- Equation $\boxed{1a}$ suggests $\bar{k} < \mathcal{O}(1)$ should provide the stable time step for this parabolic PDE, where $\mathcal{O}(1)$ is a constant number that we derive later. This number depends on the particular stencil used for the parabolic PDEs.
- Accordingly, we observe,

$$\bar{k} < \mathcal{O}(1) \qquad \Rightarrow k_{\max} \propto h^2 \qquad k_{\max} \text{ is the maximum stable time step} \tag{52}$$

That is, we observe that for parabolic PDE $k_{\max}$ is proportional to k^2 rather than k for hyperbolic PDEs.

- This implies that for small grid sizes, the explicit parabolic FD schemes (and in fact FV, FEM, *etc.*) have a much more stringent time step requirement compared to explicit hyperbolic schemes.
- FD scheme can easily be applied to 2D and 3D diffusion equations as well. The 2D, 3D diffusion equation reads as,

$$u_{,t} - \nabla.(D\nabla u) = r \quad \text{for constant } u_{,t} - D\Delta u = u_{,t} - D(u_{,11} + u_{,22} + u_{,33}) = r \tag{53}$$

- The forward time, forward space (FTFS) scheme for this equation is (2D version shown),

$$\frac{v^{n+1}_{m_x m_y} - v^n_{m_x m_y}}{k} - D\left\{\frac{v^n_{(m_x+1)m_y} + v^n_{(m_x-1)m_y} - 2v^n_{m_x m_y}}{h_x^2} + \frac{v^n_{m_x(m_y+1)} + v^n_{m_x(m_y-1)} - 2v^n_{m_x m_y}}{h_y^2}\right\} = r^n_{m_x m_y} \quad \Rightarrow \tag{54a}$$

$$v^{n+1}_m = (1 - 2\bar{k}_x - 2\bar{k}_y)v^n_m + \bar{k}_x(v^n_{(m_x-1)m_y} + v^n_{(m_x+1)m_y}) + +\bar{k}_y(v^n_{m_x(m_y-1)} + v^n_{m_x(m_y+1)}) + r^n_m \tag{54b}$$

$$\bar{k}_x = \frac{kD}{h_x^2}, \quad \bar{k}_y = \frac{kD}{h_y^2} \qquad \text{Normalized time step for parabolic PDE} \tag{54c}$$

- Finally, to obtain an implicit scheme, we write FD equations at time step $n+1$ rather than n.
- For example in 1D, backward-time central-space (BTCS) scheme for the discrete solution v gives,

$$\frac{v^{n+1}_m - v^n_m}{k} - D\frac{v^{n+1}_{m+1} + v^{n+1}_{m-1} - 2v^{n+1}_m}{h^2} = r^n_m \quad \Rightarrow \tag{55a}$$

$$(1 + 2\bar{k})v^{n+1}_m - \bar{k}(v^{n+1}_{m-1} + v^{n+1}_{m+1}) = v^n_m + r^n_m \tag{55b}$$

$$\bar{k} = \frac{kD}{h^2} \qquad \text{Normalized time step for parabolic PDE (as in } \boxed{1a}\text{)}$$

- This scheme will be stable for all $\bar{k}$.

2.1.10.1 Higher order PDEs: Hyperbolic wave equation

- Consider the wave equation,

2nd order

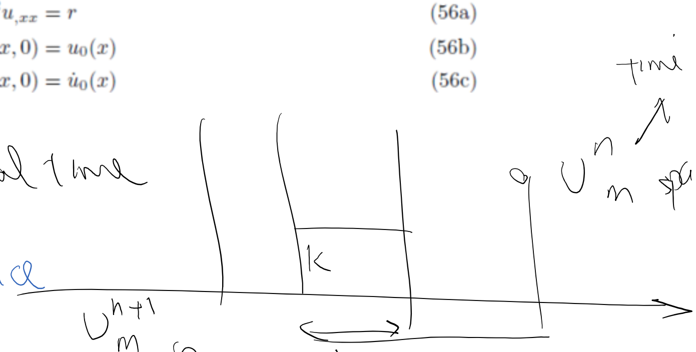
$$u_{,tt} - c^2 u_{,xx} = r \tag{56a}$$

2ICs

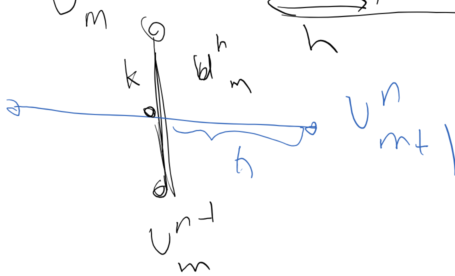
$$\text{IC 1: } 0^{\text{th}} \text{ temporal derivative} \quad u(x,0) = u_0(x) \tag{56b}$$

