

PHYSICS 410

FINAL EXAM REVIEW

Ground Rules / General Information

- The exam is completely closed book and electronics-free: no books, notes, calculators, computers or cell-phones.
- The exam will generally involve calculations of various length based on class notes, tutorials and homework/project assignments.
- Three questions, but multi-part.
- You will have 120 minutes (two hours) to complete the test.
- The review materials given below are not to be considered a complete set of notes for exam study—you are ultimately responsible for all material that was covered in class, tutorials and the homeworks and projects.
- No large-scale coding in exam, will be able to substitute pseudo-code for actual MATLAB.
- Know how to perform convergence tests! Not explicitly reviewed here.

Polynomial Interpolation

- Given n data points:

$$(x_j, f_j), \quad j = 1, 2, \dots, n$$

construct unique polynomial of maximum degree $n - 1$ that passes through all of the data points (*degree* of polynomial \equiv largest power of independent var.)

$$p(x) = \sum_{i=0}^{n-1} c_i x^i$$

- Lagrange approach

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

$$l_j(x) = \prod_{i=1, i \neq j}^n \frac{x - x_i}{x_j - x_i}$$

Barycentric Polynomial Interpolation

- Define barycentric weights

$$w_j = \frac{1}{\prod_{k=1, k \neq j}^n (x_j - x_k)}$$

- Then

$$p(x) = l(x) \sum_{j=1}^n \frac{w_j}{x - x_j} f_j$$

or

$$p(x) = \frac{\sum_{j=1}^n \frac{w_j}{x - x_j} f_j}{\sum_{j=1}^n \frac{w_j}{x - x_j}}$$

Polynomial Interpolation: Symbolic Example

- Consider 3 equispaced data points:

$$(x_0 - h, f_{-1}), (x_0, f_0), (x_0 + h, f_1)$$

- *Construct the Lagrange interpolating polynomial for these values, then evaluate the derivative at $x = x_0$.*
- Without loss of generality, we can set $x_0 = 0$, so that the data points are

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

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

- 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

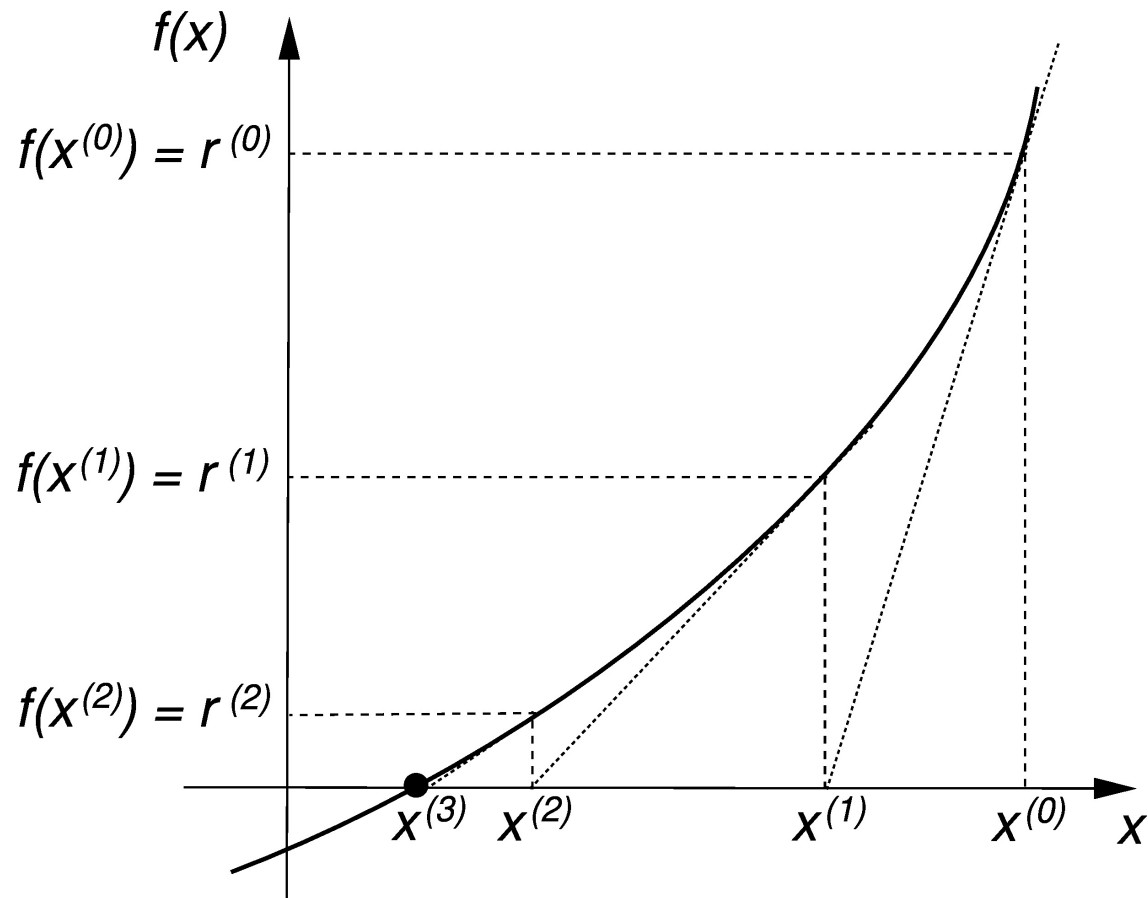
$$\left. \frac{dp}{dx} \right|_{x=0} = \frac{f_1 - f_{-1}}{2h}$$

