1 Considered hyperbolic PDEs.

Wave equation $$\frac{\partial^2 u(\vec{r},t)}{\partial t^2} = c^2 \nabla^2 u(\vec{r},t)$$

$$u(x,t) = \exp(i(kx - \omega t)) \qquad \omega = \pm ck$$

No dispersion (ω/k = const), no diffusion (ω real).

Method of lines. Second-order discretization for the 2nd derivative.

$$\frac{d^2 u_m}{dt^2} = c^2 \frac{u_{m+1} - 2u_m + u_{m-1}}{h^2}$$

Newton's equations of motion. Can use any ODE method stable for solutions of the form $\sim e^{i\omega t}$ with real ω. E.g., Euler does not work, but Verlet does.

$$\frac{u_m^{n+1} - 2u_m^n + u_m^{n-1}}{\tau^2} = c^2 \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{h^2}$$

Stable for $\alpha = \frac{c\tau}{h} \leq 1.$

Courant-Friedrichs-Lewy condition.

1^{st} order equations: $$\frac{\partial u(x,t)}{\partial t} = c\frac{\partial u(x,t)}{\partial x}$$

In free space, $u(x,t) = f(x+ct)$. $u(x,t) = \exp(i(kx-\omega t))$ $\omega = -ck$

Generalized to systems $$\frac{\partial \vec{u}(x,t)}{\partial t} = \boldsymbol{A}\frac{\partial \vec{u}(x,t)}{\partial x}$$ As part of the definition of hyperbolicity, **A** is diagonalizable and all its eigenvalues are real. Then get a set of decoupled 1^{st}-order equations.

The 2^{nd}-order wave equation can be transformed into this form.

$$\frac{\partial r}{\partial t} = c\frac{\partial s}{\partial x} \quad \Rightarrow \quad \frac{\partial^2 r}{\partial t^2} = c\frac{\partial^2 s}{\partial x \partial t}$$

$$\frac{\partial s}{\partial t} = c\frac{\partial r}{\partial x} \quad \Rightarrow \quad \frac{\partial^2 s}{\partial t \partial x} = c\frac{\partial^2 r}{\partial x^2}$$

$$\Rightarrow \quad \frac{\partial^2 r}{\partial t^2} = c^2\frac{\partial^2 r}{\partial x^2}$$

3 But such 1st order systems often arise directly in physics problems.

Consider Maxwell's equations $\frac{\partial \vec{B}}{\partial t} = -c \nabla \times \vec{E}$ and $\frac{\partial \vec{E}}{\partial t} = c \nabla \times \vec{B} - 4\pi \vec{J}$

Considering propagation along *x*, with $\vec{E} \parallel y$ and $\vec{B} \parallel z$, and assuming $\vec{J} = 0$,

$$\frac{\partial B}{\partial t} = -c \frac{\partial E}{\partial x} \qquad \frac{\partial E}{\partial t} = -c \frac{\partial B}{\partial x}$$

For acoustic waves in a fluid, $\rho_0 \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x}$

Continuity equation $\frac{\partial \rho}{\partial t} = -\rho_0 \frac{\partial v}{\partial x}$ Compressibility $\beta = \frac{1}{\rho} \frac{d\rho}{dp}$

$$\rho_0 \beta \frac{\partial p}{\partial t} = -\rho_0 \frac{\partial v}{\partial x} \Rightarrow \beta \frac{\partial p}{\partial t} = -\frac{\partial v}{\partial x}$$

$$\frac{\partial u(x,t)}{\partial t} = c\,\frac{\partial u(x,t)}{\partial x}$$

$$\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=x_m} \approx \beta\,\frac{u_{m+1}(t)-u_m(t)}{h} + (1-\beta)\,\frac{u_m(t)-u_{m-1}(t)}{h}\,.$$

β = 0 – left difference; β = 1 – right difference; β = 1/2 – centred difference.

$$\frac{d\,u_m(t)}{dt} = c\left[\beta\,\frac{u_{m+1}(t)-u_m(t)}{h} + (1-\beta)\,\frac{u_m(t)-u_{m-1}(t)}{h}\right] \qquad \gamma \equiv 2\beta - 1$$

$$= c\left[\frac{u_{m+1}(t)-u_{m-1}(t)}{2h} + \gamma\,\frac{u_{m+1}(t)-2u_m(t)+u_{m-1}(t)}{2h}\right]$$

Numerical diffusion.

5 $$\frac{d\,u_m(t)}{dt} \to \frac{u^{n+1}-u^n}{\tau}$$ Forward difference.

$$u_m^{n+1}=u_m^n+\alpha\left[\frac{u_{m+1}^n-u_{m-1}^n}{2}+\gamma\frac{u_{m+1}^n-2u_m^n+u_{m-1}^n}{2}\right] \qquad \alpha=\frac{c\tau}{h}$$

$\gamma=0.$ Centred difference. Unconditionally unstable, unlike parabolic.

Upwind schemes:

$\gamma=-1.$ $u_m^{n+1}=u_m^n+\alpha\left[u_m^n-u_{m-1}^n\right].$ Left difference. Stable for $-1\le\alpha\le 0$

$\gamma=1.$ $u_m^{n+1}=u_m^n+\alpha\left[u_{m+1}^n-u_m^n\right].$ Right difference. Stable for $0\le\alpha\le 1$

Lax-Friedrichs scheme:

$\gamma=1/\alpha.$ $$u_m^{n+1}=\frac{u_{m+1}^n+u_{m-1}^n}{2}+\alpha\frac{u_{m+1}^n-u_{m-1}^n}{2}$$ Stable for $-1\le\alpha\le 1$

These are 1st order in time and space. Damping is quite high.