$$\text{IC 2: } 1^{\text{st}} \text{temporal derivative} \quad \dot{u}(x,0) = \dot{u}_0(x) \tag{56c}$$

$$u_{tt} = \frac{U^{n+1}_m + U^{n-1}_m - 2U^n_m}{k^2} \quad \text{central time}$$



$$U_{xx} = \frac{U^n_{m+1} + U^n_{m-1} - 2U^n_m}{h^2} \quad \text{central space}$$



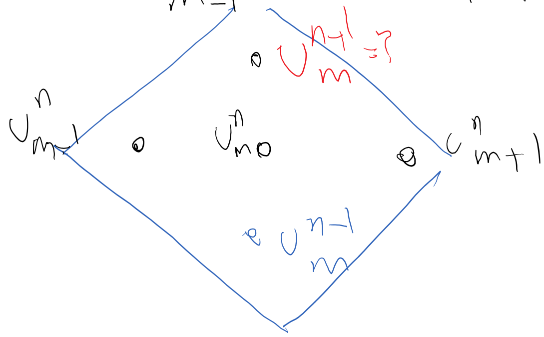
$$\frac{U^{n+1}_m + U^{n-1}_m - 2U^n_m}{k^2} - c^2\left(\frac{U^n_{m+1} + U^n_{m-1} - 2U^n_m}{h^2}\right) = r^n_m$$

multiply by k^2

$$u_m^{n+1} + u_m^{n-1} - 2u_m^n - \bar{k}^2\left(u_{m+1}^n + u_{m-1}^n - 2u_m^n\right) = k^2 r_m^n$$

$$\boxed{u_m^{n+1} = -u_m^{n-1} + 2(1-\bar{k}^2)u_m^n + \bar{k}^2 u_{m-1}^n + \bar{k}^2 u_{m+1}^n + r_m^n}$$

$$\bar{k} = \frac{ck}{h}$$



$$\frac{v_m^{n+1} + v_m^{n-1} - 2v_m^n}{k^2} - c^2\frac{v_{m+1}^n + v_{m-1}^n - 2v_m^n}{h^2} = r_m^n \quad \Rightarrow \tag{57a}$$

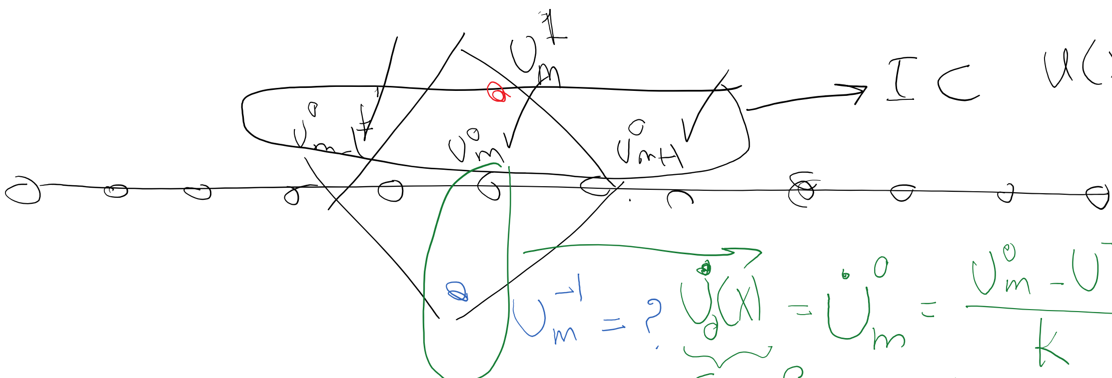
$$v_m^{n+1} = -v_m^{n-1} + 2(1-\bar{k}^2)v_m^n + \bar{k}^2(v_{m-1}^n + v_{m+1}^n) + r_m^n \tag{57b}$$

$$\bar{k} = \frac{kc}{h} \qquad \text{Normalized time step for hyperbolic wave equation} \tag{57c}$$

$n = 1$?

