Computational Physics

Partial Differential Equations

Lectures based on course notes by Pablo Laguna and Kostas Kokkotas

revamped by Deirdre Shoemaker

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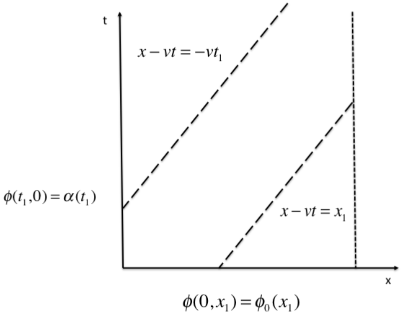
Advection or Convection Equation

- Let's consider the 1D case

$$\partial_t \phi + v\, \partial_x \phi = 0$$

  with $v = \text{const} > 0$, $t \geq 0$ and $x \in [0, 1]$
- Initial data: $\phi(0, x) = \phi_0(x)$
- Boundary conditions: $\phi(t, 0) = \alpha(t)$ and $\phi(t, 1) = \beta(t)$
- Solutions to this equation have the form $\phi(t, x) = \phi(x - v\,t)$
- Therefore, the solution $\phi(t, x)$ is constant along the lines $x - v\,t = \text{const}$ called characteristics



Forward-Time Center-Space (FTCS) Discretization

- Let's consider the following discretization of the differential operators

$$
\begin{aligned}
\partial_t \phi_i^n &= \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + O(\Delta t) \\
\partial_x \phi_i^n &= \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\,\Delta x} + O(\Delta x^2)
\end{aligned}
$$

  where we have used the notation $\phi_i^n \equiv \phi(t^n, x_i)$

- Therefore, the finite difference approximation to $\partial_t \phi + v\,\partial_x \phi = 0$ is

$$
\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v\,\frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2\,\Delta x} = 0
$$

- Notice that we are making a distinction between the solution $\phi(t, x)$ to the continuum equation and $\bar{\phi}_i^n$ the solution to the discrete equation.

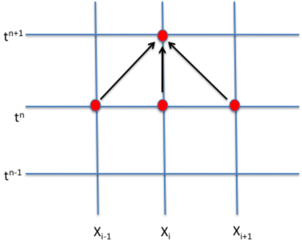
Solving

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v\,\frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2\,\Delta x} = 0$$

for $\bar{\phi}_i^{n+1}$, one gets the following relationship to update the solution

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - \frac{1}{2} C\,\left(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n\right)$$

where $C \equiv \Delta t\, v / \Delta x$



Stability

- The tendency for any perturbation in the numerical solution to decay.
- That is, given a discretization scheme, we need to evaluate the degree to which errors introduced at any stage of the computation will grow or decay.
- We are then concerned with the behavior of the solution error

$$\epsilon_i^n = \phi_i^n - \bar{\phi}_i^n$$

- Substitution of $\bar{\phi}_i^n = \phi_i^n - \epsilon_i^n$ into

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - \frac{1}{2}C\left(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n\right)$$

yields

$$\phi_i^{n+1} - \epsilon_i^{n+1} = \phi_i^n - \epsilon_i^n - \frac{1}{2}C\left(\phi_{i+1}^n - \epsilon_{i+1}^n - \phi_{i-1}^n + \epsilon_{i-1}^n\right)$$

- Substitute the following Taylor expansions

$$\begin{aligned} \phi_i^{n+1} &= \phi_i^n + \Delta t\, \partial_t \phi_i^n + O(\Delta t^2) \\ \phi_{i\pm 1}^n &= \phi_i^n \pm \Delta x\, \partial_x \phi_i^n + O(\Delta x^2) \end{aligned}$$