Lax-Wendroff scheme

$$\gamma=\alpha. \quad u_m^{n+1}=u_m^n+\alpha\left[\frac{u_{m+1}^n-u_{m-1}^n}{2}+\alpha\frac{u_{m+1}^n-2u_m^n+u_{m-1}^n}{2}\right]$$ Stable for $-1\le\alpha\le 1$

2^{nd} order in space and time. Can be viewed as quadratic interpolation.

$$u_m^{n+1}\approx u_m^n+\tau\left.\frac{\partial u}{\partial t}\right|_{x_m,t_n}+\frac{\tau^2}{2}\left.\frac{\partial^2 u}{\partial t^2}\right|_{x_m,t_n}=u_m^n+c\tau\left.\frac{\partial u}{\partial x}\right|_{x_m,t_n}+\frac{c^2\tau^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_m,t_n}$$

In principle, this can be repeated for other equations (e.g., nonlinear). But there are other, universal approaches that I will mention.

Beam-Warming – an upwind scheme based on the same principle.

Fromm – a combination of Lax-Wendroff and Beam-Warming.

7 Another, more straightforward way of getting a 2nd order scheme:

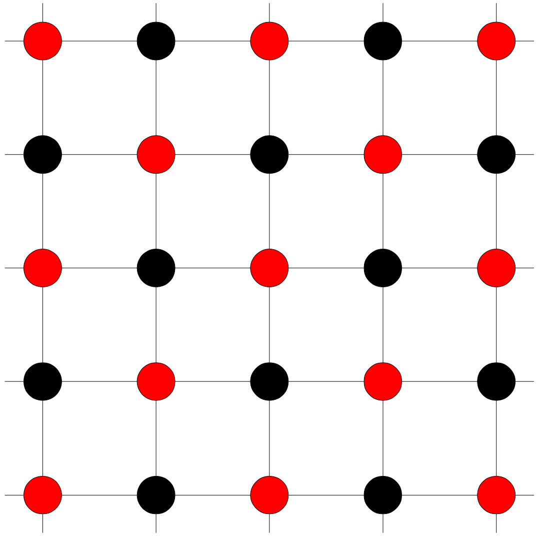
Centred-time, centred-space discretization

Unstable for the diffusion equation, but OK for the Schrödinger equation

$$\frac{u_m^{n+1}-u_m^{n-1}}{\tau}=c\,\frac{u_{m+1}^{n}-u_{m-1}^{n}}{h}$$ – leapfrog

$$u_m^{n+1}-u_m^{n-1}=\alpha\left(u_{m+1}^{n}-u_{m-1}^{n}\right) \qquad u_m^n=\exp\left(i\left(khm-\omega n\tau\right)\right)$$

$$-2i\sin(\omega\tau)=2i\alpha\sin(kh) \;\Rightarrow\; \sin(\omega\tau)=-\alpha\sin(kh)$$



Stable for $|\alpha|\leq 1,$ no dissipation in this case.

Generalized straightforwardly to nonlinear equations. But since red sites are only coupled to red sites and black to black, an instability can develop. Introduce a bit of numerical diffusion.

Recall that for the electromagnetic field

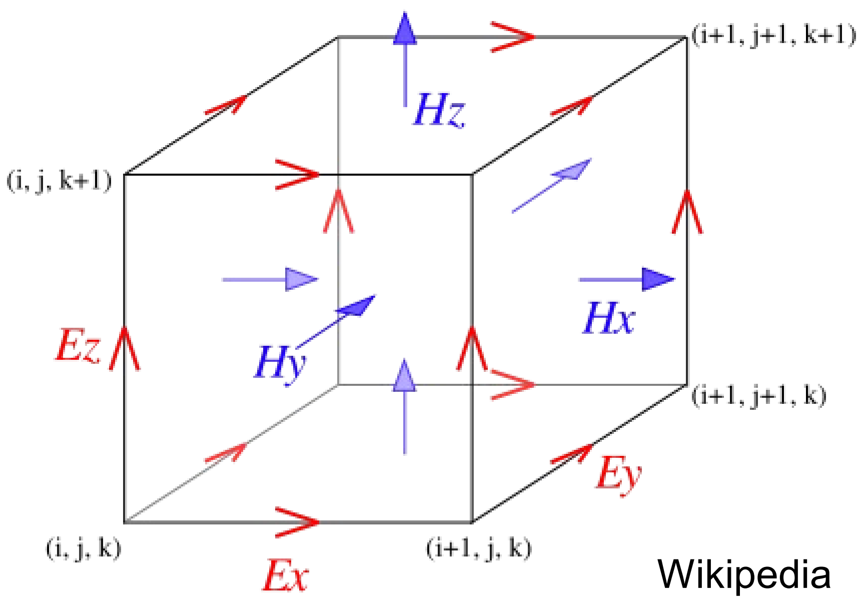
$$\frac{\partial B}{\partial t} = -c\frac{\partial E}{\partial x} \qquad \frac{\partial E}{\partial t} = -c\frac{\partial B}{\partial x}$$

$$B_m^{n+1/2} - B_m^{n-1/2} = -\frac{c\tau}{h}\left(E^n_{m+1/2} - E^n_{m-1/2}\right) \qquad E_m^{n+1/2} - E_m^{n-1/2} = -\frac{c\tau}{h}\left(B^n_{m+1/2} - B^n_{m-1/2}\right)$$

Shift:

$$B_{m+1/2}^{n+1/2} - B_{m+1/2}^{n-1/2} = -\frac{c\tau}{h}\left(E^n_{m+1} - E^n_{m}\right) \qquad E_m^{n+1} - E_m^{n} = -\frac{c\tau}{h}\left(B^{n+1/2}_{m+1/2} - B^{n+1/2}_{m-1/2}\right)$$

B and E are determined at points staggered in space and in time.



