

Attached written notes are my pseudo code for the problems.

6.9

$$\hat{H} \Psi(x) = E \Psi(x).$$

$$\hat{H} \Psi(x) = E \Psi(x).$$

$$\hat{H} \sum_{n=1}^{\infty} \Psi_n \sin \frac{n\pi x}{L} = E \sum_{n=1}^{\infty} \Psi_n \sin \frac{n\pi x}{L}$$

$$\text{given } \Psi(x) = \sum_{n=1}^{\infty} \Psi_n \sin \frac{n\pi x}{L}$$

$$\int_0^L \sin \frac{n\pi x}{L} dx \cdot \hat{H} \sum_{n=1}^{\infty} \Psi_n \sin \frac{n\pi x}{L} = \int_0^L \sin \frac{n\pi x}{L} dx \cdot E \sum_{n=1}^{\infty} \Psi_n \sin \frac{n\pi x}{L}$$

$$\sum_{n=1}^{\infty} \Psi_n \int_0^L \sin \frac{n\pi x}{L} \hat{H} \sin \frac{n\pi x}{L} dx = \sum_{n=1}^{\infty} \Psi_n E \int_0^L \sin \frac{n\pi x}{L} \cdot \sin \frac{n\pi x}{L} dx$$

since it's fourier coefficient, it's safe to put it at the front.

$$= \sum_{n=1}^{\infty} \Psi_n E \cdot \frac{1}{2} \cdot S_{mn}$$

$$\begin{cases} n \neq m & S_{mn} = 0 \\ n = m & S_{mn} = 1 \end{cases}$$

$$= \frac{1}{2} L E \Psi_m$$

$$\sum_{n=1}^{\infty} \Psi_n \underbrace{\int_0^L \sin \frac{n\pi x}{L} \hat{H} \sin \frac{n\pi x}{L} dx}_{H_{mn}} = \frac{1}{2} L E \Psi_m$$

H_{mn}

just one wavefunction.

a summation with ∞ wavefunctions.

write the equations in matrix form.

$$\hat{H} \Psi = E \Psi$$

4 is a vector.



$$\begin{aligned}
 b). \quad H_{mn} &= \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \sin \frac{m\pi x}{L} dx \\
 &= \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{a_x}{L} \right] \sin \frac{m\pi x}{L} dx \\
 &= \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} \left[+\frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2 \sin \frac{n\pi x}{L} + \frac{a_x}{L} \sin \frac{n\pi x}{L} \right] dx \\
 &= \frac{2}{L} \left[\int_0^L \frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2 \sin \frac{n\pi x}{L} \sin \frac{n\pi x}{L} dx + \int_0^L \frac{a_x}{L} \sin \frac{n\pi x}{L} \sin \frac{n\pi x}{L} dx \right] \\
 &= \frac{2}{L} \frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2 \underbrace{\int_0^L \sin \frac{n\pi x}{L} \sin \frac{n\pi x}{L} dx}_{\begin{cases} L/2 & m=n \\ 0 & m \neq n \end{cases}} + \frac{2}{L} \frac{a_x}{L} \underbrace{\int_0^L x \sin \frac{n\pi x}{L} \sin \frac{n\pi x}{L} dx}_{\begin{cases} 0 & m \neq n, \text{ both even/odd} \\ -\frac{L^2}{\pi^2} \frac{mn}{(m^2-n^2)^2} & m \neq n, \text{ even/odd} \\ L^2/4 & m=n \end{cases}}
 \end{aligned}$$

$$H_{nn} = \frac{2}{L} \frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2 \cdot \frac{L}{2} + \frac{2}{L} \frac{a_x}{L} \cdot \frac{L^2}{4} = \frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2 + \frac{a_x}{2}$$

$$H_{nn} \text{ both even/odd} = 0$$

$$H_{nn} \text{ one even, one odd} = \frac{2}{L} \frac{a_x}{L} \cdot \left[-\left(\frac{2L}{\pi} \right)^2 \frac{mn}{(m^2-n^2)^2} \right] = -\frac{8a_x}{\pi^2} \frac{mn}{(m^2-n^2)^2}$$

