Lecture 6

Paul Andries Zegeling

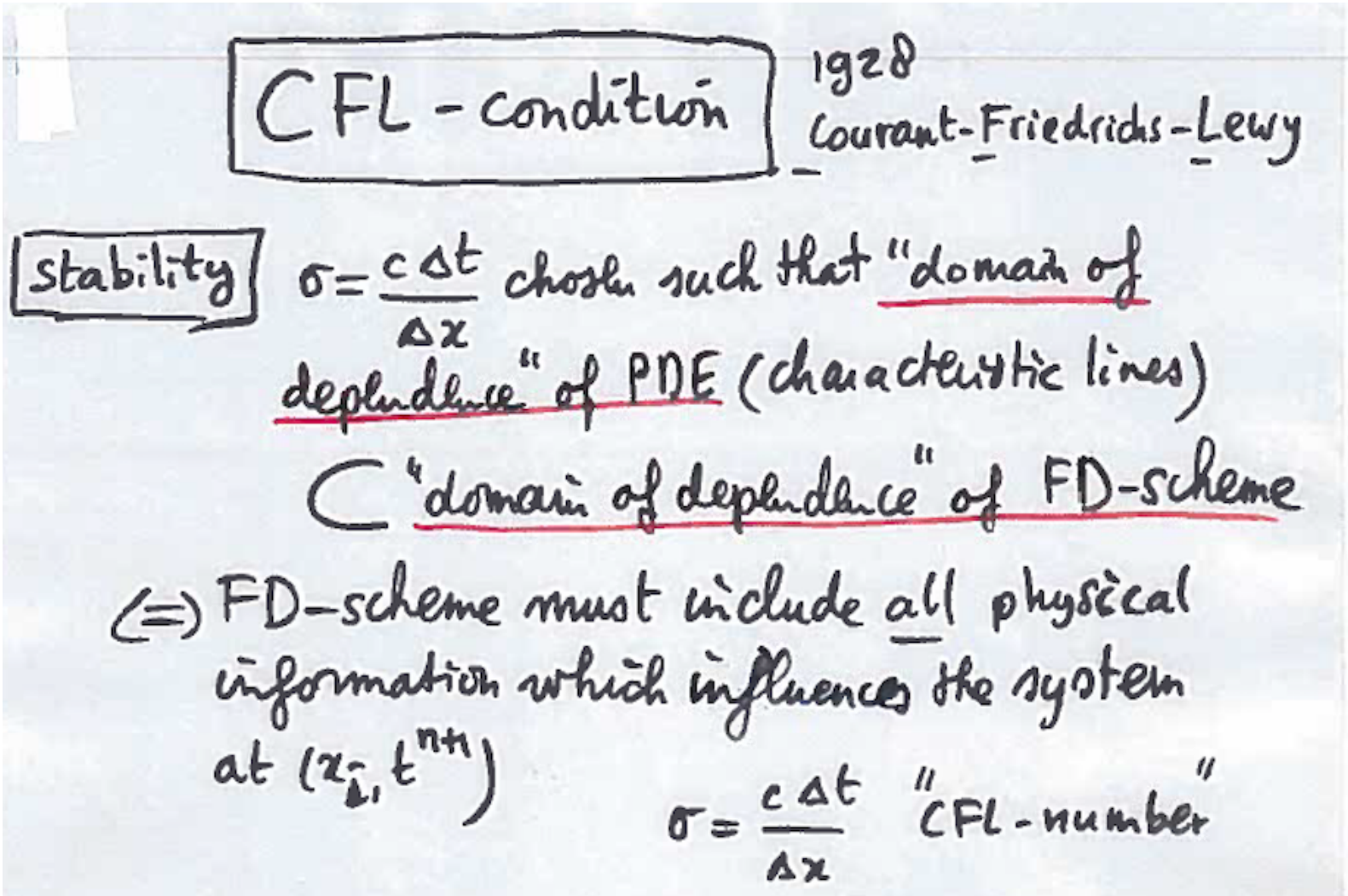
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Numerical Methods for PDEs

