Homework 4 Write-Up

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1. EXERCISE 5.3

For this exercise, I created a function that uses Simpson's methods to calculate Equ.(1). This entailed creating a function in which I first calculated the summation terms since they required a 'for loop' to loop through N.

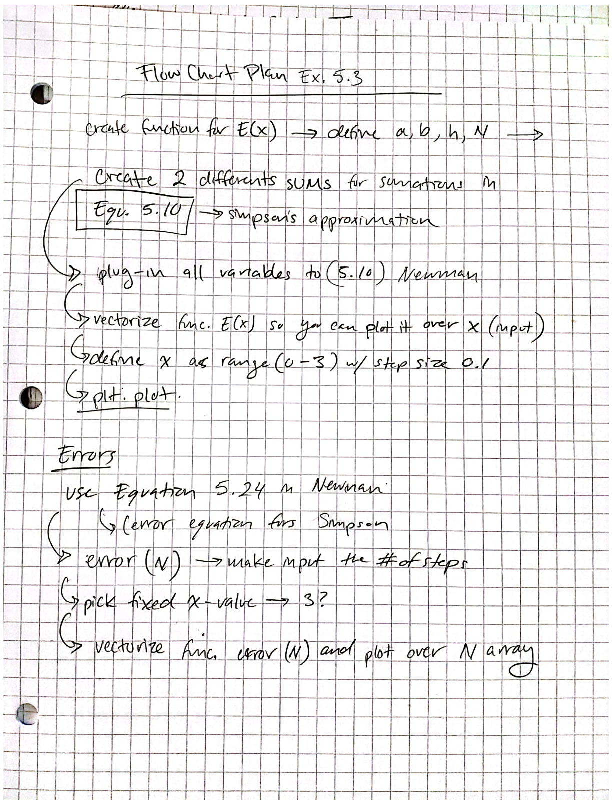

FIG. 1: Pseudo code for Exercise 5.3 Newman.

The integral must approximated because there is no way to solve the equation analytically, only numerically.

$$E(x) = \int_0^x e^{-t^2} dt \tag{1}$$

For the Simpson method of approximating an integral, I used the given Equation (5.10) from the Newman textbook listed below:

$$I(a,b) \approx \frac{h}{3}(f(a) + f(b) + 4\sum_{k=1}^{N/2} f(a + (2k-1)h) + 2 * \sum_{k=1}^{N/2-1} f(a + 2kh))$$

In Figure 2 it can be seen that E(x) plateaus when x is about 2.

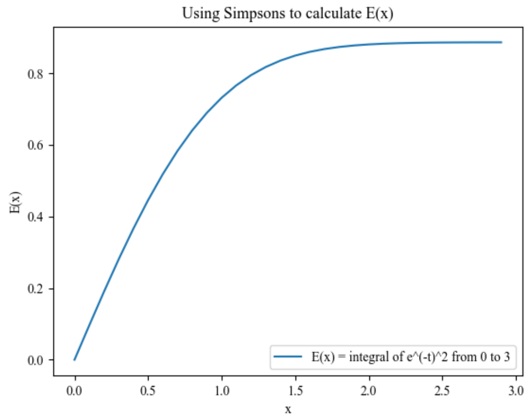

FIG. 2: Plot of Equ.(1) using Simpson's method over x.

I then created another function to calculate the error of the Simpson approximation. This was a function with N (the number of steps) as the input to see how the error decreases as step size decreases.

$$\epsilon = \frac{h^4}{90}[f'''(a) - f'''(b)] \tag{2}$$

In Figure 3. it can be seen that the total error drops to zero when N is around 3; from this we can conclude that an N=3 step size is sufficient for accurate calculations of Equation (1).

2. EXERCISE 5.9

In this exercise, we calculate the heat capacity of a solid, in this case aluminum, at a certain temperature. I first create a function to define the function inside the integral so that it is easy to call later. I then create a function for Cv (heat capacity) using Equation (3).

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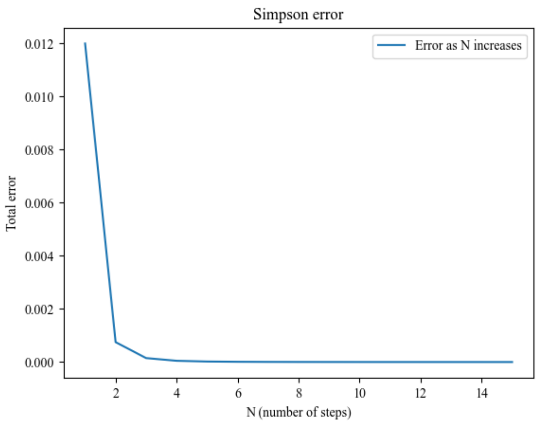

FIG. 3: Simpson error over N.

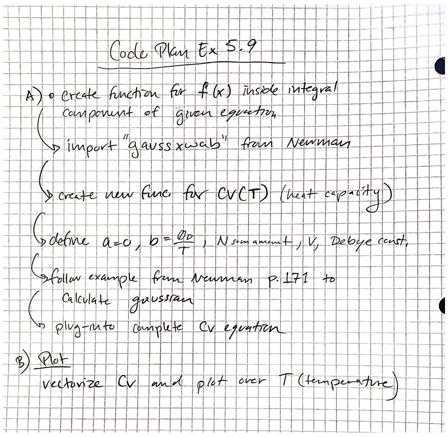

FIG. 4: Pseudo code for Exercise 5.9 Newman.

This problem uses Gaussian quadrature to approximate (basically perfectly) the integral. Fortunately, Newman provides a function for Gaussian quadrature and I did not have to write it from scratch.

$$Cv(T) = 9V\rho\kappa_B\left(\frac{T}{\theta_D}\right)^3\int_0^{\theta_D/T}\frac{x^4e^x}{(e^x-1)^2}dx \qquad (3)$$

You can see that the heat capacity begins to plateau at around 500K (Kelvins) for this material (5)

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3. SURVEY QUESTIONS

The homework this week took approximately 6 hours. I learned how to make a function for the Simpson's method which gave me a deeper understanding and I also thought it was interesting. These codes are good to have in my toolkit. I am unable to get Figure 5 to stay on this page.

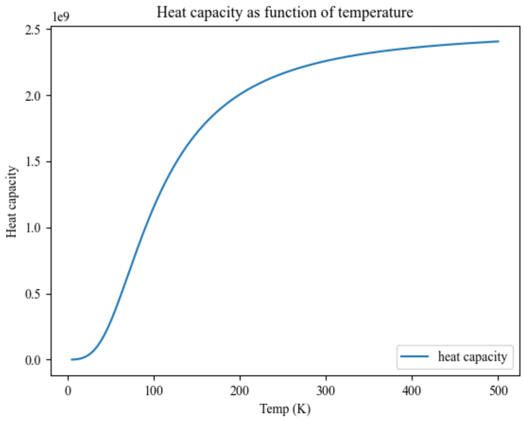

FIG. 5: Heat capacity over temperature.