Pseudocode.

```
import numpy as np.
```

```
L=5A
```

```
a=10 eV
```

```
m_e = 9.1094 E -31
```

```
c_e = 1.6022 E -19
```

```
Def Hmn (m, n, a, L) :
```

```
if m=n:
```

```
if (m%2=0 and n%2=0) or (m%2=1 and n%2=1): # both are even/odd
```

```
Hmn=0
```

```
else: # when one of m,n is even and another is odd.
```

$$H_{mn} = -\frac{8a}{\pi^2} \frac{mn}{(m^2-n^2)^2}$$

```
else:
```

$$H_{mn} = \frac{\hbar^2}{2M} \left(\frac{m\pi}{L}\right)^2 + \frac{a}{2}$$

of m & n

```
# Start a matrix
```

```
H = np.zeros ((W,W)). # W indicates the size of the matrix.
```

```
# part b.
```

```
For i in w:
```

```
for j in w:
```

```
H[i,j] = Hmn (i+1, j+1, a, L). # use i+1 & j+1
```

```
# to start from 1
```

```
# not 0.
```

```
print (H[i,j]). # which should give the entry we're interested.
```

```
# part c.
```

```
size = 10.
```

```
H = np.zeros ((size, size)).
```

```
For i in w:
```

```
for j in w:
```

```
H[i,j] = Hmn (i+1, j+1, a, L).
```

```
# Solve the eigenenergy & eigenstate.
```

```
eigenvalues, eigenvectors = np.linalg.eigh (H).
```

```
energies = eigenvalues / eV.
```

```
print ( )
```

```
# part d. # We have exactly the same thing as in part c but the  
size = 10. # size is increased to 100.
```

```
H = np.zeros ((size, size)).
```

```
For i in w:
```

```
for j in w:
```

```
H[i,j] = Hmn (i+1, j+1, a, L).
```

```
# Solve the eigenenergy & eigenstate.  
eigenvalues, eigenvectors = np.linalg.eigh(H).  
energies = eigenvalues / eV.  
print( )
```

part e.

```
x = np.linspace(0, L, 1000).
```

Set up empty array for the first three wavefunctions interested.

```
ψ₁ = np.zeros_like(x)
```

```
ψ₂ = np.zeros_like(x)
```

```
ψ₃ = np.zeros_like(x).
```

Set a loop to input values.

```
for n in range(size):
```

```
    ψ₁ += eigenvectors[n][0] · sin(nπx / L)
```

```
    ψ₂ += eigenvectors[n][1] · sin(nπx / L)
```

```
    ψ₃ += eigenvectors[n][2] · sin(nπx / L)
```

Make the plot

```
plt.plot(x, ψ₁)
```

```
plt.plot(x, ψ₂)
```

```
plt.plot(x, ψ₃).
```

6.10

(a)

$$x = 1 - e^{-cx}$$

Given $c = 2$.

$$x = 1 - e^{-2x}$$

from math import exp

$$\eta = 1.0$$

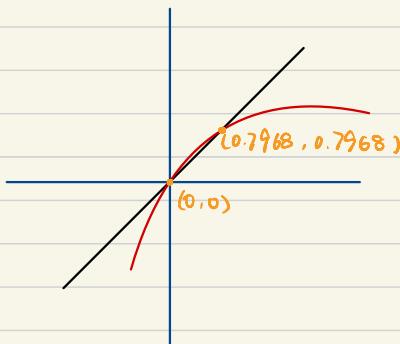
for k in range(100):

$$x = 1 - e^{-2x}$$

print(η).

After getting a converging value for x

we set new x = "that value" and repeat for higher accuracy.



$$\eta_1 = 0$$

for k in range(100):

$$x_1 = 1 - e^{-2\eta_1}$$

print(x_1).

This will generate a different answer.

(b)

Set up a set of values for c and an array for x.

$$c = np.arange(0, 3.01, 0.01)$$

$$x = np.ones_like(c)$$

Two loops needed : one for iteration in x ; the other for number of steps to

for i in range(len(x)):

calculate new x

for k in range(1000):

$$x[i] = 1 - e^{-ci} x[i]$$

Make the plot.

plt.plot(c, x).

$$53.5 \cdot 54 \cdot 5 = 112.5$$

112.5/117

PHYS 304 AS6

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(Dated: March 22, 2024)

No Collaborators. I have two python files.

PHYS_304_AS6_6.9_Xiyue_Shen.py file is the Asymmetric quantum well problem, numbered as 6.9 in the textbook.

PHYS_304_AS6_6.10_Xiyue_Shen.py is the file for the relaxation method exercise, numbered as 6.10 in the textbook.

