NATIONAL UNIVERSITY OF SINGAPORE

PC3236 – COMPUTATIONAL METHODS IN PHYSICS

(Semester II: AY 2009-10)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains FOUR questions and comprises THREE printed pages.
2. Answer any THREE questions.
3. All questions carry equal marks.
4. Answers to the questions are to be written in the answer books.
5. This is a CLOSED BOOK examination.
6. Programmable calculator is NOT allowed to be used in the examination.

1. (a) Evaluate the integral

$$\int_1^{\infty} x^{-3/2} \sin\left(\frac{1}{x}\right) \mathrm{d}x$$

by Romberg integration. Express your answer accurate to four decimal places.

(b) Solve the linear system $Ax = b$, where

$$A = \begin{pmatrix} 1 & 2 & -3 & -1 \\ 2 & 1 & -1 & 2 \\ 3 & -1 & -2 & 1 \\ -1 & 3 & 2 & 1 \end{pmatrix}, \quad \text{and} \quad b = \begin{pmatrix} -12 \\ 4 \\ 4 \\ 0 \end{pmatrix},$$

using an LU decomposition according to Crout's algorithm.

2. (a) The equations

$$\sin x + 3\cos y - 2 = 0,$$
$$\cos x - \sin y + 0.2 = 0,$$

have a solution in the vicinity of the point (1, 1). Use the Newton-Raphson method to refine the solution accurate to 4 decimal places.

(b) Evaluate the integral

$$\int_0^2 \int_0^2 \frac{x^2 \sin(y)}{x + y} \mathrm{d}x \, \mathrm{d}y$$

by applying the three-point Gauss-Legendre rule for both integrals.

Note that the Gauss-Legendre rule is given by

$$\int_{-1}^{1} f(\xi) \, \mathrm{d}\xi \approx \sum_{i=1}^{n} W_i f(\xi_i),$$

where the weights W_i and abscissas ξ_i are provided in the following table.

$\pm\xi_i$	W_i	$\pm\xi_i$	W_i
$n = 2$		$n = 5$	
0.577350	1.000000	0.000000	0.568889
$n = 3$		0.538469	0.478629
0.000000	0.888889	0.906180	0.236927
0.774597	0.555556	$n = 6$	
$n = 4$		0.238619	0.467914
0.339981	0.652145	0.661209	0.360762
0.861136	0.347855	0.932470	0.171324

3. Apply Heun's method to solve the non-linear differential equation

$$\frac{d^2y}{dx^2} + \frac{y^4}{(x+4)} = 0,$$

subject to the initial conditions $y(0) = 2$ and $y'(0) = 1$.

(i) Use a step size of 0.1 to integrate the equation from $x = 0$ to $x = 0.5$.

(ii) Use a step size of 0.05 and integrate from $x = 0$ to $x = 0.3$.

(iii) Use Richardson extrapolation to obtain better approximations for $y(0.1)$, $y(0.2)$ and $y(0.3)$.

Round your answers to four decimal places.

4. Consider the 2D Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 2(x^2 + y^2), \quad \text{for} \quad 0 < x < 1 \quad \text{and} \quad 0 < y < 1,$$

subject to the following boundary conditions

$$u(x, 0) = 0, \qquad u(0, y) = 0,$$

$$\frac{\partial u(x, 1)}{\partial y} = 2x^2, \qquad u(1, y) = y^2.$$

Use the finite difference method with a square mesh of width $h = 1/3$ to solve the Poisson equation. Give your answers either in fractions or round them to four decimal places.

LHS

– END OF PAPER –