Candidate Number

THE UNIVERSITY OF SUSSEX

F3212

BSc, MPhys END OF YEAR TWO EXAMINATIONS, 2015

SCIENTIFIC COMPUTING

Friday, 9 January 2015 — 9.30 a.m. - 11.30 a.m.

DO NOT TURN OVER UNTIL INSTRUCTED TO BY THE CHIEF INVIGILATOR

Credit will be given for the best **TWO** *answers only.*
Total time allowed: **TWO** *hours.*

Each question carries 20 marks. The approximate allocation of marks is shown in brackets by the questions.

A list of **physical constants** *is provided.*
Calculators are permitted.

Notes: *You are allowed to use your notes, as well as the course slides and codes available on Study Direct, but you must not contact other people (by email, chat or any other means). Please always explain your choice of method and code to use. Use a program that we/you wrote during the course whenever possible, and submit all programs as part of the solutions, along with a 'master sheet' write-up which summarises what you did, how to use your codes and the results that you obtained, any plots, etc. The master sheet and all programs have to be submitted (ideally in a single zip-ed file) via the drop box on the course site on Study Direct (please ensure that it worked before leaving the exam room!). The best two of the three problems count for the marks.*

1. Consider the equation $x = 1 - e^{-cx}$, where c is a known parameter and x is unknown. This equation arises in a variety of situations, including the physics of contact processes, mathematical models of epidemics, and the theory of random graphs.

   (a) Write a program to solve this equation for x using the relaxation method for the case $c = 2$. Calculate your (non-zero) solution to an accuracy of at least 10^{-6}.

   (b) Modify your program to calculate the solution for values of c from 0 to 3 in steps of 0.01 and make a plot of x as a function of c. You should see a clear transition from a regime in which $x = 0$ to a regime of nonzero x. This is an example of a phase transition. In physics this transition is known as the *percolation transition*; in epidemiology it is the *epidemic threshold*.

2. Differential equations: A projectile is fired with an initial speed of 1000 m/s at an angle α from the horizontal. A good model for the path uses an air-resistance force proportional to the square of the speed. This leads to the following equations for the acceleration in the x and y directions:

$$\begin{aligned}\ddot{x} &= -c\dot{x}\sqrt{\dot{x}^2 + \dot{y}^2}\\ \ddot{y} &= -c\dot{y}\sqrt{\dot{x}^2 + \dot{y}^2} - g\end{aligned}$$

   where an overdot signifies a derivative with respect to time, $g = 9.81\,m/s^2$ and the constant c can be taken to be $c = 0.005\,m^{-1}$. The initial conditions are $x(0) = y(0) = 0$ and $(\dot{x}(0), \dot{y}(0)) = 1000(\cos\alpha, \sin\alpha)\ m/s$.

   (a) Convert the above system of equations to 4 first-order equations. [5]

   (b) Solve the system of equations over the time interval [0,30] (using a method of your choice, e.g. scipy.integrate.odepack) for each launch angle $\alpha =$ `10, 20` and `80` degrees (convert to radians!) and default tolerance. Plot the resulting trajectories (i.e. y(x)). If the ground is flat at $x = 0$, which of the three shots reaches furthest along x? [15]

3. Numerical integration: Debye's formula for the heat capacity C_V of a solid is $C_V = 9g(u)Nk$, where

$$g(u) = u^3 \int_0^{1/u} \frac{x^4 e^x}{(e^x - 1)^2} dx,$$

N is the number of particles in the solid, k is the Boltzmann constant, $u = T/\Theta_D$, T is the absolute temperature and Θ_D is the Debye temperature. Using a method of your choice and tolerance of 1.49×10^{-8} compute $g(u)$ for $u = 0.05$ to 1.0 in intervals of 0.05 and plot the results. [20]

End of Paper