1. EXERCISE 6.9 ASYMMETRIC QUANTUM WELL

1.1. Equation Setup

According to the Schrödinger equation, we have $\hat{H}\psi = E\psi$. Given in the problem, we are given the wavefunction as $\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin \frac{\pi n x}{L}$. Substitute the wavefunction into the Schrödinger equation, then we have,

$$\hat{H} \sum_{n=1}^{\infty} \psi_n \sin \frac{\pi n x}{L} = E \sum_{n=1}^{\infty} \psi_n \sin \frac{\pi n x}{L} \quad (1)$$

We multiply a sin function on both sides and do an integral to get,

$$\begin{aligned} & \int_0^L \sin \left(\frac{\pi m x}{L} \right) \hat{H} \sum_{n=1}^{\infty} \psi_n \sin \left(\frac{\pi n x}{L} \right) dx \\ &= \int_0^L \sin \left(\frac{\pi m x}{L} \right) E \sum_{n=1}^{\infty} \psi_n \sin \left(\frac{\pi n x}{L} \right) dx \end{aligned} \quad (2)$$

Since $\sum_{n=1}^{\infty} \psi_n$ are coefficients, it's safe to put them outside the integral.

$$\begin{aligned} & \sum_{n=1}^{\infty} \psi_n \int_0^L \sin \left(\frac{\pi m x}{L} \right) \hat{H} \sin \left(\frac{\pi n x}{L} \right) dx \\ &= \sum_{n=1}^{\infty} \psi_n \int_0^L \sin \left(\frac{\pi m x}{L} \right) E \sin \left(\frac{\pi n x}{L} \right) dx \end{aligned} \quad (3)$$

Then based on the delete function illustrated in the book,

$$\int_0^L \sin \frac{\pi m x}{L} \sin \frac{\pi n x}{L} dx = \begin{cases} L/2 & \text{if } m = n, \\ 0 & \text{otherwise,} \end{cases}$$

Only when $m = n$ does the integral give nonzero values. Thus, the right-hand side of equation 3 gives,

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin \left(\frac{\pi m x}{L} \right) E \sin \left(\frac{\pi n x}{L} \right) dx = \frac{1}{2} L E \psi_m \quad (4)$$

Thus, our equation 3 is reduced to,

$$\sum_{n=1}^{\infty} \psi_n \int_0^L \sin \left(\frac{\pi m x}{L} \right) \hat{H} \sin \left(\frac{\pi n x}{L} \right) dx = \frac{1}{2} L E \psi_m \quad (5)$$

This is what we want to show.

If we have a matrix, then equation 5 is an entry of the matrix. Given in the textbook that $H_{mn} = \frac{2}{L} \int_0^L \sin \frac{\pi m x}{L} \hat{H} \sin \frac{\pi n x}{L} dx$, we substitute this into equation 5. Because of the delta function, the equation is reduced to,

$$\begin{aligned} & \sum_{n=1}^{\infty} \psi_n \frac{L}{2} \frac{2}{L} \int_0^L \sin \frac{\pi m x}{L} \hat{H} \sin \frac{\pi n x}{L} dx = \frac{1}{2} L E \psi_m \\ & \sum_{n=1}^{\infty} \psi_n H_{mn} \psi_m = E \psi_m \end{aligned} \quad (6)$$

Given matrix multiplication, when we have one row times now column, the new entry is the summation of n th entry in the row times the n th entry in the column. In equation 6, the summation on the left-hand side indicates the product of row n and column m , while the right-hand side is the product's specific value. So, equation 6 is the specific entry for a $m \times n$ matrix. In matrix form, we will have

$$\mathbf{H}\psi = E\psi \quad (7)$$

with ψ as a vector and \mathbf{H} as a matrix.