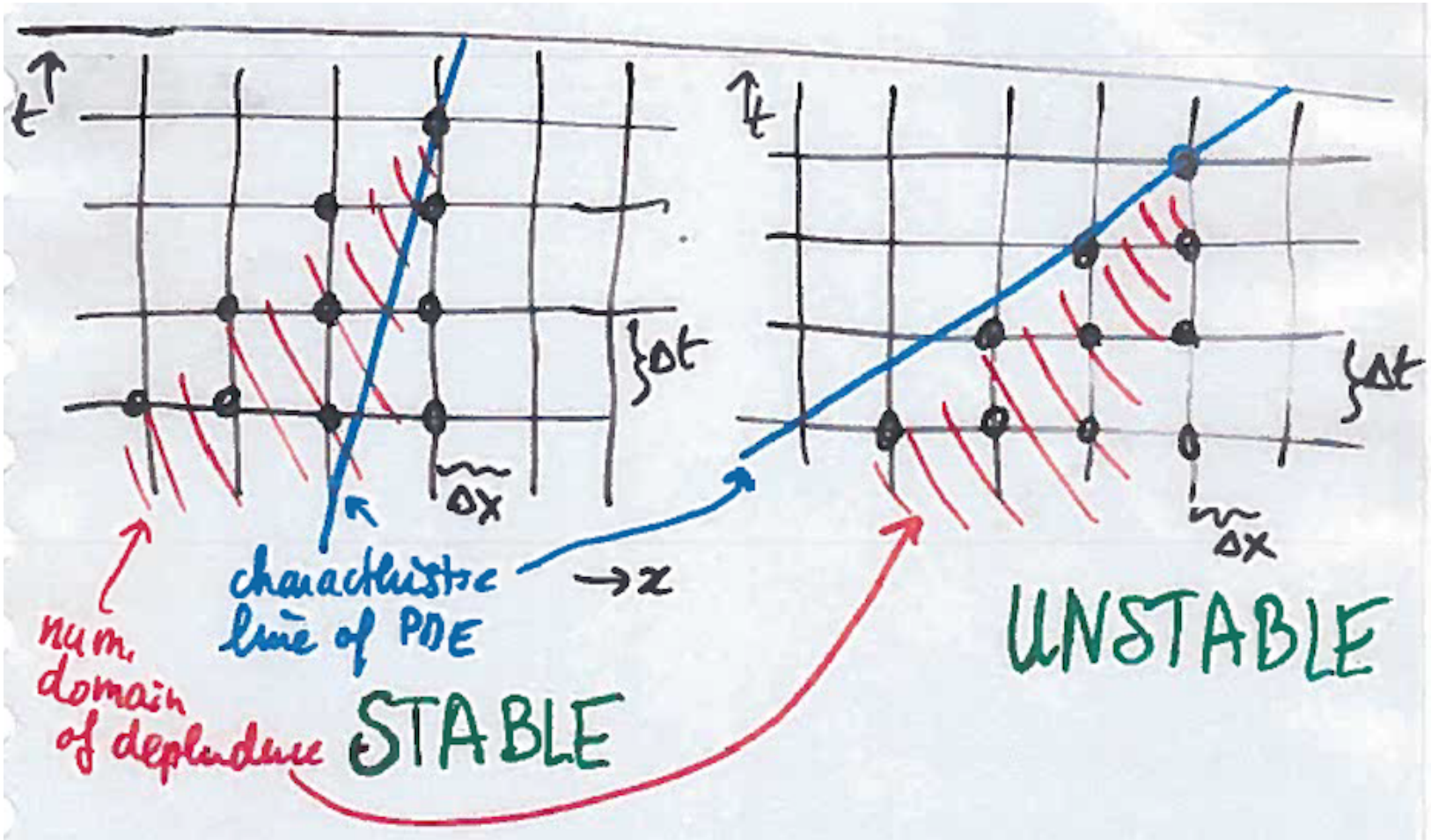
Outline of Lecture 6

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

CFL condition [1]



CFL condition [2]



CFL condition [3]

FTCS for $\frac{\partial u}{\partial t} + c \cdot \frac{\partial u}{\partial x} = 0$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \cdot \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$

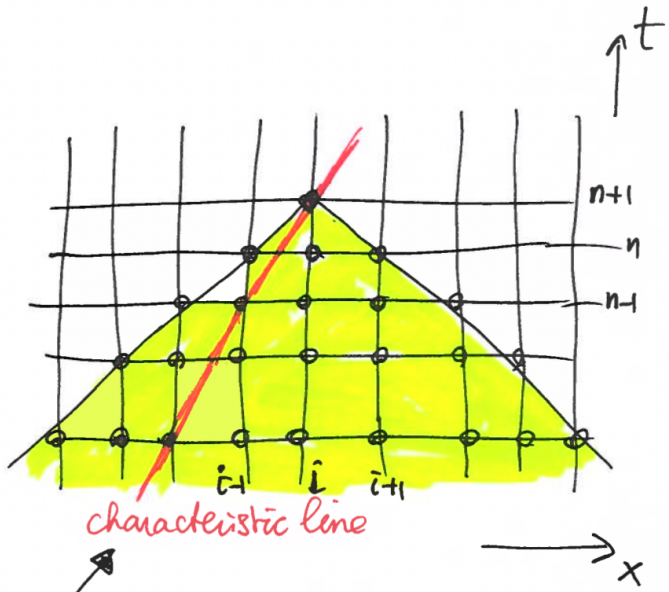
CFL-condition:

