**PhD Comprehensive Exam – Scientific Computation (June 2023)**

**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.** Consider the wave equation initial boundary value problem

$$u_{tt} = c^2 u_{xx}\,, \quad 0 < x < L, \quad u(x,0) = f(x)\,, \quad u_t(x,0) = g(x)$$

where $c$ is the wave speed. Boundary conditions are considered below.

Introduce a uniform discretization $x_j = jh, j = 0, 1, \ldots, m+1$ with grid spacing $h = L/(m+1)$. Time is discretized by $t_n = nk$ with time step $k > 0$. Consider the leapfrog scheme

$$\frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{k^2} = c^2 \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{h^2}\,,$$

where $U_j^n$ is the approximation of the solution $u(x_j, t_n)$.

(a) Show that this approximation is second-order accurate in space and time.

(b) Write down the time stepping equation. That is, rewrite the discrete system in the form $U_j^{n+1} = F(U_{j-1}^n, U_j^n, U_{j+1}^n, U_j^{n-1})$.

(c) Implement the Dirichlet boundary conditions: $u(0,t) = u_a, \quad u(L,t) = u_b$ where $u_a$ and $u_b$ are constant. Write down the time stepping equation at $x_1$ and $x_m$.

(d) Implement the Neumann boundary conditions: $u_x(0,t) = u'_a, \quad u_x(L,t) = u'_b$ where $u'_a$ and $u'_b$ are constant. Write down the time stepping equation at $x_0$ and $x_{m+1}$. Be sure to maintain the overall accuracy of the method.

(e) Implement the periodic boundary conditions: $u(L) = u(0), \quad u_x(L) = u_x(0)$. Write down the time stepping equation at $x_1$ and $x_m$.

**2.** Consider the generic one-step integration scheme

$$y_{n+1} = y_n + h\left[af(t_n, y_n) + bf(t_{n+1}, y_{n+1})\right]\,, \qquad a, b \in \mathbb{R}$$

to solve the initial value problem $y' = f(t,y), \quad y_0 = y(0)$.

(a) What is the optimal choice of $a$ and $b$ to obtain the most accurate approximation? What is the order of accuracy?

(b) Is this method zero stable?

(c) Give a set of conditions so that this method converges as $h \to 0$.

(d) Find the absolute stability of this problem when $a \neq b$ and when $a = b$. Consider both $\lambda \in \mathbb{C}$ and $\lambda \in \mathbb{R}$.

**3.** Consider the one-dimensional advection equation

$$u_t + a u_x = 0\,, \qquad u(x,0) = u_0(x)$$

where $a \neq 0, x \in \mathbb{R}$ and $t \geq 0$. Take the equally spaced spatial discretization $x_j = j\Delta x,\ j \in \mathbb{Z}$ and temporal discretization $t_n = n\Delta t$ where $n = 0, 1, \ldots$. Denote $U_j^n \approx u(x_j, t_n)$. Apply the Lax-Friedrichs finite-difference approximation

$$\frac{U_j^{n+1} - \frac{1}{2}\left(U_{j+1}^n + U_{j-1}^n\right)}{\Delta t} + a\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} = 0\,.$$

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

(b) Apply the von Neumann stability analysis to this scheme.

(c) State a theorem and conditions which guarantee convergence.

(d) Is this scheme convergent?

**4.** Consider the $n \times n$ linear system $A\mathbf{x} = \mathbf{f}$ where $A$ is invertible. Expressing $A = M - N$ for an invertible matrix $M$, the system becomes $M\mathbf{x} = N\mathbf{x} + \mathbf{f}$ which is equivalent to the fixed point problem: $\mathbf{x} = G\mathbf{x} + \mathbf{h}$ with $G = M^{-1}N$ and $\mathbf{h} = M^{-1}\mathbf{f}$. Solving the system can thus be achieved by iteration: $\mathbf{x}^{n+1} = G\mathbf{x}^n + \mathbf{h}$. The method is guaranteed to converge to $\mathbf{x}^* = A^{-1}\mathbf{f}$ if $\|G\| < 1$ for some matrix norm e.g., the spectral norm $\|G\| = \rho(G) = \max\{|\lambda|, \lambda \text{ is an eigenvalue of } G\}$ if $G$ is symmetric matrix, and $\|G\| = \rho\big((G^T G)^{1/2}\big)$ if $G$ is not symmetric.