Solution of Nonlinear Equations: Bisection

- Given $f(x_{\min})f(x_{\max}) < 0$

```
converged = false
fmin = f(xmin)
while not converged do
    xmid = (xmin + xmax) / 2
    fmid = f(xmid)
    if fmid == 0
        break
    elseif fmid * fmin < 0 then
        xmax = xmid
    else
        xmin = xmid
        fmin = fmid
    end if
    if (xmax - xmin) / abs(xmid) < epsilon then
        converged = true
    end if
end while
root = xmid
```

Newton's Method in 1 Dimension



$$x^{(n+1)} = x^{(n)} - \frac{f(x^{(n)})}{f'(x^{(n)})}$$

Newton's Method in d Dimensions

- Want to solve

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

where

$$\mathbf{x} = (x_1, x_2, \dots, x_d)$$

$$\mathbf{f} = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_d(\mathbf{x}))$$

- Newton iteration

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} - \delta\mathbf{x}^{(n)}$$

where the update vector, $\delta\mathbf{x}^{(n)}$, satisfies the $d \times d$ *linear system*

$$\mathbf{J}[\mathbf{x}^{(n)}] \delta\mathbf{x}^{(n)} = \mathbf{f}(\mathbf{x}^{(n)})$$

- Jacobian matrix, $\mathbf{J}[\mathbf{x}^{(n)}]$, has elements

$$J_{ij}[\mathbf{x}^{(n)}] = \left. \frac{\partial f_i}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}^{(n)}}$$

Finite Difference Approximation

- Taylor series

$$f(x + h) = \sum_{n=0}^{\infty} h^n \frac{f^{(n)}(x)}{n!} \quad h \text{ is the expansion parameter}$$

- Example

$$f(x + h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f''''(x) + O(h^5)$$

- Domain discretization

$$\Delta x = \frac{x_{\max} - x_{\min}}{n_x - 1}$$

$$x_j \equiv x_{\min} + (j - 1)\Delta x, \quad j = 1, 2, \dots, n_x$$

$$\Delta x = \frac{x_{\max} - x_{\min}}{2^l} \quad l \text{ is level parameter}$$

Derivation of FDAs

- Example: $O(h^2)$ centred approximation for $f'(x)$

$$\frac{1}{2} \left(\frac{f(x + \Delta x) - f(x)}{\Delta x} + \frac{f(x) - f(x - \Delta x)}{\Delta x} \right) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}$$

$$f'(x_j) \rightarrow \frac{f_{j+1} - f_{j-1}}{2\Delta x}$$

- Truncation error: Taylor series

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

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

- Gives

$$\begin{aligned}\frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} &= f'(x) + \frac{1}{6}\Delta x^2 f'''(x) + O(\Delta x^4) \\ &= f'(x) + O(\Delta x^2)\end{aligned}$$

- Example: $O(h^2)$ centred approximation for $f''(x)$

$$f''(x_j) \rightarrow \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta x^2}$$

$$f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) - \frac{\Delta x^3}{6} f'''(x) + \frac{\Delta x^4}{24} f''''(x) + O(\Delta x^5)$$

$$f(x) = f(x)$$

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) + \frac{\Delta x^3}{6} f'''(x) + \frac{\Delta x^4}{24} f''''(x) + O(\Delta x^5)$$