"stable method" $\Leftarrow$ $\frac{c \cdot \Delta t}{\Delta x} \leq 1$

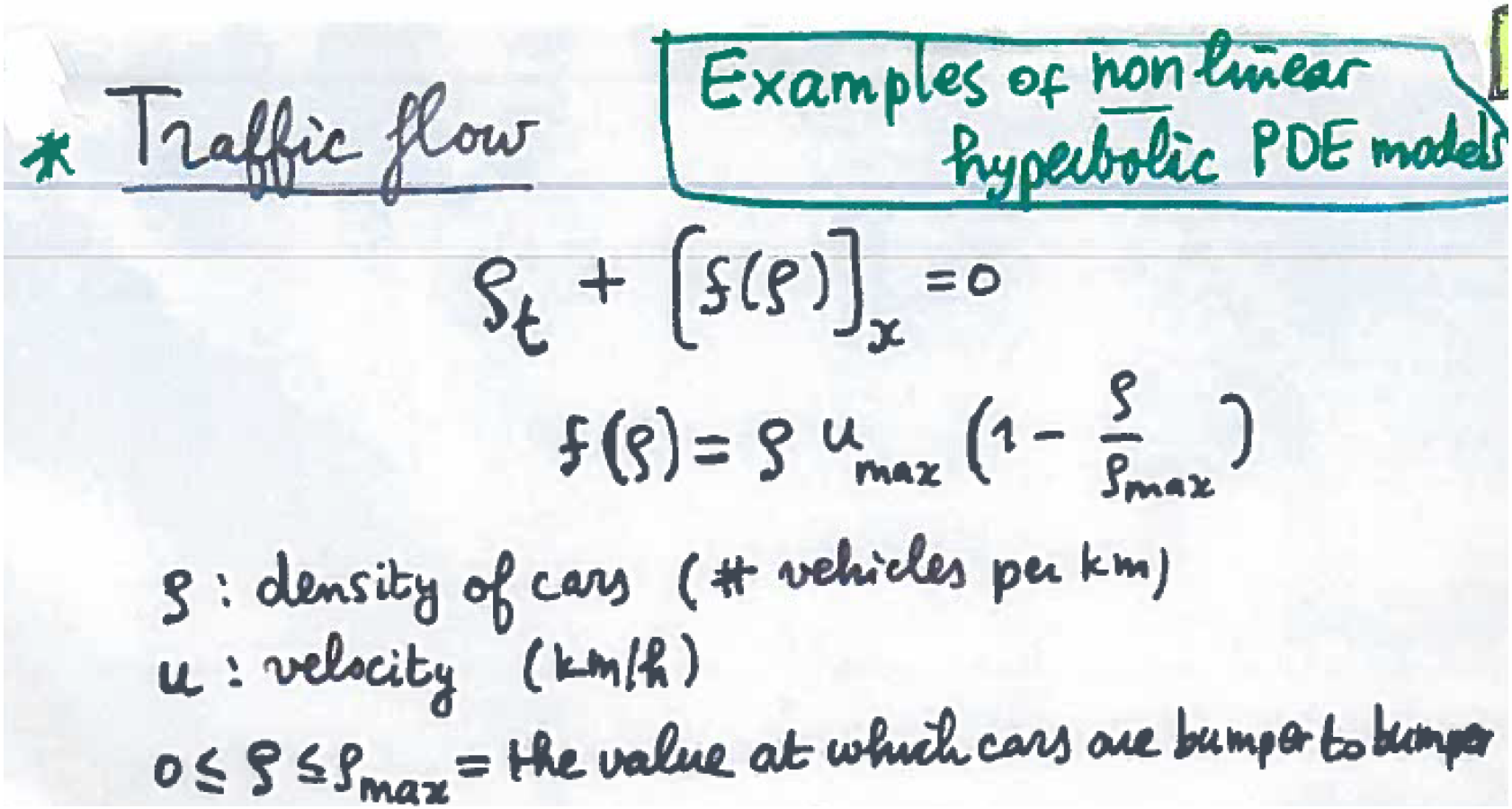
von Neumann: $|G| \geqslant 1 \Rightarrow$ always unstable

amplification factor

example: $\Delta t = \Delta x = 1$, $c = \frac{1}{2}$ $\Rightarrow$ $\frac{c\Delta t}{\Delta x} = \frac{1}{2} \leq 1$



Nonlinear hyperbolic PDEs [1]



Nonlinear hyperbolic PDEs [2]

* **Two-phase flow** (Buckley-Leverett equation)

