1 FD schemes

1.1 Taylor series expansion general formula

$f(x_i+s)=f(x_i)+f^{(1)}(x_i)\cdot s+\frac{f^{(2)}(x_i)}{2!}\cdot s^2+\frac{f^{(k)}(x_i)}{k!}\cdot s^k+...$

1.2 Check consistency

A. unknowns $=n+p-1$, $\quad n=$ derivative order, $\quad p=OOA$
B. $\lim_{\Delta t,\ \Delta x\Rightarrow 0}\frac{\Delta t}{\Delta x}=0$ (Checks for stability)

1.3 Domain

if $x\in[0,\pi]$ divided equally, $N=M+2$ grid points
$\therefore \Delta x=\frac{\pi}{M+1},\quad where\ x_i=i\Delta x,\quad where\ i=0,1,2...,M+1$

1.4 Spatial difference schemes $\quad (h\equiv\Delta x)$

Forward $\frac{\partial u}{\partial x}:\frac{f(x+\Delta x)-f(x)}{\Delta x}+O(\Delta x)$
Forward $\frac{\partial u}{\partial x}:\frac{-3f(x)+4f(x+\Delta x)+f(x-2\Delta x)}{2\Delta x}+O(\Delta x)^2$
Forward $\frac{\partial^2 u}{\partial x^2}:\frac{2f(x)-5f(x+\Delta x)+4f(x+2\Delta x)-f(x+3\Delta x)}{\Delta x^3}+O(\Delta x)^2$
Backward $\frac{\partial u}{\partial x}:\frac{f(x)-f(x-\Delta x)}{\Delta x}+O(\Delta x)$
Backward $\frac{\partial u}{\partial x}:\frac{3f(x)-4f(x-\Delta x)+f(x-2\Delta x)}{2\Delta x}+O(\Delta x)^2$
Backward $\frac{\partial^2 u}{\partial x^2}:\frac{2f(x)-5f(x-\Delta x)+4f(x-2\Delta x)-f(x-3\Delta x)}{\Delta x^3}+O(\Delta x)^2$
Central $\frac{\partial u}{\partial x}:\frac{f(x+\Delta x)-f(x-\Delta x)}{2\Delta x}+O(\Delta x)^2$
Central $\frac{\partial^2 u}{\partial x^2}:\frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{(\Delta x)^2}+O(\Delta x)^2$

1.5 Temporal difference schemes, $\quad (h\equiv\Delta t)$

Explicit euler $\quad \frac{\partial u}{\partial t}\Big|^n=\frac{u^{n+1}-u^n}{\Delta t}$
Expli Leap-frog $\quad \frac{\partial u}{\partial t}\Big|^n=\frac{u^{n+1}-u^{n-1}}{2\Delta t}$
2-step explicit $\quad \frac{\partial u}{\partial t}\Big|^n=\frac{1}{2\Delta t}\left[u^{n+1}+4u^n-5u^{n-1}\right]-\frac{1}{2}\frac{\partial u}{\partial t}\Big|^{n-1}$
(PC) Predictor $\quad u^{n+1}=\frac{1}{2}\left[u^n+\hat{u}^{n+1}+\Delta t\frac{\partial\hat{u}}{\partial t}\Big|^{n+1}\right]$
(PC) Corrector $\quad \hat{u}^{n+1}=u^n+\Delta t\frac{\partial u}{\partial t}\Big|^n$
2nd-order adams-bashforth $\quad \frac{\partial u}{\partial t}\Big|^n=\frac{2}{3h}\left[u^{n+1}-u^n\right]+\frac{1}{3}\frac{\partial u}{\partial t}\Big|^{n-1}$
Implicit Euler $\quad \frac{\partial u}{\partial t}\Big|^{n+1}=\frac{u^{n+1}-u^n}{\Delta t}$
Crank-nicholson $\quad \frac{\partial u}{\partial t}\Big|^{n+1}=\frac{2}{\Delta t}(u^{n+1}-u^n)-\frac{\partial u}{\partial t}\Big|^n$

