Lecture 18

Partial differential equations:

- Schemes that are second order in time: Staggered leapfrog and Lax-Wendroff.
- Shocks in fluids.
- Diffusive initial value problem: fully implicit and Crank-Nicholson methods.

Second order accuracy in time:

The methods we discussed up to now are first order in the discretization of the partial derivatives with respect to time. To maintain consistent accuracy in space and time discretizations one is forced to use Courant factors that are far away from 1. It is therefore better to consider the construction of schemes that are second order not only in space but also in time. Those can be pushed in many cases into the stability limit.

The staggered leapfrog method simply uses a centered scheme for the time derivative; so, for instance, for the advection we would get,

$$u_j^{n+1} - u_j^{n-1} = -\frac{v\Delta t}{\Delta x}(u_{j+1}^n - u_{j-1}^n)$$

If we perform a von Neumann stability analysis we get,

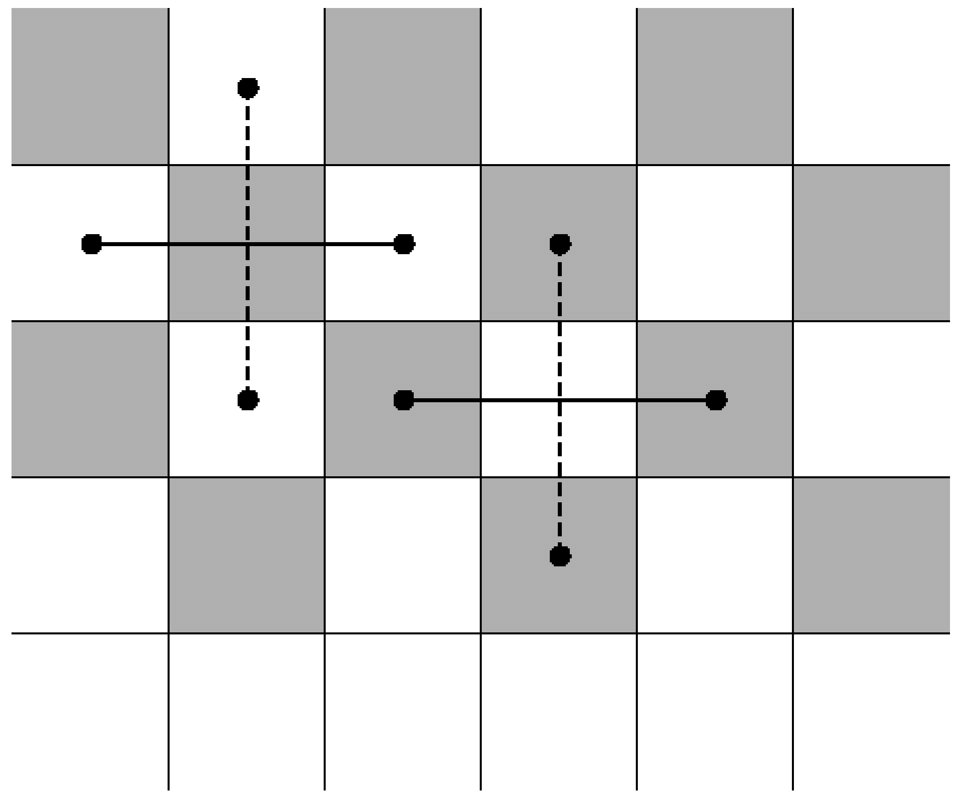
$$\xi^2 - 1 = -2i\xi\frac{v\Delta t}{\Delta x}\sin k\Delta x$$

This implies for the amplitude: $\xi = -i\frac{v\Delta t}{\Delta x}\sin k\Delta x \pm \sqrt{1-\left(\frac{v\Delta t}{\Delta x}\sin k\Delta x\right)^2}$

So we see that again the Courant condition is sufficient for stability.

It is actually even better, since for any $\Delta x < v\Delta t$ the above expression implies $|\xi|^2=1$. Therefore one can go very close to the Courant condition and still have a stable scheme, and with second order accuracy.