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

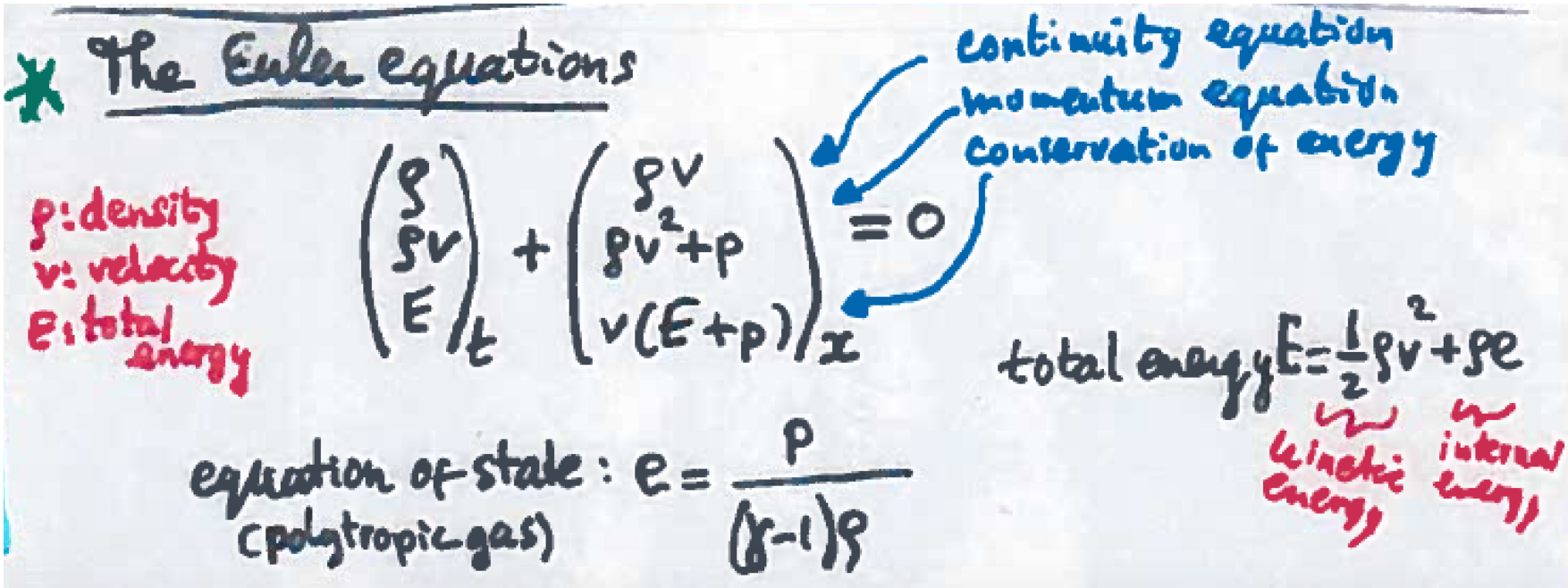
$$f(S) = \frac{S^2}{S^2 + M(1-S)^2}$$

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

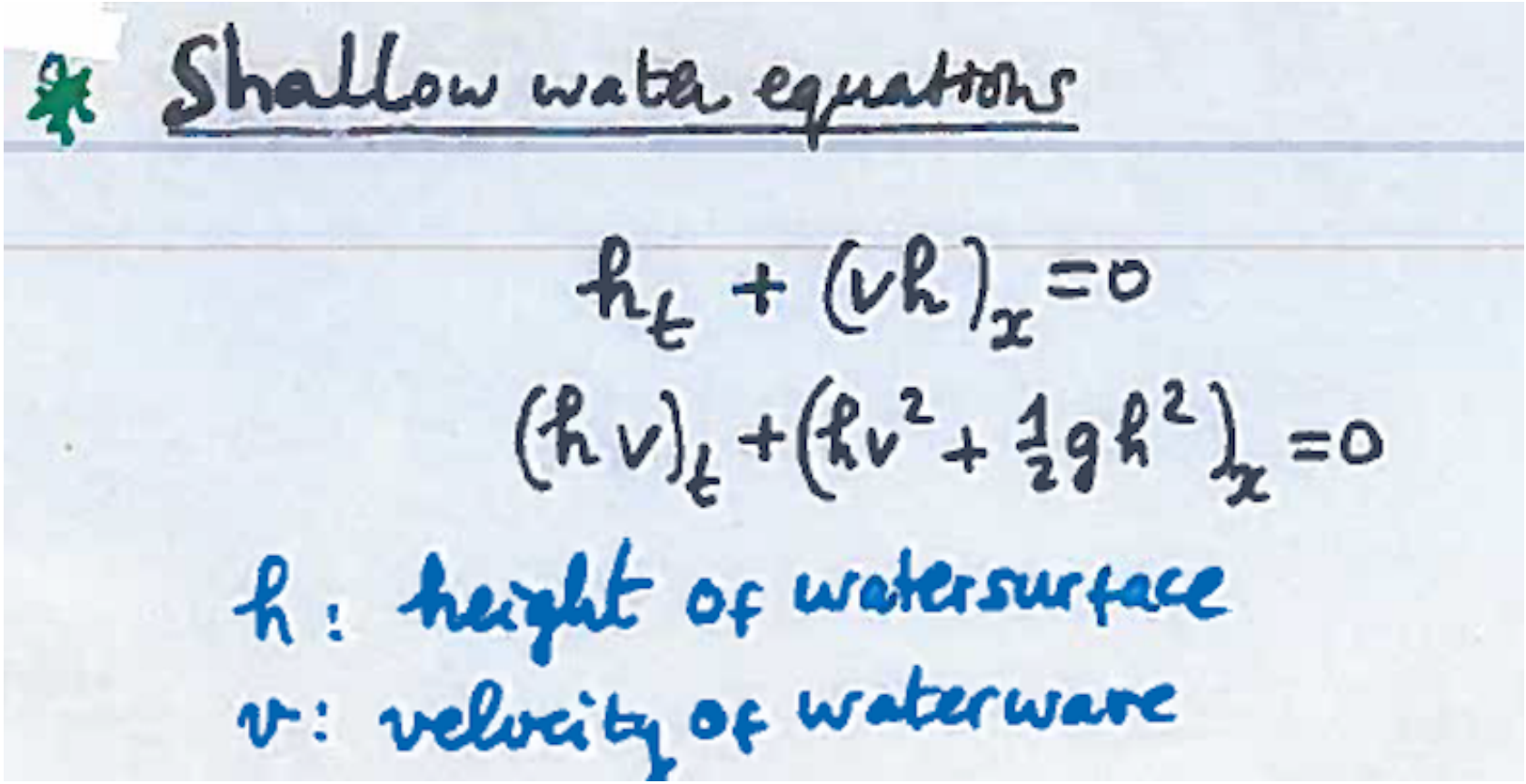
$f(S)$: fractional flow function

$$M = \frac{\mu_w}{\mu_{oxyga}} \quad \text{or} \quad = \frac{\mu_w}{\mu_{oil}} \quad \text{----}$$

