This question paper consists
of 9 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:

$$x^2 + 3\,xy = 4 \qquad (1)$$

$$x + y^2 - 2\,xy = 2 \qquad (2)$$

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]

Answer:

+——————

$\mathbf{U} = (u_1, u_2)^T = (x, y)^T$

[1 mark]

$F_1(\mathbf{U}) = u_1^2 + 3u_1u_2 - 4$
$F_2(\mathbf{U}) = u_1 + u_2^2 - 2u_1u_2 - 2$

[1 mark]

$$J = \begin{pmatrix} 2u_1 + 3u_2 & 3u_1 \\ 1 - 2u_2 & 2u_2 - 2u_1 \end{pmatrix}$$

[2 marks]

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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]

Answer:

+——————

$U = (0.5, 0)$

$F = (-3.75, -1.5)$, $|F| = 4.04$

[1 mark]

Compute $J = \begin{pmatrix} 1 & 1.5 \\ 1 & -1 \end{pmatrix}$

[1 mark]

Solve $J\delta = -F$ for $\delta = (2.4, 0.9)$

Update $U = (0.5, 0) + (2.4, 0.9) = (2.9, 0.9)$

[1 mark]

$F = (12.24, -3.5)$, $|F| = 12.73$

[1 mark]

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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]

Answer:

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Line search is used to try and prevent Newton's method from diverging [1 mark]

The update step $U = U + \delta$ is modified to a damped form [1 mark]

$U = U + \lambda\delta$, where scalar λ is chosen on the range $0 < \lambda \leq 1$ [1 mark]

A separate algorithm is required to compute λ with the goal of ensuring a reduction in $|F|$ on that step. [1 mark]

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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]

Answer:

+——————

A step-halving approach can be used.

The current solution U^k and function norm $|F^k|$ are stored

0. Set $\lambda = 1$, $tries = 0$
1. Evaluate $U^{k+1} = U^k + \lambda\delta$ and $|F^{k+1}| = F(U^{k+1})$ [1 mark]
2. If $|F^{k+1}| < |F^k|$ accept U^{k+1} and return success [1 mark]
3. Set $\lambda = \lambda/2$ and $tries = tries + 1$ [1 mark]
4. If $tries > maxTries$ return failure, else goto 1. [1 mark]

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

Answer:

+——————

From (a) $U^k = (0.5, 0)$, $|F^k| = 4.04$, $\delta = (2.4, 0.9)$

$\lambda = 1$, $U^{k+1} = (2.9, 0.9)$, $F^{k+1} = (12.24, -3.5)$, $|F^{k+1}| = 12.73$ [1 mark]

$|F^{k+1}| > |F^k|$ so set $\lambda = 1/2$ [1 mark]

$U^{k+1} = (1.7, 0.45)$, $F^{k+1} = (1.18, -1.62)$, $|F^{k+1}| = 2.02$ [1 mark]

$|F^{k+1}| < |F^k|$ so return success [1 mark]

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[20 marks total]

Question 2

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

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

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,

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

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]

Answer:
+————————

(a)

$\mathbf{F}(\mathbf{U})$ is the set of $m-2$ equations defined from (4) applied at grid points $i = 2, ..., m-1$

[1 mark]

At points $i = 2$ and $i = m-1$ boundary conditions are used to replace the values $u_1 = 0$ and $u_m = 0$.

[1 mark]

$\mathbf{U}$ is the set of $m-2$ unknown solution values u_i at the grid points $i = 2, ..., m-1$.

[1 mark]

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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]

Answer:
+————————

(b)

$t = 0$

Set initial solution U^0 from initial conditions $U_i^0 = U_0(x_i)$

[1 mark]

for k = 0 to maxSteps

$t = t + \Delta t$

Initial guess $U_0^{k+1} = U^k$ [1 mark]

$U^{k+1} =$ Newton(pdeModel, Jacobian, U_0^{k+1}, Tol) [1 mark]

end

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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]

Answer:

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(c)(i)

An equation F_i in this system only depends on 3 solution values: $F_i(u_{i-1}, u_i, u_{i+1}) = 0$

[1 mark]

Hence only Jacobian terms J_{ii-1},J_{ii},J_{ii+1} are non-zero and the system is tridiagonal

[1 mark]

There are $3N - 2$ non-zeros in the Jacobian

[1 mark]