1.6 Hybrid schemes

Dufort Frankel applied to $\frac{\partial u}{\partial t}=\alpha\frac{\partial^2 u}{\partial x^2}$
$\Rightarrow u_j^{n+1}=u_j^{n-1}+2a\frac{\Delta t}{(\Delta x)^2}\left[u_{j+1}^n-(u_j^{n+1}+u_j^{n-1})+u_{j-1}^n\right]$

Lax applied to $\frac{\partial u}{\partial t}+c\frac{\partial u}{\partial x}=0$
$\Rightarrow u_j^{n+1}=\frac{1}{2}(u_{j+1}^n+u_{j-1}^n)+\frac{c}{2}\frac{\Delta t}{\Delta x}(u_{j+1}^n+u_{j-1}^n)$

2 Matrices

For banded (tridiagonal) matrix B (a,b,c) of order M,
if $b+2\sqrt{ac}\,cos\frac{m\pi}{M+1}=0$ for $m=1,2,...,M$,
$\Rightarrow \det(\mathtt{B}(a,b,c,))=0$, $\quad\therefore$ **Non-invertible, no unique sol**

Eigenvalues : $\mathbf{det}(A-\lambda I)=0$
Eigenvectors : $(A-\lambda_1 I)\vec{v}_1=0,\ (A-\lambda_i I)\vec{v}_i=0,...$
Determinant (2x2):

3 Linear ODEs

The GS is a linear combination of all fundamental solutions.
General form will be $u^n=c^n+p^n$
Gen sol (2nd order homo): $\quad u(t)=C_1e^{\lambda_1 t}+C_2e^{\lambda_2 t}$
Gen sol (1st order non homo): $\quad u(t)=u_{cs}(t)+u_{ps}(t)$
let homogenous part = 0 $\Rightarrow$ $\quad \frac{\partial u}{\partial t}-\lambda u=0$
$\therefore u_{cs}(t)=C_1e^{\lambda_1 t}$

3.1 Coupled ODEs

$\frac{d\vec{u}}{dt}=A\vec{u}-\vec{f}$ **Idea:** $AE=ED\Rightarrow E^{-1}AE=D$
$E^{-1}\frac{d\vec{u}}{dt}=E^{-1}A\vec{u}-E^{-1}\vec{f}$
$E^{-1}\frac{d\vec{u}}{dt}=E^{-1}A(EE^{-1})\vec{u}-E^{-1}\vec{f}$ $\quad\Leftarrow$ **Use** $EE^{-1}=I$
$\Rightarrow\frac{d}{dt}(E^{-1}\vec{u})=D(\lambda)(E^{-1}\vec{u})-E^{-1}\vec{f}$ $\quad\Leftarrow$ **Use** $E^{-1}AE=D(\lambda)$
$\Rightarrow$ **Let** $\quad \vec{U}=E^{-1}\vec{u},\quad \vec{F}=E^{-1}\vec{f}$
$\frac{d\vec{U}}{dt}=D(\lambda)\vec{U}-\vec{F},\ \Rightarrow\therefore\ \frac{d\vec{U_i}}{dt}=\lambda_iU_i-Fi$

3.2 Solving coupled ODEs numerically

Solution for homogeneous uncoupled ODE is $U_i=Ce^{mt}$
For temporal derivatives, simply differentiate.
$\Rightarrow\frac{dU_i}{dt}=\frac{d}{dt}(Ce^{mt})=mCe^{mt}$

1. Uncouple the ODEs to get $\frac{d\vec{U}}{dt}=D(\lambda)\vec{U}-\vec{F}$

Note that decoupling identity matrix = 1

2. Transform eqns to, $\frac{dU_i}{dt}=\lambda_iU_i-F_i$
3. For $y^{''}+5y^{'}=8x$, homogenous part is $y^{''}+5y^{'}=0$, non-homogenous is the original eqn since it $\neq 0$.
4. Eg ODE $\frac{\partial u}{\partial t}=\lambda u+\alpha e^{st}$