- Adding series, then dividing by Δx^2 we have

$$\frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} = f''(x) + \frac{\Delta x^2}{12} f''''(x) + \dots = f''(x) + O(\Delta x^2)$$

- Subtracting the continuum expression, $f''(x)$ from the above, we have the truncation error

$$\frac{\Delta x^2}{12} f''''(x) + O(\Delta x^4) = O(\Delta x^2)$$

Derivation of FDAs Using Taylor Series

- Example: Determine approximation to $f''(x)$ that uses grid points x_{j-1} , x_j and x_{j+1} .
- Assume a linear combination of truncated Taylor series for f_{j-1} , f_j and f_{j+1} will give the formula; require

$$\alpha f_{j-1} + \beta f_j + \gamma f_{j+1} = f''(x) + \dots$$

- Taylor expanding

$$f_{j-1} = f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) - \frac{\Delta x^3}{6} f'''(x) + \frac{\Delta x^4}{24} f''''(x) + O(\Delta x^5)$$

$$f_j = f(x)$$

$$f_{j+1} = f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) + \frac{\Delta x^3}{6} f'''(x) + \frac{\Delta x^4}{24} f''''(x) + O(\Delta x^5)$$

- From requirement that first equation yields $f''(x)$ at leading order, and the Taylor expansions, we have three linear equations

$$\alpha + \beta + \gamma = 0$$

$$-\alpha + \gamma = 0$$

$$\frac{\Delta x^2}{2} (\alpha + \gamma) = 1$$

- Solving:

$$\alpha = \frac{1}{\Delta x^2}$$

$$\beta = -\frac{2}{\Delta x^2}$$

$$\gamma = \frac{1}{\Delta x^2}$$

so our FDA is

$$f''(x_j) \rightarrow \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta x^2}$$

as previously.

Richardson Extrapolation

- Basic idea: FD Approximations using different scales of discretization, h_1, h_2 , etc. but same finite difference template, can be combined to produce an approximation of higher order
- Example: forward approximation of first derivative

- Have

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

- Same formula, but applied on the scale $2\Delta x$:

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

- Take linear combination

$$\alpha L^{\Delta x} f + \beta L^{2\Delta x} f$$

so that leading order term is $f'(x)$ and leading order error term is eliminated

$$\alpha + \beta = 1$$

$$\alpha + 2\beta = 0$$

Solving this system

$$\alpha = 2$$

$$\beta = -1$$

Then

$$\begin{aligned}\alpha L^{\Delta x} f + \beta L^{2\Delta x} f &= 2 \left(\frac{f(x + \Delta x) - f(x)}{\Delta x} \right) - \left(\frac{f(x + 2\Delta x) - f(x)}{2\Delta x} \right) \\ &= \frac{-f(x + 2\Delta x) + 4f(x + \Delta x) - 3f(x)}{2\Delta x} \\ &= f'(x) - \frac{1}{3}\Delta x^2 f'''(x) + O(\Delta x^3) \\ &= f'(x) + O(\Delta x^2)\end{aligned}$$

So approximation is

$$f'(x_j) \rightarrow \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2\Delta x}$$

FDA Example: Nonlinear Pendulum

- Equation of motion, initial conditions:

$$\frac{d^2\theta}{dt^2} = -\sin\theta \quad 0 \leq t \leq t_{\max}$$

$$\theta(0) = \theta_0$$

$$\omega(0) = \omega_0$$

- $O(h^2)$ FDA (explicit):

$$\frac{\theta^{n+1} - 2\theta^n + \theta^{n-1}}{\Delta t^2} = -\sin\theta^n \quad n = 2, 3, \dots, n_t - 1)$$

or

$$\theta^{n+1} = 2\theta^n - \theta^{n-1} - \Delta t^2 \sin\theta^n \quad n = 2, 3, \dots, n_t - 1)$$

- Initialization:

$$\theta^1 = \theta(0) = \theta_0$$

and

$$\begin{aligned}\theta(\Delta t) &= \theta(0) + \Delta t \frac{d\theta}{dt}(0) + \frac{1}{2} \Delta t^2 \frac{d^2\theta}{dt^2}(0) + O(\Delta t^3) \\ &\approx \theta_0 + \Delta t \omega_0 + \frac{1}{2} \Delta t^2 \frac{d^2\theta}{dt^2}(0)\end{aligned}$$

