This question paper consists
of 5 printed pages, each of
which is identified by the
Code Number COMP5930M01

School of Computing

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COMP5930M

Scientific Computation

Time allowed: 2 hours

Answer ALL THREE Questions.

This is a closed book examination.

This means that you are not allowed to bring any material into the examination.

Calculators which conform to the regulations of the University of Leeds are permitted but all working must be shown in order to gain full marks.

Turn over for question 1

Question 1

Given functions $\mathbf{F}(\mathbf{x})$ and $\mathbf{J}(\mathbf{x})$ that return, respectively, a system of nonlinear equations and the Jacobian matrix evaluated at point $\mathbf{x}$, a Newton algorithm can be defined as follows to approximate the point $\mathbf{x}^*$ such that $\mathbf{F}(\mathbf{x}^*) = 0$. The algorithm requires a starting point $\mathbf{x}_0$ and a convergence measure Tol.

Algorithm A

[$\mathbf{x}$,$\mathbf{f}$] = Newton($\mathbf{x}_0$, Tol)

A1. $\mathbf{x} = \mathbf{x}_0$, $\mathbf{f} = \mathbf{F}(\mathbf{x}_0)$

A2. While $|\mathbf{f}| > Tol$

(i). Compute $\mathbf{A} = \mathbf{J}(\mathbf{x})$

(ii). Solve $\mathbf{A}\delta = -\mathbf{f}$

(iii). Update $\mathbf{x} = \mathbf{x} + \delta$, $\mathbf{f} = \mathbf{F}(\mathbf{x})$

A3. End

a Describe the purpose of the following two modifications to Algorithm A. In each case state the effect this modification could have on the final computed solution $\mathbf{x}$ and on the performance of the overall algorithm.

i A maximum number of Newton iterations, $maxit$, is imposed.

[3 marks]

ii A scalar parameter λ, with $0 < \lambda \leq 1$, is introduced at step A2.(iii) such that the solution is updated as $\mathbf{x} = \mathbf{x} + \lambda\delta$.

[3 marks]

b Describe an algorithm for computing an appropriate value for the scalar parameter λ during the normal execution of the Newton algorithm. This description should include criteria for completion of this step in every case.

[6 marks]

c A *homotopy continuation* approach can be defined for the nonlinear system $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ in the form

$$\mathbf{G}(\alpha, \mathbf{x}) \;=\; \mathbf{F}(\mathbf{x}) + (\alpha - 1)\mathbf{F}(\mathbf{x}_0) \tag{1}$$

with scalar parameter $\alpha \in [0, 1]$.

A practical algorithm can be constructed from Equation (1) that uses M steps of size $\Delta\alpha = 1/M$ with

$$\mathbf{x}^k \;=\; \mathbf{x}^{k-1} - \Delta\alpha\, \mathbf{J}^{-1}(\mathbf{x}^{k-1})\mathbf{F}(\mathbf{x}^0) \tag{2}$$

where $k = 1, ..., M$ and $\mathbf{x}^0 = \mathbf{x}_0$.

i Explain the use of this algorithm as an extension to Algorithm A. Your answer should include the purpose of this algorithm and the benefit of this approach.

[3 marks]

ii Describe the steps required to implement the algorithm described by Equation (2). This should be written in a similar manner to Algorithm A. Estimate the computational cost of a single step of this algorithm compared to a step of the Newton Algorithm.

[3 marks]

iii What are the issues associated with using the algorithm described by Equation (2) with respect to the step size $\Delta\alpha$ and the final computed solution, $\mathbf{x}^M$? Hence explain why the algorithm should be combined with the Newton Algorithm in practice.

[2 marks]

[20 marks total]

Question 2

A function $u(x,t)$ satisfies the following nonlinear partial differential equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(u^2\right) = \epsilon \frac{\partial}{\partial x}\left(u^2 \frac{\partial u}{\partial x}\right), \tag{3}$$

for $x \in [0,1]$ with boundary conditions $u(0,t) = 0$, $u(1,t) = 0$, and $t > 0$ with initial conditions $u(x,0) = U_0(x)$. ϵ is a known, positive constant.

