Hydrodynamics 3

Lax-Wendroff again
Geometrical source terms
Diffusion

A better Lax-Wendroff method

The Lax-Wendroff in the previous lecture can be massively improved with a better treatment of the source terms. Instead of including the source terms at the ends of the advection timesteps, we can include them at the same time.

STEP 1. Get pressure source terms at cell boundaries using central difference scheme.

$$\left(\frac{\partial P}{\partial x}\right)_{i+\frac{1}{2}} = \frac{P_{i+1} - P_i}{\Delta x} \qquad \left(\frac{\partial P v}{\partial x}\right)_{i+\frac{1}{2}} = \frac{P_{i+1}v_{i+1} - P_i v_i}{\Delta x}$$

And similarly for the i-1/2 sources

STEP 2. Do half-step Lax-Friedrich step with advection and pressure sources to get cell boundary values.

$$\rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(\rho_{i+1}^{n} + \rho_{i}^{n}\right) - \frac{\Delta t}{2\Delta x}\left(\rho_{i+1}^{n} v_{i+1}^{n} - \rho_{i}^{n} v_{i}^{n}\right)$$

$$(\rho v)_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left((\rho v)_{i+1}^{n} + (\rho v)_{i}^{n}\right) - \frac{\Delta t}{2\Delta x}\left((\rho v)_{i+1}^{n} v_{i+1}^{n} - (\rho v)_{i}^{n} v_{i}^{n}\right) - 0.5\Delta t\left(\frac{\partial P}{\partial x}\right)_{i+\frac{1}{2}}^{n}$$

$$e_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(e_{i+1}^{n} + e_{i}^{n}\right) - \frac{\Delta t}{2\Delta x}\left(e_{i+1}^{n} v_{i+1}^{n} - e_{i}^{n} v_{i}^{n}\right) - 0.5\Delta t\left(\frac{\partial P v}{\partial x}\right)_{i+\frac{1}{2}}^{n}$$

And similarly for the i-1/2 values

STEP 3. Calculate cell boundary half-timestep updated advection speeds and pressures from the above values, and then the corresponding cell center gradients for pressure sources

$$\left(\frac{\partial P}{\partial x}\right)_{i}^{n+\frac{1}{2}} = \frac{P_{i+\frac{1}{2}}^{n+\frac{1}{2}} - P_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} \qquad \left(\frac{\partial P v}{\partial x}\right)_{i}^{n+\frac{1}{2}} = \frac{P_{i+\frac{1}{2}}^{n+\frac{1}{2}} v_{i+\frac{1}{2}}^{n+\frac{1}{2}} - P_{i-\frac{1}{2}}^{n+\frac{1}{2}} v_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x}$$

STEP 4. Do full update of cell center values using half-timestep updated values including pressure source terms.

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x}\left(\rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} v_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \rho_{i-\frac{1}{2}}^{n+\frac{1}{2}} v_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

$$(\rho v)_i^{n+1} = (\rho v)_i^n - \frac{\Delta t}{\Delta x}\left((\rho v)_{i+\frac{1}{2}}^{n+\frac{1}{2}} v_{i+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i-\frac{1}{2}}^{n+\frac{1}{2}} v_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) - \Delta t \left(\frac{\partial P}{\partial x}\right)_i^{n+\frac{1}{2}}$$

$$e_i^{n+1} = e_i^n - \frac{\Delta t}{\Delta x}\left(e_{i+\frac{1}{2}}^{n+\frac{1}{2}} v_{i+\frac{1}{2}}^{n+\frac{1}{2}} - e_{i-\frac{1}{2}}^{n+\frac{1}{2}} v_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) - \Delta t \left(\frac{\partial P v}{\partial x}\right)_i^{n+\frac{1}{2}}$$

Do not forget to update the cell-centered pressure and speed values before the next timestep.

WARNING: For some reason, I could only get this method to work properly with a large courant number of a little below 1.0. This probably means that a bit of extra numerical diffusion is needed to keep the scheme stable and something could be improved with the handling of the source terms. I suggest using a larger timestep and not worrying about this issue.

