Computational Physics Homework Assignment #2

March 25, 2019; Due April 15, 2019

Reading Assignment

1. Read lecture notes and references; Study sample programs and prepare your own programs with any languages you prefer.
2. **Complete** one Lab Assignments before you lave the laboratory.

Laboratory Assignments (Total Points: 120), on April 01, 2019

1. (10 points) Consider the function $f(x) = xe^x$ at $x = 1$. Calculate its first and second derivatives for $h = 0.5, 0.45, \dots, 0.05$, using the forward and central difference formulae. Plot the log error versus $\log(h)$. Compare your results with that of Richardson extrapolation.

2. (15 points) Use the two-point, three-point, and five-point formulae to estimate the first five derivatives of f(x) at $x = 0$.

$$f(x) = \frac{e^x}{\sin^3(x) + \cos^3(x)}$$

As a check, $f^{(1)}(0) = 1, f^{(2)}(0) = 4, f^{(3)}(0) = 4,\ f^{(4)}(0) = 28,\ f^{(5)}(0) = -164$

You are recommended to change the value of h in the fashion of $\mathrm{h} = \frac{1}{2^{\mathrm{n}}}$, n = 1, 2, …

(Hint: please use forward two-point formulae to estimate first derivative, central three-point for first and second derivatives, central five-point for first four derivatives, central seven-point for fifth derivative. You can find coefficients at https://en.wikipedia.org/wiki/Finite_difference_coefficient)

3. (10 points) Use library functions and subroutines, to prove the following equalities *numerically*:

$$(\mathrm{AB})\mathrm{C} = \mathrm{A}(\mathrm{BC}) \quad (1)$$
$$\mathrm{A}(\mathrm{B}+\mathrm{C}) = \mathrm{AB} + \mathrm{AC} \quad (2)$$
$$(\mathrm{AB})^{\mathrm{T}} = \mathrm{B}^{\mathrm{T}}\mathrm{A}^{\mathrm{T}} \quad (3)$$
$$(\mathrm{AB})^{-1} = \mathrm{B}^{-1}\mathrm{A}^{-1} \quad (4)$$
$$\det(\mathrm{AB}) = \det(A)\det(B) \quad (5)$$

With

$$A = \begin{pmatrix} 1 & 1 & -1 \\ 1 & 2 & -2 \\ -2 & 1 & 1 \end{pmatrix}, B = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 1 & 0 \end{pmatrix}, C = \begin{pmatrix} 3 & 2 & 1 \\ 1 & 2 & 3 \\ 1 & -1 & 1 \end{pmatrix}$$

4. (20 points) Study the Hilbert matrix again.

$$H_n = \begin{pmatrix} \frac{1}{1} & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{1}{n} & \frac{1}{n+1} & \frac{1}{n+2} & \cdots & \frac{1}{2n-1} \end{pmatrix}$$

Diagonalizing H_n and calculate the ratio of the largest eigenvalue to the smallest eigenvalue, $\log(max|\lambda|/min|\lambda|)$, and plot it as a function of n. Discuss your results.
Do the problem for both single and double precisions. Indicate which diagonalization routine you are using.

5. **Coupled Oscillators** (35 Points: 10, 10, 15)
   Use program similar to *Oscillators* to solve the dynamics equation of motion for N=10 oscillators with the initial conditions $u_j(t=0)=0,\ v_1(t=0)=1$. Compare numerical results of $u_j(t)$ with the analytic one.
   (a) What is the maximum deviation of $u_j(t)$?
   (b) How well is the total energy conserved as function of Δt ?
   (c) How well is the total energy conserved as function of Δt if one uses Runge-Kutta 4th order algorithm?

6. (20 points) Table 3.1 lists a few values of Bessel functions. Estimate $J_1(4.5)$ by Lagrange polynomial interpolation for n = 1, 2, 3, and 5. Compare with exact value of $J_1(4.5)$ from math library. Recalculate $J_1(4.5)$ by Hermite interpolation for n 1, 3, and 5. The derivative of $J_1(x)$ is $(J_0(x) - J_2(x))/2$.

TABLE 3.1 Bessel Functions

ρ	$J_0(\rho)$	$J_1(\rho)$	$J_2(\rho)$
0.0	1.00000 00000	0.00000 00000	0.00000 00000
1.0	0.76519 76866	0.44005 05857	0.11490 34849
2.0	0.22389 07791	0.57672 48078	0.35283 40286
3.0	−0.26005 19549	0.33905 89585	0.48609 12606
4.0	−0.39714 98099	−0.06604 33280	0.36412 81459
5.0	−0.17759 67713	−0.32757 91376	0.04656 51163
6.0	0.15064 52573	−0.27668 38581	−0.24287 32100
7.0	0.30007 92705	−0.00468 28235	−0.30141 72201
8.0	0.17165 08071	0.23463 63469	−0.11299 17204
9.0	−0.09033 36112	0.24531 17866	0.14484 73415
10.0	−0.24593 57645	0.04347 27462	0.25463 03137