54 + 51 + 5 = 110

110/117

Homework 3 Write-Up

Petra Budavari*
Haverford College Department of Physics
(Dated: February 23, 2024)

1. TRIG LIBRARY

For this exercise, we created a group of functions for sine, cosine, and tangent in Python. I used Taylor series to define the trigonometric functions sine and cosine and used the resulting two functions to calculate tangent 3. Figure(1) shows my thought process. The function was set to break the Taylor series once the program could no longer tell the difference between the last Taylor series and the following one. To plot the functions to the input values of x, I had to use np.vectorize numpy function. Figure(2) gives the resulting plot.

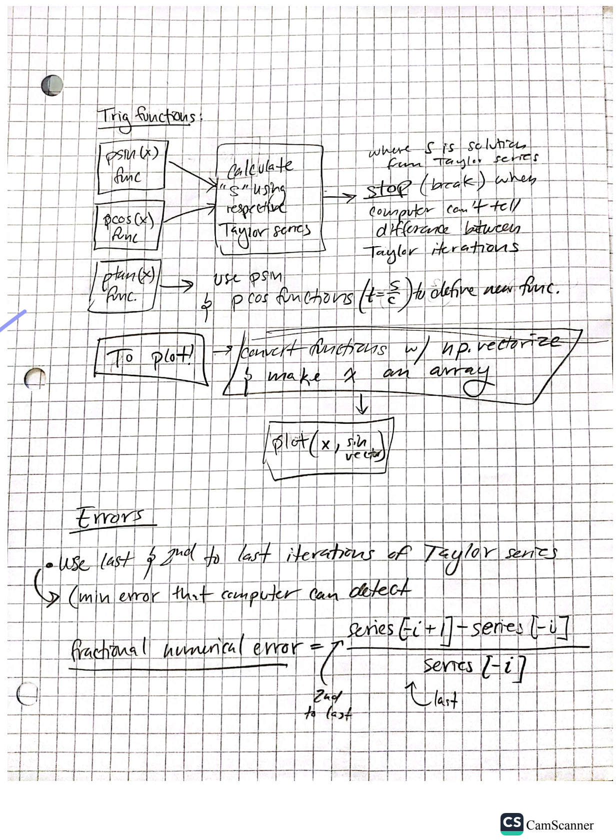
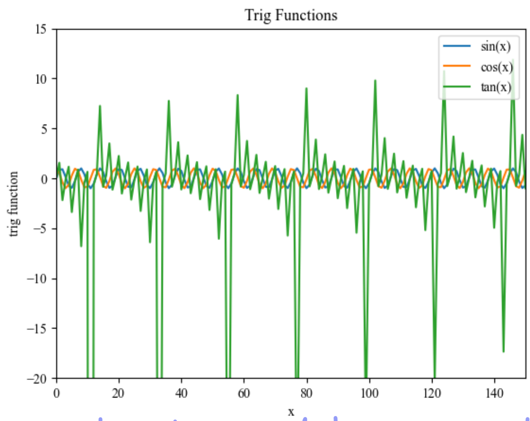


FIG. 1: Flow chart for Trig Library.

$$Sin(x) \approx \sum_{n=0}^{1000} \frac{-1^n}{(2n+1)!} x^{2n+1} \quad (1)$$

$$Cos(x) \approx \sum_{n=0}^{1000} \frac{-1^n}{(2n)!} x^{2n} \quad (2)$$

$$Tan(x) = Sin(x)/Cos(x) \quad (3)$$



Graph should be constrained to just 5 periods

FIG. 2: Plot of "homemade" trig functions over values of x.

We were then asked to calculated the fractional numerical error of the functions we created. To do this, I calculated the fractional error using the last and second to last Taylor series when the difference between the two is under some small value 4. This does introduce the problem that now the fractional error is above some fixed value - there is likely a better way to do this.

$$Error = (\text{PreviousSeries} - \text{LastSeries})/\text{LastSeries} \quad (4)$$

I then plotted the fractional errors for all of the functions in my trig library Figure(3). The error are very small (on the order of e^-11) and you can see that the error of tangent(x) is affected by cos and sin errors.