Wikipedia

Finite-difference time-domain (FDTD) method

Yee, 1966

Amplification factors for different methods

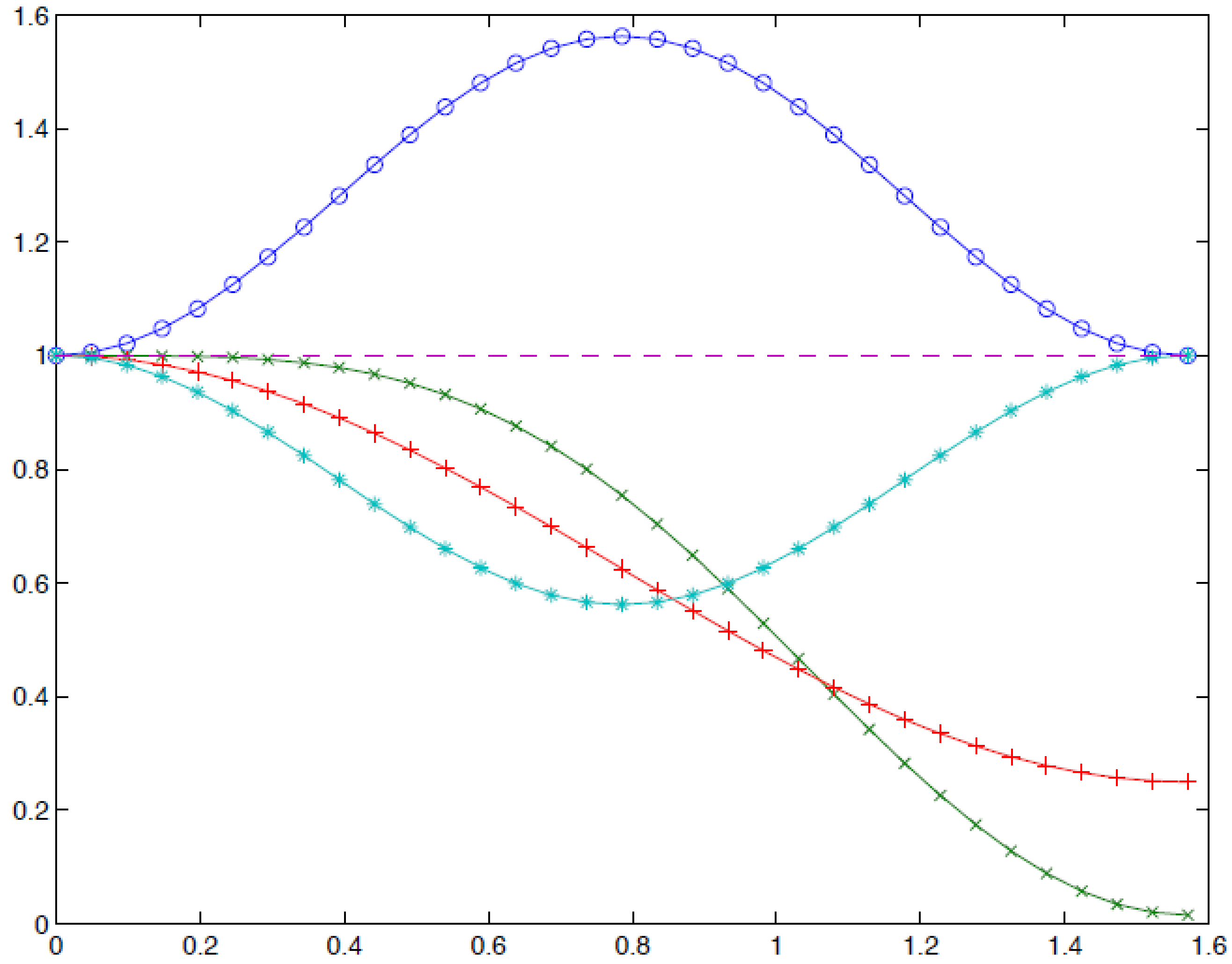


Figure 6.3.1: Magnitudes of the amplification factors when $\alpha = 0.75$ as functions of $\theta = k\pi/J$ for the centered (o), Lax-Wendroff (x), upwind (+), Lax-Friedrichs (*), and leap frog $(--)$ schemes.

