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THE NATIONAL UNIVERSITY OF IRELAND MAYNOOTH

MATHEMATICAL PHYSICS

Third Year

SEMESTER 2

2010-2011

Computational Physics I

MP354

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Time allowed: 1.5 hours

Answer two questions

All questions carry equal marks



- The following MatLab function is meant to calculate the gamma function  $\Gamma(z)$ , which is an extension of the factorial function to non-integer values, such that  $\Gamma(n) = (n - 1)!$  for all positive integers  $n$ . The code uses the following representation of the gamma function,

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt, \quad (1)$$

which is valid for  $z > 0$ . The integral is evaluated using the midpoint integral formula and terminating when the integrand becomes smaller than a given precision. To avoid problems if the integrand is 0 at  $t = 0$ , a minimum upper limit is set.

If  $z \leq 0$ , the recursion formula  $\Gamma(z + 1) = z\Gamma(z)$  is used to make the argument positive, while if  $z$  is a non-positive integer ( $0, -1, -2, \dots$ ) the function should return an error.

The code contains 10 mistakes (errors or highly inefficient ways of calculating). Find these mistakes, and write out the correct and improved code.

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1 % Gamma(z) computes the Gamma function using the integral representation
2 %           /oo  z-1  -t
3 % Gamma(z) = |  t    e    dt
4 %           /0
5 % The integral is evaluated using the midpoint method. It is terminated
6 % when the integrand drops below a given precision.
7 % A minimum cutoff Tmin is set in case the integrand is 0 at t=0
8 % If z is an integer, the factorial function is used.
9 % If z is negative, the recursion formula Gamma(z+1) = zGamma(z) is used
10 function G = Gamma(z)
11 Tmin = 10;    % minimum cutoff for integral
12 dt    = 1e-6; % grid spacing for integral
13
14 if (z > 0)
15     if (floor(z) == z) % this means that z is an integer
16         error('Gamma function undefined for non-positive integers')
17     else
18         G = Gamma(z)/z; % use the recursion formula
19     end
20
21 G = 0;
22 t = 0;
23 if ( (t < Tmin) || (fn > prec) )
24     fn = t^(z-1)*exp^-t; % evaluate integrand
25     G = G + fn*dt;
26 end

```

2. (a) Explain the difference between an integer and a floating-point number. What is meant by the *precision* of a floating-point number?
- (b) A discrete second derivative may be constructed as

$$f''(x) \approx \Delta^{(2S)} f(x) = \Delta^S(\Delta^S f(x)),$$

where  $\Delta^S f(x)$  is the symmetric first derivative.

- i. Show that

$$\Delta^{(2S)} f(x) = \frac{f(x - 2\delta) - 2f(x) + f(x + 2\delta)}{4\delta^2}.$$

- ii. By way of an appropriate Taylor expansion in  $\delta$ , determine the order of accuracy of  $\Delta^{(2S)} f(x)$ .
- iii. Explain why this derivative is in general inferior to the usual discrete second derivative.
3. (a) Explain how the second-order differential equation

$$\frac{d^2 q(t)}{dt^2} = -q(t)$$

can be reduced to two coupled first order differential equations.

- (b) Describe how the resulting equations can be solved numerically using the *Euler method*. Write out the key steps of the numerical procedure.
- (c) If we define

$$H(t) = \dot{q}^2(t) + q^2(t)$$

show that

$$H_{n+1} = (1 + \varepsilon^2)H_n,$$

where  $H_n$  is the value of  $H(t)$  after the  $n$ -th Euler step, and  $\varepsilon$  is the Euler stepsize. Discuss the implications of this result for the performance of the Euler method. How does the *Euler-Cromer* method improve on this?

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

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

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.