- Now use equation of motion to eliminate $d^2\theta/dt^2$; i.e. $d^2\theta/dt^2 = -\sin\theta$, so we have

$$\theta(\Delta t) \approx \theta_0 + \Delta t \omega_0 - \frac{1}{2} \Delta t^2 \sin \theta_0$$

Solving ODEs

- Know how to cast system of ODEs into first order form; example

$$y''(x) + q(x)y'(x) = r(x) \quad ' \equiv \frac{d}{dx}$$

- Introduce new variable $z(x) \equiv y'(x)$, then above becomes

$$\begin{aligned} y' &= z \\ z' &= r - qz \end{aligned}$$

- Know distinction between initial value and boundary value problems
- Know basic methods
 - Euler
 - Modified Euler
 - Improved Euler
 - Fourth order Runge-Kutta

Solving ODEs: Independent Residual Evaluation

- *Idea*: Attempt to directly verify that approximate solution, \hat{u} satisfies the ODE(s) through the use of an *independent discretization* of the ODE (i.e. a discretization distinct from that used by the ODE integrator).

$$\begin{aligned}L^h \hat{u}(\epsilon) &= (L + h^2 E_2 + h^4 E_4 + \dots) (u + e(\epsilon)) \\ &= Lu + h^2 E_2 u + \dots + L^h e(\epsilon) \\ &\approx h^2 E_2 [u] + L^h [e(\epsilon)] \\ &\approx h^2 E_2 [u] = h^2 r = O(h^2)\end{aligned}$$

- SHM example

$$\frac{dy_1}{dt} = y_2 \qquad \frac{dy_2}{dt} = -y_1$$

- Independent residual ($y = y_1$)

$$R_n \equiv \frac{\hat{y}_{n+1} - 2\hat{y}_n + \hat{y}_{n-1}}{h^2} + \hat{y}_n$$

ODE IVPs: Example Problems

- Understand solution approach and qualitative physics of
 - Orbiting dumbbell
 - One-dimensional Toda lattice
 - Driven Van der Pol Oscillator

ODEs: Boundary Value Problems

- Example: Toy model for deuteron ($u(r) = r\psi(r)$, $x \equiv (2m)^{1/2}r$)

$$\frac{d^2u}{dx^2} + (E - V)u = 0$$

$$V(x) = \begin{cases} -1 & 0 \leq x < x_0 \\ 0 & x > x_0 \end{cases}$$

- First order form

$$\frac{du}{dx} = w$$

$$\frac{dw}{dx} = (V - E)u$$

- Initial conditions $u(0) = 0$ (regularity), $w(0) = 1$ (arbitrary), shoot on value of $E = E(x_0)$ until solution approaches 0 for large x

PDEs: Elliptic Equations

- Model problem: Poisson equation on unit square

$$\nabla u(x, y) \equiv u_{xx} + u_{yy} = f(x, y)$$

on

$$\Omega : 0 \leq x \leq 1, 0 \leq y \leq 1$$

subject to

$$u(0, y) = u(1, y) = u(x, 0) = u(x, 1) = 0.$$

- $O(h^2)$ discretization

$$\frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{h^2} = f_{i,j} \quad 2 \leq i, j \leq n-1$$

$$u_{1,j} = u_{n,j} = u_{i,1} = u_{i,n} = 0, \quad 1 \leq i, j \leq n$$

- Solution by Gauss-Seidel relaxation

$$r_{i,j}^{(n)} = h^{-2} \left(u_{i-1,j}^{(n+1)} + u_{i+1,j}^{(n)} + u_{i,j-1}^{(n+1)} + u_{i,j+1}^{(n)} - 4u_{i,j}^{(n)} \right) - f_{i,j}$$

$$F_{i,j}^h = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{h^2} - f_{i,j} = 0$$

$$\begin{aligned} u_{i,j}^{(n+1)} &= u_{i,j}^{(n)} - r_{i,j}^{(n)} \left[\frac{\partial F_{i,j}^h}{\partial u_{i,j}} \Big|_{u_{i,j}=u_{i,j}^{(n)}} \right]^{-1} \\ &= u_{i,j}^{(n)} - \frac{r_{i,j}^{(n)}}{-4h^{-2}} \\ &= u_{i,j}^{(n)} + \frac{1}{4}h^2 r_{i,j}^{(n)} \end{aligned}$$

