University of Bath

DEPARTMENT OF PHYSICS

PH30031

Simulation Techniques

Friday, 19th January, 2018
09:30 to 11:30
2 hours

Answer ALL questions

Only calculators provided by the University may be used

PLEASE FILL IN THE DETAILS ON THE FRONT OF YOUR ANSWER BOOK/COVER AND SIGN THE SECTION ON THE RIGHT OF YOUR ANSWER BOOK/COVER, PEEL AWAY ADHESIVE STRIP AND SEAL.

TAKE CARE TO ENTER THE CORRECT CANDIDATE NUMBER AS DETAILED ON YOUR DESK LABEL.

DO NOT TURN OVER YOUR QUESTION PAPER UNTIL INSTRUCTED TO BY THE CHIEF INVIGILATOR

1. Much of mathematical science is built upon the paradigm of deriving a governing equation, then finding closed-form analytic solutions. Outline 3 types of problem where we need to go beyond this paradigm and use computational methods, giving an example that illustrates each. [6]

2. The amplitude x of free vibrations of a beam supported on an elastic foundation as a function of time t may be modelled by the equation

$$\frac{d^2x}{dt^2} + 1.49Kx^2\frac{d^2x}{dt^2} + 2Kx\left(\frac{dx}{dt}\right)^2 + \omega_o^2 x + sx^3 = 0,$$

where K is a damping parameter, s a stiffness parameter, and ω_o an angular frequency.

(a) Which term, if any, in this equation is likely to be fully empirical in origin? Which, if any, is likely to represent a non-linear contribution to the restoring force? Give a brief justification for your answers. [4]

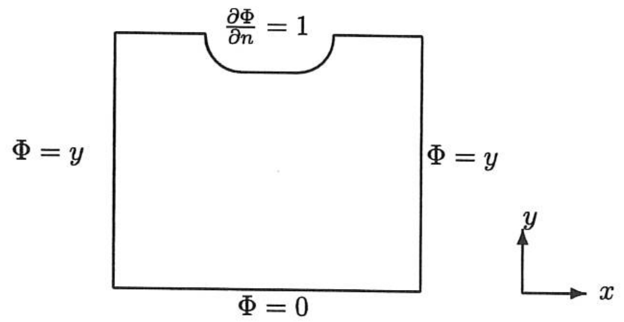
(b) De-dimensionalise the equation, choosing to keep as many terms as possible of order 1. What is the purpose of de-dimensionalising equations you wish to solve computationally? [8]

(c) Show that for very small amplitude oscillations the beam will undergo simple harmonic motion at angular frequency ω_o. Why is this a useful thing to know when solving the full equation computationally? [4]

3. This question is concerned with the computational solution of Laplace's equation

$$\nabla^2\Phi = 0$$

in two dimensions (x, y) in the region shown in the figure. Boundary conditions for the top, bottom, left and right sides of the region are indicated in the figure. $\frac{\partial\Phi}{\partial n}$ denotes the normal derivative of Φ.



(a) Starting from an appropriate Taylor Series, discretise Laplace's equation at a general point (in the interior of the region) on a square finite difference grid, defined by $x_{i+1} = x_i + h$; $y_{j+1} = y_j + h$. Ensure that your discretisation error is $O(h^2)$. [4]

(b) Choose a point close to the right hand side of the region to illustrate how Dirichlet boundary conditions are implemented in the finite difference method (FDM). [2]

(c) Why is the Neumann boundary condition along the top of the region difficult to deal with in the FDM? Briefly outline an approach (within the FDM) that might be used to deal with this Neumann condition. Explain why the finite element method (FEM) is much better at dealing with such boundary conditions. [6]

(d) Explain briefly how your finite difference discretisation will lead to a matrix equation. Show how the symmetry of this problem might be used to reduce the number of grid points needed to compute a solution of a given accuracy, and estimate the time saving involved. [5]

4. (a) What type of system tends to be studied using either the Monte Carlo or Molecular Dynamics methods? State two examples of such systems. [3]

(b) Why is the generation of random numbers so central to Monte Carlo methods, yet not to Molecular Dynamics methods? [2]

(c) Explain the reason for using Importance Sampling in Monte Carlo methods. Outline the key elements of how the Metropolis algorithm may be used to generate a sequence of deviates $\mathbf{\Gamma}_i$ drawn from a known probability density distribution $p(\mathbf{\Gamma})$. Explain why the sequence of deviates produced will contain sequential correlation, and what might be done in practical applications of the algorithm to overcome this. [10]

5. Outline the direct method of solving matrix problems of the form $\mathbf{Ax} = \mathbf{b}$ via $\mathbf{LU}$ decomposition. Illustrate the method by using it to solve the simple problem

$$\begin{pmatrix} 2 & 4 \\ 4 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 8 \\ 11 \end{pmatrix}.$$

You are given that

$$\begin{pmatrix} 2 & 4 \\ 4 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 2 & 4 \\ 0 & -5 \end{pmatrix}.$$

[6]

RJ

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FUNDAMENTAL CONSTANTS

Note: Numerical values have been rounded to four significant figures.

Quantity	Symbol	Value	Unit	Dimensions
Atomic mass unit	u	1.661×10^{-27}	kg	M
Avogadro constant	N_A	6.022×10^{23}	mol^{-1}	
Bohr magneton ($e\hbar/2m_e$)	μ_B	9.274×10^{-24}	JT^{-1}	$I\,L^2$
Bohr radius ($4\pi\hbar^2/\mu_o c^2 e^2 m_e$)	a_o	5.292×10^{-11}	m	L
Boltzmann constant	k	1.381×10^{-23}	$J\,K^{-1}$	$ML^2T^{-2}\theta^{-1}$
Charge of electron (magnitude)	e	1.602×10^{-19}	C	I T
Charge (magnitude)/rest mass ratio (electron)	e/m_e	1.759×10^{11}	$C\,kg^{-1}$	$I\,M^{-1}T$
Fine–structure constant ($\mu_o ce^2/2h$)	α	7.292×10^{-3}		
	$1/\alpha$	137.0		
Gravitational constant	G	6.672×10^{-11}	$Nm^2\,kg^{-2}$	$M^{-1}\,L^3\,T^{-2}$
Mass ratio, m_p/m_e	m_p/m_e	1836		
Molar gas constant	R	8.314	$J\,mol^{-1}K^{-1}$	$ML^2T^{-2}\theta^{-1}$
Molar volume (ideal gas, STP)	V_m	2.241×10^{-2}	m^3	L^3
Permeability of vacuum	μ_o	$4\pi \times 10^{-7}$	Hm^{-1}	$I^{-2}MLT^{-2}$
Permittivity of vacuum ($1/\mu_o c^2$)	ε_o	8.854×10^{-12}	Fm^{-1}	$I^2M^{-1}L^{-3}T^4$
	$4\pi\varepsilon_o$	1.113×10^{-10}	Fm^{-1}	$I^2M^{-1}L^{-3}T^4$
Planck constant	h	6.626×10^{-34}	Js	ML^2T^{-1}
	$\hbar$	1.055×10^{-34}	Js	ML^2T^{-1}
Rest mass of electron	m_e	9.110×10^{-31}	kg	M
Rest mass of proton	m_p	1.673×10^{-27}	kg	M
Speed of light in vacuum	c	2.998×10^8	ms^{-1}	LT^{-1}
Stefan-Boltzmann constant ($2\pi^5k^4/15h^3c^2$)	σ	5.670×10^{-8}	$Wm^{-2}K^{-4}$	$MT^{-3}\theta^{-4}$