A note on geometry

- An counterintuitive type of source term that comes into many hydrodynamic simulations when considering non-Cartesian coordinate systems are geometric source terms. Consider the simple hydro equations, including gravity, in spherical coordinates.

$$\frac{\partial \rho}{\partial t} + \frac{1}{x^2}\frac{\partial \left(x^2 \rho v\right)}{\partial x} = 0$$

$$\frac{\partial \rho v}{\partial t} + \frac{1}{x^2}\frac{\partial \left(x^2 \rho v^2\right)}{\partial x} = -\frac{\partial p}{\partial x} - \rho g$$

$$\frac{\partial e}{\partial t} + \frac{1}{x^2}\frac{\partial \left[x^2 v \left(e + p\right)\right]}{\partial x} = -\rho v g$$

- Rearranging the above equations gives

$$\frac{\partial \rho}{\partial t} + \frac{\partial\left(\rho v\right)}{\partial x} = -\frac{2\rho v}{x}$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial\left(\rho v^2\right)}{\partial x} = -\frac{\partial p}{\partial x} - \rho g - \frac{2\rho v^2}{x}$$

$$\frac{\partial e}{\partial t} + \frac{\partial\left(e v\right)}{\partial x} = -\frac{\partial\left(p v\right)}{\partial x} - \rho v g - \frac{2v\left(e+p\right)}{x}$$

- Rearranging the above equations gives

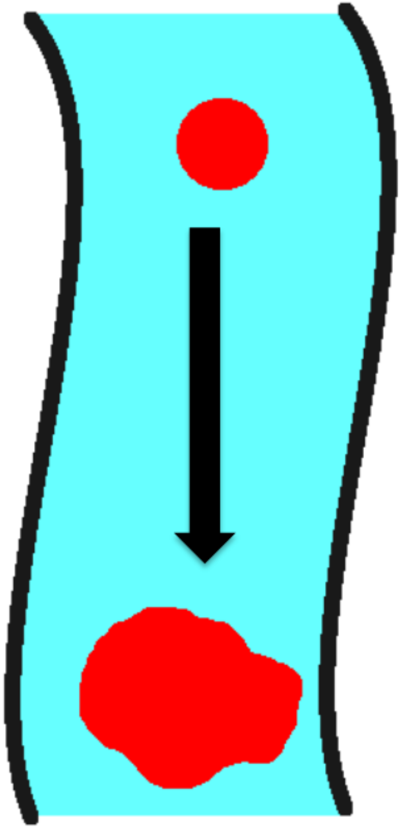
$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = -\frac{2\rho v}{x}$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial (\rho v^2)}{\partial x} = -\frac{\partial p}{\partial x} - \rho g - \frac{2\rho v^2}{x}$$

$$\frac{\partial e}{\partial t} + \frac{\partial (e v)}{\partial x} = -\frac{\partial (p v)}{\partial x} - \rho v g - \frac{2v (e + p)}{x}$$

ADDITIONAL SOURCE TERMS FOR GEOMETRY

Motion of a fluid
advection vs diffusion



Imagine you drop a blob of ink into a river. The blob will move downstream with the bulk motion of the river (advection) and will spread out in all directions (diffusion).

This is described by the following equation

$$\frac{\partial q}{\partial t} = D\nabla^2 q - \nabla \bullet \left(q\vec{v}\right)$$

where q is the quantity of interest, D is the diffusion constant that we have assumed is a constant, and v is the bulk velocity of the fluid.

$D\nabla^2 q$ ← This term corresponds to diffusion

$-\nabla \bullet \left(q\vec{v}\right)$ ← This term corresponds to advection

Diffusion

Previously we focused on the advection part of the equation

$$\frac{\partial q}{\partial t} = -\nabla \cdot (q\mathbf{v})$$ or in 1D: $$\frac{\partial q}{\partial t} = -\frac{\partial (qv)}{\partial x}$$

Let’s look at the diffusion part of this equation now and some of the methods we can use to solve it

$$\frac{\partial q}{\partial t} = D\nabla^2 q$$ or in 1D: $$\frac{\partial q}{\partial t} = D\frac{\partial^2 q}{\partial x^2}$$