$n = 0$

$n = -1$



IC $u(x, t=0) = u_0(x)$

$$u_m^{-1} = ? \quad \underbrace{\dot{u}_0(x)}_{\text{IC for velocity}} = \dot{u}_m^0 = \frac{u_m^0 - u_m^{-1}}{k}$$

$$\boxed{u_m^{-1} = u_m^0 - k\dot{u}_m^0}$$

- Notice that this is a multi-step scheme, requiring the value of v_m^{n-1}.
- For $n = 0$ (solution of first time step after IC) we need v_m^{-1} which does not exist!
- The trick is using initial 1[st] value at time step 0 by backward time difference

$$\dot{u}(mh, 0) = \dot{u}_0(mh) = (\dot{u}_0)_m = \dot{v}(x = mh, 0) \approx \nabla_k[v_m^0] = \frac{v_m^0 - v_m^{-1}}{k} \quad \Rightarrow \tag{58a}$$

$$v_m^{-1} = v_m^0 - k(\dot{u}_0)_m = u_{0m} - k(\dot{u}_0)_m \tag{58b}$$

- Same process is applied to PDEs with higher temporal derivatives: by using initial temporal derivatives v_m^{-n} are formed.
- Similar to the parabolic case, and in contrast to the 1[st] order advection equation, this FTCS scheme is conditionally stable.
- The construction of implicit schemes is also straight forward. For example, by writing equations at time step $n+1$ rather than n and using backward time central space we obtain,

$$\frac{v_m^{n+1} + v_m^{n-1} - 2v_m^n}{k^2} - c^2\frac{v_{m+1}^{n+1} + v_{m-1}^{n+1} - 2v_m^{n+1}}{h^2} = r_m^n \quad \Rightarrow \tag{59a}$$

$$-\bar{k}^2 v_{m-1}^{n+1}(1 + 2\bar{k}^2)v_m^{n+1} - \bar{k}^2 v_{m+1}^{n+1} = -v_m^{n-1} + 2v_m^n + r_m^n \tag{59b}$$

$$\bar{k} = \frac{kc}{h} \qquad \text{As in } (\boxed{1a})\text{: normalized time step} \tag{59c}$$

2.2 Finite Volume (FV)

FV methods directly work with the balance law

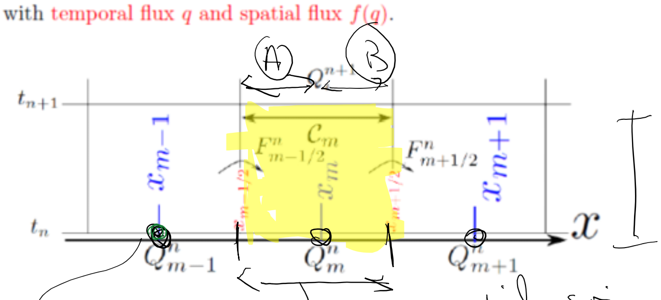
$$\dot{q} + f(q)_{,x} = r$$

1D

let's assume $r = 0$

- Consider the balance law with temporal flux q and spatial flux $f(q)$.

FVs are formed by half-distance between grid points & are extended by time step k



$k_n = t_{n+1} - t_n$

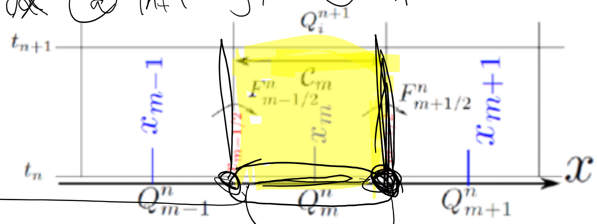
h_m = spatial size of cell m

similar to FD points

$$h_m = (A) + (B)$$
$$(A) = \frac{x_m - x_{m-1}}{2}$$
$$(B) = \frac{x_{m+1} - x_m}{2}$$

- Consider the balance law with temporal flux q and spatial flux $f(q)$.

$$\int_{t_n}^{t_{n+1}} \frac{d}{dt}\int q\,dx\;dt = \int q\,dx \;@\; t_{n+1} - \int q\,dx \;@\; t_n$$



Balance law corresponding to $\dot q + f(q)_{,x} = 0$ is $\boxed{\dot q = -f(q)_{,x}}$

$$\frac{d}{dt}\int_{C_m} q\,dx = -\left(f(q(x_{m+\frac{1}{2}},t)) - f(q(x_{m-\frac{1}{2}},t))\right)$$

integrate in time

$$\left(\int_{t_n}^{t_{n+1}}\left(\frac{d}{dt}\int_{C_m} q\,dx\right)dt = -\left(\int_{t_n}^{t_{n+1}} f(q(x_{m+\frac{1}{2}},t))\,dt - \int_{t_n}^{t_{n+1}} f(q(x_{m-\frac{1}{2}},t))\,dt\right)\right)\times\frac{1}{h_m}\cdot\frac{1}{K}$$