For more complicated, nonlinear equations, the method is stable as long as gradients are small. The reason for this is that the method has really two grids completely decoupled in the evolution, as shown in the figure.



These "mesh drifting" instabilities can be cured by adding a dissipative term that links together the two grids, as for instance, a small coefficient times $u^n_{j+1}-2u^n_j+u^n_{j-1}$

The two-step Lax-Wendroff scheme:

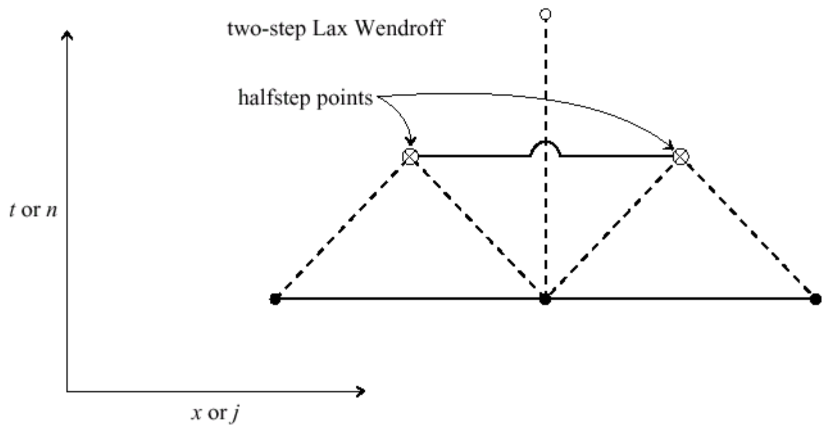
This scheme does not suffer from "mesh drifting" nor large dissipation. It is based on taking first a time evolution step towards a fictitious midpoint,

$$u^{n+1/2}_{j+1/2} = \frac{1}{2}(u^n_{j+1} + u^n_j) - \frac{\Delta t}{2\Delta x}(F^n_{j+1} - F^n_j)$$

And then using this midpoint to take a full time step with properly centered right hand sides,

$$u^{n+1}_j = u^n_j - \frac{\Delta t}{\Delta x}\left(F^{n+1/2}_{j+1/2} - F^{n+1/2}_{j-1/2}\right)$$

And then discarding the midpoint values computed.



If we now combine the two steps into a single prescription, we get the following equation,

$$u_j^{n+1} = u_j^n - \alpha\left[\frac{1}{2}(u_{j+1}^n + u_j^n) - \frac{1}{2}\alpha(u_{j+1}^n - u_j^n) - \frac{1}{2}(u_j^n + u_{j-1}^n) + \frac{1}{2}\alpha(u_j^n - u_{j-1}^n)\right]$$

$$\alpha \equiv \frac{v\Delta t}{\Delta x}$$

If we do a von Neumann analysis we get,

$$\xi = 1 - i\alpha \sin k\Delta x - \alpha^2(1 - \cos k\Delta x)$$

$$|\xi|^2 = 1 - \alpha^2(1-\alpha^2)(1 - \cos k\Delta x)^2$$

So again the Courant condition is all that is needed for stability.

You should not get the impression that the Courant condition is the only condition that can arise for stability. It just keeps appearing repeatedly for the simple equation we have chosen to study.

As long as the Courant condition holds, the amplification factor is less than one, so some dissipation occurs. However, if we study it for large wavelengths (expanding in small k), we get,

$$|\xi|^2 = 1 - \alpha^2(1-\alpha^2)\frac{(k\Delta x)^4}{4} + \ldots$$

This compares favorably to the Lax method, where you can check that,

$$|\xi|^2 = 1 - (1-\alpha^2)(k\Delta x)^2 + \ldots$$

So for long wavelengths (remember that is what you are interested in physically!) the method has two orders less dissipation than the Lax method and does not have the mesh drifting problems of the staggered leapfrog method.

