DEGREE OF MASTER OF SCIENCE

MATHEMATICAL MODELLING AND SCIENTIFIC COMPUTING

B1 Numerical Linear Algebra and Numerical Solution of Differential Equations

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HILARY TERM 2016

FRIDAY, 15 JANUARY 2016, 9.30am to 11.30am

Candidates should submit answers to a maximum of four questions that include an answer to at least one question in each section.

Please start the answer to each question on a new page.
All questions will carry equal marks.

Do not turn this page until you are told that you may do so

Section A: Numerical Solution of Differential Equations

1. The function $u(t)$, $t \geqslant 0$, with $u(0) = u_0$, is determined for $t > 0$ by

$$u' = f(t, u),$$

where f is a uniformly continuous function of the second argument satisfying a Lipshitz condition

$$|f(t, u_1) - f(t, u_2)| \leqslant L|u_1 - u_1|, \quad \forall u_1, u_2 \in \mathbb{R} \text{ and } t > 0.$$

A discrete solution is calculated at times $t_n = n\Delta t$, $n = 0, 1, 2, \ldots$, where $\Delta t > 0$ is a fixed time step. Let $u_n = u(t_n)$ and $f_n = f(t_n, u_n)$. An approximate solution for u at these times, denoted U_n, is determined for $n = 0, 1, 2, \ldots$, by Ralston's method:

$$\begin{aligned} k_1 &= f(t_n, U_n), \\ k_2 &= f(t_n + \frac{2}{3}\Delta t, U_n + \frac{2}{3}\Delta t k_1), \\ U_{n+1} &= U_n + \frac{1}{4}\Delta t(k_1 + 3k_2). \end{aligned}$$

(a) [10 marks] Show that the scheme is consistent and that the truncation error is second order in Δt.

(b) [9 marks] Prove that the error, $e_n = u_n - U_n$, tends to zero as $\Delta t \to 0$.

(c) [6 marks] Determine an estimate for the maximum error at $t = 1$ using uniform time steps $\Delta t \leqslant 1$, when

$$f(t, u) = \tan^{-1} u.$$

2. The function $u(t)$, $t \geqslant 0$ with $u(0) = u_0$, is determined for $t > 0$ by

$$u' = f(u),$$

where f is a uniformly differentiable function of u.

A linear multistep method for numerical approximation of this equation at the points $t_n = n\Delta t$, $n = 0, 1, 2, \ldots$, with $\Delta t > 0$ is defined by

$$\begin{aligned} U_0 &= u_0, \\ U_1 &= U_0 + \Delta t f(U_0), \\ U_{n+1} &= U_n + \frac{\Delta t}{12}(5F_{n+1} + 8F_n - F_{n-1}), \quad n = 1, 2, \ldots, \end{aligned}$$

where $F_n = f(U_n)$, $n = 0, 1, 2, \ldots$. Denote $u_n = u(t_n)$ and $f_n = f(u_n)$.

(a) [3 marks] Show that this method is zero stable and explain the significance of this condition.

(b) [6 marks] Define a truncation error by

$$T_n = \frac{u_{n+1} - u_n}{\Delta t} - \frac{1}{12}(5f_{n+1} + 8f_n - f_{n-1}).$$

Show that this method is third order in Δt as $\Delta t \to 0$.

(c) [10 marks] Using the function $f(u) = \lambda u$, and a characteristic polynomial, denoted $\pi(z; \overline{\Delta t})$, which you should define, describe what is meant by an interval of absolute stability. By considering values of $\overline{\Delta t} = \lambda \Delta t$ near $\overline{\Delta t} = 0$ and $\overline{\Delta t} = -6$, or values of $\frac{\mathrm{d}z}{\mathrm{d}\overline{\Delta t}}$, where z is a root of the characteristic polynomial, show that this method cannot be absolutely stable when $\overline{\Delta t}$ is small and positive or $\overline{\Delta t}$ is a little less than -6.

(d) [6 marks] The implicit method is replaced by a semi-implicit method:

$$\begin{aligned} \hat{U}_{n+1} &= U_n + \Delta t f(U_n), \\ U_{n+1} &= U_n + \frac{\Delta t}{12}(5f(\hat{U}_{n+1}) + 8F_n - F_{n-1}). \end{aligned}$$

Explain with reasons whether the interval of absolute stability has increased or decreased in extent compared to that for the fully implicit scheme.

