## Imperial College London January 2012

## COMPUTATIONAL PHYSICS TEST

## For 3rd-Year Physics Students

Monday, 9th January 2012, 14:00 to 16:00

Please attempt THREE questions.

All questions carry equal marks.

Start each question on a new page of the same answer booklet.

Continue on a new answer booklet if needed.

Marks shown on this paper are indicative of those the Examiners anticipate assigning.

## **General Instructions**

Complete the cover of each book used to answer the questions.

Please write your name on any answer book you use.

If an electronic calculator is used, write its serial number at the top of the front cover of each answer book.

You are reminded that Examiners attach great importance to legibility, accuracy and clarity of expression.

**1.** A first order, coupled ODE system with independent variable *t* is given by

(1) 
$$\frac{d}{dt} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -a & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix},$$

where a is a constant.

- (i) Derive an analytical solution for (1). [2 marks]
- (ii) Write down the update matrix **T** for a numerical integration of (1) using the Euler method. [2 marks]
- (iii) Show that, if a > 0, the Euler method is always unstable for this system.

[4 marks]

(iv) For the case where a < 0, state, without proof, the condition the solution must satisfy if the *Leapfrog* method is to be used successfully. How would this condition be enforced in practice? [2 marks]

**2.** The one dimensional heat diffusion problem is described by a Partial Differential Equation (PDE) that is first order in time *t* and second order in space *x* 

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2},$$

where u(x, t) is the solution describing e.g. the temperature along x and D is a constant diffusion coefficient.

We are to solve the system using a finite difference scheme whereby the solution u(x,t) is discretised onto a time and space lattice with indices n and j respectively i.e.  $u_i^n$ . The lattice is regular and is spaced in intervals  $\Delta t$  in time and h in space.

- (i) Describe the difference between *explicit* and *implicit* methods for numerically solving PDEs. [2 marks]
- (ii) Using a *first order*, backward difference scheme in time and a *second order* central difference scheme in space derive the following implicit method for obtaining a solution  $u_i^n$  given boundary conditions at some initial time

$$u_{i}^{n}-u_{i}^{n-1}=R\left(u_{i-1}^{n}-2u_{i}^{n}+u_{i+1}^{n}\right).$$

Make sure to define the term R that appears in the scheme. [3 marks]

(iii) Describe how you would solve the system using an iterative scheme.

[3 marks]

(iv) Show that the method is *always* stable.

[2 marks]

**3.** (i) Derive the second order, central difference scheme for the second derivative of the function u(x) discretised on a regular lattice with spacing h *i.e.* 

$$\frac{d^2u}{dx^2} = \frac{1}{h^2} \left( u_{i-1} - 2 \, u_i + u_{i+1} \right) + O(h^2) \, .$$

[2 marks]

(ii) Show that for a two-dimensional function u(x, y), discretised on a two-dimensional lattice with regular spacing h in x and y the Laplacian operator  $\nabla^2 u$  can be evaluated using the *pictorial* operator

$$\nabla^2 u = \frac{1}{h^2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix} u_{i,j} + O(h^2) .$$

[2 marks]

(iii) Write down the *two-dimensional* Taylor expansion for the function at lattice points  $u_{i+1,j+1}$ ,  $u_{i+1,j-1}$ ,  $u_{i-1,j+1}$ , and  $u_{i-1,j-1}$ , truncated at terms of order  $h^2$ .

[4 marks]

(iv) Use this to show that an alternative pictorial operator for the Laplacian is

$$\frac{1}{2 h^2} \left[ \begin{array}{ccc} 1 & 0 & 1 \\ 0 & -4 & 0 \\ 1 & 0 & 1 \end{array} \right] u_{i,j}.$$

[2 marks]

4. The generalised, one-dimensional, damped, forced oscillator problem is given by

$$m\,\frac{\partial^2 x(t)}{\partial t^2} + \gamma\,\frac{\partial x(t)}{\partial t} + \lambda\,x(t) = f(t)\,,$$

where f(t) is the time-dependent forcing term and x(t) is the solution for the displacement of the oscillator.

We seek to obtain a discrete solution for x(t) by using Discrete Fourier Transforms (DFTs) defined as

$$f_n = \frac{1}{N} \sum_{k=-N/2}^{N/2} \tilde{f}_k e^{-i 2\pi k n/N},$$

and

$$\tilde{f}_k = \sum_{n=0}^{N-1} f_n e^{i2\pi kn/N},$$

with indices n and k denoting samples in the time and frequency domain respectively. The time domain sampling is regularly spaced in steps of size  $\Delta t$ .

(i) Show that using central difference schemes for both derivatives we can write a discrete approximation for the oscillator equation as

$$\left(\frac{m}{\Delta t^2} + \frac{\gamma}{2\Delta t}\right) x_{n+1} + \left(\lambda - \frac{2m}{\Delta t^2}\right) x_n + \left(\frac{m}{\Delta t^2} - \frac{\gamma}{2\Delta t}\right) x_{n-1} \approx f_n.$$

[3 marks]

(ii) Show that, in the frequency domain, the oscillator equation can then be written as

$$\left[\frac{2m}{\Delta t^2} \left(\cos \theta - 1\right) + \lambda - i \frac{\gamma}{\Delta t} \sin \theta\right] \tilde{x}_k = \tilde{t}_k,$$

where  $\theta \equiv 2\pi k/N$ .

[4 marks]

(iii) Describe briefly how you would use the result above to obtain a solution  $x_n$  given a forcing function  $f_n$ . [3 marks]