Dispersion for different methods

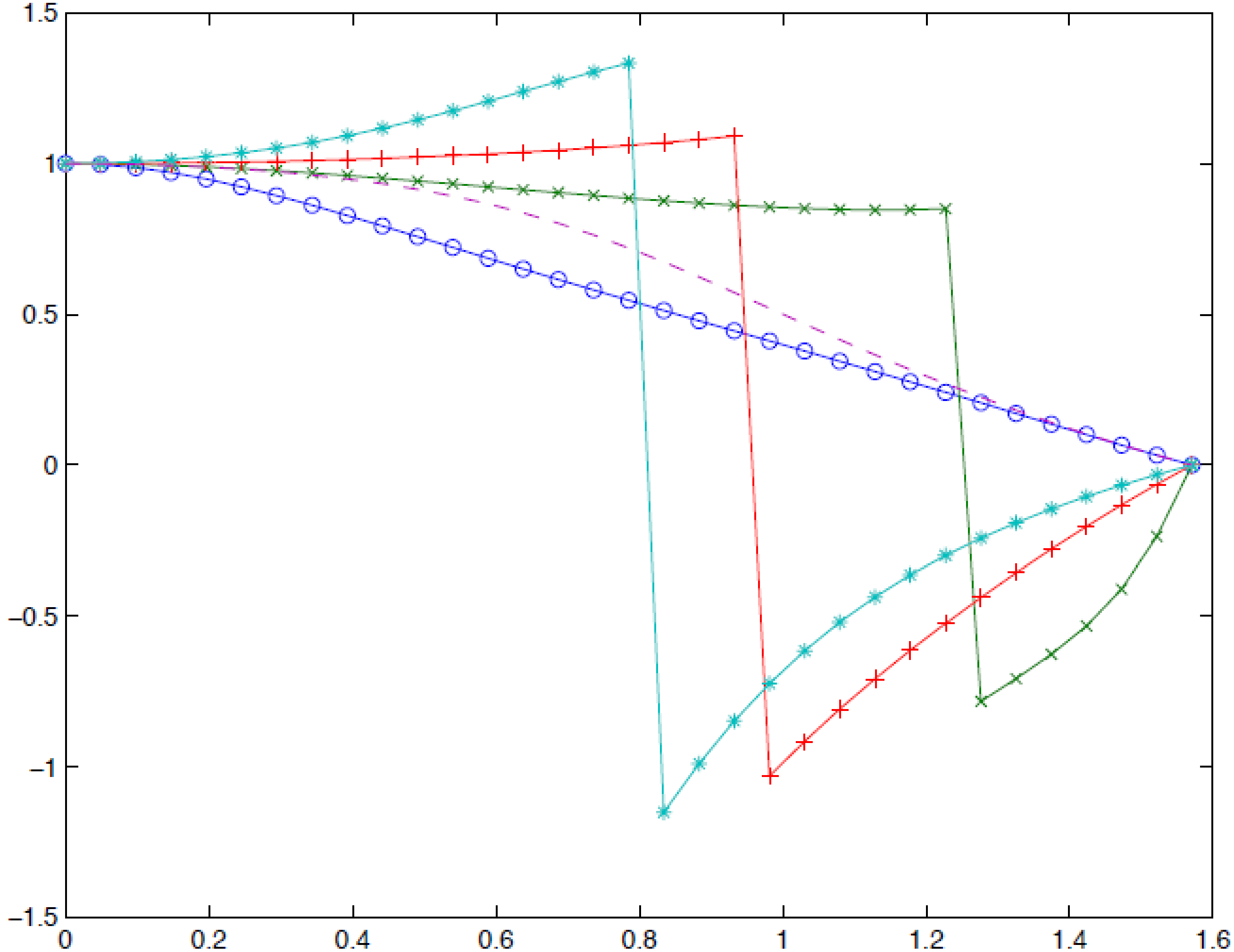
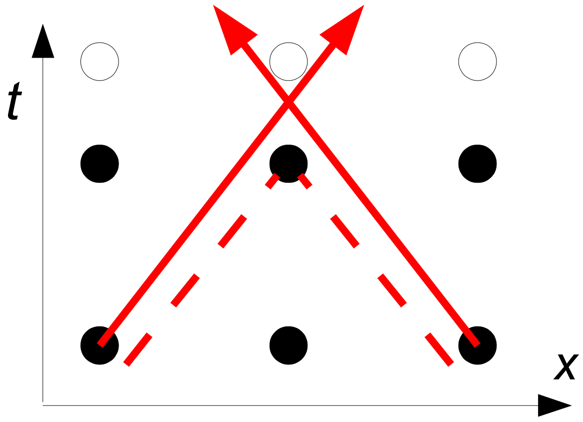


Figure 6.3.2: Normalized phase speeds γ_k/a when $\alpha = 0.75$ as functions of $\theta = k\pi/J$ for the centered (o), Lax-Wendroff (x), upwind (+), Lax-Friedrichs (*), and leap frog (−−) schemes.



$$\alpha = \frac{c\tau}{h} \le 1.$$

Much less stringent condition than we had for explicit methods for the diffusion equation ($\tau \sim h^2$).

For this reason, using implicit methods is not justified for the simple non-dispersive wave equation (2nd or 1st order). However, the situation may be different for other wave equations.

$$\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3} \qquad u(x,t) = \exp(i(kx - \omega t)) \qquad -i\omega = i^3 k^3 \;\Rightarrow\; \omega = k^3$$

For grid step h the largest possible $k \sim 1/h \;\Rightarrow$ the largest $\omega \propto 1/h^3$.

Then $\tau \sim 1/\omega \sim h^3$. For these situations implicit methods do make sense.

E.g., Crank-Nicolson constructed by analogy with the parabolic case.