2. MADELUNG CONSTANT

In this exercise, we plotted the Madelung constant. From Equ(5) you can see that the sum is taken from

*Electronic address: pbudavari@haverford

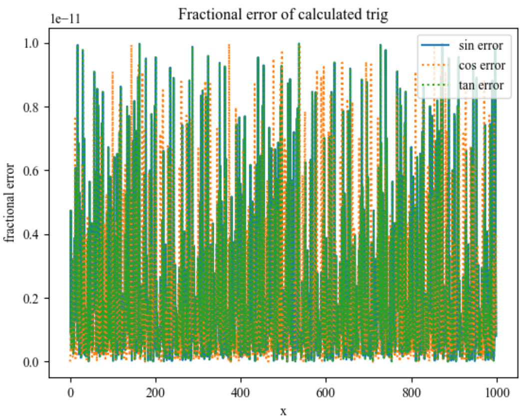


FIG. 3: Fractional error of trig functions.

negative infinity to positive infinity, however, the program cannot actually calculate this. Therefore, the lattice pattern was defined by a limited grid size. To use the sum of all three indices j,k,l, I created a system of nested for loops. Equ(5 lead to the plot seen in Figure(5) where you can see that the Madelung constant converges to the value -1.75.

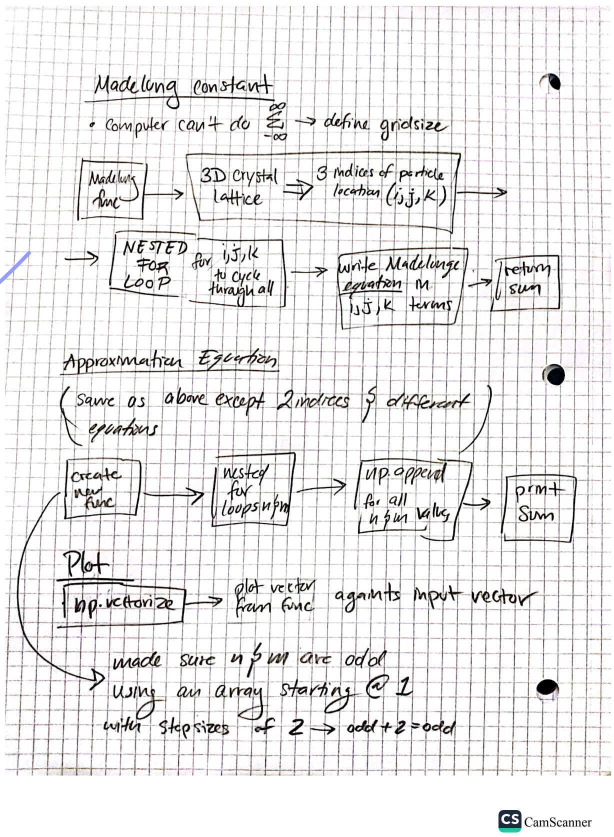


FIG. 4: Flow chart for calculating Madelung constant.

$$\text{Madelung Constant} = \sum_{j,k,l=-\infty}^{\infty} \frac{((-1)^{j+k+l}}{\sqrt{j^2+k^2+l^2}} \tag{5}$$

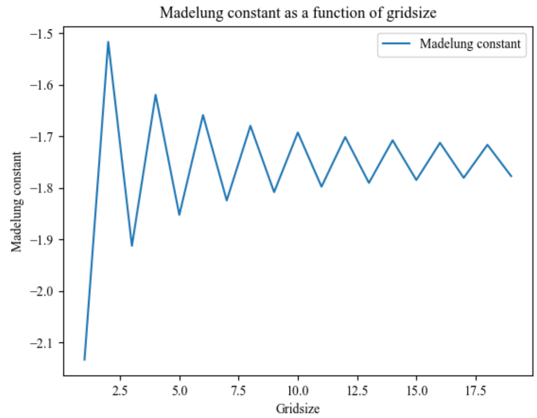


FIG. 5: Calculate Madelung constant.

