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 150 minutes (2 1/2 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; nonetheless start here first if you're short on time
- No coding in exam (could be pseudo-coding)
- No coverage of Fourier transforms
- I dropped some hints during lectures; consult classmates if you missed those

Polynomial Interpolation

- Given n data points:

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

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

$$\begin{aligned} p(x) &= \sum_{j=1}^{n} f_j \, l_j(x) \\ l_j(x) &= \prod_{i=1, i \neq j}^{n} \frac{x - x_i}{x_j - x_i} \end{aligned}$$

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

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

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

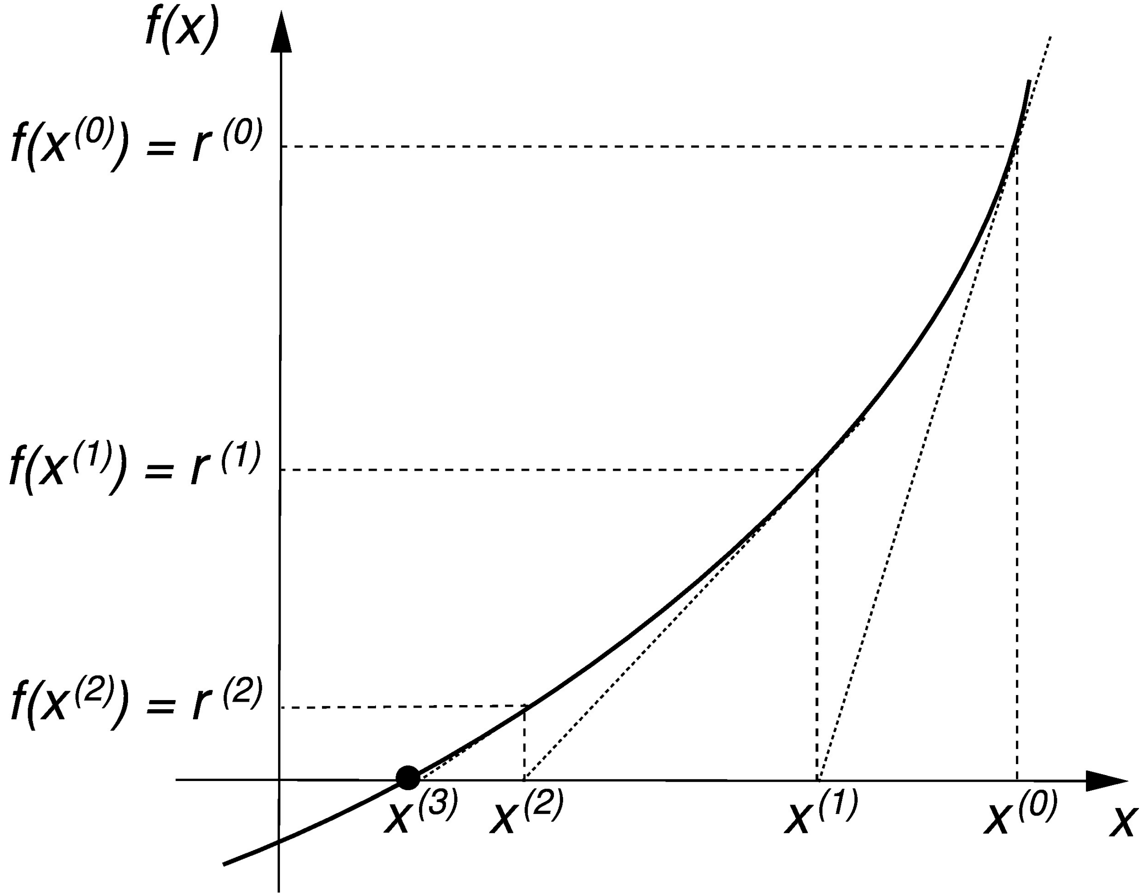
$$\left.\frac{dp}{dx}\right|_{x=0} = \frac{f_1 - f_{-1}}{2h}$$

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

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

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

- 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

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

- 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

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

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

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

Derivation of FDAs

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

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

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

- 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 $f''(x)$

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

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

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

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

- 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

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

- 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

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

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: $O(\Delta x^4)$ Centred approximation of first derivative from $O(\Delta x^2)$ formula

- Have

$$L^{\Delta x} f_j = \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta x^2} = f''(x_j) + \frac{1}{12}\Delta x^2 f''''(x_j) + O(\Delta x^4)$$

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

$$L^{2\Delta x} f = \frac{f_{j+2} - 2f_j + f_{j-2}}{(2\Delta x)^2} = f''(x_j) + \frac{1}{12}(2\Delta x)^2 f''''(x_j) + O(\Delta x^4)$$

- Take linear combination

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

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

$$\alpha + \beta = 1$$

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

Solving this system

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

Then

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

So $O(h^4)$ approximation is

$$f''(x_j) \approx \frac{-f_{j+2} + 16 f_{j+1} - 30 f_j + 16 f_{j-1} - f_{j-2}}{12\Delta x^2}$$

FDA Example: Nonlinear Pendulum

- Equation of motion, initial conditions:

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

$$\theta(0) = \theta_0$$
$$\omega(0) = \omega_0$$

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

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

or

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

- 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

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

- 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).