Nonlinear problems

Equations arising from conservation laws

If there is some quantity *u*(*x*,*t*) such that $\int u(x,t)\,dx$ is constant, and the flux of that quantity through point *x* is given by *F*(*u*(*x*,*t*)), then *u*(*x*,*t*) obeys

$$\frac{\partial u(x,t)}{\partial t}+\frac{\partial F(u(x,t))}{\partial x}=0$$

More generally,

$$\frac{\partial \vec{u}(x,t)}{\partial t}+\frac{\partial \vec{F}(\vec{u}(x,t))}{\partial x}=0$$

Example 1: 1D Maxwell's equations can be written in this form, if

$$\vec{u}=\begin{pmatrix}\vec{E}\\ \vec{B}\end{pmatrix},\ \vec{F}=\begin{pmatrix}-c\,\vec{B}\\ -c\,\vec{E}\end{pmatrix}$$

Example 2: momentum conservation for a fluid – Burgers' equation

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=0$$

13 Example 3: a toy model of traffic flow. Car density ρ, velocity *u*.

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0 \qquad u(\rho)=u_0(1-\rho/\rho_{\max})$$

Example 4: diffusion equation, if $F=-D\frac{\partial \rho}{\partial x}$

$$\frac{\partial \rho}{\partial t}-\frac{\partial}{\partial x}\left(D\frac{\partial \rho}{\partial x}\right)=0$$

We won't consider this.

$$\frac{\partial u(x,t)}{\partial t}+\frac{\partial F(u(x,t))}{\partial x}=0$$

Rewrite as $\frac{\partial u}{\partial t}+c(u)\frac{\partial u}{\partial x}=0$

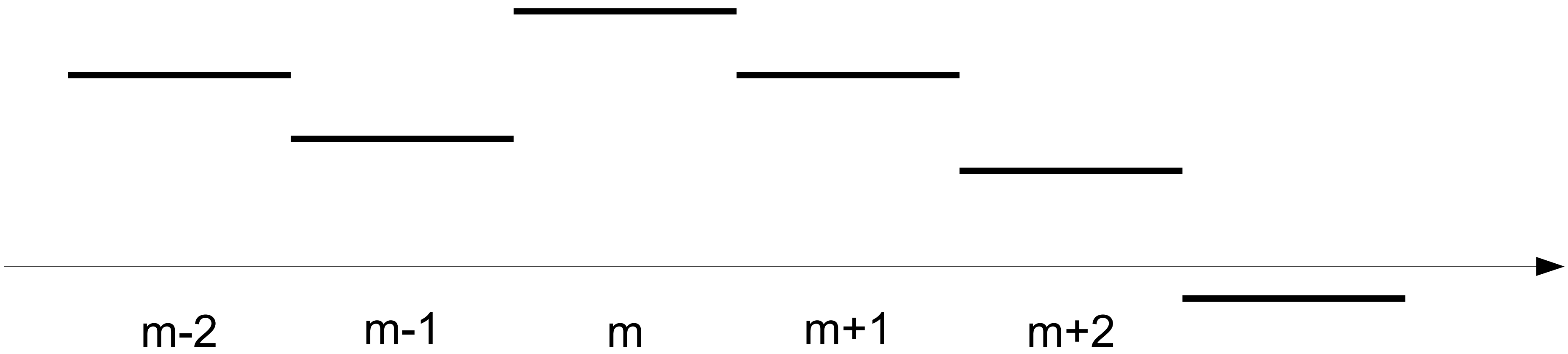
Consider an arbitrary curve *x*(*t*). The change of *u* along this curve is

$$\frac{du}{dt}=\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}\frac{dx}{dt}$$

This is zero if $\frac{dx}{dt}=c(u)$. These lines are characteristics.

Along them $u=\text{const} \Rightarrow c(u)=\text{const} \Rightarrow \text{straight lines}$

For conservation laws we can derive algorithms using the finite volume approach.



Linear case (c = const > 0). $F_{m-1/2} = c u_{m-1}$ $F_{m+1/2} = c u_m$

$$\frac{\left(u_m^{n+1} - u_m^n\right) h}{\tau} = F_{m-1/2} - F_{m+1/2} = c\left(u_{m-1} - u_m\right)$$

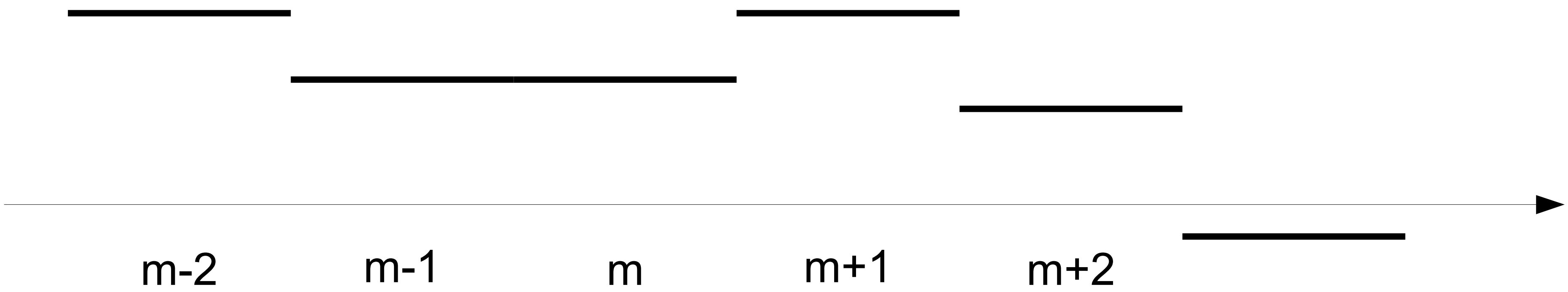
Linear case (c = const < 0). $F_{m-1/2} = c u_m$ $F_{m+1/2} = c u_{m+1}$

$$\frac{\left(u_m^{n+1} - u_m^n\right) h}{\tau} = F_{m-1/2} - F_{m+1/2} = c\left(u_m - u_{m+1}\right)$$