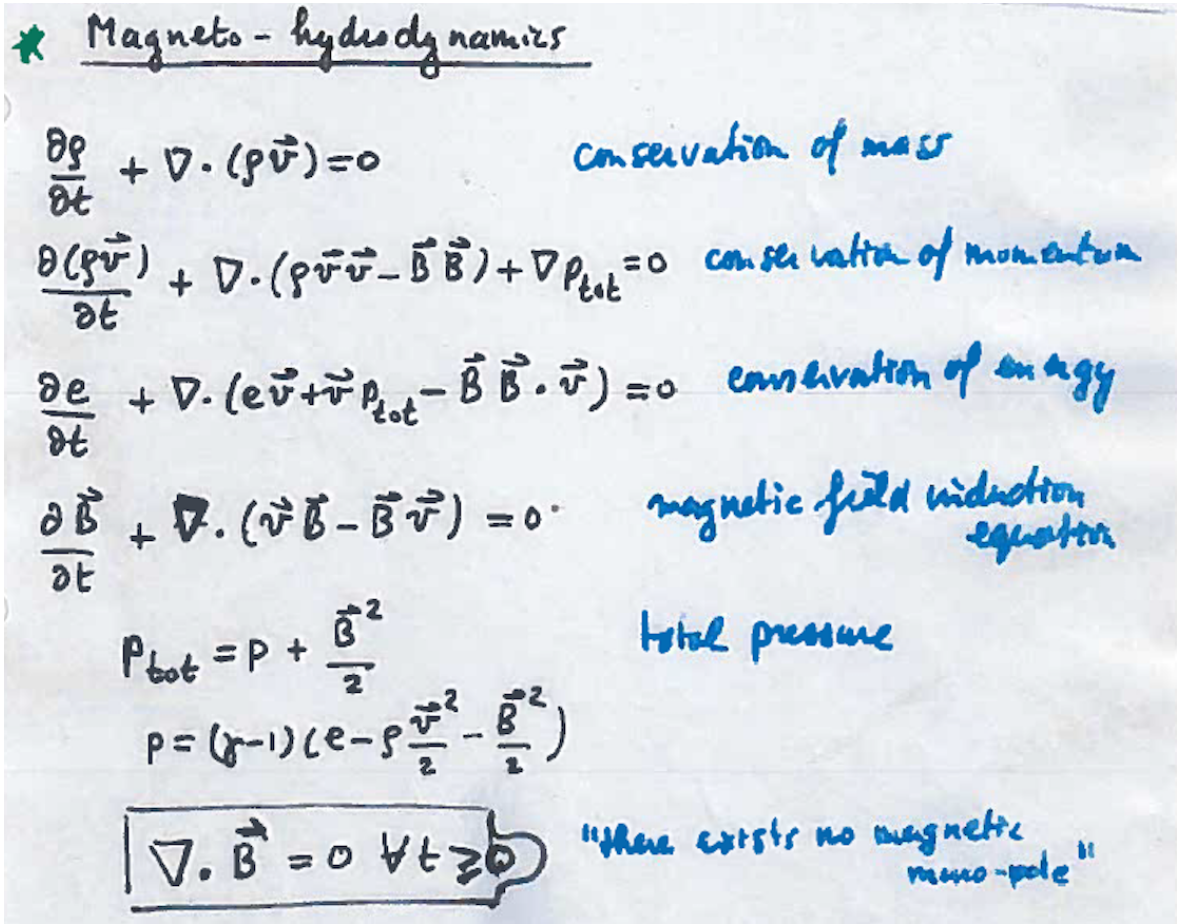
Nonlinear hyperbolic PDEs [3]



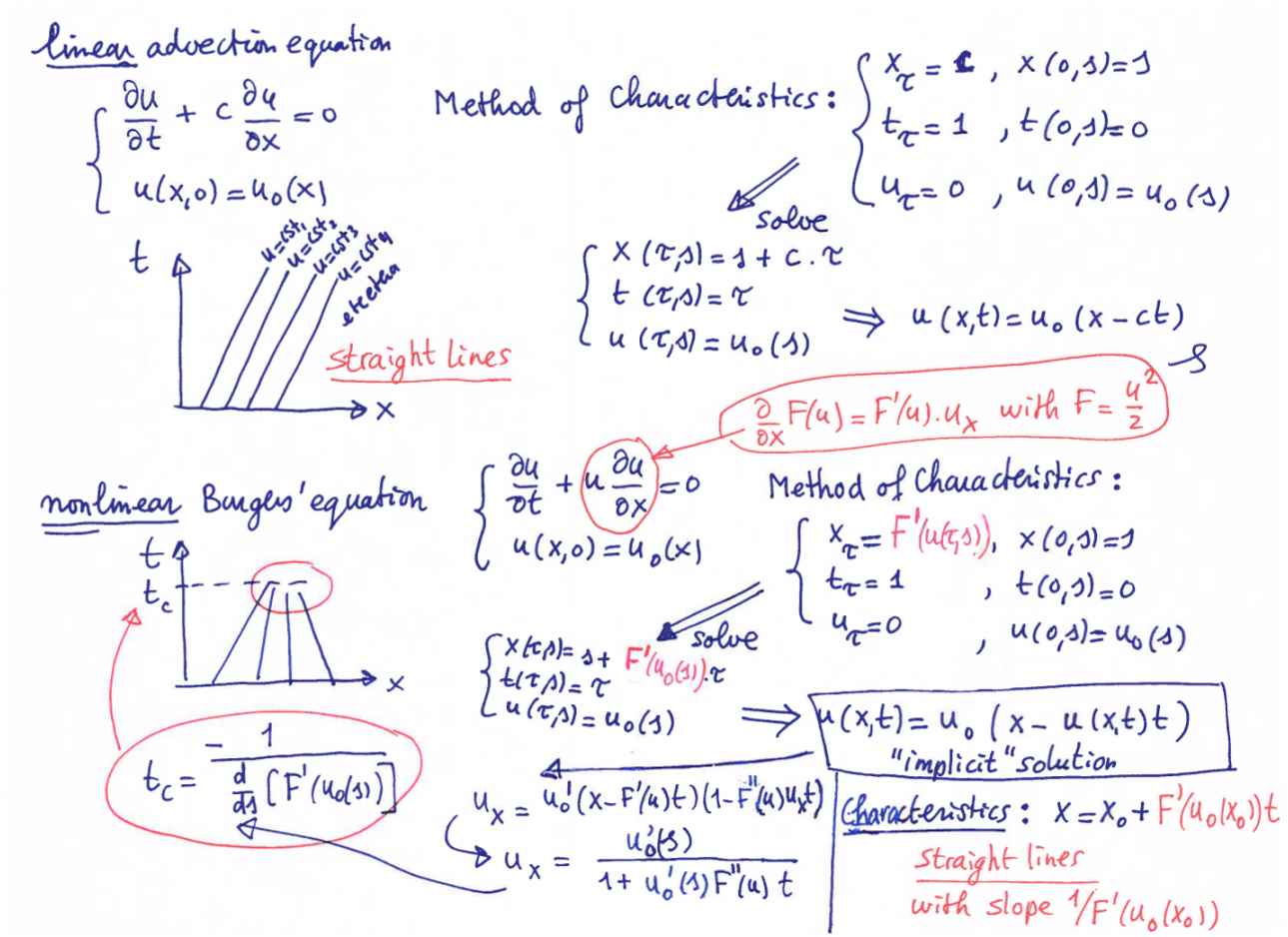
Nonlinear hyperbolic PDEs [4]



