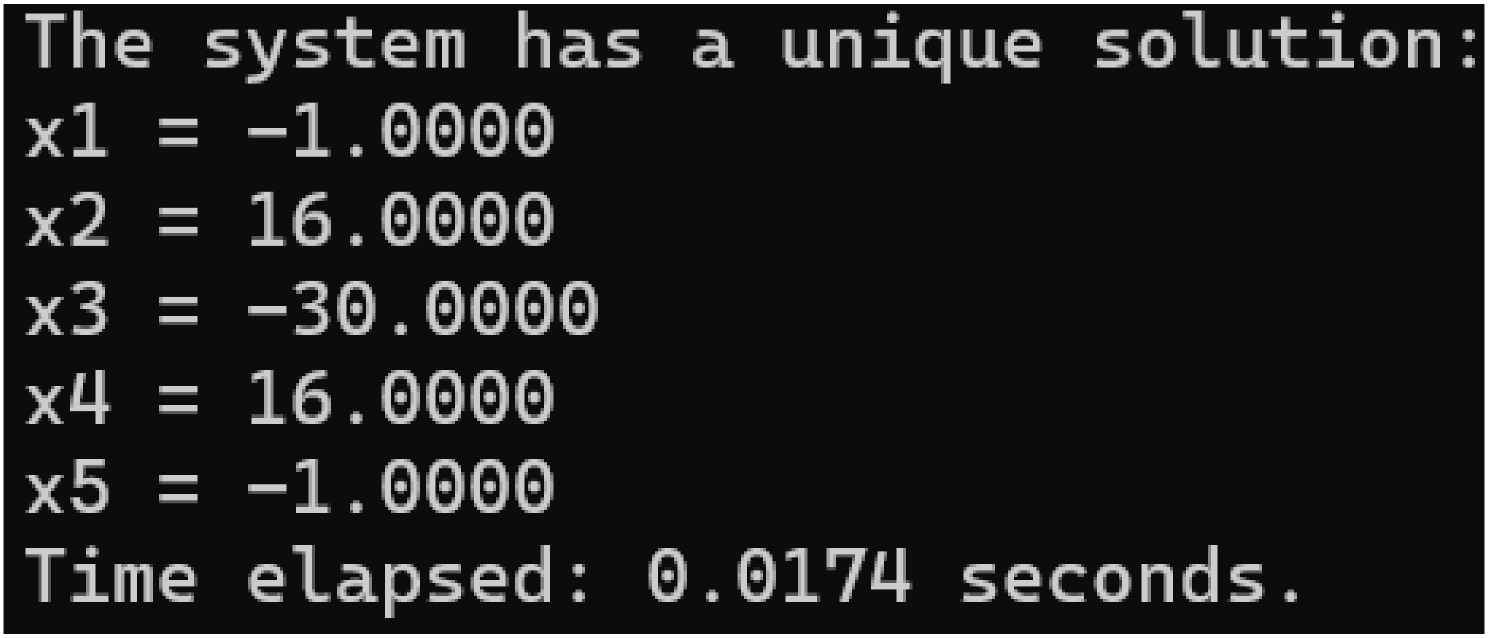

图 1: 运行结果

因此，求二阶差分的五点公式为：

$$-f_{i+2}+16f_{i+1}-30f_i+16f_{i-1}-f_{i-2}=12h^2f_i''+\mathcal{O}(h^6),$$

即，

$$\boxed{f_i''=\frac{-f_{i+2}+16f_{i+1}-30f_i+16f_{i-1}-f_{i-2}}{12h^2}+\mathcal{O}(h^4)}$$

2 ~~题目 2：Romberg 积分~~

2.1 题目描述

Consider the function $f(x)=e^{-x^2}$ on the interval $[0,1]$. Use at least four layers of Romberg integration to compute the integral of $f(x)$ over $[0,1]$ and estimate the result's precision.

浪涌，即将被 *ddl* 的海洋淹没，此拓展题无暇细究

2 题目 2：波函数 Gauss 积分

2.1 题目描述

The radial wave function of the 3s orbital is given by:

$$R_{3s}(r)=\frac{1}{9\sqrt{3}}\times\left(6-6\rho+\rho^2\right)\times Z^{3/2}\times e^{-\rho/2},$$

where:

- r: radius expressed in atomic units (1 Bohr radius = 52.9 pm),

- $e \approx 2.71828$,
- Z: effective nuclear charge for that atom,
- $\rho = \frac{2Zr}{n}$, where n is the principal quantum number (3 for the 3s orbital).

Compute the integral $\int_0^{40} |R_{3s}|^2 \, r^2 \, dr$ for a Si atom ($Z = 14$) using Simpson's rule with two different radial grids:

(1) **Equal spacing grids**:

$$r[i] = (i-1)h, \quad i = 1, \ldots, N$$

Try different values of N.

(2) **Non-uniform integration grid**: more finely spaced at small r than at large r:

$$r[i] = r_0(e^{t[i]} - 1), \quad t[i] = (i-1)h, \quad i = 1, \ldots, N$$

Typically, choose $r_0 = 0.0005$ a.u. (1 a.u. = 1 Bohr radius).

Discuss the efficiency of each approach and explain the reasons.

2.2 程序描述

2.3 伪代码

2.4 结果示例