

## 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 leave 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,  $f^{(v)}(x = 0) = -164$

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

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

$$(AB)C = A(BC) \quad (1)$$

$$A(B + C) = AB + AC \quad (2)$$

$$(AB)^T = B^T A^T \quad (3)$$

$$(AB)^{-1} = B^{-1} A^{-1} \quad (4)$$

$$\det(AB) = \det(A) \det(B) \quad (5)$$

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.

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

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  $\Delta t$  ?

(c) How well is the total energy conserved as function of  $\Delta t$  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  $(J_1(x) - J_2(x))/2$ .

<b>TABLE 3.1 Bessel Functions</b>			
$\rho$	$J_0(\rho)$	$J_1(\rho)$	$J_2(\rho)$
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