- Solution by successive overrelaxation (SOR) (\hat{u} = GS solution):

$$u_{i,j}^{(n+1)} = \omega \hat{u}_{i,j}^{(n+1)} + (1 - \omega) u_{i,j}^{(n)}$$

- Generating a test solution:
- Strategy: specify $u(x, y)$ that satisfies boundary conditions, then compute corresponding r.h.s. function, $f(x, y)$

$$u(x, y) = \sin(\omega_x x) \sin(\omega_y y)$$

where ω_x and ω_y are integer multiples of π

- Then

$$f(x, y) = -(\omega_x^2 + \omega_y^2) u(x, y)$$

- NOTE: This strategy of *specifying* a solution that satisfies appropriate conditions and then, from the governing equation, computing an effective source term can be used in many contexts, including the solution of ODEs and time-*dependent* PDEs.

Time Dependent PDEs: IVPs

- IVP nomenclature not precise; in most cases we are solving initial-boundary value problems since boundary conditions will need to be satisfied
- Understand the following terms and concepts (apply to all FDAs, including those derived for ODEs)
 - Residual
 - Truncation error
 - Consistency
 - Convergence
 - Accuracy
 - Solution Error

1-d Diffusion Equation (Forward Time, Centred Space)

- Continuum Equation

$$u(x, t)_t = \sigma u_x x, \quad u(x, 0) = u_0(x), \quad u(0, t) = u(1, t) = 0$$

- Interior FDA

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

- Truncation error

$$\tau = (\partial_t^h - \sigma \partial_{xx}^h) u = \frac{1}{2} \Delta t (u_{tt})_j^n - \frac{1}{12} \sigma \Delta x^2 (u_{xxxx})_j^n + O(\Delta t^2) + O(\Delta x^4) = O(\Delta t, \Delta x^2)$$

- Discretized boundary conditions and initial conditions

$$u_1^{n+1} = u_J^{n+1} = 0, \quad u_j^0 = u_0(x_j)$$

Von Neumann Stability Analysis

- Consider update operation in Fourier space (k -space)

$$\tilde{\mathbf{u}}^{n+1}(k) = \tilde{\mathbf{G}}[\tilde{\mathbf{u}}^n(k)],$$

where

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

- For a general difference scheme, we will find ($\xi \equiv kh \equiv k\Delta x$)

$$\tilde{\mathbf{u}}^{n+1}(k) = \tilde{\mathbf{G}}(\xi) \tilde{\mathbf{u}}^n(k),$$

- Determining stability conditions \equiv determining conditions such that $\tilde{\mathbf{G}}(\xi)$'s eigenvalues lie within or on the unit circle for all conceivable ξ
- Appropriate range for ξ is

$$-\pi \leq \xi \leq \pi ,$$

Diffusion Equation: Stability Analysis

- Define a (non-divided) difference operator D^2 as follows:

$$D^2 u(x) = u(x + h) - 2u(x) + u(x - h).$$

- Suppress spatial grid index, difference equation is

$$u^{n+1} = u^n + \alpha D^2 u^n,$$

where $\alpha \equiv \sigma \Delta t / h^2 = \sigma \Delta t / \Delta x^2$ (but $\sigma = 1$ below).

- Need to know the action of D^2 in Fourier-space. Using the inverse transform have

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

so

$$\begin{aligned}
D^2 u(x) = u(x+h) - 2u(x) + u(x-h) &\propto \int_{-\infty}^{+\infty} (e^{ikh} - 2 + e^{-ikh}) e^{ikx} \tilde{u}(k) dk \\
&\propto \int_{-\infty}^{+\infty} (e^{i\xi} - 2 + e^{-i\xi}) e^{ikx} \tilde{u}(k) dk.
\end{aligned}$$

- Now consider the quantity $-4 \sin^2(\xi/2)$:

$$\begin{aligned}
-4 \sin^2 \frac{\xi}{2} &= -4 \left(\frac{e^{i\xi/2} - e^{-i\xi/2}}{2i} \right)^2 \\
&= \left(e^{i\xi/2} - e^{-i\xi/2} \right)^2 = e^{i\xi} - 2 + e^{-i\xi},
\end{aligned}$$

so

$$D^2 u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(-4 \sin^2 \frac{\xi}{2} \right) e^{ikx} \tilde{u}(k) dk.$$