Complimentary solution* $\Rightarrow\frac{\partial u}{\partial t}-\lambda u=0\quad\therefore u_{cs}(t)=\beta_1e^{\lambda_1 t}$
***If polynomial**, use $c^n=\beta\sigma^n\approx\beta e^{\lambda h}$ for every root
Particular solution $\Rightarrow$ Guess a similar form to non-homo part of ODE E.g. $\alpha e^{st}\ \Rightarrow\ \therefore u_{ps}(t)=C_2e^{st}$
***If polynomial**, use $u_i^n=\gamma c_i$

5. Form characteristic polynomial
6. Recouple $\vec{u}=E\vec{U}$ and solve for constants

Example: $u^{n+2}-4u^{n+1}+3u^n=\alpha a^n$
Characteristic poly: $u^n=\beta\sigma^n\Rightarrow\sigma^2-4\sigma+3=0$
Since polynomial has 2 roots, **Compli sol**: $c^n=\beta_1\sigma_1^n+\beta_2\sigma_2^n$
Particular sol: $\frac{\alpha}{a^2-4a+3}a^n$
$G(S)=\beta_1\sigma_1^n+\beta_2\sigma_2^n+\frac{\alpha}{a^2-4a+3}a^n$

3.3 Solving coupled ODEs analytically

1. Uncouple ODEs to get $\frac{d\vec{U}}{dt}=D(\lambda)\vec{U}-\vec{F}$
2. Decouple into $\frac{dU_i}{dt}=\lambda_iU_i+F_i$ for i=λ_i...
3. If have constant F after decoupling, particular solution exist, becomes $U_i=C_ie^{\lambda_i}t+\frac{1}{\lambda_i}$, else $U_i=C_ie^{\lambda_i}t$
4. Convert back to $\vec{u}\quad\Rightarrow\quad\vec{u}=E\vec{U}$

3.4 Isolation Theorem

1. Multiply E^{-1} to all terms.
2. Add EE^{-1} to right of A matrix, since $EE^{-1}=1$.
2. Sub $E^{-1}AE=D$ into equation.

3.5 Exact solution of non-homogenous FDE

Complimentary solution is a **fluctuating** component, $\sigma\approx e^{\lambda h}$ and particular solution is **steady state** solution.
$\sigma=e^{\lambda h}=1+\lambda h+\frac{1}{2!}(\lambda h)^2+\frac{1}{3!}(\lambda h)^3+...+O(h)^k$
Leapfrog will have 2 roots, principal and spurious.
Principal roots matches the $e^{\lambda h}$ term while spurious does not. Numerical methods with spurious roots are not self-starting, require additional initial condition.

3.6 Accuracy of temporal discretization

Transient solution error	$\epsilon_\lambda=e^{\lambda\Delta t}-\sigma_{principal}$
Amplitude error	$\epsilon_{\lvert\lambda\rvert}=1-\sqrt{\sigma_r^2+\sigma_i^2}$
Phase error	$\epsilon_w=wh-\tan^{-1}(\frac{\sigma_i}{\sigma_r})$
Particular solution error	$\epsilon_{PS}=p_{numerical}-p_{exact}$
Exact ODE solution	$u(t)=ce^{\lambda t}+\frac{a}{\mu-\lambda}e^{\mu t}$

3.7 Stability analysis

****$|\sigma_i|\leq 1$ where the root can be real or complex
Gerschogrin's Circle $|\lambda_i-A_{ii}|\leq r_i$
Need to do $A_{11},A_{22},..$ Plot and find largest circle.