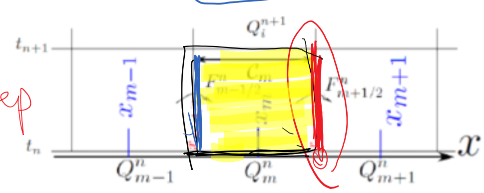
cell average at t_{n+1} | cell average @ t_n

$$\frac{1}{K}\left(\frac{1}{h_m}\int_{C_m} q\,dx\,\Big|_{t_{n+1}} - \frac{1}{h_m}\int_{C_m} q\,dx\,\Big|_{t_n}\right) = \frac{-1}{h_m}\left(\frac{1}{K}\int_{t_n}^{t_{n+1}} f(q(x_{m+\frac{1}{2}},t))\,dt - \frac{1}{K}\int_{t_n}^{t_{n+1}} f(q(x_{m-\frac{1}{2}},t))\,dt\right)$$

Q^{n+1}_m

average of q of the cell

time step n



$x_{m+\frac{1}{2}}$

$$\boxed{\begin{gathered} Q^{n+1}_m - Q^n_m = -\frac{K}{h_m}\left(F^n_{m+\frac{1}{2}} - F^n_{m-\frac{1}{2}}\right) \\ F^n_{m\pm\frac{1}{2}} = \frac{1}{K_n}\int_{t_n}^{t_{n+1}} f(q(x_{m\pm\frac{1}{2}},t))\,dt \end{gathered}}$$

cell average

average of spatial flux at $x_{m+\frac{1}{2}}$

average of spatial flux @ $x_{m-\frac{1}{2}}$

$$\boxed{Q^{n+1}_m = Q^n_m - \frac{K}{h_m}\left(F^n_{m+\frac{1}{2}} - F^n_{m-\frac{1}{2}}\right)}$$

known from previous step

How to calculate average spatial fluxes

$F^n_{m-\frac{1}{2}}$ & $F^n_{m+\frac{1}{2}}$

$$Q_m^{n+1} = Q_m^n - \frac{k}{h_m}(F^n_{m+1/2} - F^n_{m-1/2}), \text{ where} \tag{65a}$$

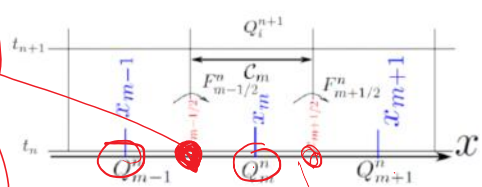
$$k = t_{n+1} - t_n \qquad \text{time step size (which can easily be nonuniform)} \tag{65b}$$

$$\underline{F^n_{m\pm1/2} \approx \frac{1}{k}\int_{t_n}^{t_{n+1}} f(q(x_{m\pm1/2}, t))\,\mathrm{d}t} \qquad \text{some approximation of the average flux along } x_{m\pm1/2} \tag{65c}$$

In explicit FV methods the average spatial flux is written as a function of Q values @ the beginning of the time step

$F^n_{m-\frac{1}{2}} = \mathcal{F}(Q^n_{m-1}, Q^n_m)$

$F^n_{m+\frac{1}{2}} = \mathcal{F}(Q^n_m, Q^n_{m+1})$



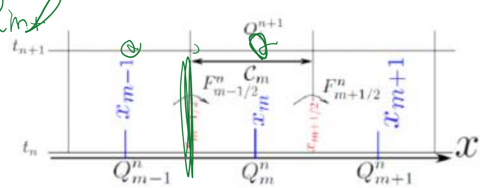
- For hyperbolic problems information propagates with finite speed, so it is reasonable to assume that we can obtain $F^n_{m-1/2}$ based on the values Q^n_{m-1} and Q^n_m: the cell averages on the two sides at the beginning of the time step,

$$F^n_{m-1/2} = \mathcal{F}(Q^n_{m-1}, Q^n_m), \qquad F^n_{m+1/2} = \mathcal{F}(Q^n_m, Q^n_{m+1}) \tag{66}$$

where $\mathcal{F}$ is some numerical flux function.