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

- 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

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

$$u(x,t)_t = \sigma u_{xx}\,, \quad u(x,0) = u_0(x)\,, \quad u(0,t) = u(1,t) = 0$$

- 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

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

- Discretized boundary conditions and initial conditions

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

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

$$-\pi \le \xi \le \pi\,,$$

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

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

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

$$D^2\, u(x) = u(x+h) - 2u(x) + u(x-h) \;\propto\; \int_{-\infty}^{+\infty} \left(e^{ikh} - 2 + e^{-ikh}\right) e^{ikx}\, \tilde{u}(k)\, dk$$

$$\propto\; \int_{-\infty}^{+\infty} \left(e^{i\xi} - 2 + e^{-i\xi}\right) e^{ikx}\, \tilde{u}(k)\, dk\,.$$

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

$$-4\sin^2\frac{\xi}{2} \;=\; -4\left(\frac{e^{i\xi/2} - e^{-i\xi/2}}{2i}\right)^2$$

$$=\; \left(e^{i\xi/2} - e^{-i\xi/2}\right)^2 = e^{i\xi} - 2 + e^{-i\xi}\,,$$

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

$$\mathbf{u}(x) \;\longrightarrow\; \tilde{\mathbf{u}}(k)\,,$$

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

- 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 $(x, t) = (x_j, t^{n+1/2})$)

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

- 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

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

- Apply Crank-Nicholson differencing

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

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

- Truncation error

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

- Stability

- *In stability analysis, can neglect terms that do not involve spatial or temporal derivatives (theorem)*

- Thus can ignore potential term in stability analysis

- Write scheme (without V) as

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

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

- Under Fourier transform, this becomes

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

- Thus, the amplification factor is

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

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` (codeless description).

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

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

- 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

$$
\begin{aligned}
u_j^0 \quad , \qquad & j = 1, 2, \cdots, J \\
u_j^1 \quad , \qquad & j = 1, 2, \cdots, J
\end{aligned}
$$

- 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 $O(\Delta t^2)$:

$$
\begin{aligned}
u_j^1 &= u_j^0 + \Delta t \, (u_t)_j^0 + \frac{1}{2} \Delta t^2 \, (u_{tt})_j^0 + O(\Delta t^3) \\
&= u_j^0 + \Delta t \, (u_t) + \frac{1}{2} \Delta t^2 \, (u_{xx})_j^0 + O(\Delta t^3) \\
&\approx u_0(x_j) + \Delta t \, v_0(x_j) + \frac{1}{2} \Delta t^2 u_0''(x_j)
\end{aligned}
$$

- 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

$$
\left[\begin{array}{c} u \\ v \end{array} \right]^{n+1} = \left[\begin{array}{cc} 2 + \lambda^2 D^2 & -1 \\ 1 & 0 \end{array} \right] \left[\begin{array}{c} u \\ v \end{array} \right]^{n}
$$

- Under Fourier transformation this becomes

$$
\left[\begin{array}{c} \tilde{u} \\ \tilde{v} \end{array} \right]^{n+1} = \left[\begin{array}{cc} 2 - 4\lambda^2 \sin^2 \xi/2 & -1 \\ 1 & 0 \end{array} \right] \left[\begin{array}{c} \tilde{u} \\ \tilde{v} \end{array} \right]^{n}
$$

- 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

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

or equivalently

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

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

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

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

- Define operators

$$\partial^h_{xx} u^n_{i,j} = \frac{u^n_{i+1,j} - 2u^n_{i,j} + u^n_{i-1,j}}{\Delta x^2}$$

$$\partial^h_{yy} u^n_{i,j} = \frac{u^n_{i,j+1} - 2u^n_{i,j} + u^n_{i,j-1}}{\Delta y^2}$$

- FDA

$$\frac{u^{n+1}_{i,j} - u^n_{i,j}}{\Delta t} = \frac{1}{2}\left(\partial^h_{xx} + \partial^h_{yy}\right)\left(u^{n+1}_{i,j} + u^n_{i,j}\right)$$

- Truncation error

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

- ADI solution

$$\left(1 - \frac{\Delta t}{2}\partial^h_{xx}\right)\left(1 - \frac{\Delta t}{2}\partial^h_{yy}\right) u^{n+1}_{i,j} = \left(1 + \frac{\Delta t}{2}\partial^h_{xx}\right)\left(1 + \frac{\Delta t}{2}\partial^h_{yy}\right) u^{n}_{i,j}$$

- Retains $O(\Delta x^2, \Delta t^2)$ truncation error

- System can be solved in stages by introducing an intermediate gridfunction, $u^{n+\frac{1}{2}}_{i,j}$, then solving in turn

$$\left(1 - \frac{\Delta t}{2}\partial^h_{xx}\right) u^{n+\frac{1}{2}}_{i,j} = \left(1 + \frac{\Delta t}{2}\partial^h_{xx}\right)\left(1 + \frac{\Delta t}{2}\partial^h_{yy}\right) u^{n}_{i,j}$$

$$\left(1 - \frac{\Delta t}{2}\partial^h_{yy}\right) u^{n+1}_{i,j} = u^{n+\frac{1}{2}}_{i,j}$$

- Solve via
  - *Stage 1*: For each $j = 2, 3, \ldots n-1$ solve a tridiagonal system for $u^{n+\frac{1}{2}}_{i,j}$, $i = 1, 2, \ldots n$
  - *Stage 2*: For each $i = 2, 3, \ldots n-1$ solve a tridiagonal system for $u^{n+1}_{i,j}$, $j = 1, 2, \ldots n$

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

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

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

- Solution by Gauss-Seidel relaxation

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

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

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

- 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

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

- 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.

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
```

Monte Carlo Algorithm

```
set T and H
initialize all spins s_i (i = 1, 2, ...n^2)
for desired number of Monte Carlo sweeps through lattice
   for each spin
      calculate E_flip
      if E_flip <= 0
         flip spin
      else
         generate r = random(0,1)
         if r <= exp(-E_flip/(k_B T))
            flip spin
         else
            leave spin as is
         end
      end
   end
   compute new energy, magnetization, ...
end
```