This question paper consists of 4 printed pages, each of which is identified by the Code Number COMP5930M01.

This is a closed book examination. No material is permitted.

School of Computing

January 2018

COMP5930M

Scientific Computation

Answer ALL questions

Time allowed: 2 hours

TURN OVER FOR QUESTIONS

Question 1

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

$$\begin{aligned} x^2 y &= 2 \quad (1) \\ x + y^2 &= 1 \quad (2) \end{aligned}$$

(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 $(x, y) = (1, 1)$. **[4 marks]**

(c) The standard Newton algorithm can be extended to include a Line Search algorithm.

(i) Describe the purpose of Line Search as part of the overall algorithm.

(ii) State the modification to the Newton algorithm in this case.

(iii) Describe a practical Line Search algorithm that could be used.

(iv) Include a description of the successful and unsuccessful termination of the Line Search algorithm.

[6 marks]

(d) Compute one step of the Newton algorithm including Line Search, starting from the point $(x, y) = (1, 1)$ as before. **[4 marks]**

(e) Explain why combining Newton's Method with the Bisection Method is preferred to Line Search in the case of scalar nonlinear equations. **[2 marks]**

[question 1 total: 20 marks]

Question 2

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

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

for $x \in [0,1]$ with boundary conditions $u(0,t) = 0$, $u(1,t) = 0$, and $t > 0$ with initial conditions $u(x,0) = U_0(x)$. $g(u)$ is a known, always positive, function of the solution u.

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,

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \frac{1}{h^2}\left(g(u_{i+\frac{1}{2}}^{k+1})(u_{i+1}^{k+1} - u_i^{k+1}) - g(u_{i-\frac{1}{2}}^{k+1})(u_i^{k+1} - u_{i-1}^{k+1})\right) + \left(u_i^{k+1}\right)^2 \tag{4}$$

(a) State two alternative, consistent forms for the discretisation of the factor $g(u_{i+\frac{1}{2}}^{k+1})$. **[2 marks]**

(b) State the size of the nonlinear system that would be solved in this case, 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.

(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.

[7 marks]

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

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

[6 marks]

[question 2 total: 20 marks]

Question 3

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

$$\frac{\partial}{\partial x}\left(u^4 \frac{\partial u}{\partial x}\right) + \frac{\partial^2 u}{\partial y^2} \;=\; 0 \tag{5}$$

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).

$$\frac{1}{16h^2}\Big((u_{i+1j} + u_{ij})^4 (u_{i+1j} - u_{ij}) - (u_{ij} + u_{i-1j})^4 (u_{ij} - u_{i-1j})\Big) + \frac{1}{h^2}(u_{ij+1} - 2u_{ij} + u_{ij-1}) \;=\; 0 \tag{6}$$

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

(a) 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.

[4 marks]

(b) The Jacobian matrix is determined to be numerically symmetric and positive definite.

Assuming the Jacobian can be computed, describe an efficient iterative solution strategy for the linear equations system at each Newton iteration. **[3 marks]**

(c) 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]**

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

(e) State two advantages and two disadvantages of iterative linear algebra, compared to direct linear algebra for these problems. **[4 marks]**

[question 3 total: 20 marks]

[grand total: 60 marks]