$F^n_{m-\frac{1}{2}} = \mathcal{F}(Q^{n+1}_{m-1}, Q^{n+1}_{m})$

Implicit



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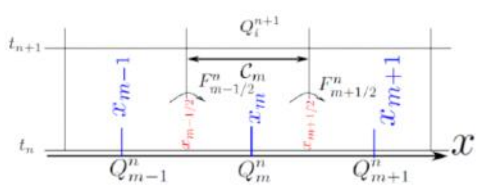
$$F^n_{m-1/2} = \mathcal{F}(Q^n_{m-1}, Q^n_m), \qquad F^n_{m+1/2} = \mathcal{F}(Q^n_m, Q^n_{m+1}) \tag{66}$$

where $\mathcal{F}$ is some numerical flux function.

Continuing with explicit scheme:



- For hyperbolic problems information propagates with finite speed, so it is reasonable to assume that we can obtain $F^n_{m-1/2}$ based on the values Q^n_{m-1} and Q^n_m: the cell averages on the two sides at the beginning of the time step,

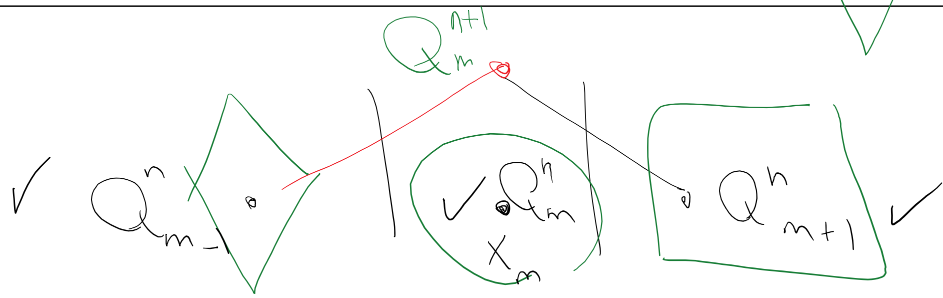
$$F^n_{m-1/2} = \mathcal{F}(Q^n_{m-1}, Q^n_m), \qquad F^n_{m+1/2} = \mathcal{F}(Q^n_m, Q^n_{m+1}) \tag{66}$$

where $\mathcal{F}$ is some numerical flux function.

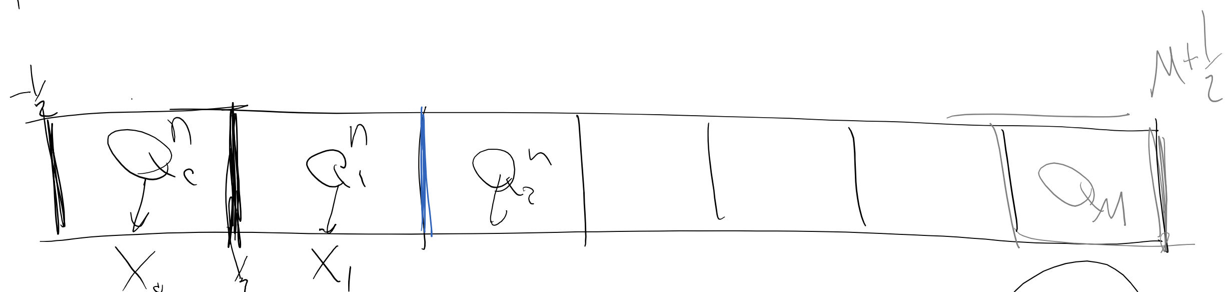
$$Q_m^{n+1} = Q_m^n - \frac{k}{h}\left(F^{n}_{m+\frac{1}{2}} - F^{n}_{m-\frac{1}{2}}\right)$$

$$\boxed{Q_m^{n+1} = Q_m^n - \frac{k}{h}\left(\mathcal{F}(Q_m^n, Q_{m+1}^n) - \mathcal{F}(Q_{m-1}^n, Q_m^n)\right)}$$

3 pt stencil



Balance property of FV methods



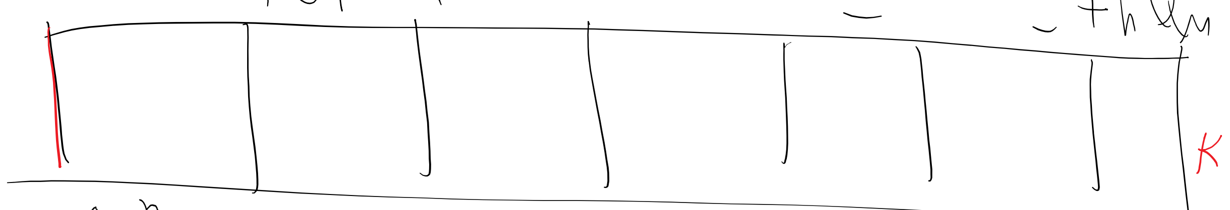
$h^0(Q_0^{n+1} - Q_0^n)$ $\quad h^1(Q_1^{n+1} - Q_1^n)$ $\quad h^M(Q_M^{n+1} - Q_M^n)$