Upwind scheme

For arbitrary c, $F_{m+1/2} = \frac{1}{2} c\left(u_{m+1} + u_m\right) - \frac{1}{2}|c|\left(u_{m+1} - u_m\right)$

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=0$$



In the nonlinear case, $$F_{j+1/2}=\frac{1}{2}(f_{j+1}+f_j)-\frac{1}{2}\left|\frac{f_{j+1}-f_j}{u_{j+1}-u_j}\right|(u_{j+1}-u_j)$$

Other schemes, e.g., Lax-Wendroff, can also be derived as conservative schemes.

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=0$$

Two-stage nonlinear extensions of Lax-Wendroff

Linear Lax-Wendroff is unique in the sense of being the only possible 1-step 2nd-order scheme (leapfrog is 2-step). But in the nonlinear case different extensions are possible.

1. Lax-Wendroff-Richtmyer (aka “2-step Lax-Wendroff” - more properly, 2-stage). Lax-Friedrichs + leapfrog.

$$u_{m+1/2}^{n+1/2}=\frac{u_{m+1}^{n}+u_{m}^{n}}{2}+\frac{\tau}{h}\frac{f_{m+1}^{n}-f_{m}^{n}}{2}$$

$$\frac{u_{m}^{n+1}-u_{m}^{n}}{\tau}=\frac{f_{m+1/2}^{n+1/2}-f_{m-1/2}^{n+1/2}}{h}$$

In the linear case ($f = cu$), $$u_{m}^{n+1}=u_{m}^{n}+\alpha\left(\frac{u_{m+1}^{n}-u_{m-1}^{n}}{2}+\alpha\frac{u_{m+1}^{n}-2u_{m}^{n}+u_{m-1}^{n}}{2}\right)$$

(Lax-Wendroff)

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=0$$

2. MacCormack method: (FTFS+BTBS)/2

$$\tilde{u}_m^{n+1}=u_m^n-\frac{\tau}{h}\left(f_{m+1}^n-f_m^n\right)$$

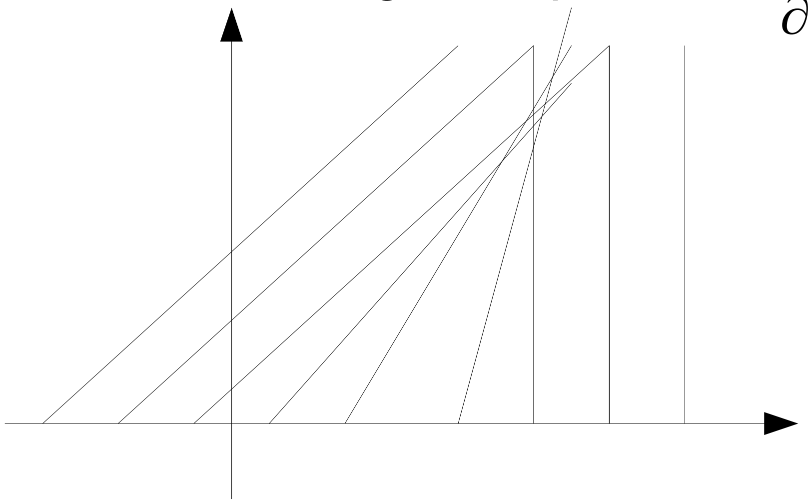
$$\tilde{\tilde{u}}_m^{n+1}=u_m^n-\frac{\tau}{h}\left(\tilde{f}_m^{n+1}-\tilde{f}_{m-1}^{n+1}\right)$$

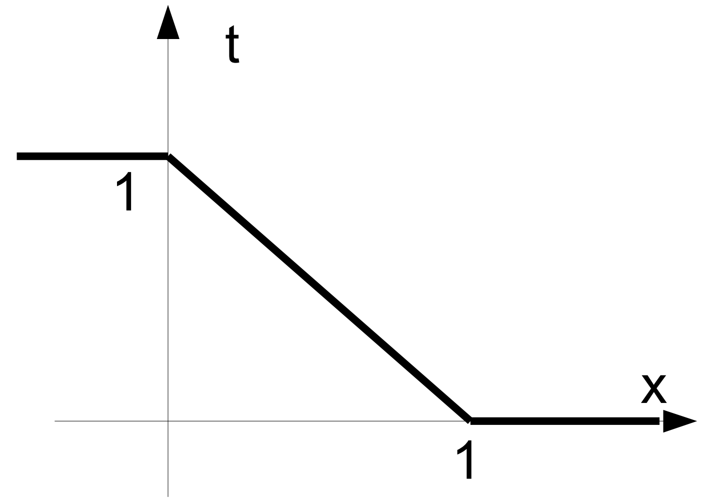
$$u_m^{n+1}=\frac{1}{2}\left(\tilde{u}_m^{n+1}+\tilde{\tilde{u}}_m^{n+1}\right)$$

The first stage by itself would be unstable for f ' > 0, but the second stage compensates.