On a uniform grid of m nodes, with nodal spacing h, covering the domain $x \in [0,1]$, we can write a numerical approximation to the PDE (3) at a typical internal node i as,

$$\begin{aligned}\frac{u_i^{k+1} - u_i^k}{\Delta t} \quad = \quad & \frac{1}{h}\left(\frac{(u_{i+1}^{k+1})^2 + (u_i^{k+1})^2}{2}\left(-1 + \frac{\epsilon}{h}\left(u_{i+1}^{k+1} - u_i^{k+1}\right)\right)\right. \\ & \left. - \frac{(u_i^{k+1})^2 + (u_{i-1}^{k+1})^2}{2}\left(-1 + \frac{\epsilon}{h}\left(u_i^{k+1} - u_{i-1}^{k+1}\right)\right)\right) \end{aligned} \tag{4}$$

a Describe the compact finite difference method and the steps required to approximate the PDE (3) in the discrete form (4). [2 marks]

b State the size of the nonlinear system that would be solved, and the precise form of the solution vector $\mathbf{U}$ that would be required. [2 marks]

c Describe the algorithm required to advance the model in time. This should include:

- initialisation of the time stepping;
- a suitable initial state for Newton's method at each time step.

[3 marks]

d i Explain why the Jacobian for this nonlinear system has tridiagonal structure.
State the precise number of non-zero entries (nz) as a function of the number of equations in your system N.

[3 marks]

ii State which steps of the Newton algorithm can be made more efficient, in terms of memory and CPU time, for a problem with a tridiagonal Jacobian. In each case give a reason for your answer.

[4 marks]

e i Describe an efficient numerical approximation to the Jacobian matrix that could be made assuming the tridiagonal sparse structure.

[4 marks]

ii State one advantage and one disadvantage of an analytical form of the Jacobian in this case.

[2 marks]

[20 marks total]

Question 3

A two-dimensional nonlinear PDE for $u(x, y)$ is defined as

$$\frac{\partial}{\partial x}\left(u^2 \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(u^2 \frac{\partial u}{\partial y}\right) \;=\; 0 \tag{5}$$

for the spatial domain $(x, y) \in [0, 1] \times [0, 1]$. On the boundary of the domain, boundary conditions $u(x, y) = U_b(x, y)$ are known.

A uniform mesh of m nodes is used in each coordinate direction, with nodal spacing h.

Applying standard finite difference approximations in space a possible discretised form of this problem is given by Equation (6).

$$\begin{aligned}\frac{1}{4h^2}\Big(& (u_{i+1j} + u_{ij})^2 (u_{i+1j} - u_{ij}) - (u_{ij} + u_{i-1j})^2 (u_{ij} - u_{i-1j}) \\ & + (u_{ij+1} + u_{ij})^2 (u_{ij+1} - u_{ij}) - (u_{ij} + u_{ij-1})^2 (u_{ij} - u_{ij-1}) \Big) \;=\; 0\end{aligned} \tag{6}$$

where $u_{ij} \equiv u(x_i, y_j)$, $i, j = 2, ..., m - 1$.

a Describe the steps that are required to approximate the PDE (5) in the discrete form (6).

[5 marks]

b Deduce the sparse structure of the Jacobian matrix for this problem, stating a realistic bound on the number of non-zero entries in the matrix.

[3 marks]

c The Jacobian matrix is determined to be numerically symmetric and positive definite.

Describe an efficient iterative solution strategy for the linear equations system at each Newton iteration. [3 marks]

d If the discrete system (6) is written in the form $\mathbf{F}(\mathbf{U}) = \mathbf{0}$ describe a pseudo-timestepping solution algorithm for this problem.

State one advantage and one disadvantage of this approach. [6 marks]

e How would your answers to parts (b)-(d) change if the three-dimensional form of the PDE (5) was to be solved? [3 marks]

[20 marks total]