This question paper consists
of 4 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

A nonlinear system is defined by 2 equations in 2 variables x, y:

$$x^2 + 3\,xy = 4 \tag{1}$$
$$x + y^2 - 2\,xy = 2 \tag{2}$$

a Formulate the problem as a system of nonlinear equations $\mathbf{F}(\mathbf{U}) = \mathbf{0}$, stating the precise form for $\mathbf{U}$ and $\mathbf{F}(\mathbf{U})$.

Derive the analytical form of the Jacobian for this problem. [4 marks]

b Using a single step of Newton's Method compute an approximation to a root of this equation system starting from the point $(x, y) = (0.5, 0)$. [4 marks]

c Describe the purpose of the line-search algorithm as part of a solution algorithm for nonlinear systems. Explain the modifications to the basic Newton algorithm in this case. [4 marks]

d Describe a line-search algorithm that could be used with Newton's method. Include a description of the successful and unsuccessful termination of the algorithm. [4 marks]

e Compute one step of the Newton algorithm including line search starting from the point $(x, y) = (0.5, 0)$ as before. [4 marks]

[20 marks total]

Question 2

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

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

for $x \in [0,1]$ with boundary conditions $u(0,t) = 0$, $u(1,t) = 0$, and $t > 0$ with initial conditions $u(x,0) = U_0(x)$.

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,

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \frac{1}{h^4}\left((u_{i+1}^{k+1} - u_i^{k+1})^3 - (u_i^{k+1} - u_{i-1}^{k+1})^3\right) \tag{4}$$

a Define a nonlinear system, in the form $\mathbf{F}(\mathbf{U}) = \mathbf{0}$, that can be solved at each time step $[t^k, t^{k+1}]$. State the precise form of the equations $\mathbf{F}(\mathbf{U})$ and solution vector $\mathbf{U}$. [3 marks]

b 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]

c 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.

ii Describe how the solution algorithm for the nonlinear system can be made more efficient in terms of memory and CPU time for a problem with a tridiagonal Jacobian.

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

[10 marks]

d Explain how you would modify the numerical model to achieve second order accuracy in time.

What changes would this make to your numerical algorithm for solving the problem?

[4 marks]

[20 marks total]

Question 3

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

$$-\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+u^3 \;=\; 0 \tag{5}$$

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).

$$-\frac{1}{h^2}\left(u_{ij-1}+u_{i-1j}-4u_{ij}+u_{i+1j}+u_{ij+1}\right)+u_{ij}^3 \quad=\quad 0 \tag{6}$$

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).

[3 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.

Analytically derive the entries of the Jacobian matrix for a typical equation in this system.

[5 marks]

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

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

d A pseudo-continuation form of the problem is defined as

$$-\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+\alpha u^3 \;=\; 0, \tag{7}$$

with free parameter α, where $0\leq\alpha\leq 1$.

Explain how a continuation approach could be used, in this form, as part of a solution strategy for the original PDE (5).

State one advantage and one disadvantage of this approach. [5 marks]

e How would your answers to parts (b)-(d) change if the three-dimensional form of the PDE (5) was to be solved? [4 marks]

[20 marks total]