$k(\cancel{F^n_{\frac{1}{2}}} - F^n_{-\frac{1}{2}})$ $= k(\cancel{F^n_{\frac{3}{2}}} - \cancel{F^n_{\frac{1}{2}}})$ $= k(F^n_{M+\frac{1}{2}} - F^n_{M-\frac{1}{2}})$

$h^0 Q_0^{n+1} + h^1 Q_1^{n+1} + \dots + h^M Q_M^{n+1}$

we get

$-kF^n_{-\frac{1}{2}}$

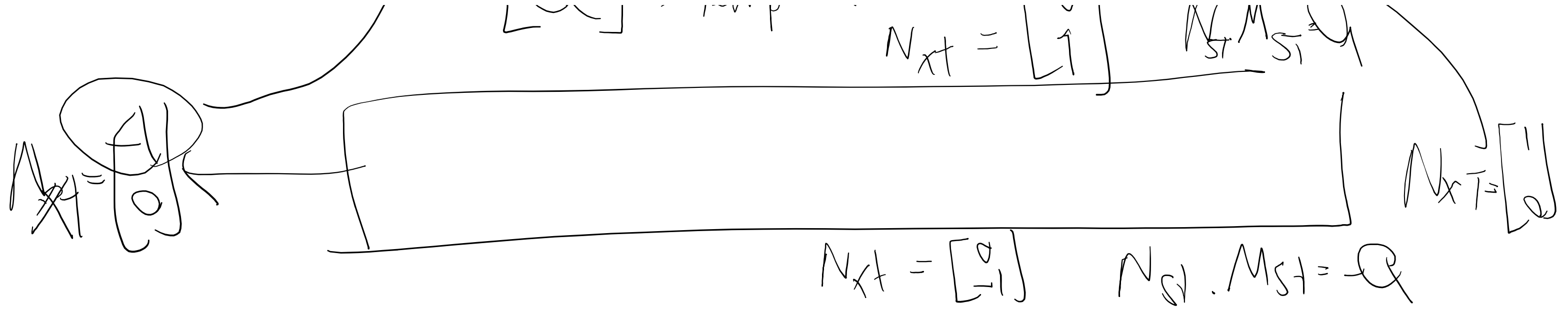


$-$ $\quad h^0 Q_0^n + h^1 Q_1^n + \dots + h^M Q_M^{n+1}$ $\quad kF^n_{M+\frac{1}{2}}$

this is the integral of spacetime flux over the boundary of these cells

$$M_{ST} = \begin{bmatrix} F \\ Q \end{bmatrix} \begin{matrix} \rightarrow \text{spatial} \\ \rightarrow \text{temporal} \end{matrix}$$

$N_{xt} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ $\quad N_{ST} M_{ST} = Q$



So, the nice thing is that each FV and the entire domain satisfy the balance law

Another advantage of FV over FD method is the flexibility in defining numerical flux F

2.2.2 FV examples from 1st order hyperbolic PDEs

- To illustrate the importance of numerical flux function (66) we consider three difference options.
- We consider the hyperbolic system (62),

$$q_{,t} + \{f(q)\}_{,x} = 0 \qquad \text{PDE} \qquad (70a)$$
$$q(x, t=0) = q_0(x) \qquad \text{IC} \qquad (70b)$$

- Specifically, we consider the linear case of (70a) which is the advection equation,

$$q_{,t} + a q_{,x} = 0 \qquad f(q) = aq \qquad (71)$$

where for simplicity it is assumed the wave speed $a(x,t) = a > 0$ is constant and positive. That is we consider a right-going wave. If $a(x,t)$ we get a source term of the form $-a_{,x}(x,t)q$ which is ignored here as it does not change the nature of the influence of different flux options (lower order derivatives).

