PhD Comprehensive Exam – Scientific Computation (August 2025)

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 approximating the solution of the IVP $u'(t) = f(u(t))\,,\ u(0) = u_0$ by the predictor-corrector method

$$\widehat{U}^{n+1} = U^n + kf(U^n)\,, \qquad U^{n+1} = U^n + \frac{k}{2}\left[f(U^n) + f(\widehat{U}^{n+1})\right]\,.$$

Here the grid is $t_n = nk$ with time step $k > 0$ and $U^n \approx u(t_n)$.

(a) Is the method explicit or implicit? What initial data is needed to advance the time step?

(b) Show the method is consistent. What is the order of accuracy?

(c) Find the region of absolute stability. What is the interval of absolute stability along the real axis? Does the region of absolute stability include a subset of the imaginary axis? Is this method zero stable?

2. Consider the linear system $A\mathbf{x} = \mathbf{f}$ given explicitly as

$$2x_1 - x_2 = 1, -x_1 + 2x_2 - x_3 = 0, -x_2 + 2x_3 = 1,$$

with exact solution $\mathbf{x} = (1, 1, 1)^T$.

(a) Write down the Jacobi iterative method. Using $\mathbf{x}^{(0)} = \mathbf{0}$ as an initial guess, take one step. Compute the errors $\|\mathbf{e}^{(0)}\|_2, \|\mathbf{e}^{(1)}\|_2$ where $\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}$.

(b) Repeat part (a) for the Gauss-Seidel method. Which method gives a smaller errors? Based on known convergence results, does this make sense?

(c) Prove that the Jacobi method converges. Derive an error equation whose solution you can bound. What is convergence rate?

3. Consider the boundary value problem

$$-u''(x) = f(x)\,, \quad 0 < x < 1\,, \quad u(0) = 0\,,\ u(1) = 0\,.$$

(a) Put this problem in a weak formulation. Identify the energy inner product. Identify an appropriate vector space in which to work. Are the boundary conditions essential or natural?

(b) Discretize this problem using 5 equally spaced grid points (4 subintervals). Using a piecewise linear Lagrange basis, formulate the finite element approximation. Identify the appropriate subspace and its dimension. Make a sketch of the interval and basis functions.

(c) Derive the stiffness matrix and load vector for $f(x) = 1$. You do *not* need to solve. Compare your system to a standard finite difference approximation.

(d) What is the expected rate of convergence in the L^2 norm and in the Energy norm?

4. Create and analyze a finite difference method approximation for the heat equation $u_t(x,t) = u_{xx}(x,t)\,,\ (x,t) \in (0,1) \times (0,T)$ with periodic boundary conditions

$$u(0,t) = u(1,t), \qquad u_x(0,t) = u_x(1,t) \quad \text{and} \quad u(x,0) = \phi(x)\,.$$

(a) Take equally spaced grid in x with n points i.e., $\Delta x = \frac{1}{n}$. Denote by $U_j(t) \approx u(x_j,t)$. Using the centered second difference for u_{xx}, write down a system of n first-order ODEs in time for $U_j(t)$ and express it as $U'(t) = MU(t)$. Describe the entries and structure of matrix M.

(b) Take an equally spaced grid in t with $m+1$ points i.e., $\Delta t = \frac{T}{m}$. Denote by $U_j^k \approx u(x_j,t_k)$. Use a leapfrog scheme to discretize the system of part (a) in time. Write down a system of equations to compute U_j^{k+1}, $0 \le j \le n-1$ in terms of U_r^k and U_s^{k-1} for appropriate r, s.

(c) Verify the method is consistent. What is the order of accuracy?

(d) Perform von Neumann stability analysis. Is this method stable?

5. Suppose $p_k(x)$ are polynomials of degree k satisfying the orthogonality conditions

$$\int_{-1}^{1} p_k(x)p_m(x)w(x)dx = 0 \qquad m \neq k\,.$$

Furthermore, let $-1 = x_0 < x_1 < \cdots < x_N$ be the $N+1$ ordered roots of the polynomial $q(x) = p_{N+1}(x) + ap_N(x)$ where a is chosen such that $q(-1) = 0$, and $w_0, w_1, \ldots, w_N$ be the solution of the linear system

$$\sum_{j=0}^{N} (x_j)^k w_j = \int_{-1}^{1} x^k w(x)dx\,, \qquad 0 \le k \le N\,.$$

(a) Denote the vector space of polynomials of degree k by $\mathbb{P}_k$. Prove Gaussian quadrature for all polynomials $p \in \mathbb{P}_{2N}$

$$\sum_{j=0}^{N} p(x_j)w_j = \int_{-1}^{1} p(x)w(x)dx\,.$$

(b) Let $u, v \in \mathbb{P}_N$. Define the discrete inner product $(u,v)_N = \sum_{j=0}^{N} u_j v_j w_j$, where $u_j := u(x_j)$ and $v_j := v(x_j)$ are values at the collocation points $\{x_j\}_{j=0}^{N}$. Prove that $(u,v)_N = (u,v)$ where

$$(u,v) := \int_{-1}^{1} u(x)v(x)w(x)dx\,.$$

(c) Consider a Legendre ($w(x) = 1$) spectral approximation of the advection equation

$$\left.\frac{\partial u^N}{\partial t} + \frac{\partial u^N}{\partial x}\right|_{x=x_j} = 0\,, \quad -1 < x < 1\,, \qquad u^N(-1,t) = 0\,.$$

where the approximate solution $u^N \in \mathbb{P}_N$. Show that the solution is stable with respect to the discrete norm for all $t > 0$.

6. Consider the initial-boundary value problem with periodic boundary conditions

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 2\pi, \quad u(0,t) = u(2\pi,t), \; u_x(0,t) = u_x(2\pi,t)$$

with $u(x,0) = u_0(x) \in H_p^m(0,2\pi)$ which is defined as the periodic subspace

$$H_p^m(0,2\pi) = \left\{ u : ||u||_{H^m(0,2\pi)} < \infty, \quad u^{(k)}(x+2\pi) = u^{(k)}(x), \quad k = 0,1,\ldots,m-1 \right\},$$

where the Sobolev norm of order m is defined by

$$||u||_{H^m(0,2\pi)} = \left(\sum_{k=0}^{m} \int_0^{2\pi} |u^{(k)}(x)|^2 dx \right)^{1/2},$$

(a) Consider a function $f \in H_p^m(0,2\pi)$. Give an intuitive argument for decay rate of the Fourier coefficients.

(b) Derive a Fourier-Galerkin method. Approximate the solution $u(x,t)$ by the truncated Fourier series

$$u^N(x,t) = \sum_{k=-N/2}^{N/2} \widehat{u}_k(t) e^{ikx}, \qquad \widehat{u}_k(t) = \frac{1}{2\pi} \int_0^{2\pi} u(x,t) e^{-ikx} dx.$$

Derive the equation describing the evolution of the Fourier coefficients $\widehat{u}_k(t)$.

(c) Write down the explicit solution of the Galerkin problem.

(d) Show that the Galerkin method is stable. That is, show that the energy of the solution is bounded for $t \geq 0$.

(e) Instead of the exact solution in part (c), approximate the evolution of the Fourier coefficients by the backward Euler method. Show that this method is absolutely stable.