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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

MATHEMATICAL PHYSICS

Third Year

AUTUMN REPEAT EXAMINATION

2008-2009

Computational Physics I

MP354

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Time allowed: 1.5 hours

Answer two questions

All questions carry equal marks

1. The following MatLab function is meant to calculate the series

$$S(x) = \sum_{n=1}^{\infty} \frac{(2x)^n}{n(n!)^2}\,,$$

by computing each term from the previous one. It should return an error if x is not a positive number. The code contains 10 mistakes (errors or highly inefficient ways of calculating). Find these mistakes, and write out the correct and improved code.

```
function S = series(x)
% function to evaluate the series
%     --
%     \    ___(2x)^n___
%     /_     n (n!)^2
%     n=1
%
% to a given precision. x must be a positive number.
% Set the precision
prec = 1000;
% check for valid arguments
if ( x > 0 )
    error('x must be a positive number')
% compute the first term t_1
t = 2x;
n = 0;
if ( t>prec )
    S = S+t;
    % compute the next term t_(n+1) from t_n
    t = t*2n*x/n+1^2;
    n = n+1;
end
```

2. (a) Explain the difference between *rounding errors* (precision) and *truncation errors* (accuracy), giving examples of both. You may illustrate the notion of truncation errors with reference to numerical differentiation or integration schemes.

   (b) By way of an appropriate Taylor expansion in δ, determine the order of accuracy of the discrete first-order derivative

$$f'(x) \approx \frac{1}{6\delta}\Big[-2f(x-\delta) - 3f(x) + 6f(x+\delta) - f(x+2\delta)\Big]\,.$$

3. The formula for the midpoint method for solving a general first-order ODE,

$$\frac{dy}{dx} = F(x, y)$$

is given by

$$y(x + \varepsilon) = y(x) + \varepsilon F(x_{\text{mid}}, y_{\text{mid}})$$

with

$$x_{\text{mid}} = x + \frac{\varepsilon}{2}, \qquad y_{\text{mid}} = y(x) + \frac{\varepsilon}{2} F(x, y(x)) .$$

By means of appropriate Taylor expansions obtain the accuracy of this formula.

4. (a) Explain the difference between a *boundary value problem* and an *initial value problem* for an ordinary differential equation. Which complications may you encounter for a boundary value problem that are not present in an initial value problem?

   (b) Describe how the boundary value problem

$$\frac{d^2y}{dx^2} = f(x, y), \qquad y(x_1) = y_1, \quad y(x_2) = y_2$$

   where $f(x, y)$ is a given function and x_1, y_1, x_2, y_2 are given numbers, may be solved using the *shooting method*. Write out the key steps of the numerical procedure.