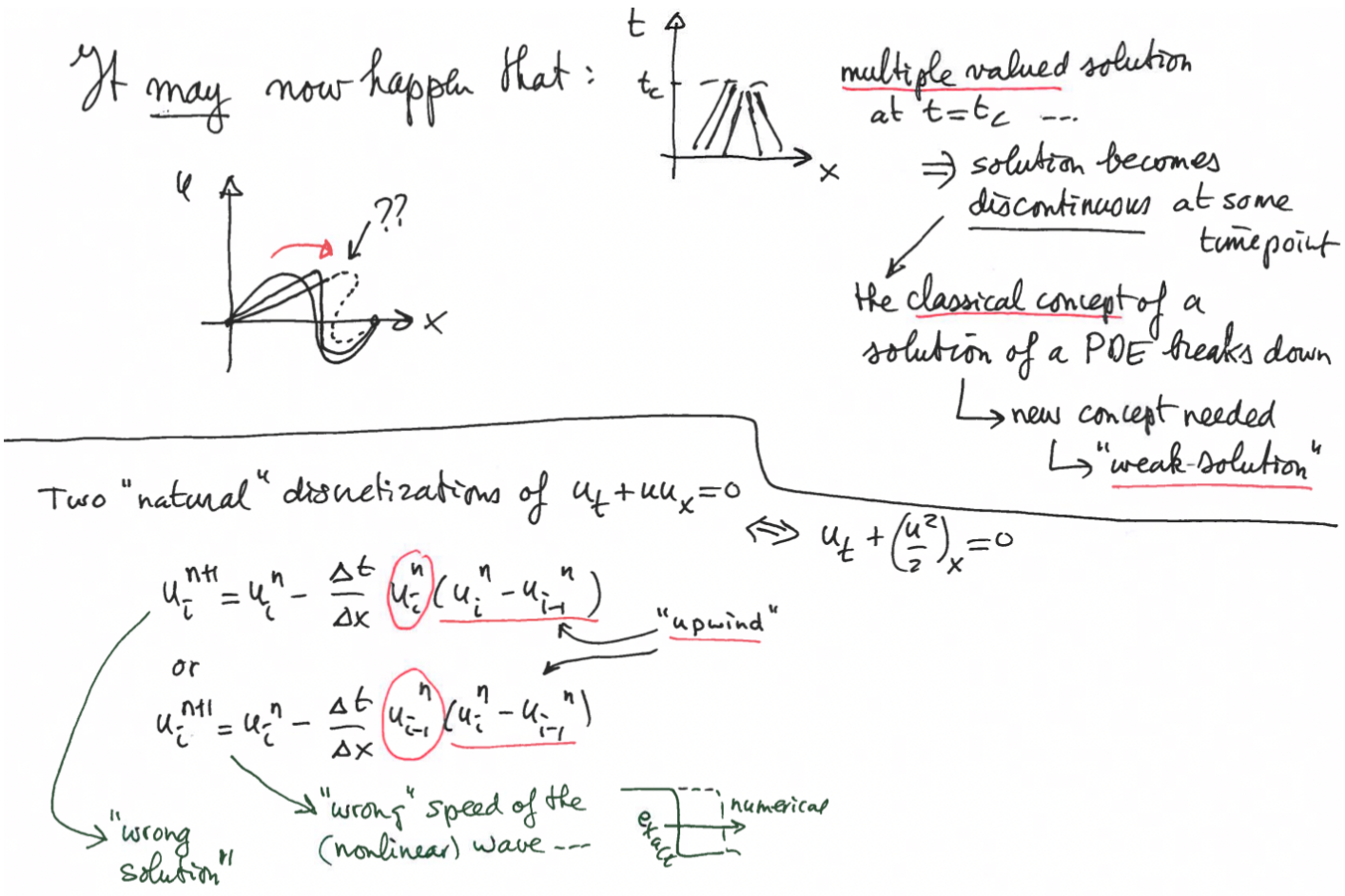
Nonlinear hyperbolic PDEs [5]