In what follows $A = D - L - U$ where $D$ denotes the diagonal part of $A$ while $-U$ and $-L$ denote the strictly upper and lower triangular parts of $A$, respectively. Note that

- Forward Gauss-Seidel method corresponds to the choice $M = D - L, N = U$. Hence the iteration matrix is $G_f = (D - L)^{-1}U$.
- Backward Gauss-Seidel method corresponds to $M = D - U, N = L$. Hence the iteration matrix is $G_b = (D - U)^{-1}L$.
- Symmetric Gauss-Seidel method corresponds to a forward Gauss-Seidel iteration followed by a backward Gauss-Seidel iteration. Hence the iteration matrix is

$$G_s = G_b G_f = (D - U)^{-1}L(D - L)^{-1}U\,.$$

Define $B = (D - U)^{-1}D(D - L)^{-1}$.

(a) Verify that $G_s = I - BA$. (Hence the symmetric Gauss-Siedel method is the same iteration method as that of $BA\mathbf{x} = B\mathbf{f}$: $\mathbf{x}^{n+1} = (I - BA)\mathbf{x}^n + B\mathbf{f}$).

(b) Show that if $A$ is symmetric: $A = A^T$ (equivalently $U = L^T$) then $B$ is also symmetric. Does this imply $G_s$ is symmetric matrix?

(c) Consider the Poisson equation $-u''(x) = f(x)$ on $(0, 1)$ with Dirichlet boundary conditions: $u(0) = u(1) = 0$. Use centered differences to discretize the boundary value problem on $[0, 1]$ with $n = 2$ interior, equi-distant nodes. Derive a linear system $A\mathbf{u} = \mathbf{f}$ where $\mathbf{u} = [u_1, u_2]^T$ are the approximate values of $u(x)$ at the interior nodes, $A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$, and a suitable $\mathbf{f}$. Compute $G_s$ in this case and show that $\|G_s\| < 1$ (for a matrix norm of your choosing). Hence the symmetric Gauss-Seidel method converges.

**5.** In polar coordinates Poisson equation on unit disk $\Omega = \{(r,\theta)\,\big|\,0 \le r \le 1, 0 \le \theta < 2\pi\}$ reads as

$$\Delta u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = f(r,\theta), \quad 0 < r < 1\,, \quad u(r=1,\theta) = 0\,.$$

In this problem, we assume $f = f(r)$ is $\theta$-independent. By uniqueness, the solution is also $\theta$-independent, hence radially symmetric: $u = u(r)$.

(a) Derive the following equation: $\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = rf(r), \quad 0 < r < 1$. Then write down an explicit boundary value problem on the interval $[-1,1]$. (Hint: Extend $f(r)$ to $-1 < r < 1$, by even extension $f(-r) = f(r)$).

(b) Discretize the boundary value problem using the collocation method: use Chebyshev nodes $r_j = \cos(j\pi/N)$, $j = 0,\ldots N$ on the interval $[-1,1]$ and $(N+1)\times(N+1)$ Chebyshev differentiation matrix $D_N$ satisfying $p'(r_k) = \sum_j (D_N)_{kj}p(r_j)$, $p(r)$ being the interpolating polynomial for $(r_j,u_j)$ where $u_j$ approximates $u(r_j)$. Express your answer as a linear system: $A\mathbf{U} = \mathbf{F}$, $\mathbf{U}$ being the vector of 'unknowns' $u_j$. Make sure to correctly impose the boundary conditions.

(c) Show that $p(r)$, the interpolating polynomial obtained in part (b), is an even function, i.e., $p(-r) = p(r)$, and conclude that $p'(0) = 0$. Explain why this is consistent with the radially symmetric property of the exact solution $u$.

**6.** This problem deals with the Radial Basis Function (RBF) method applied to solving the linear Schrodinger equation for the complex function $q(x,t)$

$$iq_t + q_{xx} + V(x)\,q = 0\,, \qquad q(x,0) = q_0(x)$$

where $x \in [0,L]$, $t \ge 0$, and $V = V(x)$ is a real valued (potential) function.

(a) Consider first $V(x) = 0$. Choosing an appropriate radial function $\phi = \phi(r)$, $r > 0$ and discretization nodes $x_j$, find the approximate solution of the form

$$q(x,t) = \sum_j c_j(t)\phi(|x - x_j|)$$

Comment on the invertibility of the matrices involved.

(b) Redo part (a) for a general potential function $V(x)$.

(c) The nonlinear Schrodinger equation is

$$iq_t + q_{xx} + |q|^2 q = 0, \quad q(x,0) = q_0(x),$$

where $V(x)$ is replaced by $|q(x,t)|^2$. Using the explicit Euler time discretization, describe the algorithm by which one can solve this equation numerically using the RBF-PS (pseudo-spectral) method.