PHYS 410: Computational Physics Fall 2023

FINAL EXAM

Friday, December 15, 8:30–11:00 AM, IBLC 182

Please do not read past this page until you are instructed to begin the exam.

Please note the following:

1. This exam is completely closed book and electronics free: no books, notes, calculators, computers or cell phones are allowed.
2. You have 2 1/2 hours to complete the test. It is recommended that you read quickly through the exam before you start working on it.
3. The exam has 3 problems. Problems 1 and 2 are worth 10 points each; Problem 3 is worth 12 points, so there are a total of 32 points available. Marks for individual subproblems are given at the beginning of each subproblem.
4. Answer all questions in the exam booklets provided. Ensure that your name and student number are legibly entered on the front of each booklet that you use. Don't worry about the course section number.

Problem 1: [10 pts]

Problem 1.1: Lagrange Interpolation [5 pts]

Using the Lagrange interpolating formula, compute the unique second degree polynomial, $p(x)$, which passes through the following (x_i, f_i) pairs (i.e. $p(x)$ must satisfy $p(x_i) = f_i$ for $i = 1, 2, 3$).

$$(0, -9) \qquad (3, -3) \qquad (6, -15)\,.$$

Recall that the standard representation of the Lagrange interpolating formula is

$$p(x) = \sum_{j=1}^{n} f_j l_j(x)\,,$$

where the maximum degree of the interpolating polynomial is $n - 1$, the polynomials $l_j(x)$ satisfy

$$l_j(x_i) = \delta_{ji}\,,$$

and δ_{ji} is the Kronecker delta function.

Problem 1.2: Richardson extrapolating an $O(h)$ finite difference approximation (FDA) [5 pts]

Let x_j be a uniform finite difference mesh, such that $x_{j+1} - x_j = \Delta x$ for all j, and let $u_j \equiv u(x_j)$. Then the following approximation:

$$\frac{d^2u}{dx^2}(x_j) \approx \frac{u_j - 2u_{j+1} + u_{j+2}}{\Delta x^2} \tag{1}$$

satisfies

$$\frac{u_j - 2u_{j+1} + u_{j+2}}{\Delta x^2} = \frac{d^2u}{dx^2}(x_j) + \Delta x \frac{d^3u}{dx^3}(x_j) + O(\Delta x^2)\,. \tag{2}$$

Note that, despite appearances, this is a *forward*, not *centred*, difference approximation which is *first order* accurate ($O(\Delta x)$) at $x = x_j$.

Using (2) and Richardson extrapolation, construct an $O(\Delta x^2)$ approximation of the second derivative d^2u/dx^2 at $x = x_j$ that uses the grid function values u_j, u_{j+1}, u_{j+2}, and u_{j+4}.

Problem 2: [10 pts]

Consider the following system of ODEs for the functions $P \equiv P(t)$ and $Q \equiv Q(t)$.

$$\frac{d^2P}{dt^2} + \frac{dP}{dt}\frac{dQ}{dt} = 0\,, \tag{3}$$

$$\frac{d^2Q}{dt^2} + \frac{dQ}{dt}\left(\frac{dP}{dt}\right)^2 = 0\,. \tag{4}$$

Equations (3)–(4) are to be solved on the domain $0 \le t \le t_{\max}$ subject to initial conditions:

$$P(0) = P_0\,,$$
$$\frac{dP}{dt}(0) = P_1\,,$$
$$Q(0) = Q_0\,,$$
$$\frac{dQ}{dt}(0) = Q_1\,.$$

Replace the continuum domain with a uniform finite difference grid t^n, satisfying $t^n - t^{n-1} = \Delta t$ for all n, and adopt the usual grid function notation where, for example, P^n approximates the continuum value $P(t^n)$.

Problem 2.1: Finite difference approximation of the ODE [2 pts]

Using the usual centred, second-order approximations for the first and second derivatives, write an $O(\Delta t^2)$ FDA for the system (3)–(4).

Problem 2.2: Initialization of the ODE [4 pts]

To initialize the FDA you wrote down, values for $P^1 \equiv P(0)$, $P^2 \equiv P(\Delta t)$, $Q^1 \equiv Q(0)$ and $Q^2 \equiv Q(\Delta t)$, must be computed up to and including terms of $O(\Delta t^2)$, so that the overall scheme is $O(\Delta t^2)$.

Specify appropriate values of P^1, P^2, Q^1 and Q^2 in terms of P_0, P_1, Q_0, Q_1 and Δt.

Problem 2.3: Determining P^{n+1} and Q^{n+1} [4 pts]

Describe in detail how you would use the FDA that you wrote down, in conjunction with a two-dimensional Newton's method, to determine P^{n+1} and Q^{n+1} from P^n, P^{n-1}, Q^n, Q^{n-1} and other relevant quantities. Ensure that you fully define all elements of the Jacobian matrix associated with the Newton iteration.

Problem 3: [12 pts]

Consider the following PDE for the function $u \equiv u(t, x)$:

$$u_{tt} = u_{xx} + \frac{1}{2} m^2 u^2 + \frac{1}{4} \sigma^4 u^4 \,. \tag{5}$$

Here m and σ are real-valued parameters. Equation (5) is to be solved on the spatial domain $0 \le x \le 1$, with $x = 0$ and $x = 1$ identified (periodic boundary conditions) and for $0 \le t \le t_{\max}$. The initial conditions are

$$u(0, x) = u_0(x) \,,$$
$$u_t(0, x) = v_0(x) \,.$$

Problem 3.1: FDA of the PDE [2 pts]

Using the standard, centred, second order FDA for a second derivative, write a second order FDA of (5). (Adopt the usual finite difference notation $u_j^n \equiv u(x_j, t^n)$.)

Problem 3.2: Truncation Error of the FDA [4 pts]

Using Taylor series expansion about the point (t^n, x_j), determine the truncation error of the FDA. Your answer must include the full leading order terms in the truncation error, which will contain Δt and Δx raised to some power(s).

Problem 3.3: Stability Analysis of the FDA [6 pts]

Your final task is to perform a von Neumann stability analysis of the scheme you wrote down for Problem 3.1. You can make the usual assumptions, which in this case amounts to assuming that we are solving the problem on the unbounded domain $-\infty < x < \infty$. You may find the following formulae useful:

Fourier transform

$$\tilde{\mathbf{u}}^n(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx}\, \mathbf{u}^n(x)\, dx \,.$$

Inverse Fourier transform

$$\mathbf{u}^n(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx}\, \tilde{\mathbf{u}}^n(k)\, dk \,.$$

Perform a von Neumann analysis of the finite difference scheme you wrote down for Problem 3.1. Your analysis should result in a condition on $\lambda \equiv \Delta t / \Delta x$ for stability of the scheme.