Euler forward	$\lvert\sigma_{principal}\rvert=\lvert 1+\lambda h\rvert\leq 1,\ \lambda_{max}=-\frac{4\nu}{(\Delta x)^2}$
Leapfrog	Unstable if leaves circle. Gives 1 spurious, 1 principal
MC Pred-corrector	Same as Euler forward, but with a higher OOA for small λh

Matrix method

1. Discretize spatial derivatives, reduce PDE to a set of coupled ODEs in the form of: $\frac{d\vec{u}}{dt}=A\vec{u}+\vec{f}$.
2. Choose typical eigenvalue of **A**, called λ_T, you get $\frac{du}{dt}=\lambda_T\cdot u$.
3. Choose temporal FD scheme and sub ODE into FD scheme.
4. Add shift operator, $S\approx\frac{u^{n+1}}{u^n}$
5. Find dispersion relation, $\sigma_i=\sigma_i(\lambda_T\Delta T)$
6. Check FDE stability is met for all roots, $|\sigma_i|\leq 1$
7. For OOA, binomial exp:

$(1+x)^n=1+nx+n(n-1)\frac{x^2}{2!}+n(n-1)(n-2)\frac{x^3}{3!}+...$
- σ_i could be real or complex. If ODE is unstable, FDE stability doesn't matter.
- Numerical methods are Adams-type if all spurious roots lie at origin when $\Delta t=0$. E.g. Adams-Bashforth, Adam-Moulton
- Methods of Milne-type (e.g. leap-frog method) have spurious roots at unit circle when $\Delta t=0$. Typically, Milne-type are more accurate but less stable than Adams-type.

ODE Stability criteria $\Rightarrow Re(\lambda_m)\leq 0$

von Neumann method

Sub $u_j^n=v^ne^{ikxj},\ u_{j+1}^n=v^ne^{ik(xj+\Delta x)}\quad,k\Delta x=\theta$
Amplication factor, $|G|=|\frac{\nu^{n+1}}{\nu^n}\leq 1$
Courant number, $c\frac{\Delta t}{\Delta x}\leq 1$
Diffusion number, S, $\nu\frac{\Delta t}{(\Delta x)^2}\leq\frac{1}{2}$

4 Boundary Conditions

Periodic $i=0,1,2,...,Npoints$ $U_0=U_{N-1}$ $,U_1=U_N$

Neumann Derivative value at points

Dirichlet Fixed value at points

5 Examples

5.1 Derive PDE of Burger's eqn

$\frac{\partial u}{\partial t}+C\frac{\partial u}{\partial x}=\nu\frac{\partial^2 u}{\partial x^2}$

3 point central, 2nd order:

$\frac{\partial u}{\partial t}=(\frac{\nu}{\Delta x^2}-\frac{c}{2\Delta x})u_{i+1}-\frac{2\nu}{\Delta x^2}u_i+(\frac{\nu}{\Delta x^2}+\frac{c}{2\Delta x})u_{i-1}+O(\Delta x)^2$

Domain $x\in[0,1]$, $Grid=0,1,2,...,N$

For Interior points $i=1,2,3...N-1$,

$i=1,\quad (\frac{\nu}{\Delta x^2}-\frac{c}{2\Delta x})u_2-\frac{2\nu}{\Delta x^2}u_1+(\frac{\nu}{\Delta x^2}+\frac{c}{2\Delta x})u_0$

$i=2,\quad (\frac{\nu}{\Delta x^2}-\frac{c}{2\Delta x})u_3-\frac{2\nu}{\Delta x^2}u_2+(\frac{\nu}{\Delta x^2}+\frac{c}{2\Delta x})u_1$

...

$i=N-2,(\frac{\nu}{\Delta x^2}-\frac{c}{2\Delta x})u_{N-1}-\frac{2\nu}{\Delta x^2}u_{N-2}+(\frac{\nu}{\Delta x^2}+\frac{c}{2\Delta x})u_{N-3}$