- In summary, under Fourier transformation, we have

$$\begin{aligned}
\mathbf{u}(x) &\longrightarrow \tilde{\mathbf{u}}(k), \\
D^2 \mathbf{u}(x) &\longrightarrow -4 \sin^2 \frac{\xi}{2} \tilde{\mathbf{u}}(k).
\end{aligned}$$

- Difference scheme is

$$u^{n+1} = u^n + \alpha D^2 u^n$$

- Using these results in the Fourier transform of the update, we have (cancelling all of the $1/\sqrt{2\pi}$'s)

$$\int_{-\infty}^{+\infty} e^{ikx} \tilde{\mathbf{u}}(k)^{n+1} dk = \int_{-\infty}^{+\infty} e^{ikx} \tilde{\mathbf{u}}(k)^n dk - \alpha \int_{-\infty}^{+\infty} e^{ikx} 4 \sin^2 \frac{\xi}{2} \tilde{\mathbf{u}}(k)^n dk$$

- So *amplification factor* in Fourier space is

$$\tilde{G}(\xi) = 1 - 4\alpha \sin^2 \frac{\xi}{2}$$

- Thus, for stability— $|\tilde{G}(\xi)| \leq 1$ —we must have

$$4\alpha \sin^2 \frac{\xi}{2} \leq 2 \quad \rightarrow \quad \alpha \leq \frac{1}{2} \quad \rightarrow \quad \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

Diffusion Equation: Crank-Nicolson Scheme

- Average spatial operators at t^n and t^{n+1}

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{1}{2}\sigma \left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} \right)$$

- Truncation error (note expansion about $(x, t) = (x_j, t^{n+1/2})$)

$$\begin{aligned} \tau &= \frac{1}{24}\Delta t^2 (u_{tttt})_j^{n+1/2} - \frac{1}{8}\sigma\Delta t^2 (u_{ttxx})_j^{n+1/2} - \frac{1}{12}\sigma\Delta x^2 (u_{xxxx})_j^{n+1/2} \\ &\quad + O(\Delta t^4) + O(\Delta x^4) + O(\Delta t^2\Delta x^2) \\ &= O(\Delta t^2, \Delta x^2) \end{aligned}$$

- Stability: Write scheme as

$$\left(1 - \frac{\alpha}{2}D^2\right) u_j^{n+1} = \left(1 + \frac{\alpha}{2}D^2\right) u_j^n$$

- Now apply Fourier transform. Get

$$\left(1 + 2\alpha \sin^2 \frac{\xi}{2}\right) \tilde{\mathbf{u}}(k)^{n+1} = \left(1 - 2\alpha \sin^2 \frac{\xi}{2}\right) \tilde{\mathbf{u}}(k)^n$$

- So amplification factor is

$$\tilde{G}(\xi) = \frac{1 - 2\alpha \sin^2(\xi/2)}{1 + 2\alpha \sin^2(\xi/2)}$$

- This is of the form

$$\frac{1 - X}{1 + X}$$

with $X \geq 0$, which we can show satisfies

$$\left| \frac{1 - X}{1 + X} \right| \leq 1$$

- Thus, we have

$$\tilde{G}(\xi) \leq 1$$

for all ξ and α , so this scheme is unconditionally stable

1-d Schrödinger Equation

- Continuum equation: (ψ complex)

$$i\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V(x, t)\psi$$

- Non-dimensionalize, solve on unit interval with homogeneous Dirichlet conditions

$$\begin{aligned}i\psi_t &= -\psi_{xx} + V\psi \\ \psi(x, 0) &= \psi_0(x) \\ \psi(0, t) &= \psi(1, t) = 0\end{aligned}$$

- Apply Crank-Nicholson differencing

$$i \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = - \frac{1}{2} \left(\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\Delta x^2} + \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} \right) + \frac{1}{2} V_j^{n+1/2} (\psi_j^{n+1} + \psi_j^n)$$

$$\psi_1^{n+1} = \psi_J^{n+1} = 0$$

- Truncation error

$$\tau = O(\Delta t^2, \Delta x^2)$$

- Stability
- *In stability analysis, can neglect terms that do not involve spatial derivatives (theorem)*
- Thus can ignore potential term in stability analysis

