Numerical Lecture #18: Implicit Timestepping Schemes

I. Implicit Timestepping

A. Diffusion Equation (parabolic equation)

① 1. $$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

2. Standard Forward Euler Time, Centered space differencing

$$\boxed{\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}\right]} \quad \text{FTCS}$$

3. Stability: a. For a hyperbolic equation, FTCS is unstable.

b. Van Neumann Stability Analysis shows

$$\xi = 1 - \frac{4D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) \rightarrow \text{Stable for } \frac{2D\Delta t}{(\Delta x)^2} \leq 1$$

c. Physical interpretation: $\Delta t \leq \frac{(\Delta x)^2}{2D}$ approximately diffusion time across a cell of Δx.

d. But, we often want to measure diffusion across much larger scales with $\lambda \gg \Delta x$ (many cells)

→ Number of timesteps needed by this <u>explicit</u> FTCS scheme is prohibitive.

I. (Continued)

B. Implicit schemes

1. We want to take much larger timesteps in a way that is stable.

2. By taking much larger timesteps:
   a. Evolution on small scales may be inaccurate
   b. We want these scales to do something "innocuous," hopefully physically reasonable.

3. Approaches:
   a. Design a scheme that drive small-scale features to equilibrium forms.
   b. Or, let small scales maintain their initial amplitudes
   $\Rightarrow$ The second approach yields a scheme that is 2nd-order accurate in time $\Rightarrow$ Crank-Nicholson scheme

4. Fully implicit scheme: Evaluate RHS of Eq (1) at step $n+1$

a.
$$\boxed{\frac{U_j^{n+1} - U_j^n}{\Delta t} = D\left[\frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{(\Delta x)^2}\right]}$$
Fully Implicit, or Backward Euler

b. Define: $\alpha \equiv \frac{D\Delta t}{(\Delta x)^2}$

c. To solve, requires solving N_x simultaneous linear equations, where $j = 1, 2, \ldots, N_x$

$$\Rightarrow -\alpha \underbrace{U_{j-1}^{n+1}}_{\text{unknowns}} + (1+2\alpha) U_j^{n+1} - \alpha U_{j+1}^{n+1} = U_j^n \leftarrow \text{known}$$

I. B. (Continued)

4. (Continued)

d. Need to solve a tridiagonal matrix:

$$
\begin{pmatrix}
1+2\alpha & -\alpha & 0 & & & & \\
-\alpha & 1+2\alpha & -\alpha & 0 & \cdots & & 0 \\
0 & -\alpha & 1+2\alpha & -\alpha & 0 & & \vdots \\
 & 0 & -\alpha & 1+2\alpha & -\alpha & 0 & \vdots \\
\vdots & & & \ddots & \ddots & \ddots & \\
0 & \cdots & & 0 & -\alpha & 1+2\alpha & -\alpha \\
 & & & & 0 & -\alpha & 1+2\alpha
\end{pmatrix}
\begin{pmatrix}
U_1^{n+1} \\ U_2^{n+1} \\ U_3^{n+1} \\ \vdots \\ \vdots \\ U_{N_x-1}^{n+1} \\ U_{N_x}^{n+1}
\end{pmatrix}
=
\begin{pmatrix}
U_1^{n} \\ U_2^{n} \\ U_3^{n} \\ \vdots \\ \vdots \\ U_{N_x-1}^{n} \\ U_{N_x}^{n}
\end{pmatrix}
$$

Known — Depends on BCs — Unknown — Known (Current Timestep)

e. Tridiagonal matrices can be solved very efficiently numerically (using LU decomposition and back substitution).

f. Requires appropriate boundary conditions at $j=1$, $j=N_x$.