Shocks in fluids

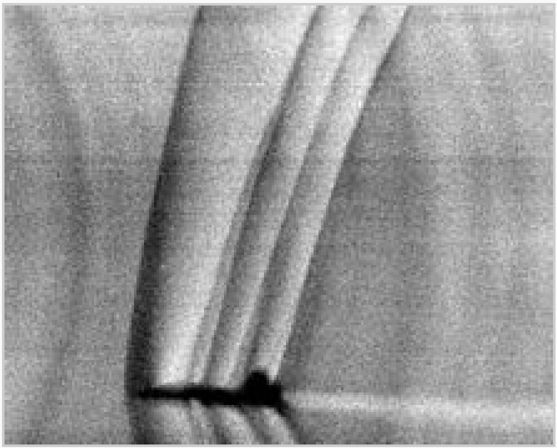
Navier–Stokes equations *(Incompressible flow)*

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=-\nabla p+\mu\nabla^2\mathbf{v}+\mathbf{f}.$$

As we mentioned last class, the Navier-Stokes equation that describes fluid motion is non-linear and coupling of modes of high and low frequency lead to solutions that have discontinuities in the variables known as shocks. These are real physical effects, not mathematical artifacts, that are challenging to model numerically.

Broadly speaking, the are three main approaches to handling shocks.

1) Add artificial viscosity. In nature shocks are not real discontinuities because fluids have viscosity. One can ameliorate the effect of the shock adding more viscosity.



Shock waves produced by a T-38 Talon during flight

2) Combine numerical schemes. For instance use a low order scheme to model the shock and a high accuracy one for the smooth regions. Typically one combines the schemes with weights that are determined by the magnitude of derivatives. When derivatives become large, indicating a shock, one switches to low accuracy.

3) Godunov's methods. Here one goes away from finite differencing. Consider the equation:

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0,$$

Integrating in space:

$$\frac{d}{dt}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x,t)dx = \mathbf{F}(\mathbf{U}(x_{i-1/2},t)) - \mathbf{F}(\mathbf{U}(x_{i+1/2},t)) \, ,$$

And then in time:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x,t^{n+1})dx = \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x,t^{n})dx + \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{U}(x_{i-1/2},t))dt - \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{U}(x_{i+1/2},t))dt\ , \tag{1.12}$$

Defining:

$$\mathbf{U}_i^n = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x,t^n)dt$$

$$\mathbf{F}_{i\pm 1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \mathbf{F}[\mathbf{U}(x_{i\pm 1/2},t)]dt$$

The equation becomes:

$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n + \frac{\Delta t}{\Delta x}(\mathbf{F}_{i-1/2} - \mathbf{F}_{i+1/2}).$$

This becomes a numerical scheme when one proposes an approximation for F’s.

Diffusive initial value problem:

Consider the diffusion equation: $$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)$$

This is a flux-conservative equation like the ones we considered before, with,

$$F = -D\frac{\partial u}{\partial x}$$

And D>0, otherwise the continuum equation has solutions that blow up, and that of course cannot be cured by any numerical method!

It is worthwhile discussing this equation separately since it has special features that distinguish it from the hyperbolic cases we considered before. In a nutshell, since the physics itself has dissipation, the numerics will end up being much more benign than in the hyperbolic case.

To see this, let us consider the maligned FTCS scheme, for the case of D=constant,

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \qquad \frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}\right]$$

Let us now consider the von Neumann stability analysis,

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

Which implies stability if, $\frac{2D\Delta t}{(\Delta x)^2} \leq 1$

Physically, this just means that the maximum timestep allowed should be smaller than the diffusion time across a cell of length Δx. For a region of size λ, the diffusion time is, $\tau \sim \frac{\lambda^2}{D}$

However, this points to a problem. Normally we are interested in scales λ that are much bigger than Δx. This implies that we need to take $(\lambda/\Delta x)^2$ steps before anything interesting happens physically, if we wish a stable scheme. This is usually prohibitive.

Normally, we would like to construct a scheme that is stable and that can take steps of order λ, that is following the time scale of the physics of the problem.

