

Lecture 6

Paul Andries Zegeling

Department of Mathematics, Utrecht University

Numerical Methods for Time-Dependent PDEs

Outline of Lecture 6

- ⌈ exercises of Lecture 5
- ⌋ nonlinear hyperbolic PDEs
- ⌈ CFL-condition
- ⌋ wave equation
- ⌈ CTCS
- ⊕ extra IC & CFL-condition
- ⌋ outlook to Lecture 7

CFL condition [1]

CFL - condition ¹⁹²⁸
 Courant-Friedrichs-Lewy

stability $\sigma = \frac{c \Delta t}{\Delta x}$ chosen such that "domain of dependence" of PDE (characteristic lines)

\subset "domain of dependence" of FD-scheme

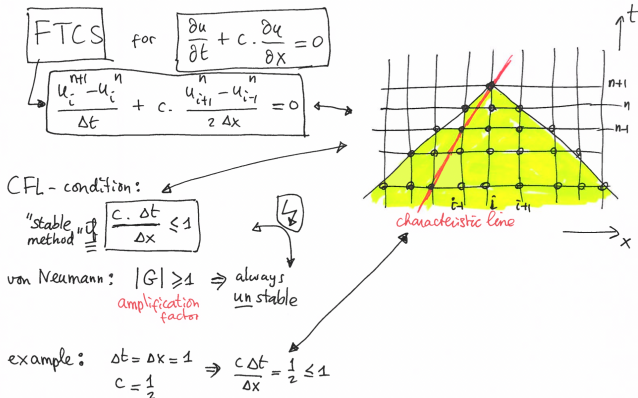
\Leftrightarrow FD-scheme must include all physical information which influences the system at (z_i, t^{nn})

$\sigma = \frac{c \Delta t}{\Delta x}$ "CFL-number"

The diagrams illustrate the CFL condition on a grid with time t on the vertical axis and space z on the horizontal axis. The grid spacing is Δx and Δt .

- Left Diagram (STABLE):** A blue line represents a characteristic line of the PDE. A red shaded region represents the numerical domain of dependence. The characteristic line is within the numerical domain, meaning the FD-scheme includes all information that influences the system at that point.
- Right Diagram (UNSTABLE):** The characteristic line is outside the numerical domain (steeper than the CFL limit). Red arrows point to grid points that influence the system but are not included in the numerical domain, leading to instability.

CFL condition [2]



Nonlinear hyperbolic PDEs [1]

* Traffic flow

Examples of non-linear hyperbolic PDE models

$$S_t + [f(S)]_x = 0$$

$$f(S) = S u_{\max} \left(1 - \frac{S}{S_{\max}}\right)$$

S : density of cars (# vehicles per km)

u : velocity (km/h)

$0 \leq S \leq S_{\max}$ = the value at which cars are bumper to bumper

* Two-phase flow (Buckley-Leverett equation)

$$S_t + [f(S)]_x = 0$$

$$f(S) = \frac{S^2}{S^2 + M(1-S)^2}$$

S : water saturation level ; $0 \leq S \leq 1$

$f(S)$: fractional flow function

$$M = \frac{\mu_w}{\mu_{\text{oxygen}}} \quad \text{or} \quad \frac{\mu_w}{\mu_{\text{oil}}} \quad \dots$$

* The Euler equations

ρ : density
 v : velocity
 E : total energy

$$\begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix}_t + \begin{pmatrix} \rho v \\ \rho v^2 + p \\ v(E+p) \end{pmatrix}_x = 0$$

continuity equation
momentum equation
conservation of energy

total energy $E = \frac{1}{2} \rho v^2 + \rho e$
kinetic energy internal energy

equation of state: $e = \frac{p}{(\gamma-1)\rho}$
(polytropic gas)

Nonlinear hyperbolic PDEs [2]