3. The function $u(x,t)$, defined for $0 \leqslant x \leqslant 1$ and $t \geqslant 0$, satisfies

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},$$

with intial data $u(x,0) = u_0(x)$ and boundary data $u(0,t) = u(1,t) = 0$.

For some integer $M > 0$, $h = 1/M$, the partial differential equation is discretised on a uniform mesh $x_r = rh$, $r = 0,1,2,\cdots,M$ and $t_n = n\Delta t$, $n = 0,1,2,\cdots$. Denote U_r^n as an approximation for $u_r^n = u(x_r,t_n)$ and

$$||U^n||_{l_\infty} = \max_{r\in[1,\dots,M-1]} |U_r^n|, \qquad ||U^n||_{l_2} = \left(\sum_{r=1}^{M-1} (U_r^n)^2\right)^{1/2}.$$

Let $\mu = \Delta t/h^2$.

(a) [8 marks] For $0 \leqslant \theta \leqslant 1$, $r = 1,\dots,M-1$, the equation is discretised by a θ-method:

$$U_r^{n+1} = U_r^n + \theta\mu(U_{r+1}^{n+1} - 2U_r^{n+1} + U_{r-1}^{n+1}) + (1-\theta)\mu(U_{r+1}^n - 2U_r^n + U_{r-1}^n).$$

Use a maximum principle, which you should state but not prove, to show that provided $2\mu(1-\theta) \leqslant 1$, then

$$||U^{n+1}||_{l_\infty} \leqslant ||U^0||_{l_\infty},\ n = 1,2,\dots.$$

(b) [8 marks] The method in (a) is replaced by a predictor-corrector method, for $r = 1,\dots,M-1$,

$$\hat{U}_r^{n+1} = U_r^n + \mu(U_{r+1}^n - 2U_r^n + U_{r-1}^n),$$
$$U_r^{n+1} = U_r^n + \mu(\hat{U}_{r+1}^{n+1} - 2\hat{U}_r^{n+1} + \hat{U}_{r-1}^{n+1}).$$

Show that provided $\mu \leqslant 1/4$,

$$||U^{n+1}||_{l_\infty} \leqslant ||U^0||_{l_\infty},\ n = 1,2,\dots.$$

(c) [9 marks] A third discretisation is given for $r = 1,\dots,M-1$, by

$$U_{r+1}^{n+1} + 4U_r^{n+1} + U_{r-1}^{n+1} = U_{r+1}^n + 4U_r^n + U_{r-1}^n + 6\mu(U_{r+1}^n - 2U_r^n + U_{r-1}^n).$$

Formulate this discrete representation as a matrix problem. Using the vectors $\mathbf{z}^p = (z_r^p)$ with $z_r^p = \sin pr\pi h$, $p, r = 1,\dots M-1$, or otherwise, show that for this method

$$||U^n||_{l_2} \leqslant ||U^0||_{l_2},\ n = 1,2,\dots,$$

provided $\mu \leqslant 1/3$.

4. The functions $u(x,t)$, $v(x,t)$, defined for $x \in \mathbb{R}$ and $t \geqslant 0$, satisfy, for real α, β and $t > 0$, the evolutionary equations

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \alpha^2 u - \beta^2 v, \tag{1}$$

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2}, \tag{2}$$

with initial data $u(x,0) = u_0(x) \geqslant 0$, $v(x,0) = v_0(x) \geqslant 0$ where $|u_0| \to 0$, $|v_0| \to 0$ as $|x| \to \infty$. The continuous system is discretised on a uniform mesh $x_r = rh$, $r = 0, \pm 1, \pm 2, \cdots$, and $t_n = n\Delta t$, $n = 1, 2, \cdots$ with $h > 0$ and $\Delta t > 0$ such that U_r^n, V_r^n are approximations for $u_r^n = u(x_r, t_n)$ and $v_r^n = v(x_r, t_n)$ respectively.

Define the l_2-norm of data $\{U_r\}$ by $||U^n||_{l_2} = \left(h \sum_{r=-\infty}^{\infty} |U_r|^2\right)^{1/2}$, and semi-discrete Fourier transform, $\hat{U}(k)$ by $\hat{U}(k) = h \sum_{r=-\infty}^{\infty} \mathrm{e}^{-ikrh} U_r$.