(c)(ii)

The Jacobian matrix can be computed analytically, requiring only the non-zero entries to be computed with $\mathcal{O}(N)$ work [1 mark]

The Jacobian can be stored in a sparse matrix structure requiring $\mathcal{O}(N)$ storage [1 mark]

The Jacobian system can be solved with a tridiagonal solution algorithm (Thomas algorithm) with $\mathcal{O}(N)$ work

[1 mark]

(c)(iii)

A term of the Jacobian can be approximated numerically by the difference

$$J_{ij} = \frac{\partial F_i}{\partial u_j} = \frac{F_i(\mathbf{u} + \epsilon u_j) - F_i(\mathbf{u})}{\epsilon}$$

[1 mark]

Each column of the Jacobian has only 3 non-zero entries hence we can form 3 non-overlapping sets of Jacobian columns [1 mark]

The numerical approximation can be applied to each set as one function evaluation $F_(\mathbf{u}+\epsilon u_j)$ where u_j varies depending which Jacobian column we are computing. [1 mark]

The columns of the Jacobian can be extracted from the resulting vector in groups of 3. [1 mark]

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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]

Answer:

+——————

The first-order Backward Euler time approximation could be replaced with second-order BDF2

[1 mark]

In (4) the approximation $\frac{u_i^{k+1}-u_i^k}{\Delta t}$ is replaced by $\frac{3u_i^{k+1}-4u_i^k+u_i^{k-1}}{2\Delta t}$

[1 mark]

This requires storing one extra vector U^{k-1} [1 mark]

The nonlinear function and Jacobian are modified for the new approximation in time. [1 mark]

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[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).

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

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]

Answer:

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(a) At grid point ij use the following approximations

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2} &= \frac{1}{h^2}\left(u_{i-1j} - 2u_{ij} + u_{i+1j}\right)\\
\frac{\partial^2 u}{\partial y^2} &= \frac{1}{h^2}\left(u_{ij-1} - 2u_{ij} + u_{ij+1}\right)
\end{aligned}$$

[1 mark]

In the PDE

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

[1 mark]

Rearrange to the required form [1 mark]

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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]

Answer:

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(b)

An equation F_{ij} depends on 5 solution values $F_{ij}(u_{ij-1}, u_{i-1j}, u_{ij}, u_{i+1j}, u_{ij+1})$

There are $N = (m-2)^2$ equations and a realistic bound is $nz < 5N$ [1 mark]

If a row-by-row numbering system is adopted, the structure of the Jacobian is an $(n-2) \times (n-2)$ array of blocks each of size $(n-2) \times (n-2)$ [1 mark]

The blocks on the diagonal are tridiagonal, first off-diagonal blocks are diagonal, all other blocks are zero. [1 mark]

$J_{ij-1} = \frac{-1}{h^2}$, $J_{i-1j} = \frac{-1}{h^2}$, $J_{ij+1} = \frac{-1}{h^2}$, $J_{i+1j} = \frac{-1}{h^2}$ [1 mark]

$J_{ii} = \frac{4}{h^2} + 3u_{ij}^2$ [1 mark]

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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]

Answer:

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(c)

The Conjugate Gradient method would be the most appropriate choice [1 mark]

Preconditioning should be used to increase efficiency [1 mark]

For this system an Incomplete Choleski decomposition could be used [1 mark]

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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]

Answer:

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(d) The continuation approach can be used to set up a series of nonlinear problems for which we have more precise initial data [1 mark]

Define a series of steps from $\alpha = 0$ (linear Laplace equation) to $\alpha = 1$ (the target nonlinear system) [1 mark]

The $\alpha = 0$ system can be solved directly and each subsequent step uses the previous computed solution as initial data [1 mark]

Advantage: Removes problems associated with the initial state for Newton's method [1 mark]

Disadvantage: The initial step from $\alpha = 0$ (linear Laplace equation) to any non-zero α may be problematic. [1 mark]

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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]

Answer:

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(e)

The sparsity pattern would change. The overall structure would expand to reflect the 3D finite difference grid. [1 mark]

The number of non-zeros is bounded by $nz < 7N$ [1 mark]

The matrix would still be SPD and preconditioned CG in the form described in (c) could be used. [1 mark]

The continuation approach (d) would still be valid and work in the same way [1 mark]

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[20 marks total]