- Then

$$\phi_i^n + \Delta t\, \partial_t \phi_i^n - \epsilon_i^{n+1} = \phi_i^n - \epsilon_i^n$$
$$-\frac{1}{2} C \left(\phi_i^n + \Delta x\, \partial_x \phi_i^n - \epsilon_{i+1}^n - \phi_i^n + \Delta x\, \partial_x \phi_i^n + \epsilon_{i-1}^n \right)$$

or

$$\Delta t\, \partial_t \phi_i^n - \epsilon_i^{n+1} = -\epsilon_i^n - \frac{1}{2} C \left(2\, \Delta x\, \partial_x \phi_i^n - \epsilon_{i+1}^n + \epsilon_{i-1}^n \right)$$
$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2} C \left(\epsilon_{i+1}^n - \epsilon_{i-1}^n \right) + \Delta t\, \partial_t \phi_i^n - C\, \Delta x\, \partial_x \phi_i^n$$
$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2} C \left(\epsilon_{i+1}^n - \epsilon_{i-1}^n \right) + \Delta t \left(\partial_t \phi_i^n - v\, \partial_x \phi_i^n \right)$$
$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2} C \left(\epsilon_{i+1}^n - \epsilon_{i-1}^n \right)$$

- That is, the solution error satisfies also the discrete finite differences approximation

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2} C \left(\epsilon_{i+1}^n - \epsilon_{i-1}^n \right)$$

- Von Neumann stability analysis: Assume that the errors satisfy a "separation-of-variables" of the form

$$\epsilon_i^n = \xi^n \, e^{I\, x_j} = \xi^n \, e^{I\, k\, \Delta x\, j}$$

  where $I = \sqrt{-1}$, $k = 2\,\pi/\lambda$ and ξ is a complex amplitude. The n in ξ^n is understood to be a power.
- The condition of stability is $|\xi| \leq 1$ for all k.

Substitution of $\epsilon_i^n = \xi^n \, e^{I\,k\,\Delta x\,i}$ into the finite difference equation yields

$$\xi^{n+1}\, e^{I\,k\,\Delta x\,i} = \xi^n\, e^{I\,k\,\Delta x\,i} - \frac{1}{2} C \left(\xi^n\, e^{I\,k\,\Delta x\,(i+1)} - \xi^n\, e^{I\,k\,\Delta x\,(i-1)} \right)$$

$$\xi^{n+1} = \xi^n - \frac{1}{2} C \left(\xi^n\, e^{I\,k\,\Delta x} - \xi^n\, e^{-I\,k\,\Delta x} \right)$$

$$\xi = 1 - \frac{1}{2} C \left(e^{I\,k\,\Delta x} - e^{-I\,k\,\Delta x} \right)$$

$$\xi = 1 - \frac{1}{2} C\, 2\, I\, \sin\left(k\,\Delta x\right)$$

$$\xi = 1 - I\, C\, \sin\left(k\,\Delta x\right)$$

$$|\xi|^2 = 1 + C^2\, \sin^2\left(k\,\Delta x\right)$$

Therefore FTCS discretization applied to the advection equation is unstable.

Forward-Time Forward-Space (FTFS) Discretization

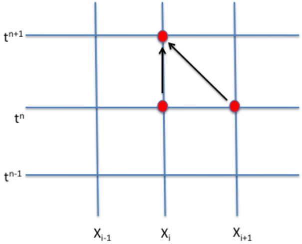
Approximate the advection equation as

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v \, \frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_i^n)}{\Delta x} = 0$$

thus

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - C \, \left(\bar{\phi}_{i+1}^n - \bar{\phi}_i^n\right)$$

where $C \equiv \Delta t \, v / \Delta x$



FTFS Stability

Substitute $\epsilon_i^n = \xi^n e^{I k \Delta x i}$ into

$$\epsilon_i^{n+1} = (1 + C)\epsilon_i^n - C\,\epsilon_{i+1}^n$$
$$\xi^{n+1} e^{I k \Delta x i} = (1 + C)\xi^n e^{I k \Delta x i} - C\,\xi^n e^{I k \Delta x (i+1)}$$
$$\xi^{n+1} = (1 + C)\xi^n - C\,\xi^n e^{I k \Delta x}$$
$$\xi = (1 + C) - C\,e^{I k \Delta x}$$
$$|\xi|^2 = \left[(1 + C) - C\,e^{I k \Delta x}\right]\left[(1 + C) - C\,e^{-I k \Delta x}\right]$$
$$|\xi|^2 = (1 + C)^2 + C^2 - (1 + C)C\,(e^{I k \Delta x} + e^{-I k \Delta x})$$
$$|\xi|^2 = (1 + C)^2 + C^2 - 2\,(1 + C)C\,\cos(k\,\Delta x)$$
$$|\xi|^2 = 1 + 2\,(1 + C)C\,[1 - \cos(k\,\Delta x)] \geq 1$$