2

* Shallow water equations

$$h_t + (vh)_x = 0$$

$$(hv)_t + (hv^2 + \frac{1}{2}gh^2)_x = 0$$

h : height of watersurface
 v : velocity of waterwave

* Magneto-hydrodynamics

$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$ conservation of mass

$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v} - \vec{B} \vec{B}) + \nabla p_{\text{tot}} = 0$ conservation of momentum

$\frac{\partial e}{\partial t} + \nabla \cdot (e \vec{v} + \vec{v} p_{\text{tot}} - \vec{B} \vec{B} \cdot \vec{v}) = 0$ conservation of energy

$\frac{\partial \vec{B}}{\partial t} + \nabla \cdot (\vec{v} \vec{B} - \vec{B} \vec{v}) = 0$ magnetic field induction equation

$p_{\text{tot}} = p + \frac{\vec{B}^2}{2}$ total pressure

$$p = (\gamma - 1) \left(e - \rho \frac{\vec{v}^2}{2} - \frac{\vec{B}^2}{2} \right)$$

$\nabla \cdot \vec{B} = 0 \quad \forall t \geq 0$

"there exists no magnetic monopoles"

$$\vec{v}^2 \stackrel{\text{def}}{=} \vec{v}^T \vec{v}$$

$$\vec{B}^2 = \vec{B}^T \vec{B}$$

Nonlinear hyperbolic PDEs [5]

FTBS for Burgers' equation in the quasilinear form (non-conservative)

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

Assume: $u_i^n \geq 0 \quad \forall i, n$

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} u_i^n (u_i^n - u_{i-1}^n) \quad (*)$$

consider the IC: $u_i^0 = \begin{cases} 1, & i < 0 \\ 0, & i \geq 0 \end{cases}$

check this!

$$u_i^1 = u_i^0 \quad \forall i$$

$$u_i^2 = u_i^1 = u_i^0 \quad \forall i$$

etcetera (via induction): $u_i^n = u_i^0 \quad \forall i, n$

a "stationary" wave independent of $t, \Delta x$.

WRONG SOLUTION

Conservative form [1]

$$u_t + (F(u))_x = 0$$

example: $F(u) = \frac{u^2}{2}$

$\left(\frac{u^2}{2}\right)_x$ conservative form
 uu_x non-conservative form

$$1) u_i^{n+1} = u_i^n - \frac{\Delta t}{4 \Delta x} \left((u_{i+1}^n)^2 - (u_{i-1}^n)^2 \right)$$

$$2) u_i^{n+1} = u_i^n - \Delta t u_i^n \frac{(u_{i+1}^n - u_{i-1}^n)}{2 \Delta x}$$

$$3) u_i^{n+1} = u_i^n - \Delta t u_i^n \frac{(u_i^n - u_{i-1}^n)}{\Delta x}$$

$$4) u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \frac{\Delta t}{4 \Delta x} \left((u_{i+1}^n)^2 - (u_{i-1}^n)^2 \right) \quad \text{"Lax-Friedrichs"}$$

et cetera (it matters!)

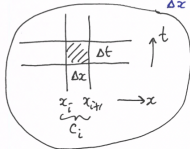
Finite volumes [1]

Finite Volumes

Rather than viewing u_i^n as an approximation to the single value $u(x_i, t^n)$, we will now view it as an approximation to the average value of u over an interval $C_i = [x_i, x_{i+1}]$

"cell", "volume"
with $x_i = x_L + \frac{i-1}{N}$, $i=1, \dots, N$
 $\Delta x = x_{i+1} - x_i$

$$u_i^n \approx \frac{\int_{x_i}^{x_{i+1}} u(x, t^n) dx}{\Delta x} = \frac{1}{\Delta x} \int_{C_i} u(x, t^n) dx$$



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

$$\iint (u_t + (F(u))_x) dx dt = \iint 0 dx dt$$

$$\Leftrightarrow \int_{x_i}^{x_{i+1}} \int_{t^n}^{t^{n+1}} u_t dt dx + \int_{t^n}^{t^{n+1}} \int_{x_i}^{x_{i+1}} (F(u))_x dx dt = 0$$