(a) [7 marks] The equation (2) is discretised by

$$\frac{V_r^{n+1} - V_r^n}{\Delta t} = \frac{1}{h^2}(V_{r+1}^n - 2V_r^n + V_{r-1}^n).$$

Define practical stability and von Neumann stability for a discrete method in terms of the l_2-norm and show that this discretisation is practically stable provided $\Delta t < \frac{1}{2}h^2$.

(b) [7 marks] Equation (1) is discretised by

$$\frac{U_r^{n+1} - U_r^n}{\Delta t} = \frac{1}{h^2}(U_{r+1}^n - 2U_r^n + U_{r-1}^n) - \alpha^2 U_r^n - \beta^2 V_r^n.$$

Define

$$\mathbf{W}^n = \begin{pmatrix} \hat{U}^n(k) \\ \hat{V}^n(k) \end{pmatrix}$$

Determine the matrix A such that $\mathbf{W}^{n+1} = A\mathbf{W}^n$.

(c) [6 marks] Deduce that the solutions of the combined scheme will reduce to zero as $n \to \infty$ provided

$$\Delta t \leqslant \frac{2h^2}{4 + \alpha^2 h^2}.$$

(d) [5 marks] If the equation (2) was replaced by

$$\frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2},$$

with real $D > 0$, determine the time step restriction that would be required to guarantee that the numerical approximations for u and v both decay to zero for a large number of time steps.

You may use without proof Parseval's Identity $||U^n||_{l_2} = \frac{1}{\sqrt{2\pi}}||\hat{U}^n||_{L_2}$.

Section B: Numerical Linear Algebra

5. (a) [8 marks] State the Jacobi algorithm for computing an approximate solution to the square system of equations $Ax = b$. State and prove conditions such that the Jacobi algorithm converges to $A^{-1}b$. Give an example of a matrix for which the prior conditions given are sharp, in that if they are not satisfied then the Jacobi algorithm need not converge to $A^{-1}b$.

   (b) [8 marks] Consider the QR factorisation of $A \in \mathbb{R}^{m\times n}$ where A has the properties that: $m \geqslant n$, the columns of A are linearly independent, and $A_{ij} = 0$ unless $j = i$ or $j = i - 1$. Which entries of Q and R should be exactly zero?

   (c) [9 marks] State an efficient algorithm using Givens rotations for computing the matrix R in the QR factorisation of $A \in \mathbb{R}^{m\times n}$ where A has the properties in part (b) of this question. What is, to leading order, the number of floating point operations used in the stated algorithm? (Consider the evaluation of a trigonometric function to be a single floating point operation and assigning a value to be without cost.)

6. (a) [9 marks] Design and state an algorithm to approximately solve the square linear system of equations $Ax = b$, for A symmetric ($A = A^*$), by updating the estimate $x^{(k)}$ along the direction $Ap^{(k)}$ where $p^{(k)} = b - Ax^{(k)} - \beta_{k-1}p^{(k-1)}$, β_{k-1} is selected so that $Ap^{(k)}$ and $Ap^{(k-1)}$ are orthogonal, and $p^{(0)} = b - Ax^{(0)}$ where $x^{(0)}$ is the initial approximate solution.

(b) [8 marks] State and describe the GMRES algorithm; specifically discuss: the subspace minimised over, the class of matrices for which the method is designed, and any stability issues.

(c) [8 marks] The algorithm GMRES requires solving the least squares subproblem

$$\min_y \left\| \|b\|_2 e_1 - \tilde{H}_k y \right\|_2$$

at iteration k where: e_1 is the vector of all zeros except the first entry which is equal to one, b is the vector in the equation $Ax = b$ being approximately solved, and $\tilde{H}_k \in \mathbb{R}^{k+1,k}$ is in upper-Hessenberg form, in that $\tilde{H}_k(i,j) = 0$ for $i > j + 1$. Assume a QR factorisation of $\tilde{H}_k$ has already been computed, $\tilde{H}_k = \tilde{Q}_k \tilde{R}_k$ where $Q_k \in \mathbb{R}^{k+1,k+1}$ is unitary and $\tilde{R}_k = \begin{pmatrix} R_k \\ 0 \end{pmatrix}$ where R_k is upper triangular. State an efficient algorithm for computing the QR factorisation of $\tilde{H}_{k+1} = \begin{pmatrix} \tilde{H}_k & h_{k+1} \\ 0 & h_{k+2,k+1} \end{pmatrix}$ and calculate, to leading order, the number of floating point operations required.