Computational Physics - Final Exam

Date: 30-06-2020

Name:

ID:

Class:

Instructions

1. Time schedule
   9:30-10:00: preparation
   10:00-12:00: exam
   12:00-12:10: submission & uploading
2. There are two parts of the exam
   - Part I: single-choice problems
   - Part II: questions and coding problems
3. You are required to submit your answers to Part I direcly via *Canvas* platform. Beaware: You have only **ONE** trial!
4. You are required to download the file `CP_final_yourname_ID.ipynb` of Part II. **Please modify the file name to include your name!**. **Please write your name and ID in the file.**
5. You are required to write your answers (including the brief descriptions, the codes, the results and the plots) to Part II in the file during the exam session, and upload your file via *Canvas* platform after the exam session. Beaware: You have only **ONE** trial!

Part I

1. (4 points) The finite difference formula to approximate the first-order derivative of $f(x)$ is given as

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}$$

   Which of the following statements is True?

2. (4 points) Imagine a different universe in which Newton's second law has the form, $F(x,t) = m\frac{d^3x}{dt^3}$. If the force is given as $F(x) = kx^3$. Express this equation in the dynamical form appropriate for a Runge-Kutta algorithm:
3. (5 points) You are given the following data:

```
x = np.linspace(0,5.5,12)
y = np.array([9.882e-01, -7.000e-03, -3.852e-01, -1.018, -6.358e-02,  \
              1.633,  3.513,  6.121, 9.525,  1.407e+01,  1.805e+01, 2.387e+01])
```

   Using the central difference formulas, the approximate values of the first-order and the second-order derivative of y with respective to x at $x = 3.5$ would be
4. (4 points) The most effecive method to calculate the integrals is

$$I = \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx$$

5. (4 points) What of the following statements is True?
6. (5 points) The following table shows the data of Romberg integration.

$O(h^2)$	$O(h^4)$	$O(h^6)$
0.69393872		?
0.71337009		
0.72928425		

   The final result of sixth-order accuracy would be:
7. (5 points) The following code aims to generate a series of random numbers. The probability density function $p(x)$ should be

```
N = 10000
u = np.random.rand(N)
x = np.cbrt(8*u)
```

8. (5 points) How many errors can you find in the following code?

```
% Determine the period of an anharmonic oscillator

from scipy_integrate import solve_ivp

def anharmonic_oscillator(t,y)
    return [y[1], -np.sin(y[0])]

tspan = np.linespace(0,30,1000)
yinit = [np.pi/6; 0]
sol = solve_ivp(anharmonic_oscillator, [tspan[0],tspan[end]], yinit,t_eval=tspan)    t = sol.t
y = sol.y(0,:)

tmax = np.zeros()
for n in np.arange(1,len(t)):
    if y[n] > y[n-1] AND y[n] > y[n+1]
        tmax = np.append(tmax,t[n])

period = np.mean(np.dif(tmax))
print('period = {:d}'.format(period)
```

9. (4 points) Which of the following methods can NOT be used to solve the energy eigenvalues of hydrogen atom?

Part II

1. (25 points) A single particle is in the state of

$$\psi(x) = \begin{cases} Ae^{\cos(x)}, & 0 \le x \le 4\pi \\ 0, & \text{otherwise} \end{cases}$$

where $\psi(x)$ is the wave function.
(1) (5 points) Write the **vectorized** code to implement the trapezoid's rule to determine the normalization factor A. The total number N of x nodes is set as $N = 10$. How much is the step size Δx?
(2) (2 points) Define the wave function using `lamda`.
(3) (3 points) Compare your result of (1) with the result from the built-in function of `scipy.integrate` package. Calculate the relative error (You can take the average value of both results as the exact value).
(4) (4 points) Plot the normalized wave function. The figure size is set to be (10,7). The fontsize of title to be 16, the fontsize of axis labels to be 12. Set the range of x-axis to be $[0, 4\pi]$. Turn on the grid.

(5) (4 points) Write the code to approximate Fourier transform, the variable is called `phi`. The total number N of x nodes is set as $N = 101$. How much is the step size Δk in the $k-$space?
(6) (4 points) The code below employs `scipy.fftpack` package to calculate FFT of the wavefunction, the variable is called `G`. Please write the comments to each line.
(7) (3 points) If you compare the results from (5) and (6), you will see big differences between the two. Can you modify the code of (6) so that the power spectrum of `phi` and `G` agrees with each other?

2. (25 points) The conservation of heat can be used to develop a heat balance for a long, thin rod. If the rod is not insulated along its length and the system is at a steady state, the equation that results is

$$\frac{d^2T}{dx^2} + \kappa(T_a - T) = 0$$

The total length of the rod $L = 10$ m. $\kappa = 0.01$ m^2. $T_a = 20$. The boundary conditions are given as $T(0) = 40$, $T(10) = 200$.
(1) (3 points) Apply the shooting method in combination of RK4 to solve the BVP again. Please first define the drive function, the returning variable is of data type `list`.
(2) (4 points) The code `rk4` for the implementation of Rk4 is provided as follows. Complete the test function `rod_rk4_app` to plot the values of $T(10)$ vs $T'(0)$. Take the step size $\Delta x = 2$.
(3) (6 points) Following (1) and (2), define the root-finding function `rod_root`. Use the built-in function of `scipy.optimize` package to solve the BVP. Print out the results of Ts at $x = 2, 4, 6, 8$
.
(4) (8 points) The finite-difference approach yields the linear system of equations as $AT = b$. Take the step size $\Delta x = 2$. Calculate the coefficients and generate A and b via `diag`. Write the code and print out the results of Ts at $x = 2, 4, 6, 8$.
(5) (4 points) The exact solution is $T = 73.4523e^{0.1x} - 53.4523e^{-0.1x} + 20$. Comment on the comparison of your results of (3) and (4) with the exact solution. What are the maximum relative errors concerning the two methods?

3. (10 points) Find the volume of a four-dimensional sphere of radius 2. A sphere is defined to be the set of points such that:

$$\sum_{i=1}^{D} x_i^2 \leq R^2$$

where D is the dimension of the space, R is the radius of the sphere, and the set $\{x_i\}_{i=1}^{D}$ are the coordinates (so, for example, in $D = 2$, we have $x_1 = x$, $x_2 = y$).
(1) (2 points) You must first find the “area” of the enclosing cube.

(2) (5 points) Use the condition above to determine if a dart has hit or missed. Set the number N of darts in one trial to be $N = 1000$. Determine the volume for one trial. Please test your code with $D = 3$.

(3) (3 points) Repeat the hit-or-miss experiment 100 times, determine the mean value of the volume and its standard deviation. To test your code, set the seed of random generator to be one.

4. (**optional**, 5 points bonus) Calculate the energy of the ground state, and plot the associated wave function for a potential of the form

$$V(x) = \begin{cases} -10\cos(\pi x), & -\frac{1}{2} \le x \le \frac{1}{2} \\ 0, & \text{otherwise} \end{cases}$$

Take the step size $\Delta x = 0.002$ if you employ the central finite difference formula.