the method is unstable

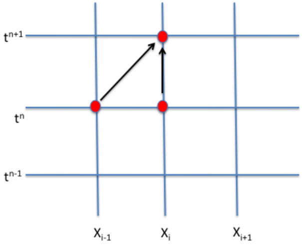
Approximate the advection equation as

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v\,\frac{(\bar{\phi}_i^n - \bar{\phi}_{i-1}^n)}{\Delta x} = 0$$

thus

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - C\,\left(\bar{\phi}_i^n - \bar{\phi}_{i-1}^n\right)$$

where $C \equiv \Delta t\, v/\Delta x$



FTBS Stability

Substitute $\epsilon_i^n = \xi^n e^{I\,k\,\Delta x\,i}$ into

$$\epsilon_i^{n+1} = (1-C)\epsilon_i^n + C\,\epsilon_{i-1}^n$$
$$\xi^{n+1}\,e^{I\,k\,\Delta x\,i} = (1-C)\xi^n\,e^{I\,k\,\Delta x\,i} + C\,\xi^n\,e^{I\,k\,\Delta x\,(i-1)}$$
$$\xi^{n+1} = (1-C)\xi^n + C\,\xi^n\,e^{-I\,k\,\Delta x}$$
$$\xi = (1-C) + C\,e^{-I\,k\,\Delta x}$$
$$|\xi|^2 = \left[(1-C) + C\,e^{-I\,k\,\Delta x}\right]\left[(1-C) + C\,e^{I\,k\,\Delta x}\right]$$
$$|\xi|^2 = (1-C)^2 + C^2 + (1-C)C\,(e^{I\,k\,\Delta x} + e^{-I\,k\,\Delta x})$$
$$|\xi|^2 = (1-C)^2 + C^2 + 2\,(1-C)C\,\cos(k\,\Delta x)$$
$$|\xi|^2 = 1 - 2\,(1-C)C\,[1-\cos(k\,\Delta x)]$$

Given

$$\xi|^2 = 1 - 2(1-C)C\,[1-\cos(k\,\Delta x)]$$

in order to have $|\xi|^2 \leq 1$

$$-1 \leq 1 - 2(1-C)C\,[1-\cos(k\,\Delta x)] \leq 1$$
$$-2 \leq -2(1-C)C\,[1-\cos(k\,\Delta x)] \leq 0$$
$$1 \geq (1-C)C\,[1-\cos(k\,\Delta x)] \geq 0$$

thus

$$\begin{aligned} 1 - C &\geq 0 \\ C &\leq 1 \\ \frac{v\,\Delta t}{\Delta x} &\leq 1 \end{aligned}$$

Thus for stablility we need to pick a time-step

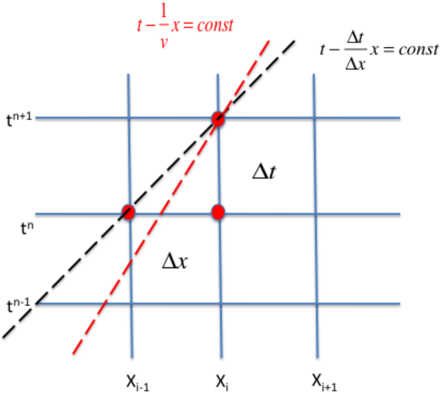
$$\Delta t \leq \frac{\Delta x}{v}$$

The stablility condition

$$\Delta t \leq \frac{\Delta x}{v}$$

implies that the numerical characteristics are contained within the physical characteristics since

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{v}$$



How does FTBS prevent the onset of instabilities?