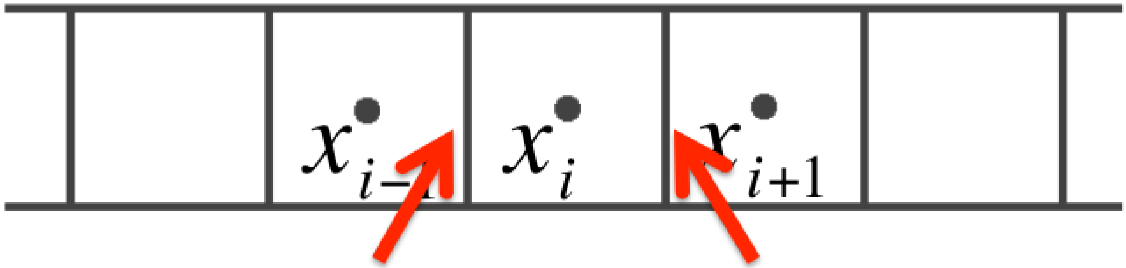
Note: Laplace operator

- The 3D version of the diffusion equation is valid in different coordinate systems with the definition of the Laplace operator being the difference

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial^2 \phi}$$

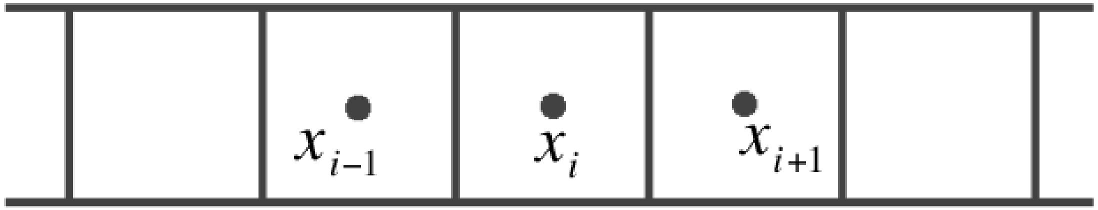
Second Derivative of Space



$$\frac{\partial q_{i-1/2}}{\partial x} = \frac{q_i - q_{i-1}}{x_i - x_{i-1}} \qquad \frac{\partial q_{i+1/2}}{\partial x} = \frac{q_{i+1} - q_i}{x_{i+1} - x_i}$$

$$\frac{\partial^2 q_i}{\partial x^2} \approx \frac{\frac{\partial q_{i+1/2}}{\partial x} - \frac{\partial q_{i-1/2}}{\partial x}}{\Delta x} = \frac{q_{i+1}^n - 2q_i^n + q_{i-1}^n}{\Delta x^2}$$

Second space derivative



As in previous lecture, can approximate second derivative as central difference of central difference

$$\frac{\partial q_{i-1/2}}{\partial x} = \frac{q_i - q_{i-1}}{x_i - x_{i-1}} \quad \leftarrow \text{Left cell gradient}$$

$$\frac{\partial q_{i+1/2}}{\partial x} = \frac{q_{i+1} - q_i}{x_{i+1} - x_i} \quad \leftarrow \text{Right cell gradient}$$

$$\frac{\partial^2 q_i}{\partial x^2} \approx \frac{\frac{\partial q_{i+1/2}}{\partial x} - \frac{\partial q_{i-1/2}}{\partial x}}{\Delta x} = \frac{q_{i+1}^n - 2q_i^n + q_{i-1}^n}{\Delta x^2}$$

The same result can be achieved by doing alternate left/right derivatives for d/dx terms

$$\begin{aligned}
\left(\frac{\partial^2 q}{\partial x^2}\right)_i &= \frac{\partial}{\partial x}\left(\frac{\partial q}{\partial x}\right)_i \\
&= \frac{1}{\Delta x}\left[\left(\frac{\partial q}{\partial x}\right)_{i+1} - \left(\frac{\partial q}{\partial x}\right)_i\right] \\
&= \frac{1}{\Delta x}\left[\frac{q_{i+1} - q_i}{\Delta x} - \frac{q_i - q_{i-1}}{\Delta x}\right] \\
&= \frac{q_{i+1} - 2q_i + q_{i-1}}{\Delta x^2}
\end{aligned}$$

A simple explicit scheme

Let’s first try a simple scheme to solve the diffusion equation. As with the advection problem, let’s first use a forward Euler method for the time discretisation, and let’s use the above method for the spacial discretisation. This scheme is called ‘forward time centered space’ (FTCS)

$$\frac{q_i^{n+1} - q_i^n}{\Delta t} = D\frac{q_{i+1}^n - 2q_i^n + q_{i-1}^n}{\Delta x^2}$$

This leads to the basic equation for the scheme

$$q_i^{n+1} = q_i^n + \frac{D\Delta t}{\Delta x^2}\left(q_{i+1}^n - 2q_i^n + q_{i-1}^n\right)$$

Can this scheme be stable? Unlike the similar scheme for advection, this can be stable for diffusion under appropriate conditions.