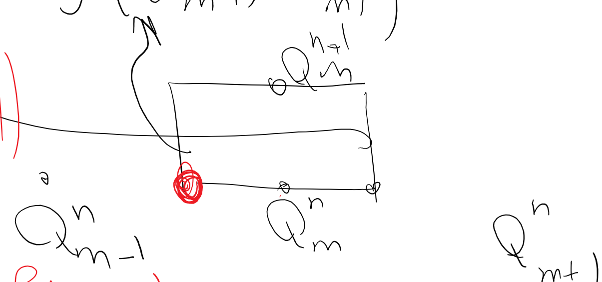
2.2.2.1 1. Average fluxes

- The average flux option means that we use the average of the fluxes from the two sides,

$$\mathcal{F}(Q^n_{m-1}, Q^n_m) = \frac{1}{2}\left(f(Q^n_{m-1}) + f(Q^n_m)\right) \qquad \Rightarrow \mathcal{F}(Q^n_m, Q^n_{m+1}) = \frac{1}{2}\left(f(Q^n_m) + f(Q^n_{m+1})\right)$$

$$Q^{n+1}_m = Q^n_m - \frac{k}{h}\left(\mathcal{F}(Q^n_m, Q^n_{m+1}) - \mathcal{F}(Q^n_{m-1}, Q^n_m)\right)$$

$$\mathcal{F}(Q^n_{m-1}, Q^n_m) = \frac{1}{2}\left(f(Q^n_{m-1}) + f(Q^n_m)\right)$$



$$Q^{n+1}_m = Q^n_m - \frac{k}{h}\left(\frac{1}{2}\left(\cancel{f(Q^n_m)} + f(Q^n_{m+1})\right) - \frac{1}{2}\left(\cancel{f(Q^n_m)} + f(Q^n_{m-1})\right)\right)$$

spatial flux $f(Q^n_{m-1})$ $f(Q^n_m)$

$$\boxed{Q^{n+1}_m = Q^n_m - \frac{k}{2h}\left(f(Q^n_{m+1}) - f(Q^n_{m-1})\right)} \quad 1$$

Update eqn for average flux

Update eqn for average flux

Advection eqn $q_t + a q_{,x} = 0$ $\quad \boxed{f(q) = aq}$ plug in (1)

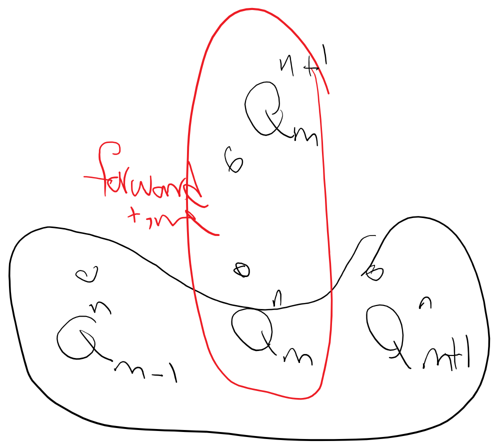
$$\boxed{Q_m^{n+1} = Q_m^n - \frac{ka}{2h}\left(Q_{m+1}^n - Q_{m-1}^n\right)}$$

can write it as

$$\frac{Q_m^{n+1} - Q_m^n}{k} + a\left(\frac{Q_{m+1}^n - Q_{m-1}^n}{2h}\right) = 0$$

forward time

Central Space



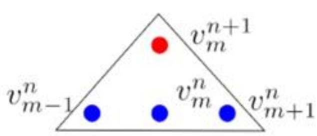
FV for advection equation with average fluxes is the same as FD with CSFT difference scheme.
Is this scheme stable (conditionally stable)

Unfortunately, this is UNCONDITIONALLY UNSTABLE.

- Specifically, if we consider the simple linear advection PDE (71), equation (74) becomes,

$$\frac{Q_m^{n+1} - Q_m^n}{k} + a\frac{Q_{m+1}^n - Q_{m-1}^n}{2h_m} = 0 \qquad (75)$$

which is forward-time, central-space (FTCS) scheme discussed in (27c). As discussed under (34) this scheme is unconditionally unstable!



- So simply using the average fluxes not only may affect the accuracy (compared to correct fluxes) may also render the method unstable!

2.2.2.2 2. Lax-Friedrichs fluxes

- To simplify the discussion, we assume that the spatial grid is uniform (extensions to nonuniform can be done easily).
- To address the problem with average fluxes, Lax-Friedrichs fluxes modify them by adding a jump part of q values.