- Write scheme (without V) as

$$\left(\frac{i}{\Delta t} + \frac{1}{2}\alpha D^2 \right) \psi^{n+1} = \left(\frac{i}{\Delta t} - \frac{1}{2}\alpha D^2 \right) \psi^n$$

where D^2 is as defined for the diffusion equation and $\alpha = \Delta t / \Delta x^2$

- Under Fourier transform, this becomes

$$\left(\frac{i}{\Delta t} - 2\alpha \sin^2 \frac{\xi}{2} \right) \tilde{\psi}^{n+1}(k) = \left(\frac{i}{\Delta t} + 2\alpha \sin^2 \frac{\xi}{2} \right) \tilde{\psi}^n(k)$$

- Thus, the amplification factor is

$$\tilde{G}(\xi) = \frac{i/\Delta t + 2\alpha \sin^2 \frac{\xi}{2}}{i/\Delta t - 2\alpha \sin^2 \frac{\xi}{2}}$$

which has unit modulus for all α and ξ

- Thus, the scheme is unconditionally stable.

Implicit Schemes

- The Crank-Nicholson schemes for the diffusion and Schrödinger equation are implicit
- Written as a linear system for the advanced unknown vector, \mathbf{u}_j^{n+1}

$$\mathbf{A}\mathbf{u}_j^{n+1} = \mathbf{b}$$

the matrix \mathbf{A} is *tridiagonal*

- Know how to identify such systems (including the boundary conditions), and how to set up and solve them in MATLAB.

1-d Wave Equation

- Continuum equation (non-dimensionalized, $c = 1$)

$$u(x, t)_{tt} = u_{xx}, \quad u(x, 0) = u_0(x), \quad u_t(x, 0) = v_0(x), \quad u(0, t) = u(1, t) = 0$$

- Interior FDA

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\Delta t^2} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} \quad j = 2, 3, \dots, J - 1$$

- Truncation error

$$\tau = \frac{1}{12} \Delta t^2 (u_{tttt})_j^n - \frac{1}{12} \Delta x^2 (u_{xxxx})_j^n + O(\Delta t^4) + O(\Delta x^4) = O(\Delta t^2, \Delta x^2) = O(h^2)$$

- Discrete boundary conditions

$$u_1^{n+1} = u_J^{n+1} = 0$$

- Discrete initial conditions

$$u_j^0, \quad j = 1, 2, \dots, J$$

$$u_j^1, \quad j = 1, 2, \dots, J$$

- First time level comes from $u_0(x)$

$$u_j^0 = u_0(x_j)$$

- u_j^1 must be initialized up to and including terms of order $O(\Delta t^2)$:

$$u_j^1 = u_j^0 + \Delta t (u_t)_j^0 + \frac{1}{2} \Delta t^2 (u_{tt})_j^0 + O(\Delta t^3)$$

$$= u_j^0 + \Delta t (u_t)_j^0 + \frac{1}{2} \Delta t^2 (u_{xx})_j^0 + O(\Delta t^3)$$

$$\approx u_0(x_j) + \Delta t v_0(x_j) + \frac{1}{2} \Delta t^2 u_0''(x_j)$$

- Stability analysis
- First rewrite difference equation in “first order” form; introduce $v_j^n = u_j^{n-1}$:

$$\begin{aligned} u_j^{n+1} &= 2u_j^n - v_j^n + \lambda^2 \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right), \\ v_j^{n+1} &= u_j^n, \end{aligned}$$

or, in matrix form

$$\begin{bmatrix} u \\ v \end{bmatrix}^{n+1} = \begin{bmatrix} 2 + \lambda^2 D^2 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}^n$$

- Under Fourier transformation this becomes

$$\begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}^{n+1} = \begin{bmatrix} 2 - 4\lambda^2 \sin^2 \xi/2 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}^n$$

- We must now determine conditions under which above matrix has eigenvalues that lie within or on the unit circle

- Characteristic equation (whose roots are the e.v.'s) is

$$\begin{vmatrix} 2 - 4\lambda^2 \sin^2(\xi/2) - \mu & -1 \\ 1 & -\mu \end{vmatrix} = 0$$

or

$$\mu^2 + \left(4\lambda^2 \sin^2 \frac{\xi}{2} - 2\right) \mu + 1 = 0.$$

- Equation has roots

$$\mu(\xi) = \left(1 - 2\lambda^2 \sin^2 \frac{\xi}{2}\right) \pm \left(\left(1 - 2\lambda^2 \sin^2 \frac{\xi}{2}\right)^2 - 1\right)^{1/2}.$$

- Need sufficient conditions for

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

or equivalently

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

- Can write

$$\mu(\xi) = (1 - Q) \pm ((1 - Q)^2 - 1)^{1/2},$$

where

$$Q \equiv 2\lambda^2 \sin^2 \frac{\xi}{2},$$

is *real* and *non-negative* ($Q \geq 0$).