Finite volumes [2]

$$\Leftrightarrow \int_{x_i}^{x_{i+1}} [u(x, t^{n+1}) - u(x, t^n)] dx + \int_{t^n}^{t^{n+1}} [F(u(x_{i+1}, t)) - F(u(x_i, t))] dt = 0$$

$$\Leftrightarrow \int_{C_i} u(x, t^{n+1}) dx - \int_{C_i} u(x, t^n) dx = \int_{t^n}^{t^{n+1}} F(u(x_i, t)) dt - \int_{t^n}^{t^{n+1}} F(u(x_{i+1}, t)) dt$$

still exact!!!

Re-arranging and dividing by Δx :

$$\frac{1}{\Delta x} \int_{C_i} u(x, t^{n+1}) dx = \frac{1}{\Delta x} \int_{C_i} u(x, t^n) dx - \frac{1}{\Delta x} \left\{ \int_{t^n}^{t^{n+1}} F(u(x_{i+1}, t)) dt - \int_{t^n}^{t^{n+1}} F(u(x_i, t)) dt \right\}$$

$u_i^{n+1} \approx$ (at time level t^{n+1})

$u_i^n \approx$ (at time level t^n)

$$\Rightarrow u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} (F_{i+1}^n - F_i^n) \quad \text{with} \quad F_i^n \approx \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F(u(x_i, t)) dt$$

"in conservative form"

↑ approximation

Finite volumes [3]

Note (!)
"exact"

$$u_t + (F(u))_x = 0 \Leftrightarrow \int_0^t \int_{-\infty}^{\infty} u_t(x,s) dx ds + \int_0^t \int_{-\infty}^{\infty} (F(u))_x dx ds$$

$$\Leftrightarrow \int_0^t \int_{-\infty}^{\infty} u_t(x,s) ds dx + \int_0^t (F(u)) \Big|_{x=-\infty}^{x=\infty} ds = 0$$

$$\Leftrightarrow \int_{-\infty}^{\infty} [u(x,t) - u(x,0)] dx + \int_0^t [F(u(\infty,s)) - F(u(-\infty,s))] ds = 0$$

suppose = 0

$$\Leftrightarrow \int_{-\infty}^{\infty} [u(x,t) - u(x,0)] dx = 0$$

$$\Leftrightarrow \int_{-\infty}^{\infty} u(x,t) dx = \int_{-\infty}^{\infty} u(x,0) dx$$

initial condition

$\forall t \geq 0$

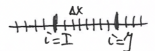
"conservation of mass"

*or $u|_{\pm\infty} = 0$
or $u|_{\infty} = u|_{-\infty}$
example: $F(u) = u^2$
or F is an even function*

Finite volumes [4]

Note ("numerical") sum $\Delta x u_i^{n+1}$ from $i=I$ to J over any set of grid cells:

$$\begin{aligned}
 \Delta x \sum_{i=I}^J u_i^{n+1} &= \Delta x \sum_{i=I}^J u_i^n - \Delta t \sum_{i=I}^J (F_{i+1}^n - F_i^n) \\
 &= \Delta x \sum_{i=I}^J u_i^n - \Delta t \left\{ \cancel{F_{I+1}^n} - \cancel{F_I^n} + \cancel{F_I^n} - \cancel{F_{I+1}^n} + \dots + \cancel{F_{J-1}^n} - \cancel{F_J^n} \right\} \\
 &= \Delta x \sum_{i=I}^J u_i^n - \Delta t \left[\underbrace{F_{J+1}^n - F_I^n}_{\text{"boundary" terms}} \right] \quad \left\{ \begin{array}{l} \text{all terms} \\ \text{disappear} \\ \text{except} \end{array} \right.
 \end{aligned}$$



Conserved quantity $\sim \left[\int u \, dx \right]^{t^{n+1}}$ and $\sim \left[\int u \, dx \right]^{t^n}$

$$I=0 \quad \text{and} \quad J=N \quad \text{with} \quad F_{J+1} - F_I = F_{N+1} - F_0 = 0$$

(initial index) (final index)

as for continuous case

CFL vs von Neumann

Remark: ① for many (not all) FD methods:

CFL-condition \Leftrightarrow von Neumann stability criterion

② CFL-condition can be extended to non-linear hyperbolic PDEs!