There are two possibilities. In one of them we set up a scheme such that fluctuations of scale much smaller than λ are driven to their equilibrium state, that is, satisfying the equation with LHS=0. We will discuss a method ("fully implicit") that achieves this but is first order in time only. The other possibility is to allow stuff that happens at small scales to fluctuate around their initial values without growing or decreasing. This will lead to a second order method ("Crank-Nicholson").

Fully implicit method:

Suppose we try a FTCS scheme but with the RHS evaluated at n+1,

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

To get the quantities at n+1 we have to solve a system of linear equations (for this simple equation). The system is tri-diagonal, we can immediately see this by grouping terms,

$$-\alpha u_{j-1}^{n+1} + (1+2\alpha)u_j^{n+1} - \alpha u_{j+1}^{n+1} = u_j^n, \qquad j = 1, 2 \ldots J-1$$

$$\alpha \equiv \frac{D\Delta t}{(\Delta x)^2}$$

If we now study what happens for large timesteps (large α), we see that we are discretizing the equilibrium condition,

$$\frac{\partial^2 u}{\partial x^2} = 0$$

And a von Neumann stability analysis shows, Scheme is stable for any timestep.

$$\xi = \frac{1}{1 + 4\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}$$

The details of the small scale fluctuations are obviously wrong for large timesteps, but they correspond to the requested equilibrium state.

Crank-Nicholson method:

This method consists in taking an average of the explicit and fully implicit FTCS schemes,

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

Both sides are correctly centered at n+1/2 so the method is second order accurate. The von Neumann stability analysis shows that the method is stable for any timestep,

$$\xi = \frac{1 - 2\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}{1 + 2\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}$$

The method therefore does not suppress nor amplify small scale fluctuations. It is a widely used method.

Iterated Crank-Nicholson:

Choptuik proposed solving for u^{n+1} in the Crank-Nicholson method iteratively, turning the method into an explicit one.

One first computes an intermediate variable using FTCS,

$$\frac{{}^{(1)}\tilde{u}_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

Then another intermediate variable, by averaging,

$${}^{(1)}\bar{u}_j^{n+1/2} = \tfrac{1}{2}\left({}^{(1)}\tilde{u}_j^{n+1} + u_j^n\right).$$

Final step is obtained by FTCS again,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{{}^{(1)}\bar{u}_{j+1}^{n+1/2} - {}^{(1)}\bar{u}_{j-1}^{n+1/2}}{2\Delta x}.$$

If one wishes more than one iteration,

$$\frac{{}^{(2)}\tilde{u}_j^{n+1} - u_j^n}{\Delta t} = \frac{{}^{(1)}\bar{u}_{j+1}^{n+1/2} - {}^{(1)}\bar{u}_{j-1}^{n+1/2}}{2\Delta x},$$
$${}^{(2)}\bar{u}_j^{n+1/2} = \tfrac{1}{2}\left({}^{(2)}\tilde{u}_j^{n+1} + u_j^n\right).$$

And again FTCS to take the final step. If you want to take more Steps, you get the idea.

Teukolsky noted that the von Neumann analysis yields,

$$\begin{aligned}
{}^{(0)}\xi &= 1 + 2i\beta, \\
{}^{(1)}\xi &= 1 + 2i\beta - 2\beta^2, \\
{}^{(2)}\xi &= 1 + 2i\beta - 2\beta^2 - 2i\beta^3, \\
{}^{(3)}\xi &= 1 + 2i\beta - 2\beta^2 - 2i\beta^3 + 2\beta^4,
\end{aligned}$$

$$\beta = (\alpha/2)\sin k\Delta x$$

Now the surprise:
Levels 0 and 1-> unstable
Levels 2 and 3 -> stable if $\beta^2<1$
Levels 4 and 5 ->unstable
Levels 6 and 7 ->stable

Bottomline: use 2 levels!

Summary

- Staggered leapfrog and Lax-Wendroff provide second order accuracy in time.
- Shocks are handled with special techniques.
- For the diffusive initial value problems, the implicit and Crank-Nicholson method work well.