Stability of the FTCS scheme

von Neumann stability analysis shows that the forward time center space scheme is stable for the diffusion equation when

$$\frac{2\Delta t D}{\Delta x^2} \leq 1$$

This gives a good method for determining the timestep to use in this scheme. Define c and as the courant number and make it less than 1 (e.g. 0.2 is a decent choice)

$$\Delta t = c\frac{\Delta x^2}{2D}$$

For a derivation of this, see https://en.wikipedia.org/wiki/Von_Neumann_stability_analysis)

Backward Euler method

For stability reasons, diffusion problems are often better solved using implicit methods which typically have the advantage that they can be used for much longer timesteps. If we use backward Euler, the scheme is called backward time centered space (BTCS)

$$\frac{q_i^{n+1} - q_i^n}{\Delta t} = D\frac{q_{i+1}^{n+1} - 2q_i^{n+1} + q_{i-1}^{n+1}}{\Delta x^2}$$

We could rearrange this in the normal way to get

$$q_i^{n+1} = q_i^n + \frac{D\Delta t}{\Delta x^2}\left(q_{i+1}^{n+1} - 2q_i^{n+1} + q_{i-1}^{n+1}\right)$$

However, this is not helpful since much of what is on the right-hand side is unknown to us.

A more useful way to write the above equations is

$$-\frac{D\Delta t}{\Delta x^2}q_{i+1}^{n+1} + \left(1 + \frac{2D\Delta t}{\Delta x^2}\right)q_i^{n+1} - \frac{D\Delta t}{\Delta x^2}q_{i-1}^{n+1} = q_i^n$$

Or

$$aq_{i+1}^{n+1} + bq_i^{n+1} + cq_{i-1}^{n+1} = d$$

Where

$$a = c = -\frac{D\Delta t}{\Delta x^2} \qquad b = \left(1 + \frac{2D\Delta t}{\Delta x^2}\right) \qquad d = q_i^n$$

Note that if D and Δx are variable spatially, then a, b, c, and d should be replaced with a_i, b_i, c_i, and d_i in the above equations.

What about stability? A similar von Neumann analysis shows the BTCS scheme is stable if

$$\left| \frac{1}{1 + \frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{1}{2}k\Delta x\right)} \right| \leq 1$$

It can be quite easily seen from this that this scheme is unconditionally stable. The scheme is stable for all timestep lengths, even very large timesteps. This of course does not mean it is accurate for very large timesteps!

It is useful to write these equations in matrix notation

$$\begin{pmatrix} b & c & 0 & \dots & 0 & 0 \\ a & b & c & \dots & 0 & 0 \\ 0 & a & b & \dots & 0 & 0 \\ 0 & 0 & a & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & a & b \end{pmatrix} \begin{pmatrix} q_1^{n+1} \\ q_2^{n+1} \\ q_3^{n+1} \\ q_4^{n+1} \\ \vdots \\ q_N^{n+1} \end{pmatrix} = \begin{pmatrix} q_1^{n} \\ q_2^{n} \\ q_3^{n} \\ q_4^{n} \\ \vdots \\ q_N^{n} \end{pmatrix}$$

This type of matrix is called a tridiagonal matrix and can solved quickly and easily using the tridiagonal matrix algorithm.

Tridiagonal matrix algorithm

This algorithm is based on a special case of Gaussian elimination

$$a_i x_{i+1} + b_i x_i + c_i x_{i+1} = d_i$$

Where $x_i = q_i^{n+1}$

STEP 1:

$$c'_i = \begin{cases} \dfrac{c_i}{b_i} & ; \quad i = 1 \\ \dfrac{c_i}{b_i - a_i c'_{i-1}} & ; \quad i = 2, 3, \dots, n-1 \end{cases}$$

STEP 2:

$$d'_i = \begin{cases} \dfrac{d_i}{b_i} & ; \quad i = 1 \\ \dfrac{d_i - a_i d'_{i-1}}{b_i - a_i c'_{i-1}} & ; \quad i = 2, 3, \dots, n. \end{cases}$$

STEP 3:

$$x_n = d'_n$$

$$x_i = d'_i - c'_i x_{i+1} \qquad ; \; i = n-1, n-2, \dots, 1.$$

Source: Wikipedia