• Three cases to consider:

1. $(1 - Q)^2 - 1 = 0$,
2. $(1 - Q)^2 - 1 < 0$,
3. $(1 - Q)^2 - 1 > 0$.

• Case 1: $Q = 0$ or $Q = 2$; in both cases $|\mu(\xi)| = 1$

• Case 2: $((1 - Q)^2 - 1)^{1/2}$ is purely imaginary, so

$$|\mu(\xi)|^2 = (1 - Q)^2 + (1 - (1 - Q)^2) = 1.$$

• Case 3: $(1 - Q)^2 - 1 > 0 \longrightarrow (1 - Q)^2 > 1 \longrightarrow Q > 2$, then

$$1 - Q - ((1 - Q)^2 - 1)^{1/2} < -1,$$

so stability criterion will *always* be violated.

- Thus, necessary condition for Von-Neumann stability is

$$(1 - Q)^2 - 1 \leq 0 \longrightarrow (1 - Q)^2 \leq 1 \longrightarrow Q \leq 2.$$

- But $Q \equiv 2\lambda \sin^2(\xi/2)$ and $\sin^2(\xi/2) \leq 1$, so have

$$\lambda \equiv \frac{\Delta t}{\Delta x} \leq 1,$$

for stability of our scheme

2-d Diffusion Equation: ADI Solution

- Continuum equation: $u = u(x, y, t)$, $\sigma = 1$

$$u_t = u_{xx} + u_{yy}, \quad 0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad t \geq 0$$

$$u(x, y, t) = u_0(x, y), \quad u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0$$

- Define operators

$$\partial_{xx}^h u_{i,j}^n = \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2}$$

$$\partial_{yy}^h u_{i,j}^n = \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}$$

- FDA

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \frac{1}{2} (\partial_{xx}^h + \partial_{yy}^h) (u_{i,j}^{n+1} + u_{i,j}^n)$$

- Truncation error

$$\tau = O(\Delta x^2, \Delta t^2)$$

- ADI solution

$$\left(1 - \frac{\Delta t}{2} \partial_{xx}^h\right) \left(1 - \frac{\Delta t}{2} \partial_{yy}^h\right) u_{i,j}^{n+1} = \left(1 + \frac{\Delta t}{2} \partial_{xx}^h\right) \left(1 + \frac{\Delta t}{2} \partial_{yy}^h\right) u_{i,j}^n$$

- Retains $O(\Delta x^2, \Delta t^2)$ truncation error
- System can be solved in stages by introducing an intermediate gridfunction, $u_{i,j}^{n+\frac{1}{2}}$, then solving in turn

$$\left(1 - \frac{\Delta t}{2} \partial_{xx}^h\right) u_{i,j}^{n+\frac{1}{2}} = \left(1 + \frac{\Delta t}{2} \partial_{xx}^h\right) \left(1 + \frac{\Delta t}{2} \partial_{yy}^h\right) u_{i,j}^n$$

$$\left(1 - \frac{\Delta t}{2} \partial_{yy}^h\right) u_{i,j}^{n+1} = u_{i,j}^{n+\frac{1}{2}}$$

- Solve via

- *Stage 1:* For each $j = 2, 3, \dots, n-1$ solve a tridiagonal system for $u_{i,j}^{n+\frac{1}{2}}$, $i = 1, 2, \dots, n$
- *Stage 2:* For each $i = 2, 3, \dots, n-1$ solve a tridiagonal system for $u_{i,j}^{n+1}$, $j = 1, 2, \dots, n$

Generation of Non-uniform Pseudo-Random Numbers

- Given a probability distribution function $p(x)$, and a uniform pseudo-random number generator, the following pseudo-code describes an algorithm that will generate random numbers distributed according to $p(x)$

```
accept = false
until accept do
  x = random(xmin, xmax)
  y = random(0, pmax)
  if y < p(x) then
    rand = x
    accept = true
  end if
end do
```