Can be reversed: FTBS, then BTFS.

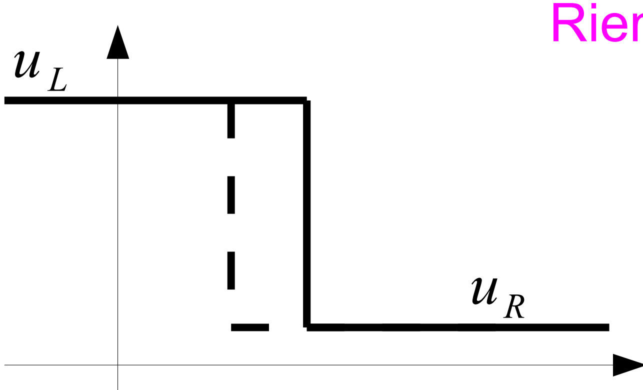
18 Consider Burgers' equation $$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=0$$





Lines cross at t = 1 – ambiguity. Does not make sense. An infinitely sharp jump (or a shock wave).

What happens next? The shock wave propagates. The equation does not make sense anymore, but the conservation law does.



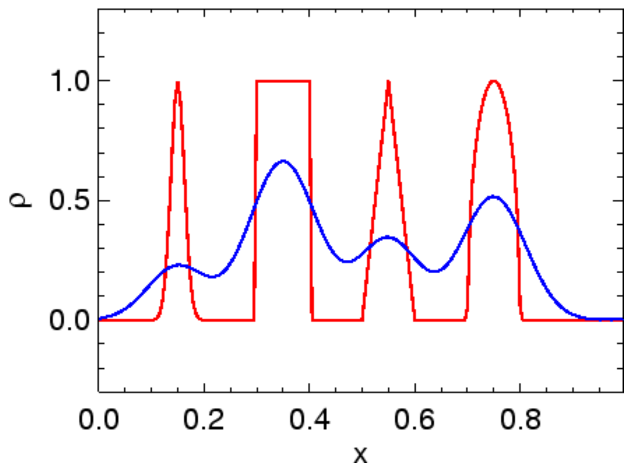
Riemann problem

$$(u_L-u_R)\Delta x=\left(\frac{u_L^2}{2}-\frac{u_R^2}{2}\right)\Delta t$$

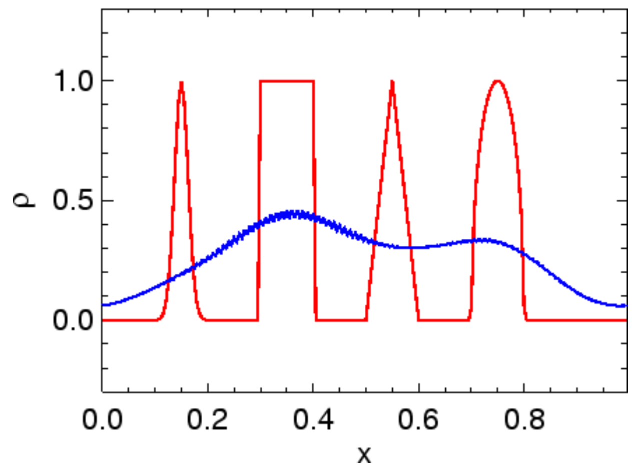
$$\frac{\Delta x}{\Delta t}=\frac{u_L+u_R}{2}$$

19 So it is very desirable to have methods that are able to reproduce and propagate shocks correctly

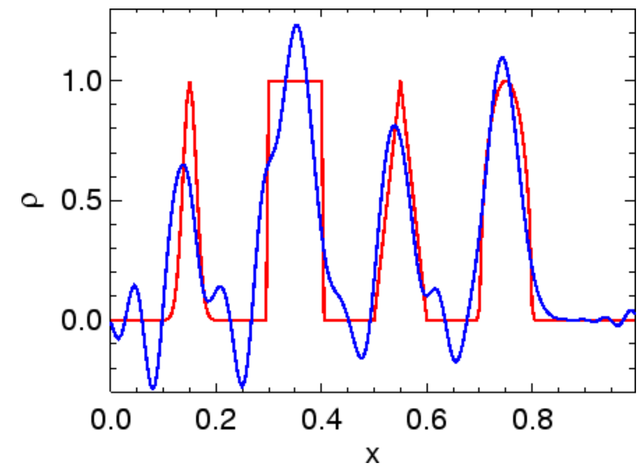
Some results for the simple linear case (200 grid points, 500 time steps, α = 0.4): http://www.astro.uu.se/~bf/course/numhd_course/



