NATIONAL UNIVERSITY OF SINGAPORE

PC3236 – COMPUTATIONAL METHODS IN PHYSICS

(Semester II: AY 2017-18)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

1. Please write your student number only. **Do not write your name**.
2. This examination paper contains FOUR questions and comprises FOUR printed pages.
3. Answer ALL questions.
4. All questions carry equal marks.
5. Answers to the questions are to be written in the answer books.
6. Show all working steps clearly and box each answer.
7. Please start each question on a new page.
8. This is a CLOSED BOOK examination.
9. Programmable or graphic calculators are **NOT** allowed to be used in this examination.
10. The last page contains a list of formulae.

1. (a) Calculate $f'(1.5)$, as accurately as possible, from the following data.

x	1.0	1.5	2.0	2.5
$f(x)$	3.7183	5.4817	8.3891	13.1825

(b) Calculate the following improper integral numerically

$$\int_1^2 \frac{\ln x}{(x-1)^{1/5}}\,\mathrm{d}x.$$

Express your answer accurate to at least three decimal places.

2. (a) Given

$$f(x) = -2x^6 - 1.5x^4 + 10x + 2,$$

determine the maximum of this function. Perform iterations until the relative error falls below 0.5%.

(b) Consider the following differential equation

$$y' = \frac{1}{t^2} - \frac{y}{t} - y^2, \quad \text{with } y(1) = -1.$$

Use a third-order Taylor series method (with a local truncation error of $\mathcal{O}(\tau^4)$) to approximate the solution for the first two time steps. Use a time step of 0.05.

3. Solve the following initial-value problem

$$y''(x) + xy^2(x) = 0, \quad y(0) = 1, \quad y'(0) = 3$$

using the modified Euler method.

(i) Integrate from $x = 0$ to $x = 1.5$, using a step size of 0.5.

(ii) Repeat with a step size of 0.25.

(iii) Based on the above results, obtain better approximations for $y(0.5)$, $y(1.0)$ and $y(1.5)$.

Round your answers to four decimal places.

4. Consider the 2D Laplace equation

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

subject to the following boundary conditions

$$u(x,0) = \sin(x), \qquad u(x,1) = e\sin(x),$$
$$u(0,y) = 0, \qquad u(1,y) = e^y \sin(1).$$

Employ the Gauss-Seidel method with a square mesh of width $h = 1/3$ to solve the Laplace equation. Set all starting trial values to 0.5. Give your answers accurate to at least two decimal places.

LHS

Formulae Sheet

Taylor series:

$$f(x) = f(a)+(x-a)f'(a)+\frac{(x-a)^2}{2!}f''(a)+\cdots+\frac{(x-a)^{n-1}}{(n-1)!}f^{[n-1]}(a)+\frac{(x-a)^n}{n!}f^{[n]}(\xi)$$

Inverse quadratic interpolation:

$$x(f) = \frac{(f-f_2)(f-f_3)}{(f_1-f_2)(f_1-f_3)}x_1 + \frac{(f-f_1)(f-f_3)}{(f_2-f_1)(f_2-f_3)}x_2 + \frac{(f-f_1)(f-f_2)}{(f_3-f_1)(f_3-f_2)}x_3$$

Secant method: $x_{i+1} = x_i - f(x_i)\dfrac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$

Newton's method for system of equations: $\boldsymbol{J}(\boldsymbol{x})\Delta\boldsymbol{x} = -\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{J}$ is the Jacobian matrix

Central difference: $f'(x) = \dfrac{f(x+h)-f(x-h)}{2h}$, $f''(x) = \dfrac{f(x+h)-2f(x)+f(x-h)}{h^2}$

Richardson extrapolation: $F = \dfrac{(h_1/h_2)^p D(h_2) - D(h_1)}{(h_1/h_2)^p - 1}$

Padé: $R_{n,m}(x) = \dfrac{\sum_{i=0}^{n} p_i x^i}{1+\sum_{j=1}^{m} q_j x^j}$, $\displaystyle\sum_{i=0}^{k} a_i q_{k-i} = p_k$, $k = 0, 1, \ldots, N$ and $N = n+m$

Lagrange: $p(x) = \displaystyle\sum_{j=1}^{n} l_{j,n}(x) f(x_j)$, $l_{j,n}(x) = \dfrac{(x-x_1)(x-x_2)\cdots(x-x_{j-1})(x-x_{j+1})\cdots(x-x_n)}{(x_j-x_1)(x_j-x_2)\cdots(x_j-x_{j-1})(x_j-x_{j+1})\cdots(x_j-x_n)}$

Simpson's 1/3 rule: $\displaystyle\int_a^b f(x)\,\mathrm{d}x = \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]\frac{h}{3}$

Monte Carlo: $\displaystyle\int_a^b f(x)\,\mathrm{d}x \approx (b-a)(\langle f\rangle_N \pm \sigma_N)$, $\sigma_N = \sqrt{\dfrac{\frac{1}{N}\sum_i f(x_i)^2 - \left(\frac{1}{N}\sum_i f(x_i)\right)^2}{N-1}}$

Modified Euler: $y(x_0+h) = y(x_0) + hf(x_{\text{mid}}, y_{\text{mid}})$

Heun's method: $y(x_0+h) = y(x_0) + h\dfrac{f_0 + f(x_0+h, y_0+hf_0)}{2}$

Crank-Nicolson method: $y(x_0+h) = y(x_0) + \dfrac{h}{2}(f_0 + f_1)$

Leibniz Integral Rule: $\dfrac{\mathrm{d}}{\mathrm{d}x}\displaystyle\int_{a(x)}^{b(x)} f(x,y)\,\mathrm{d}y = \int_{a(x)}^{b(x)} \frac{\partial f}{\partial x}\,\mathrm{d}y + f(x,b(x))\frac{\mathrm{d}b}{\mathrm{d}x} - f(x,a(x))\frac{\mathrm{d}a}{\mathrm{d}x}$

Gauss-Legendre quadrature:

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

$\pm\xi_i$	W_i	$\pm\xi_i$	W_i
$n=2$		$n=3$	
$\frac{1}{\sqrt{3}}$	1	0	$\frac{8}{9}$
		$\sqrt{\frac{3}{5}}$	$\frac{5}{9}$

– END OF PAPER –