Recall

$$\phi_i^{n+1} = \phi_i^n - C\,\left(\phi_i^n - \phi_{i-1}^n\right)$$

where $C \equiv \Delta t\, v/\Delta x$. Substitute

$$\begin{aligned}
\phi_i^{n+1} &= \phi_i^n + \Delta t\,\partial_t\phi_i^n + \frac{\Delta t^2}{2}\,\partial_t^2\phi_i^n + O(\Delta t^3) \\
\phi_{i-1}^n &= \phi_i^n - \Delta x\,\partial_x\phi_i^n + \frac{\Delta x^2}{2}\,\partial_x^2\phi_i^n + O(\Delta x^3)
\end{aligned}$$

then

$$\begin{aligned}
\phi_i^n + \Delta t\,\partial_t\phi_i^n + \frac{\Delta t^2}{2}\,\partial_t^2\phi_i^n &= \phi_i^n \\
-C\,\left[\phi_i^n - \phi_i^n + \Delta x\,\partial_x\phi_i^n - \frac{\Delta x^2}{2}\,\partial_x^2\phi_i^n\right]
\end{aligned}$$

Then

$$\Delta t\,\partial_t\phi + \frac{\Delta t^2}{2}\,\partial_t^2\phi = -v\frac{\Delta t}{\Delta x}\,\left[\Delta x\,\partial_x\phi - \frac{\Delta x^2}{2}\,\partial_x^2\phi\right]$$

$$\partial_t\phi + \frac{\Delta t}{2}\,\partial_t^2\phi = -v\left[\partial_x\phi - \frac{\Delta x}{2}\,\partial_x^2\phi\right]$$

$$\partial_t\phi + v\,\partial_x\phi + \frac{\Delta t}{2}\,\partial_t^2\phi - v\frac{\Delta x}{2}\,\partial_x^2\phi = 0$$

but from $\partial_t\phi = -v\,\partial_x\phi$ we have that

$$\partial_t^2\phi = -v\,\partial_t\partial_x\phi = -v\,\partial_x\partial_t\phi = v^2\,\partial_x^2\phi$$

thus

$$\partial_t\phi + v\,\partial_x\phi + v^2\frac{\Delta t}{2}\,\partial_x^2\phi - v\frac{\Delta x}{2}\,\partial_x^2\phi = 0$$

$$\partial_t\phi + v\,\partial_x\phi + \left(v^2\frac{\Delta t}{2} - v\frac{\Delta x}{2}\right)\,\partial_x^2\phi = 0$$

$$\partial_t\phi + v\,\partial_x\phi + \left(v^2\frac{\Delta t}{2} - v\frac{\Delta x}{2}\right)\,\partial_x^2\phi = 0$$

$$\partial_t\phi + v\,\partial_x\phi - v\frac{\Delta x}{2}\left(1 - v\frac{\Delta t}{\Delta x}\right)\,\partial_x^2\phi = 0$$

$$\partial_t\phi + v\,\partial_x\phi - v\frac{\Delta x}{2}\,(1 - C)\;\partial_x^2\phi = 0$$

This equation has the form

$$\partial_t\phi + v\,\partial_x\phi - \alpha\,\partial_x^2\phi = 0$$

advection-diffusion equation with

$$\alpha \equiv v\frac{\Delta x}{2}\,(1 - C)$$

Recall that for stability $C \leq 1$, thus $\alpha \geq 0$.

Given

$$\phi(t,x) = \phi_0\, e^{-pt}\, e^{-i\,k(x-q\,t)}$$

Substitution into

$$\partial_t\phi + v\,\partial_x\phi = 0 \quad\Rightarrow\quad p = 0 \quad q = v$$

$$\partial_t\phi + v\,\partial_x\phi - \alpha\,\partial_x^2\phi = 0 \quad\Rightarrow\quad p = \alpha\,k^2 \quad q = v \quad \text{dissipation}$$

$$\partial_t\phi + v\,\partial_x\phi - \beta\,\partial_x^3\phi = 0 \quad\Rightarrow\quad p = 0 \quad q = v - \beta\,k^2 \quad \text{dispersion}$$

- That is, the FTBS discretization introduces artificial numerical dissipation to prevent the growth of instabilities.
- Notice that the dissipation coefficient $\alpha \propto \Delta t$.
- Therefore, in the continuum limit $\lim_{\Delta x\to 0}\alpha = 0$