$i=N-1,(\frac{\nu}{\Delta x^2}-\frac{c}{2\Delta x})u_N-\frac{2\nu}{\Delta x^2}u_{N-1}+(\frac{\nu}{\Delta x^2}+\frac{c}{2\Delta x})u_{N-2}$

$$\frac{\partial u}{\partial t}=\left[\frac{\nu}{\Delta x^2}\begin{bmatrix}-2&1&0&&0\\1&-2&1&&\\0&1&-2&1&\\&&\ddots&\ddots&1\\0&&0&1&-2\end{bmatrix}-\frac{c}{2\Delta x}\begin{bmatrix}0&1&0&&0\\-1&0&1&&\\0&-1&0&1&\\&&\ddots&\ddots&1\\0&&0&-1&0\end{bmatrix}\right]\begin{bmatrix}u_1\\u_2\\\vdots\\u_{N-2}\\u_{N-1}\end{bmatrix}+\begin{bmatrix}\frac{ca}{2\Delta x}+\frac{\nu a}{(\Delta x)^2}\\0\\\vdots\\0\\\frac{-cb}{2\Delta x}+\frac{\nu b}{(\Delta x)^2}\end{bmatrix}$$

Expressed in the form of $\frac{\partial\vec{u}}{\partial t}=A\vec{u}+\vec{f}$

5.2 Solve coupled ODE numerically, find u_1,u_2 (Crank Nic)

$\frac{du_1}{dt}=-\frac{3}{2}u_1-\frac{1}{2}u_2-1$, $\frac{du_2}{dt}=-\frac{1}{2}u_1-\frac{3}{2}u_2+1$

A=$\begin{bmatrix}-1.5&-0.5\\-0.5&-1.5\end{bmatrix}$ $\lambda=det(A-\lambda I)$ $\Rightarrow\lambda_1=-1,\lambda_2=-2$

E=$\begin{bmatrix}1&1\\1&-1\end{bmatrix}$ D=$\begin{bmatrix}-2&0\\0&-1\end{bmatrix}$

$u^{n+1}=u^n 0.5h\left[\frac{\partial u}{\partial t}\Big|^{n+1}+\frac{\partial u}{\partial t}\Big|^{n}\right]$

Sub $\Rightarrow$ $\frac{\partial\vec{u}}{\partial t}=A\vec{u}+\vec{f}$

$\vec{u}^{n+1}=\vec{u}^n+0.5h\left[(A\vec{u}^{n+1}+\vec{f})+(A\vec{u}^n+\vec{f})\right]$

$(I-0.5hA)\vec{u}^{n+1}=(I+0.5hA)\vec{u}^n+h\vec{f}$

$E^{-1}\vec{u}^{n+1}-\frac{h}{2}DE^{-1}\vec{u}^{n+1}=E^{-1}\vec{u}^n+\frac{h}{2}DE^{-1}\vec{u}^n+hE^{-1}\vec{f}$

Sub $\Rightarrow$ $E^{-1}\vec{u}^n=\vec{U}^n$, $\vec{F}=E^{-1}\vec{f}$

$(I-0.5hD)\vec{U}^{n+1}=(I+0.5D)\vec{U}^n+h\vec{F}$

Change to i $\Rightarrow(1-0.5h\lambda_i)U_i^{n+1}=(I+0.5\lambda_i)U_i^n+hF_i$

Complimentary sol, sub $U_i^n=\beta_i\sigma_i^n$

$\Rightarrow(1-0.5h\lambda_i)\sigma_i-(I+0.5\lambda_i)=0$

Particular sol, sub $U_i^n=c_i$

$\Rightarrow(1-0.5h\lambda_i)c_i=(I+0.5\lambda_i)c_i+hF_i$

$G(S)=\beta_i\sigma_i^n-\frac{F_i}{\lambda_i}\Rightarrow U_{1,2}^n=\beta_1(\frac{1-h}{1+h})^n-0,\ \beta_2(\frac{1-0.5h}{1+0.5h})^n-1$

5.3 Solve coupled ODE analytically

$\frac{du_1}{dt}=-\frac{3}{2}u_1-\frac{1}{2}u_2-1$, $\frac{du_2}{dt}=-\frac{1}{2}u_1-\frac{3}{2}u_2+1$