(von Neumann can not)

$$\max_u \left| F'(u) \frac{\Delta t}{\Delta x} \right| \leq 1$$

for $u_t + (F(u))_x = 0$

③ for Lax-Friedrichs, it is also a sufficient condition (i.e. \Leftrightarrow)

for upwind ($c > 0$) " " " " "

for downwind ($c < 0$) " " " " "

④ Note that for $F(u) = c \cdot u$ (linear advection): $F'(u) = c$

$$\downarrow \left| c \frac{\Delta t}{\Delta x} \right| \leq 1$$

Wave equation [1]

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Introduce new variables: $\xi = x - ct$, $\eta = x + ct$

$$\text{chain rule: } \begin{cases} \frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x} \cdot \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x} \cdot \frac{\partial}{\partial \eta} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial t} = \frac{\partial \xi}{\partial t} \cdot \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial t} \cdot \frac{\partial}{\partial \eta} = -c \cdot \frac{\partial}{\partial \xi} + c \cdot \frac{\partial}{\partial \eta} \end{cases}$$

$$\Rightarrow \begin{cases} \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial \xi^2} + 2 \cdot \frac{\partial^2 u}{\partial \xi \partial \eta} + \frac{\partial^2 u}{\partial \eta^2} \\ \frac{\partial^2 u}{\partial t^2} = c^2 \cdot \frac{\partial^2 u}{\partial \xi^2} - 2c^2 \frac{\partial^2 u}{\partial \xi \partial \eta} + c^2 \frac{\partial^2 u}{\partial \eta^2} \end{cases}$$

substitute in wave equation $\frac{\partial^2 u}{\partial \xi \partial \eta} = 0$

integrating twice

$$\begin{aligned} u(x,t) &= G(\xi) + F(\eta) \\ &= G(x-ct) + F(x+ct) \end{aligned}$$

d'Alembert (1717-1783)

Wave equation [2]

Example: $\begin{cases} u(x,0) = f(x) \\ u_t(x,0) = g(x) \end{cases}$ initial conditions

$$\Rightarrow \begin{cases} f(x) = G(x) + F(x) \\ g(x) = -c G'(x) + c F'(x) \end{cases}$$

Solve for F and G in terms of f and g

(two equations with two unknowns)

$$\begin{aligned} \xrightarrow{\text{integrating from } 0 \text{ to } x} & \begin{cases} F(x) = \frac{1}{2} f(x) + \frac{1}{2c} \int_0^x g(s) ds - \frac{1}{2} (G(0) - F(0)) \\ G(x) = \frac{1}{2} f(x) - \frac{1}{2c} \int_0^x g(s) ds + \frac{1}{2} (G(0) - F(0)) \end{cases} \\ \swarrow \text{from general solution} & \end{aligned}$$

$$\begin{aligned} u(x,t) &= G(x-ct) + F(x+ct) \\ &= \frac{1}{2} f(x-ct) - \frac{1}{2c} \int_0^{x-ct} g(s) ds + \frac{1}{2} (G(0) - F(0)) \\ &\quad + \frac{1}{2} f(x+ct) + \frac{1}{2c} \int_0^{x+ct} g(s) ds - \frac{1}{2} (G(0) - F(0)) \\ &= \frac{1}{2} (f(x-ct) + f(x+ct)) + \frac{1}{2c} \int_{x-ct}^{x+ct} g(s) ds \end{aligned}$$

Wave equation [3]

If $u_t(x,0) = g(x) = 0$, then: $u(x,t) = \frac{1}{2} f(x-ct) + \frac{1}{2} f(x+ct)$

The lines $x-ct = \text{constant}$ and $x+ct = \text{constant}$ are the characteristics of this PDE.