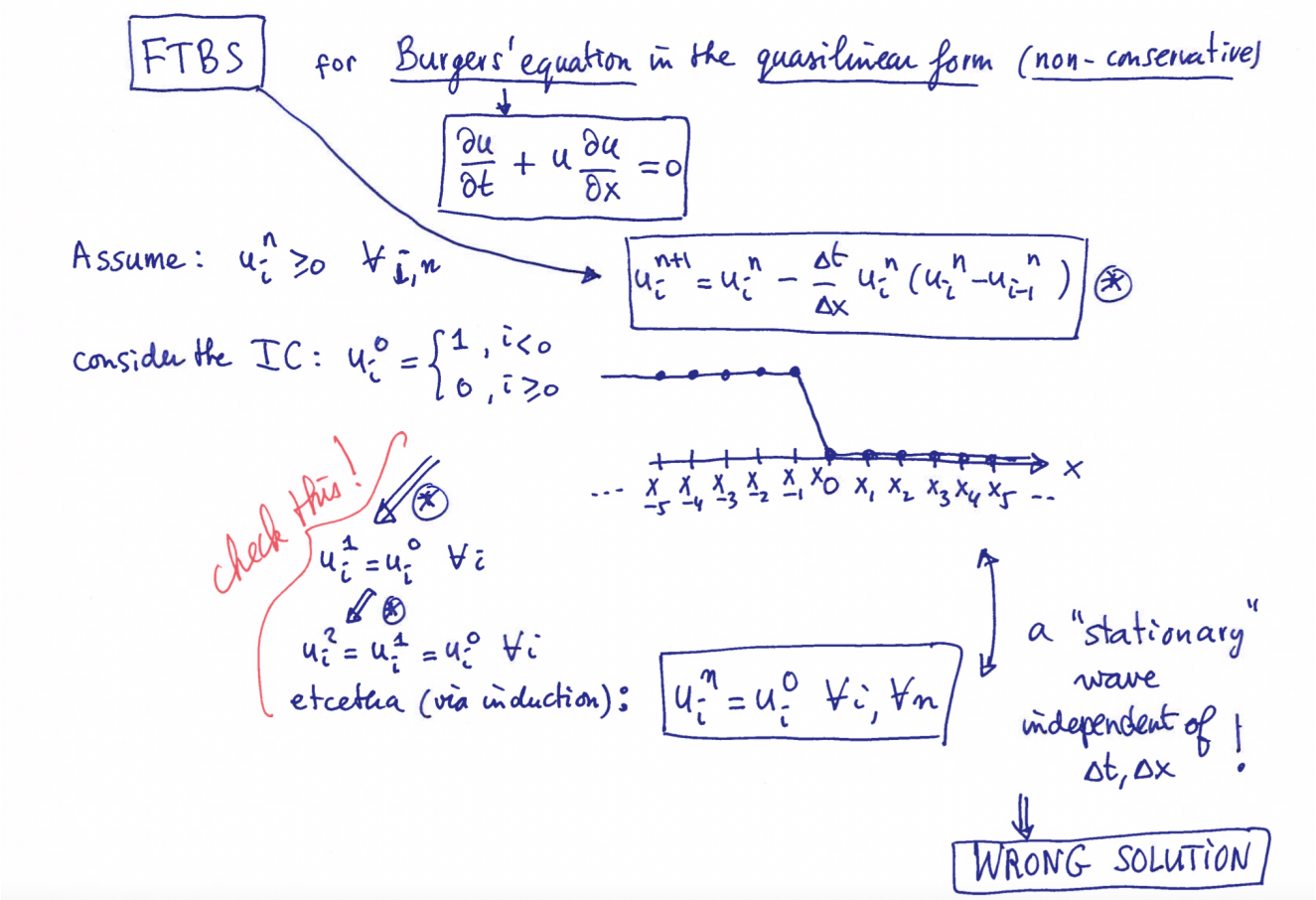
Nonlinear hyperbolic PDEs [6]



Nonlinear hyperbolic PDEs [7]



Nonlinear hyperbolic PDEs [8]



Conservative form [1]

$u_t + \left(F(u)\right)_x = 0$

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

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

uu_x non-conservative form

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

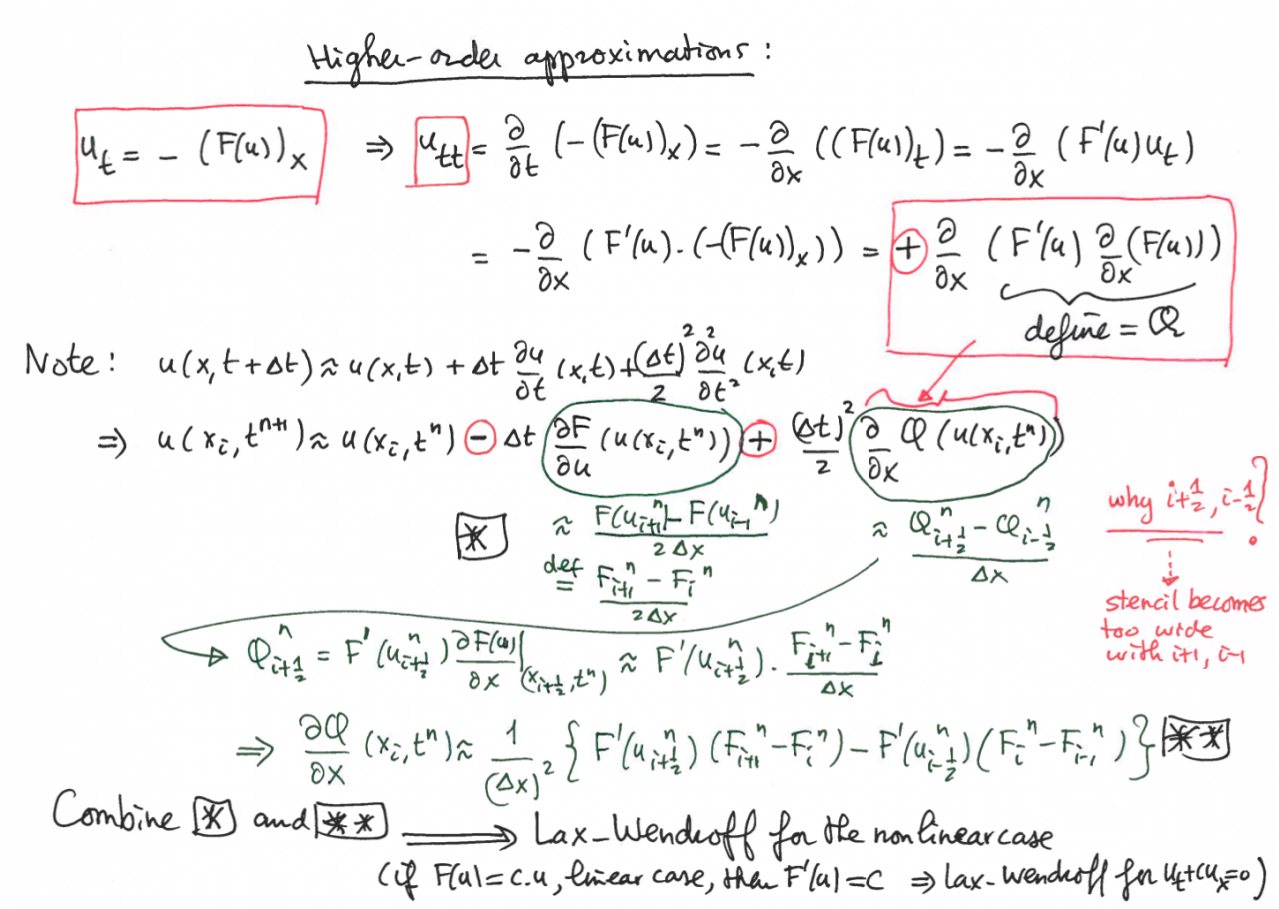
2) $u_i^{n+1} = u_i^n - \Delta t\, u_i^n \frac{\left(u_{i+1}^n - u_{i-1}^n\right)}{2\Delta x}$