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b Given H_{mn} as,

$$H_{mn} = \frac{2}{L} \int_0^L \sin \frac{\pi mx}{L} \left[-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + V(x) \right] \sin \frac{\pi nx}{L} dx \quad (8)$$

We have $V = ax/L$, and substitute it into H_{mn} ,

$$\begin{aligned} H_{mn} &= \frac{2}{L} \int_0^L \sin \frac{\pi mx}{L} \left[-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + ax/L \right] \sin \frac{\pi nx}{L} dx \\ &= \frac{2}{L} \int_0^L \sin \frac{\pi mx}{L} \left[-\frac{\hbar^2}{2M} \frac{d^2(\sin \frac{\pi nx}{L})}{dx^2} + \frac{ax}{L} \sin \frac{\pi nx}{L} \right] dx \\ &= \frac{2}{L} \int_0^L \sin \frac{\pi mx}{L} \left[\frac{\hbar^2}{2M} \left(\frac{\pi n}{L} \right)^2 \frac{\sin \frac{\pi nx}{L}}{dx^2} + \frac{ax}{L} \sin \frac{\pi nx}{L} \right] dx \\ &= \frac{2}{L} \frac{\hbar^2}{2M} \left(\frac{\pi n}{L} \right)^2 \int_0^L \sin \frac{\pi mx}{L} \sin \frac{\pi nx}{L} dx \\ &\quad + \frac{2}{L} \frac{a}{L} \int_0^L \sin \frac{\pi mx}{L} \sin \frac{\pi nx}{L} dx \end{aligned} \quad (9)$$

We have H_{mn} in two parts; one is $\frac{2}{L} \frac{\hbar^2}{2M} \left(\frac{\pi n}{L} \right)^2 \int_0^L \sin \frac{\pi mx}{L} \sin \frac{\pi nx}{L} dx$, while the other is $\frac{2}{L} \frac{a}{L} \int_0^L \sin \frac{\pi mx}{L} \sin \frac{\pi nx}{L} dx$. According to the hint given, we have three different situations,

- (a) $m = n$, we have $H_{mn} = \frac{\hbar^2}{2M} \left(\frac{\pi n}{L} \right)^2 + \frac{a}{2}$
- (b) $m \neq n$ and both even or both odd; we have $H_{mn} = 0$
- (c) $m \neq n$ and one is even, one is odd; we have $H_{mn} = -\frac{8a}{\pi^2} \frac{mn}{(m^2 - n^2)^2}$

Once we have the analytical value for H_{mn} and given the constant values, we can form our matrix. As the pseudocode shows, I used an if statement for $m = n$ and $m \neq n$. I set another if statement inside the $m \neq n$ case to distinguish the odd and even cases. Then, an empty matrix is created. A for loop is set to specify the exact entry we want. Since all constants we used are real numbers, the entries are also real. And as indicated by the footnotes, we would have the same value for H_{mn} and H_{nm} . A quick test of the code generates the same values for H_{45} and H_{54} .

c In this part, I set the matrix size to 10. The whole matrix can be generated following what I have set up in part b. Then, using np.linalg.eigh, the eigenvalues and eigenvectors can be obtained. The ground state energy is 5.83660289eV, as expected.

d This follows the same logic as the previous part. Instead, the matrix size was increased to 100, and only the first 10 energy states were printed. We

can compare the value with part c. The ground-level energy is 5.83660248eV. The energies I got from 100×100 matrix are generally smaller than 10 arrays on the order of 10^{-7} . The accuracy is increased since we consider more eigenstates. However, based on the difference in the order of 10^{-7} , the first then eigenstates provide very good results.

e In this part, we want to calculate the wavefunction related to the matrix's eigenvectors. For the nth wavefunction, we only want the nth row, which represents the coefficients of the eigenstate in that wavefunction. The wavefunction is the summation of a bunch of components from each eigenstate. Figure 1 shows the first three states' probability density.

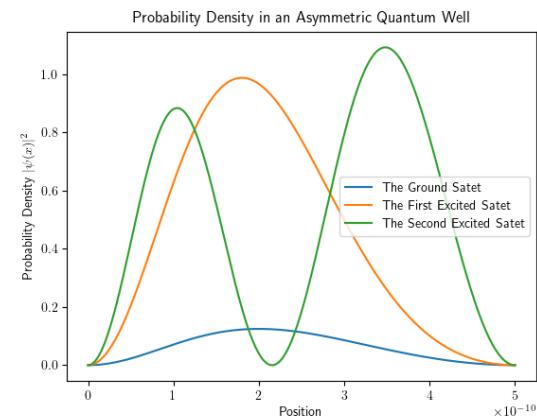


FIG. 1: [Probability Density of the First Three States.]

The second excited state is a bit confusing. Since we have an increasing potential, the peak on the right is expected to be lower than on the left. However, given that the plot has a probability density, the square of the original wavefunction is at a lower valley for the right part. This makes sense and agrees with our plot.