Same A, D, E as 5.2. $\Rightarrow\lambda_1=-1,\lambda_2=-2$

$\frac{d\vec{U}}{dt}=D(\lambda)\vec{U}+\vec{F}$ where, $\vec{F}=E^{-1}\vec{f}=\begin{bmatrix}0\\-1\end{bmatrix}$

$\frac{dU_1}{dt}=\lambda_1U_1+0,\quad\frac{dU_2}{dt}=\lambda_2U_2-1$

$U_1=\frac{1}{\lambda_1}\frac{dU_1}{dt}=C_1e^{\lambda_1t}$

$U_2=\frac{1}{\lambda_2}\frac{dU_2}{dt}+\lambda_2=C_2e^{\lambda_2t}+\frac{1}{\lambda_2}$

Recouple back $\vec{u}=E\vec{U}=\begin{bmatrix}1&1\\1&-1\end{bmatrix}\begin{bmatrix}C_1e^{\lambda_1t}\\C_2e^{\lambda_2t}+\frac{1}{\lambda_2}\end{bmatrix}$

$u_1(t)=e^{-2t}+e^{-t}-1$

$u_2(t)=e^{-2t}+e^{-t}+1$

5.4 Find dispersion relationship

Model eqn: $\frac{\partial u}{\partial t}=\lambda u+ae^{\mu t}$

FDE: $u^{n+1}=u^n+0.5h\left[3(\frac{\partial u}{\partial t})^n-(\frac{\partial u}{\partial t})^{n-1}\right]$

Sub FDE into eqn,

$u^{n+1}-(1+1.5h\lambda)u^n+0.5h\lambda u^{n-1}=0.5ahe^{\mu hn}(3-e^{-\mu h})$

Add shift op $s\equiv\frac{u^{n+1}}{u^n}\equiv u$, $s^2=(1+1.5h\lambda h)s-0.5\lambda h$

$P(\sigma)=P(s)=0,\quad\sigma^2-(1+1.5\lambda h)\sigma+0.5\lambda h=0$

$\sigma=\frac{(1+1.5\lambda h\pm\sqrt{(1+1.5\lambda h)^2-2\lambda h}}{2}$

$\sigma_{positive}$ is principal root as it matches binom exp of $e^{\lambda h}$

5.5 Fourier series stability neumann

Sub $u_j^n=v^ne^{ikxj}$, $u_{j+1}^n=v^ne^{ik(xj+\Delta x)}$ $,k\Delta x=\theta$

Sub in G, courant, diffusion constants to simplify eqn.

Express in G

$\nu^{n+1}e^{ikx_j}=\nu^ne^{ikx_j}\left[1+\frac{\Delta t}{\Delta x^2}(1-\frac{3}{2}\Delta x)\right]+$

$\nu^ne^{ik(x_j+\Delta x)}\left[2\frac{\Delta t}{\Delta x^2}(\Delta x-1)\right]+\nu^ne^{ik(x_j+2\Delta x)}\left[\frac{\Delta t}{\Delta x^2}(1-\frac{1}{2}\Delta x)\right]$

$G\nu^ne^{ikx_j}=\nu^ne^{ikx_j}\left[1+P-\frac{3}{2}Q)\right]+\nu^ne^{ik(x_j+\Delta x)}\left[2(Q-P)\right]+$

$\nu^ne^{ik(x_j+2\Delta x)}(P-\frac{1}{2}Q)$

Divide by $\nu^ne^{ikx_j}$ and apply Euler, $e^{i\theta}=\cos\theta+sin\theta$

$G=(1-\frac{1}{2}P)+e^{i2k\Delta x}(\frac{1}{2}P)=$

$(1-\frac{1}{2}P+\frac{1}{P}\cos(2k\Delta x))+i\frac{1}{2}P\sin(2k\Delta x)$

Square G and solve inequality.

$1+P(1-\frac{1}{2}P)\left[cos(2k\Delta x)-1\right]\le1$

Since $cos(2k\Delta x)$ is negative, middle term must be +

$1-\frac{1}{2}P\ge0\Rightarrow\quad P\le2,\quad\Rightarrow\Delta t\le2$