Numerical approximation:

(suppose Dirichlet BCs $u(0,t) = \alpha(t)$ and $u(L,t) = \beta(t)$, $t \geq 0$)
and $c > 0$

$t^n = n \Delta t$, $x_i = i \Delta x$

$$\text{CTCS} \quad u_{tt}(x_i, t^n) \approx \frac{u(x_i, t^{n+1}) - 2u(x_i, t^n) + u(x_i, t^{n-1}))}{(\Delta t)^2} \quad (+ O((\Delta t)^2))$$

$$u_{xx}(x_i, t^n) \approx \frac{u(x_{i+1}, t^n) - 2u(x_i, t^n) + u(x_{i-1}, t^n))}{(\Delta x)^2} \quad (+ O((\Delta x)^2))$$

substitute in PDE

define $\sigma = \frac{c \Delta t}{\Delta x} > 0$

$$u_i^{n+1} = \sigma^2 u_{i+1}^n + 2(1 - \sigma^2) u_i^n + \sigma^2 u_{i-1}^n - u_i^{n-1} \quad \begin{matrix} i = \dots \\ n = \dots \end{matrix}$$

Wave equation [5]

$$\begin{aligned} \text{Taylor: } \frac{u(x_i, \Delta t) - u(x_i, 0)}{\Delta t} &= \frac{\partial u}{\partial t}(x_i, 0) + \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2}(x_i, 0) + \mathcal{O}((\Delta t)^3) \\ &= \frac{\partial u}{\partial t}(x_i, 0) + \frac{c^2 \Delta t}{2} \frac{\partial^2 u}{\partial x^2}(x_i, 0) + \mathcal{O}((\Delta t)^3) \end{aligned}$$

$$\begin{aligned} \rightsquigarrow u_i^1 = u(x_i, \Delta t) &\approx u(x_i, 0) + \Delta t \frac{\partial u}{\partial t}(x_i, 0) + \frac{c^2 (\Delta t)^2}{2} \frac{\partial^2 u}{\partial x^2}(x_i, 0) \\ &\approx f_i + \Delta t \cdot g_i + \frac{c^2 (\Delta t)^2}{2} f''(x_i, 0) \\ &\approx f_i + \Delta t \cdot g_i + \frac{c^2 (\Delta t)^2}{2 (\Delta x)^2} (f_{i+1} - 2f_i + f_{i-1}) \\ &= \frac{1}{2} \sigma^2 f_{i+1} + (1 - \sigma^2) f_i + \frac{1}{2} \sigma^2 f_{i-1} + \Delta t \cdot g_i \end{aligned}$$

$$\text{in matrix-vector form: } \begin{cases} \vec{u}^0 = \vec{f} \\ \vec{u}^1 = \frac{1}{2} B \vec{u}^0 + \Delta t \vec{g} + \frac{1}{2} \vec{b}^0 \end{cases}$$

$$\rightsquigarrow \boxed{\mathcal{O}((\Delta t)^2) + \mathcal{O}((\Delta x)^2)}$$

Wave equation [8]

2D wave equation: $u_{tt} = c^2 \Delta u$

CTCS
 $\Delta x = \Delta y = h$

$$\sigma_x = \frac{c \Delta t}{\Delta x}$$

$$\sigma_y = \frac{c \Delta t}{\Delta y}$$

Stability criterion:

$$\frac{c \Delta t}{h} \leq \frac{1}{\sqrt{2}}$$

in d space dimensions:

$$\frac{c \Delta t}{h} \leq \frac{1}{\sqrt{d}}$$

Outlook to Lecture 7

- ⤴ prepare exercises of Lecture 6 (see webpage!)
- ⤴ Lecture 7: exact and nonstandard finite differences
- ⤴ splitting and explicit-implicit methods (optional)
- ⤴ exponential integrators (optional)