54 + 51 + 5 = 110

110/117

Homework 4 Write-Up

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(Dated: March 5, 2024)

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.

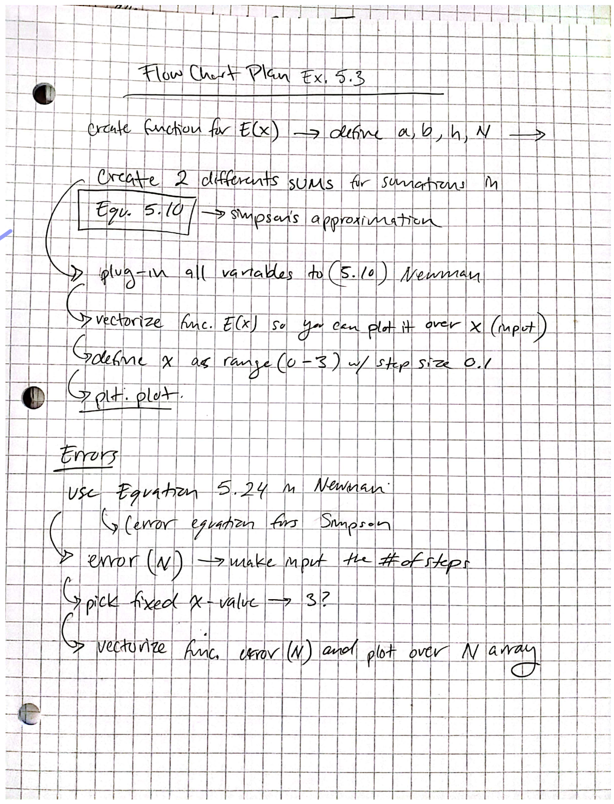

FIG. 1: Pseudo code for Exercise 5.3 Newman.

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.

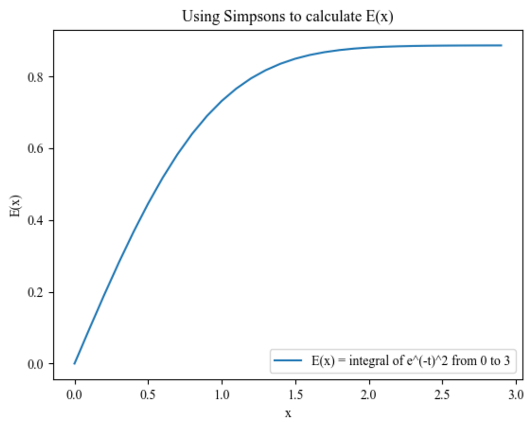

FIG. 2: Plot of Equ.(1) using Simpson's method over x.

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

define?

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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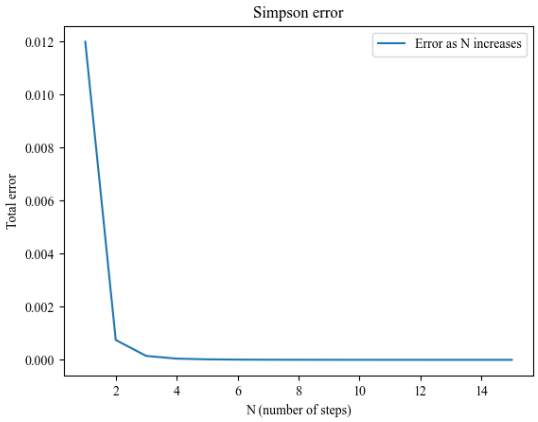
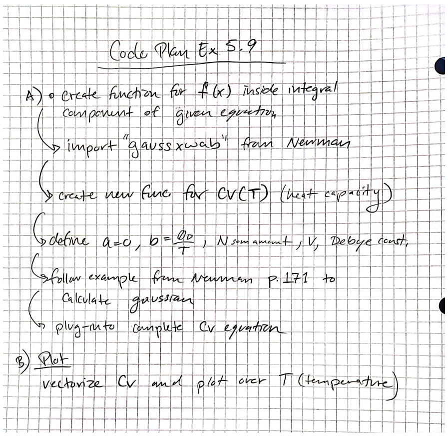


FIG. 3: Simpson error over N.



Code Plan Ex 5.9

A) • create function for f(x) inside integral component of given equation
→ import "gaussxwab" from Newman
→ create new func for CV(T) (heat capacity)
→ define a=0, b=$\frac{\theta_D}{T}$, N sam amount, V, Debye const,
→ follow example from Newman p.171 to Calculate gaussian
→ plug-into complete Cv equation

B) Plot
vectorize Cv and plot over T (temperature)

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.

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

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

+5

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.

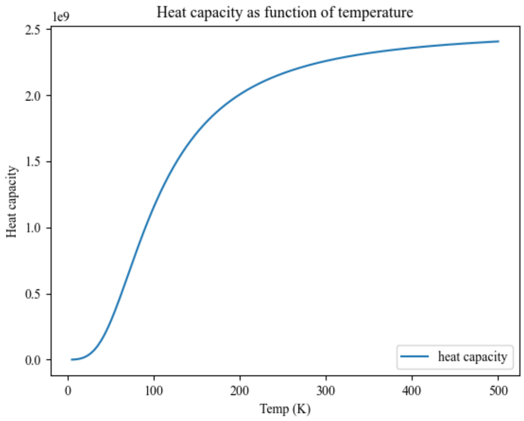

FIG. 5: Heat capacity over temperature.

5.3 54/56

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 56 points will be available per problem. Partial credit available on all non-1 items.

3 1. Does the program complete without crashing in a reasonable time frame? (+4 points) −1

comment out plt.savefig() before submission. creates an error and prevents me from running your code

1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points) must include plt.show() otherwise graphs aren't produced −1

3 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points)

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

4 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

4 6. Is the output answer correct? (+4 points).

3 7. Is the code readable? (+3 points)

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

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[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

. 5.3. Are units explained (if necessary)?

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

3 8. Is the code well documented? (+3 points)

. 6.1. Is the code author named?

. 6.2. Are the functions described and ambiguous variables defined?

. 6.3. Is the code functionality (i.e. can I run it easily enough?) documented?

9. Write-up (up to 28 points)

5 . Is the problem-solving approach clearly indicated through a flow-chart, pseudo-code, or other appropriate schematic? (+5 points)

✓ . Is a clear, legible LaTeX type-set write up handed in?

3 . Are key figures and numbers from the problem given? (+ 3 points)

4 . Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points)

3 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)

2 . Is a brief explanation of physical context given? (+2 points)

1 . If relevant, are helpful analytic scalings or known solutions given? (+1 point)

3 . Is the algorithm used explicitly stated and justified? (+3 points)

2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

2 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

1 . Are collaborators clearly acknowledged? (+1 point)

2 . Are any outside references appropriately cited? (+2 point)

5.9 51/56

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V must be in m^3 -1

3 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

3 6. Is the output answer correct? (+4 points).

graph slightly off due to error above -1

2 7. Is the code readable? (+3 points)

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Please include the units for v, ρ, θ_D, k_B −1

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1 . Is a brief explanation of physical context given? (+2 points) Define heat capacity −1

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