I then plotted another equation of a very good approximation of the Madelung constant 6. This only took one nested for loop as there are only two variables. This result converges to approximately 1.75 (Fig.(6). I suspect that there is a change in sign because of the new assumption that all of the particle around the center particle are positively charges rather than negatively. Otherwise, the plots converge to the same Madelung constant.

$$\text{Madelung Approx.} = 12\pi \sum_{n,m\geq 1,odd} sech^2\left(\frac{\pi}{2}\sqrt{m^2+n^2}\right) \tag{6}$$

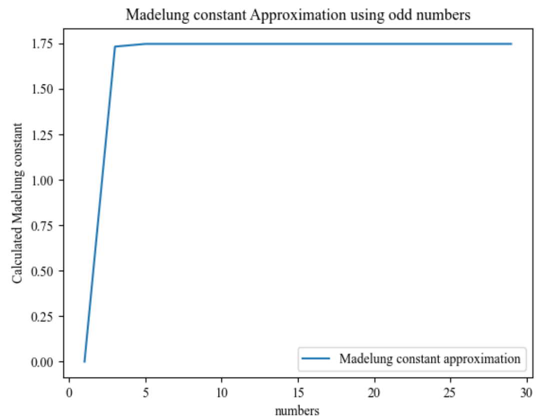


FIG. 6: Approximation for Madelung constant.

Lastly, I re-plotted the original Madelung equation but with changes to the lattice parameters. Now, the distance between particles along the j axis is ten times the original distance, twice the length for particles along the k axis and also t,he particles along the j vector have the same charge as the point we are measuring the Madelung constant from 7. This new Madelung constant converges to -1.4 as seen in Figure(7).

$$\text{My Madelung Constant} = \sum_{j,k,l=-\infty}^{\infty} \frac{((-1)^{-j+k+l}}{\sqrt{10j^2 + 2k^2 + l^2}} \tag{7}$$

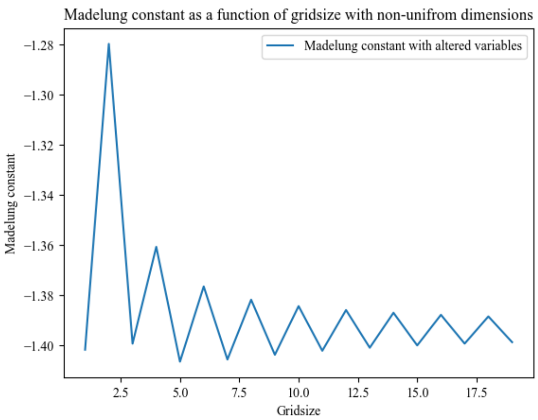


FIG. 7: Madelung constant with varied parameters.

The Madelung constant can be used the measure the electrostatic potential of any ion in a crystal lattice by approximated the charge density as a point charge [1]. This has very important application for understanding and characterizing crystal structures. It takes into account the attraction and repulsion forces between the ions and there have been many approximations for this calculation [2].

Great write-up!

3. SURVEY QUESTIONS

.5

The homework this week took approximately 8 hours (I was stuck on a bug for about 1.5 hours of that). I learned how to use nested for loops, how to build functions and vectorize them, and more general problem solving techniques. This homework was reasonable and useful.

[1] *Madelung constant*, URL https://en.wikipedia.org/wiki/Madelung_constant.
[2] *Libre texts, 5.11: Lattice energy - madelung constants*, URL https://chem.libretexts.org/Courses/Northern_Michigan_University/CH_215%3A_Chemistry_of_the_Elements_Fall_2023/05%3A_Solids_and_Solid-State_Chemistry/5.11%3A_Lattice_Energy_-_Madelung_Constants#:~:text=The%20Madelung%20constant%20takes%20in,from%20the%20distance%20between%20ions.

Q. 1

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.

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

[this prevents me from seeing your plots]

1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

comment out plt.savefig() before you submit, otherwise code produces an error because that directory does not exist on my computer -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?

---

[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?

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

. 6.1. Is the code author named? Please comment your name at the top of your code -1

. 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)

Q. 2 51/56

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.

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

[this prevents me from seeing your plots]

1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points) comment out plt.savefig() before you submit, otherwise code produces an error because that directory does not exist on my computer -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)

2 6. Is the output answer correct? (+4 points). Make sure to include plt.show(), otherwise plots won't show -2

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

. 5.1. Are variables named reasonably?

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

---

[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?

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

. 6.1. Is the code author named? please comment your name at the top of your code -1

. 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)

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

could expand on why, despite the first result being negative, we can compare their magnitudes -1

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)