

计算物理作业 5

杨远青 22300190015



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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:

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

目标是构造一个线性组合以消除一阶导数 f'_i 及三阶导数 f'''_i , 不妨设:

$$Af_{i+2} + Bf_{i+1} + Cf_i + Df_{i-1} + Ef_{i-2} = Kf''_i + \mathcal{O}(h^5),$$

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

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

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The system has a unique solution:
x1 = -1.0000
x2 = 16.0000
x3 = -30.0000
x4 = 16.0000
x5 = -1.0000
Time elapsed: 0.0174 seconds.

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图 1: 运行结果

因此，求二阶差分的五点公式为：

$$-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2} = 12h^2 f_i'' + \mathcal{O}(h^5),$$

即，

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

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:

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

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:**

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

Try different values of N .

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

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

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