PHYS 410: Computational Physics Fall 2022
Final exam key

Problem 1: [10 pts]

Problem 1.1: Derivative of a polynomial interpolant [5 pts]

Consider 3 equispaced data points:

$$(-h, f_{-1}),\ (0, f_0),\ (h, f_1)$$

Construct the Lagrange interpolating polynomial for these values, then evaluate the derivative at $x = 0$.

$$\begin{aligned}
p(x) &= \sum_{j=1}^{3} f_j\, l_j(x) = \sum_{j=1}^{3} f_j \prod_{i=1, i\neq j}^{3} \frac{x - x_i}{x_j - x_i} \\
&= f_{-1}\frac{x(x-h)}{(-h)(-2h)} + f_0\frac{(x+h)(x-h)}{(h)(-h)} + f_1\frac{(x+h)(x)}{(2h)(h)} \\
&= f_{-1}\frac{x^2 - hx}{2h^2} - f_0\frac{x^2 - h^2}{h^2} + f_1\frac{x^2 + hx}{2h^2}
\end{aligned}$$

Now, since the above expression is a polynomial in x, to determine the derivative evaluated at $x = 0$, we simply need to read off the coefficient of the linear term of the polynomial. Thus we have

$$\left.\frac{dp}{dx}\right|_{x=0} = \frac{f_1 - f_{-1}}{2h}$$

Problem 1.2: Richardson extrapolating an $O(h^2)$ FDA [5 pts]

We are given

$$\frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} = \frac{d^2u}{dx^2} + \frac{1}{12}\Delta x^2 \frac{d^4u}{dx^4} + O(\Delta x^4)$$

Truncating at the $O(\Delta x^2)$ term, we have at scales Δx and $2\Delta x$

$$L^{\Delta x}u_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} \sim \frac{d^2u}{dx^2} + \Delta x^2 e_2(x)$$

$$L^{2\Delta x}u_j \frac{u_{j+2} - 2u_j + u_{j-2}}{4\Delta x^2} \sim \frac{d^2u}{dx^2} + 4\Delta x^2 e_2(x)$$

We now want to take a linear combination such that

$$\alpha L^{\Delta x}u_j + \beta L^{2\Delta x}u_j = \frac{d^2u}{dx^2} + O(\Delta x^4)$$

We thus must have

$$\alpha + \beta = 1$$
$$\alpha + 4\beta = 0$$

Solving, we have

$$\alpha = \frac{4}{3}$$
$$\beta = -\frac{1}{3}$$

Assembling results:

$$\frac{4}{3}L^{\Delta x}u_j - \frac{1}{3}L^{2\Delta x}u_j = \frac{16u_{j+1} - 32u_j + 16u_{j-1}}{12\Delta x^2} - \frac{u_{j+2} - 2u_j + u_{j-2}}{12\Delta x^2}$$

So our $O(h^4)$ approximation is

$$\boxed{\frac{-u_{j+2} + 16u_{j+1} - 30u_j + 16u_{j-1} - u_{j-2}}{12\Delta x^2}}$$

Problem 2: [10 pts]

The differential equation is

$$\frac{d^2x}{dt^2} + \left(x\frac{dx}{dt}\right)^3 = s(t)$$

with initial conditions

$$x(0) = x_0$$

$$\frac{dx}{dt}(0) = v_0$$

Problem 2.1: FDA [2 pts]

The FDA is

$$\boxed{\frac{x^{n+1} - 2x^n + x^{n-1}}{\Delta t^2} + \left((x^n)\,\frac{x^{n+1} - x^{n-1}}{2\Delta t}\right)^3 = s^n}$$

Problem 2.2: Initialization [4 pts]

We need to determine values for $x^1 = x(0)$ and $x^2 = x(\Delta t)$. The latter must be computed up to and including terms of $O(\Delta t^2)$ so that the overall scheme is $O(\Delta t^2)$. We have

$$\boxed{x^1 = x_0}$$

and using the equation of motion to eliminate the second time derivative in the Taylor series expansion

$$\begin{aligned} x^2 &= x^1 + \Delta t\frac{dx}{dt}(0) + \frac{1}{2}\Delta t^2\frac{d^2x}{dt^2}(0) + O(\Delta t^3) \\ &\approx x_0 + \Delta t v_0 + \frac{1}{2}\Delta t^2\left(s(0) - \left(x(0)\frac{dx}{dt}(0)\right)^3\right) \end{aligned}$$

so

$$\boxed{x^2 = x_0 + \Delta t v_0 + \frac{1}{2}\Delta t^2\left(s(0) - (x_0 v_0)^3\right)}$$

Problem 2.3: Determining x^{n+1} [4 pts]

The FDA is a *nonlinear* equation in x^{n+1}:

$$F(x^{n+1}) = \frac{x^{n+1} - 2x^n + x^{n-1}}{\Delta t^2} + \left((x^n)\,\frac{x^{n+1} - x^{n-1}}{2\Delta t}\right)^3 - s^n = 0$$

We can determine x^{n+1} iteratively

$$x^{n+1}_{(0)} \to x^{n+1}_{(1)} \to \ldots x^{n+1}_{(m)} \to x^{n+1}_{(m+1)} \to \ldots$$

using Newton's method. Start with the initial estimate

$$\boxed{x^{n+1}_{(0)} = x^n}$$

then generate the iterates via

$$\boxed{x^{n+1}_{(m+1)} = x^{n+1}_{(m)} - \frac{F(x^{n+1}_{(m)})}{dF/dx^{n+1}|x = x^{n+1}_{(m)}}}$$

where

$$\boxed{\frac{dF}{dx^{n+1}} = \frac{1}{\Delta t^2} + \frac{3(x^n)^3}{8\Delta t^3}\left(x^{n+1} - x^{n-1}\right)^2}$$

