NATIONAL UNIVERSITY OF SINGAPORE

PC3236 – COMPUTATIONAL METHODS IN PHYSICS

(Semester II: AY 2016-17)

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) Use the secant method to determine the root of

$$-x^3 + 5x^2 - 2 = 0$$

that lies in the interval $(4, 6)$. Express your answer accurate to at least three decimal places.

(b) i. Find the Padé approximation $R_{1,1}(x)$ for $f(x) = \tan(\sqrt{x})/\sqrt{x}$. You may use the Maclaurin expansion

$$f(x) = 1 + \frac{x}{3} + \frac{2x^2}{15} + \cdots$$

ii. Hence show that

$$\tan(x) \approx R_{3,2}(x) = \frac{15x - x^3}{15 - 6x^2}$$

2. (a) Use the following data to approximate $\int_1^5 f(x)\,dx$ as accurately as possible.

x	1	2	3	4	5
$f(x)$	2.4142	2.6734	2.8974	3.0976	3.2804

(b) Consider the following differential equation

$$\frac{dy}{dt} = 1 + (t - y)^2, \quad \text{with } y(2) = 1$$

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 τ of 0.5.

3. Solve the following boundary-value problem

$$\frac{d^2y}{dx^2} + y^2 = 2x^2, \quad y(0) = 0, \quad y'(2) = 1$$

with the finite difference method. Discretize the spatial domain using a step size of $\frac{2}{3}$. Ensure that your answers have converged to at least 1 decimal place.

4. Solve the heat equation

$$\frac{\partial u}{\partial t} - \frac{1}{16}\frac{\partial^2 u}{\partial x^2} = 0, \quad 0 < x < 1$$

subject to the initial and boundary conditions

$$\begin{aligned} u(x,0) &= 2\sin(2\pi x), \\ u(0,t) &= 0, \\ u(1,t) &= 0 \end{aligned}$$

Integrate for one time step using the Crank-Nicolson method with a spatial step size of 0.2 and a time step of 0.1. Give your answers rounded off to four 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: $y(x_0+h) = y(x_0) + hf(x_{\mathrm{mid}}, y_{\mathrm{mid}})$

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 –