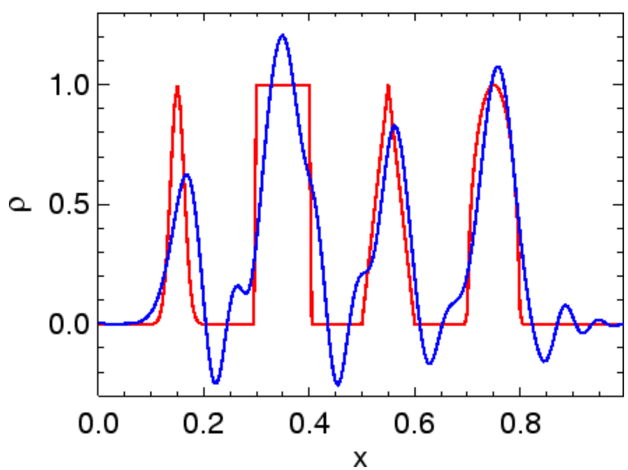
Upwind



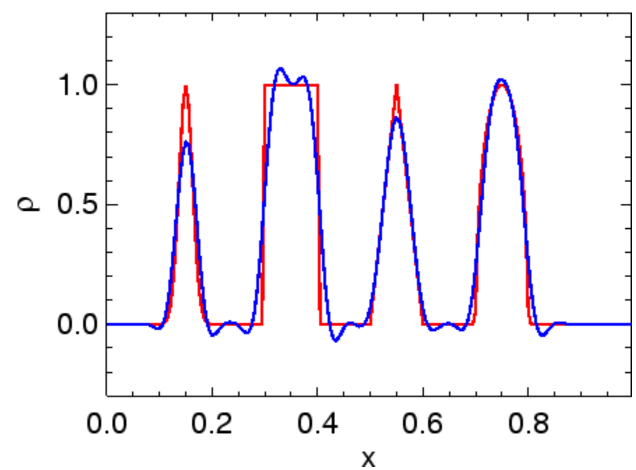
Lax-Friedrichs



Lax-Wendroff



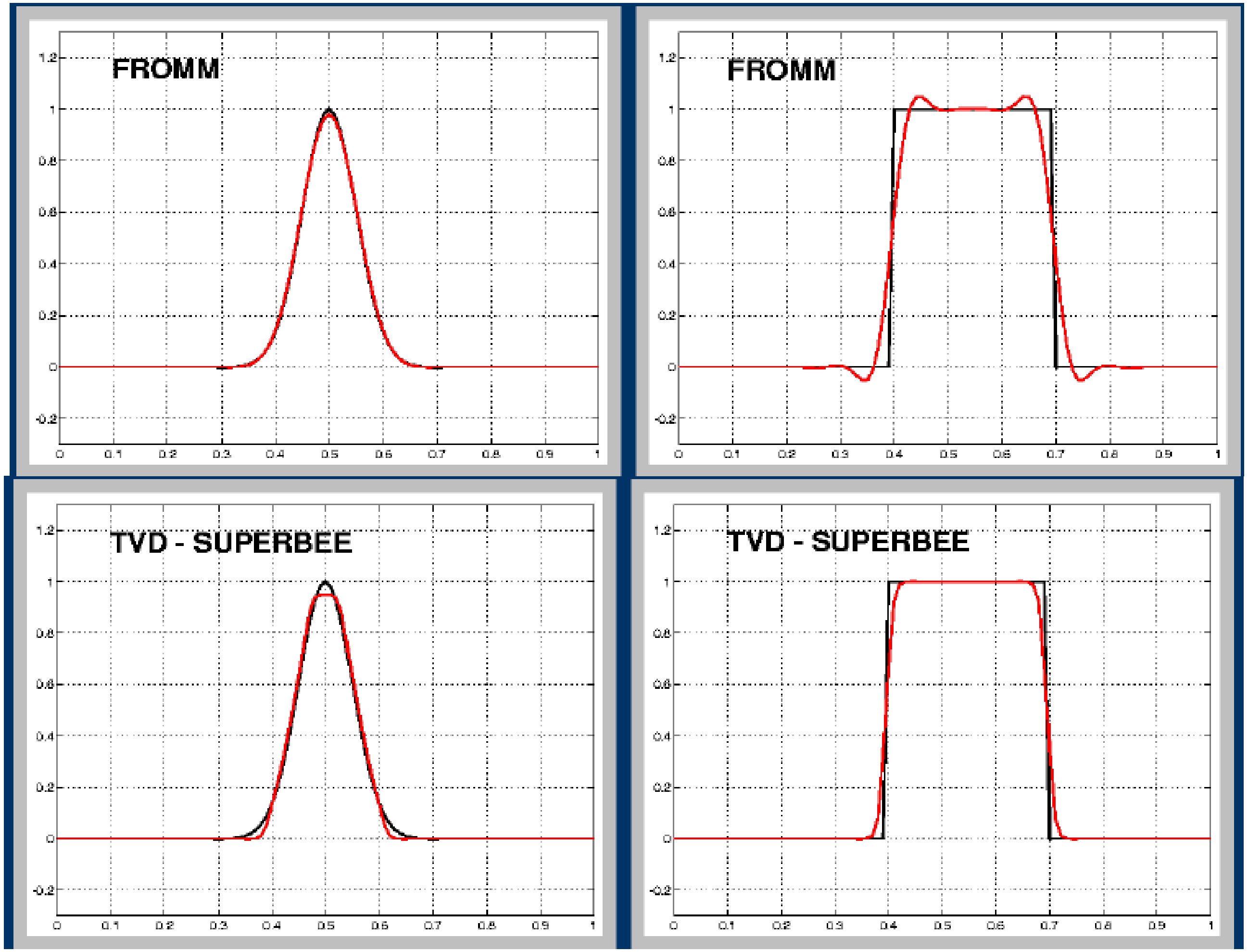
Beam-Warming



Fromm

20 Godunov's theorem: there are no linear methods of order >1 that are "monotone" (meaning they don't produce extra peaks).

Nonlinear flux limiters interpolating between Lax-Wendroff for smooth functions and upwind for "nasty" functions.



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