Problem 3 [15 pts]

Problem 3.1: FDA [2 pts]

Adopting the usual finite difference notation, the FDA is

$$\boxed{\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \alpha u_j^n}$$

Problem 3.2: Truncation Error [4 pts]

Compute the truncation error for the $O(h^2)$ approximation to the first derivative

$$u(x+\Delta x) = u(x) + \Delta x u'(x) + \frac{1}{2}\Delta x^2 u''(x) + \frac{1}{6}\Delta x^3 u'''(x) + O(\Delta x^4)$$
$$u(x-\Delta x) = u(x) - \Delta x u'(x) + \frac{1}{2}\Delta x^2 u''(x) - \frac{1}{6}\Delta x^3 u'''(x) + O(\Delta x^4)$$

so

$$\frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} = u'(x) + \frac{1}{6}\Delta x^2 u'''(x) + O(\Delta x^4)$$

Writing the difference approximation in the form

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} - \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} - \alpha u_j^n = 0$$

the truncation error is

$$\boxed{\tau = \frac{1}{6}\Delta t^2 u_{ttt} - \frac{1}{6}\Delta x^2 u_{xxx}}$$

Problem 3.3: Initialization [4 pts]

To guarantee an $O(h^2)$ accurate solution at any fixed (t, x) we need to know u_j^2 to $O(\Delta t^2)$ accuracy. Taylor series expanding, we have

$$u(x, \Delta t) = u(x, 0) + \Delta t u_t(x, 0) + \frac{1}{2}\Delta t^2 u_{tt}(x, 0) + O(\Delta t^3) \tag{1}$$

Now, from the initial conditions we have $u(x, 0) = u_0(x)$, and from the governing PDE we have

$$u_t(x, 0) = u_x(x, 0) + \alpha u(x, 0) = u_0' + \alpha u_0$$

$$\begin{aligned} u_{tt}(x, 0) &= (u_x(x, 0) + \alpha u(x, 0))_t = u_{xt}(x, 0) + \alpha u_t(x, 0) = u_{tx}(x, 0) + \alpha u_t(x, 0) \\ &= u_0'' + \alpha u_0' + \alpha u_0' + \alpha^2 u_0 = u_0'' + 2\alpha u_0' + \alpha^2 u_0 \end{aligned}$$

Substituting in (1) we have

$$\boxed{\begin{aligned} u_j^1 &= u_{0_j} \\ u_j^2 &= u_{0_j} + \Delta t \left(u_0' + \alpha u_0\right)_j + \frac{1}{2}\Delta t^2 \left(u_0'' + 2\alpha u_0' + \alpha^2 u_0\right)_j \end{aligned}}$$

Problem 3.4: Stability Analysis [5 pts]

First, according to a theorem quoted without proof in class, we can neglect undifferentiated terms when performing a von Neummann stability analysis.

Second, rewrite the difference equation in "first order" form, introducing $v_j^n = u_j^{n-1}$:

$$\begin{aligned} u_j^{n+1} &= v_j^n + \lambda \left(u_{j+1}^n - u_{j-1}^n \right) , \\ v_j^{n+1} &= u_j^n , \end{aligned}$$

where $\lambda = \Delta t / \Delta x$. In matrix form

$$\begin{bmatrix} u \\ v \end{bmatrix}^{n+1} = \begin{bmatrix} \lambda D_0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}^n$$

where $D_0 u_j^n = u_{j+1}^n - u_{j-1}^n$. Under Fourier transformation this becomes

$$\begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}^{n+1} = \begin{bmatrix} 2i\lambda \sin\xi & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}^n$$

where $\xi = kh$ as usual. We must now determine conditions under which the above matrix has eigenvalues that lie within or on the unit circle. The characteristic equation is

$$\begin{vmatrix} 2i\lambda \sin\xi - \mu & 1 \\ 1 & -\mu \end{vmatrix} = 0$$

or

$$\mu^2 - (2i\lambda \sin\xi)\, \mu - 1 = 0 \, .$$

This equation has roots at

$$\mu(\xi) = i\lambda \sin\xi \pm \sqrt{1 - \lambda^2 \sin^2\xi} \, ,$$

Need sufficient conditions for

$$|\mu(\xi)| \leq 1,$$

or equivalently

$$|\mu(\xi)|^2 \leq 1.$$

Two cases to consider

1. $1 - \lambda^2 \sin^2\xi \geq 0 \rightarrow \lambda \leq 1$
2. $1 - \lambda^2 \sin^2\xi < 0 \rightarrow \lambda > 1$

Case 1

$|\mu(\xi)|^2 = \lambda^2 \sin^2\xi + 1 - \lambda^2 \sin^2\xi = 1$, so we have von Neumann stability.

Case 2

The argument of the square root is negative for sufficiently large ξ so the square root itself is purely imaginary. Together with the fact that $|i\lambda \sin(\xi)| > 1$ this implies that $\mu(\xi) > 1$ for large ξ, so we have von Neumann instability.

Thus, the von Neumann stability criterion for this scheme is

$$\boxed{\lambda \leq 1}$$