CHEN 2450
HOMEWORK 7

NUMERICAL DIFFERENTIATION & INTEGRATION

Submit all your homework using Jupyter notebooks. You are expected to include proper text and discussion for each and every problem including appropriate headings and formatting. You will lose points if your reports are not readable or just include code with a few print out statements. No exceptions.

Problem 1 (50 pts)

The amount of energy required to change a compound from temperature T_1 to T_2 at constant pressure can be written as

$$q = \int_{T_1}^{T_2} c_p \mathrm{d}T, \tag{1}$$

where q is the required energy and c_p is the compound's *heat capacity*, which is a function of temperature.

1. Using the data for $c_p(T)$ from Table 1, determine how much energy is required to heat one kg of CO_2, steel and graphite from $T_1 = 400$ K to $T_2 = 1000$ K. Do this using the Trapezoid rule (implement your own). You may use Python's `trapz` functions to check your results, but you **must implement your own version of this**. Submit a brief report or a Jupyter Notebook describing how you solve the problem (with appropriate equations) and with a table summarizing the heat required for each compound.

Table 1: Heat capacity (c_p) in $\frac{\mathrm{kJ}}{\mathrm{kg \cdot K}}$ as a function of temperature.

Temperature (K)	400	450	500	550	600	650	700	750	800	850	900	950	1000
c_p CO_2	0.942	0.981	1.02	1.05	1.08	1.10	1.13	1.15	1.17	1.187	1.204	1.220	1.234
c_p Steel	487				559				685				1169
c_p Graphite	992				1406				1650				1793

Problem 2 (50 pts)

In this problem, you will explore the effect of the spacing, h, and the order of accuracy of a few numerical differentiation approximations we discussed in class. Consider the function

$$f(x) = \sin(x)\exp\left(-x/20\right). \tag{2}$$

1. Plot the absolute true error, E_t, in $f'(2)$ as a function of h for the following approximations to $f'(x)$

   - First-order forward difference, $f'(x_i) \approx \frac{f(x_{i+1})-f(x_i)}{h}$
   - First-order backward difference, $f'(x_i) \approx \frac{f(x_i)-f(x_{i-1})}{h}$
   - Second-order forward difference $f'(x_i) \approx \frac{-3f(x_i)+4f(x_{i+1})-f(x_{i+2})}{2h}$
   - Second order central difference, $f'(x_i) \approx \frac{f(x_{i+1})-f(x_{i-1})}{2h}$
   - Fourth-order central difference $f'(x_i) \approx \frac{\frac{1}{4}f(x_{i-2})-2f(x_{i-1})+2f(x_{i+1})-\frac{1}{4}f(x_{i+2})}{3h}$

Use spacings from $h = 10$ to $h = 10^{-5}$, with choices for h spaced logarithmically over that range (h=np.logspace(1,-5)). You should measure the error in $f'(2)$ by comparing to the analytic derivative. Your plot should show E_t versus h on a loglog plot, (`plt.loglog(E,h)}`),where E is the absolute true error. ***Discuss your findings***. Recall that $x_{i+k} = x_i + kh$. For example: $x_{i+1} = x_i + h$, $x_{i+2} = x_i + 2h$.