1.2. Physical Meaning

This system provides many insights into studying the small oscillations around an equilibrium point. We can stimulate the harmonic oscillators at the quantum level with an arbitrary potential energy. For example, we can set up a model for the vibration of a single electron in a strongly correlated system. With collective behavior, we can study emergent phenomena.

2. EXERCISE 6.10 RELAXATION METHOD

a Given the equation $x = 1 - e^{-cx}$, we can plot where the steady points are located, as shown in

INCLUDE RESULTS ↗

figure 2. There are steady points; one is $(0, 0)$, while the other is $(0.7968, 0.7968)$. Following the example code in the textbook, I input the function and set an initial value for x . Then, set a for loop to run the function for 100 times. Each run will assign a new value to x , closer to one of the steady points. Initially, I set $x = 1$, and then it ends at 0.7968121300200202 . Then I set x to 0.7968121 and got 0.7968121300200199, which should be more accurate since our initial values are closer.

From figure 2, we know there'll be two steady points. I started another run and set the initial value very close to zero. Until I went to 10^{-17} , the values converge to 0.

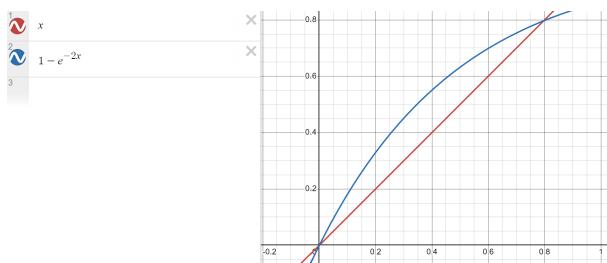


FIG. 2: [Sketch of $x = 1 - e^{-2x}$]

b For this one, I created an array of values for c as indicated in the problem. Then, for every c , I run the function 1000 times, the same as what we did in part a. Then, fill the empty x array with the values we just got. The plot is shown below,

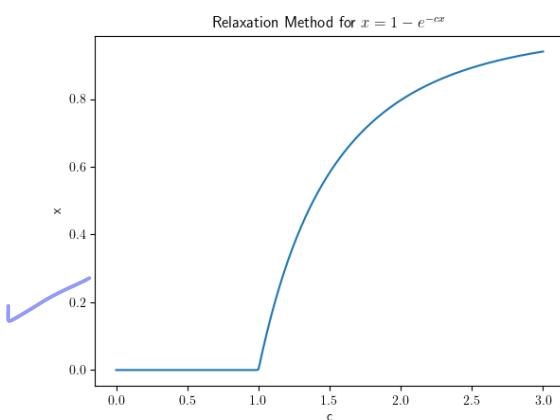


FIG. 3: [x as a function of c]

We can obviously, around $c = 1$, x jumps from zero to the regime of nonzero values. ✓

2.1. Physical Meaning

The relaxation method can estimate the electric potential in electrodynamics in two dimensions. The electric potential at a specific point is the average of the points around it. Just as we did in this problem, we start with a particular value at the boundary and then take a small step around based on Laplace's equation. Each point will be the average value of the neighbors. After running this several times, our estimate will become increasingly accurate; the values start approaching the steady points.

great write-up!

3. SURVEY ✓, 5

I spent roughly 5 hours on this homework. I learned more about how computers use numerical methods to solve differential equations. I like the Asymmetrica Quantum Potential Well problem since it provides many insights into quantum mechanics. Moreover, the relaxation method reminds me of the Laplace equation in electrodynamics. I think this set is about the right length.

4. UNGRADED PART

I have done all of the required and ungraded work.

6.9

53.5/56

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics¹

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)

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

2.5 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points) -0.5
PLOT should be $|\Psi|^2$ (yours is just Ψ)

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)

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

An indexing error and missing normalization - 1

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? *MISSING name -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?
1. Are key figures and numbers from the problem given? (+ 3 points) *include final outputs and define variables*
4. Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points) *(h, a, etc)*
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)

6.10

54 / 56

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics¹

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)
- 1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points) *All printed answers need a description, such as "for c=2, x = ..."* - 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

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 - . 5.4. Are algorithms found on the internet/book/etc. properly attributed?
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- . 6.1. Is the code author named? *MISSING name -/*
 - . 6.2. Are the functions described and ambiguous variables defined?
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- 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)
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- 2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

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- 1 . Are collaborators clearly acknowledged? (+1 point)
- 2 . Are any outside references appropriately cited? (+2 point)