5. For more complicated systems, such as fluid systems like hydrodynamics or magnetohydrodynamics (MHD), results in band diagonal systems that can also be efficiently solved.

a. LAPACK is a Linear Algebra Package of optimized routines for solving matrix equations

I, B, Continued)

6. Stability: a. Von-Neumann analysis: $\xi = \dfrac{1}{1 + 4\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}$

i) For large scales $k\Delta x \ll 1$, $\xi \sim 1$

ii) For small scales $k\Delta x \to 1$ $\xi \to 0$ as α goes large.

b. Stable for any value of $\alpha \Rightarrow$ any Δt. $\boxed{\text{Unconditionally Stable}}$

c. When $\alpha \to \infty$, what is the associated numerical solution?

i. Dividing by $\alpha \Rightarrow$ $-U_{j-1}^{n+1} + \cancel{\frac{1}{\alpha} U_j^{n+1}}^{\,0} + 2U_j^{n+1} - U_{j+1}^{n+1} = \cancel{\frac{U_j^n}{\alpha}}^{\,0}$

ii. This corresponds to $\dfrac{\partial U}{\partial x^2} = 0$

$\Rightarrow$ Drives small scales to equilibrium $\left(\frac{\partial U}{\partial t} = 0\right)$

7. But, Backward Euler is only first-order accurate in time.

C. Crank-Nicholson scheme

1. Average implicit and explicit schemes:

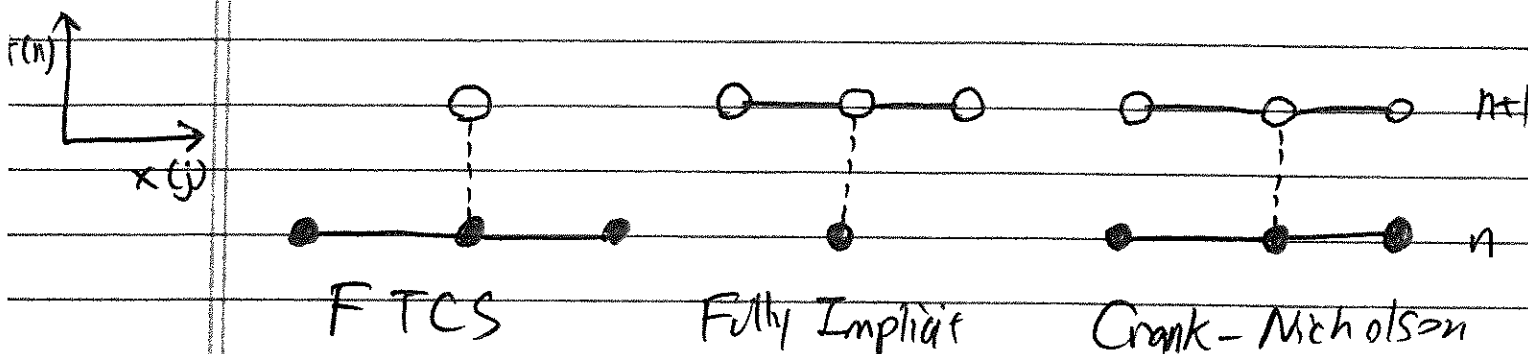
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{D}{2}\left[\frac{\left(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}\right) + \left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)}{(\Delta x)^2}\right]$$

a. Second-order accurate in time

b. Stability $\xi = \dfrac{1 - 2\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}{1 + 2\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}$ $\boxed{\text{Unconditionally Stable}}$

I. (Continued)

D. Stencils for FTCS, Fully Implicit, Crank-Micholson



1. In general, for diffusion problems, recommended approach is Crank-Micholson scheme, followed by a few fully implicit steps at the end to drive small scales into equilibrium.

E. Complications

1. Nonlinear Equations: For plasma physics, most systems of interest are nonlinear
a. Implicit schemes then require solving coupled system of nonlinear equations, which is very challenging/expensive.

$\Rightarrow$ Newton-Krylov methods (nonlinear couplings iterated to convergence)

2. Can also use operator splitting:
a. Linear terms (waves) are advanced implicitly
b. Nonlinear terms are advanced explicitly.