PhD Comprehensive Exam – Scientific Computation (June 2017)

Attempt ANY 5 of the following 6 problems. CROSS OUT any problem that you do not want to be graded. Please write only on one side of the page and start each problem on a new page.

1. (a) The standard second order finite difference approximation to the ODE $u''(x) = f(x)$ can schematically be written as $\frac{1}{h^2}[1 \quad -2 \quad 1]u = [1]f + O(h^2)$. Verify that the following approximation is indeed fourth order accurate

$$\frac{1}{h^2}[1 \quad -2 \quad 1]u = [1 \quad 10 \quad 1]f/12 + O(h^4)\,.$$

(b) The fourth order accurate finite difference scheme in 2-D for approximating the Poisson equation $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y)$ is given by

$$\frac{1}{6h^2}\begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix} u = \begin{bmatrix} & 1 & \\ 1 & 8 & 1 \\ & 1 & \end{bmatrix} f + O(h^4)\,.$$

Sketch the structure and give the entries of the linear system that is obtained when using the scheme given above to solve a Poisson equation with Dirichlet boundary conditions on the square domain $[0,1] \times [0,1]$.

(c) When $f(x,y) \equiv 0$ (i.e. Laplace's equation) in part (b), the accuracy of the above scheme (remarkably) jumps to $O(h^6)$ from $O(h^4)$. Without working through the details, outline an approach for verifying this increased order of accuracy.

2. Consider the heat equation $\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2}$ where a is a constant.

(a) Give a formula for each of the following finite difference approximations:

(i) Forward Euler: Centered differences in space, forward difference in time.

(ii) Backward Euler: Centered differences in space, backward difference in time.

(iii) Leapfrog: Centered difference in space and centered difference in time.

(b) What is the order of accuracy of each method in part (a)?

(c) Use a von Neumann analysis (or any appropriate analysis, such as Lax-Richtmyer) to determine the stability of each method in part (a).

3. Consider the ODE $u'(t) = f(u(t))$ solved by the explicit Runge Kutta method

$$U^* = U^n + 1/2kf(U^n)\,, \qquad U^{n+1} = U^n + kf(U^*)\,.$$

(a) Determine the order of accuracy of this method.

(b) Determine the absolute stability region. Is it A-stable? Is it L-stable?

(c) Use this method to solve the initial value problem $u'(t) = 2u(t) + 1$, $u(1) = 0$.

4. Let $x_1, x_2, \dots, x_N$ be N *distinct* real numbers. Consider the Lagrange interpolation basis $\{\ell_j(x)\}_{j=1}^N$, where each

$$\ell_j(x) = \prod_{n=1, n\neq j}^{N} \frac{x - x_n}{x_j - x_n}$$

is a polynomial of degree $N-1$ satisfying $\ell_j(x_k) = 0$ if $j \neq k$ and $\ell_j(x_j) = 1,\ j,k = 1,2,\dots N$. Let $u(x)$ be a polynomial of degree at most $N-1$.

(a) Show that the coefficients $\hat{u}_j$ in the expansion $u(x) = \sum_{j=1}^N \hat{u}_j \ell_j(x)$ are uniquely defined. Write formulas for these coefficients, in terms of the polynomial $u(x)$ and the nodes $x_1, \dots, x_N$.

(b) Let $\hat{u} = (\hat{u}_1, \dots, \hat{u}_N)^T$ and $\hat{v} = (\hat{v}_1, \dots, \hat{v}_N)^T$ be vectors such that $u(x) = \sum_{j=1}^N \hat{u}_j \ell_j(x)$ and its derivative $u'(x) = \sum_{j=1}^N \hat{v}_j \ell_j(x)$. Consider the $N \times N$ matrix D defined componentwise by $D_{jk} = {\ell_k}'(x_j)$. Show that $\hat{v} = D\hat{u}$.

(c) Let $\hat{w} = (\hat{w}_1, \dots, \hat{w}_N)^T$ be defined by $u''(x) = \sum_{j=1}^N \hat{w}_j \ell_j(x)$, where $u''(x)$ is the second derivative of $u(x)$. Show that $\hat{w} = D^2\hat{u}$ where the vector $\hat{u}$ is defined in part (b).

5. Let $|X|$ denote the usual Euclidean norm of the vector $X \in \mathbb{R}^N$, and for real, $N \times N$ matrices B define the norm

$$\|B\| = \sup_{|X|=1} |BX|\,.$$

Suppose A and C_0 are $N \times N$ real-valued matrices, satisfying $AC_0 = I - R_0$, where $\|R_0\| < 1$.

(a) Show that A is invertible, with $A^{-1} = C_0 \sum_{n=0}^{\infty} R_0^n$.

(b) Starting with C_0 and R_0, define sequences of matrices $\{C_m\}$ and $\{R_m\}$ by

$$C_{m+1} = C_m(I + R_m), \quad R_{m+1} = I - AC_{m+1}\,.$$

Show that $R_{m+1} = R_m^2$.

(c) Relate $A^{-1} - C_m$ to R_m and conclude that the sequence C_m converges to A^{-1}.

6. Let $f : (a,b) \to \mathbb{R}$ be *five* times differentiable on (a,b) with bounded fifth derivative, i.e. there exists a positive number $M > 0$ such that $|f^{(5)}(x)| \le M$ for all x in (a,b).

(a) Let $x_0 \in (a,b)$. Using Taylor's theorem, derive a fourth order accurate finite difference approximation $f_1(x_0,h)$ of $f'(x_0)$ that uses the values $f(x_0), f(x_0 \pm h)$ and $f(x_0 \pm 2h)$, where $h > 0$ is a number such that $x_0 \pm 2h \in (a,b)$. Prove that your approximation $f_1(x_0,h)$ yields the absolute error $O(h^4)$.

(b) Suppose that there exists $\varepsilon > 0$ such that for every $x \in (a,b)$, the computational error $|f(x) - \overline{f(x)}| < \varepsilon$, where $\overline{f(x)}$ is the computer representation of $f(x)$. Derive an estimate for the computational error $|f'(x_0) - \overline{f_1(x_0,h)}|$ by an expression $e(M,\varepsilon,h)$ that involves M, ε and h. Given that M and ε are fixed, for what value of h is this expression $e(M,\varepsilon,h)$ minimal?

(c) Let $f(x) = \sin x$ and $x_0 = 1.2$. Write a formula for the computational error in the approximation $f'(x_0) \approx f_1(x_0,h)$. What is the dominant term of the absolute error in the approximation $f'(x_0) \approx f_1(x_0,h)$?