$$\mathcal{F}(Q_{m-1}^n, Q_m^n) = \frac{1}{2}\left(f(Q_{m-1}^n) + f(Q_m^n)\right) - \frac{h}{2k}\left(Q_m^n - Q_{m-1}^n\right) \quad \Rightarrow \qquad (76a)$$

$$\mathcal{F}(Q_m^n, Q_{m+1}^n) = \frac{1}{2}\left(f(Q_m^n) + f(Q_{m+1}^n)\right) - \frac{h}{2k}\left(Q_{m+1}^n - Q_m^n\right) \qquad (76b)$$

$$Q_m^{n+1} = Q_m^n - \frac{k}{h}\left(F(Q_m^n, Q_{m+1}^n) - F(Q_{m-1}^n, Q_m^n)\right) =$$

$$Q_m^n - \frac{k}{h}\left(\underbrace{\frac{1}{2}\left(f(Q_{m+1}^n) - f(Q_{m+1}^n)\right)}_{\text{already did this}} - \frac{h}{2k}\left(Q_{m+1}^n - Q_m^n\right) + \frac{h}{2k}\left(Q_m^n - Q_{m-1}^n\right)\right)$$

$$Q_m^{n+1} = Q_m^n - \frac{k}{2h}\left(f(Q_{m+1}^n) - f(Q_{m-1}^n)\right) \qquad \left(Q_{m+1}^n + Q_{m-1}^n - 2Q_m^n\right)$$

$$\boxed{Q_m^{n+1} = Q_m^n - \frac{k}{2h}\left(f(Q_{m+1}^n) - f(Q_{m-1}^n)\right) + \left(\frac{Q_{m+1}^n + Q_{m-1}^n - 2Q_m^n}{2}\right)}$$

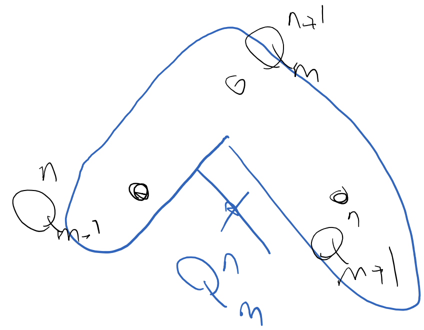
(2a)

$$Q_m^{n+1} = \frac{Q_{m+1}^n + Q_{m-1}^n}{2} - \frac{k}{2h}\left(f(Q_{m+1}^n) - f(Q_{m-1}^n)\right)$$

for advection eqn $\quad f(Q) = aQ$

$$Q_m^{n+1} = \frac{Q_{m+1}^n + Q_{m-1}^n}{2} - \frac{ka}{2h}\left(Q_{m+1}^n - Q_{m-1}^n\right)$$

$$\frac{Q_m^n - \frac{Q_{m+1}^n + Q_{m-1}^n}{2}}{k} + \frac{Q_{m+1}^n - Q_{m-1}^n}{2h} = 0$$



Similar to central Space Forward time

but $\quad Q_m^n \longrightarrow \dfrac{Q_{m-1}^n + Q_{m+1}^n}{2}$

the same exact Lax Friedrichs FD scheme we covered before

I mentioned before that this scheme is conditionally stable.

$$f(Q) = aQ$$

(2a)

$$\boxed{Q_m^{n+1} = Q_m^n - \frac{k}{2h}\left(f(Q_{m+1}^n) - f(Q_{m-1}^n)\right) + \left(\frac{Q_{m+1}^n + Q_{m-1}^n - 2Q_m^n}{2}\right)}$$

$$\frac{Q_m^{n+1} - Q_m^n}{k} = -a\left(\frac{Q_{m+1}^n - Q_{m-1}^n}{2h}\right) + \frac{h^2}{k}\left(\frac{Q_{m+1}^n + Q_{m-1}^n - 2Q_m^n}{h^2}\right)$$

$$Q_{,t} = -aQ_{,x} + \frac{h^2}{k} Q_{,xx}$$

We are really solving

$$\overline{\left| Q_{,t} + \underbrace{aQ_{,x}}_{\text{advection}} - \frac{h^2}{k} Q \quad = 0 \right|}$$

Numerical Diffusion ← added

advection

$$\boxed{Q_{,t} + aQ_{,x} - \frac{h^2}{k} Q_{,xx} = 0}$$

added diffusion

Original eqn $\boxed{Q_{,t} + aQ_{,x} = 0}$

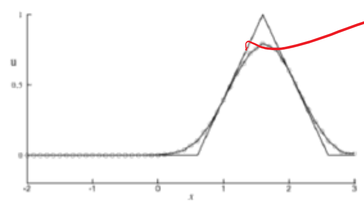


Figure 1.6. *A solution of the Lax–Friedrichs scheme,* $\lambda = 0.8$.

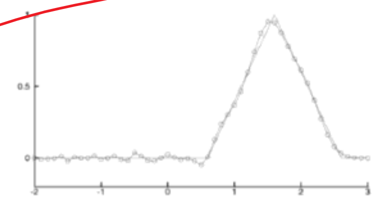


Figure 1.8. *A solution computed with leapfrog scheme,* $\lambda = 0.8$.