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

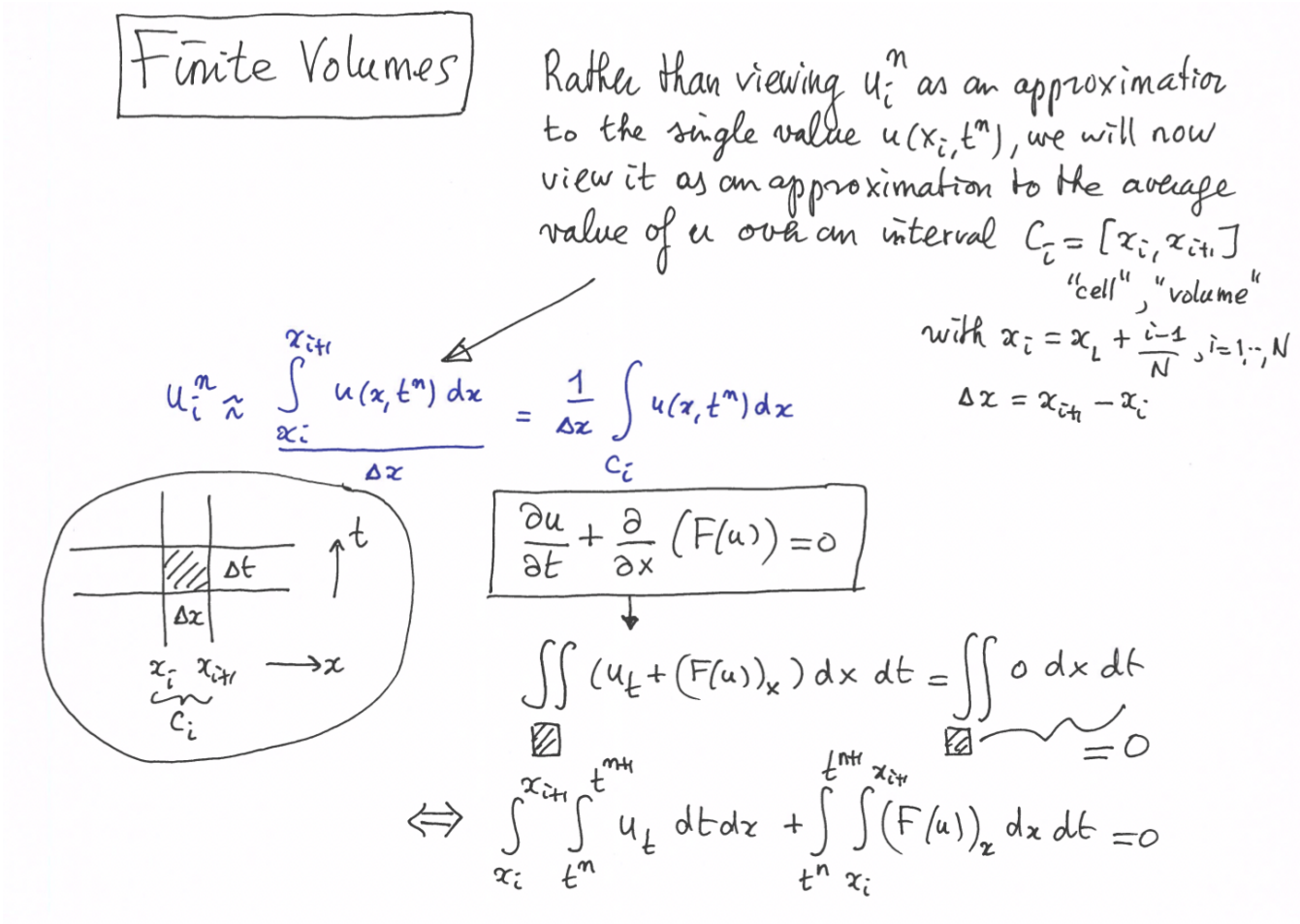
4) $u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \frac{\Delta t}{4\Delta x}\left(\left(u_{i+1}^n\right)^2 - \left(u_{i-1}^n\right)^2\right)$ "Lax-Friedrichs"

etcetera (it matters!)

Conservative form [2]



Finite volumes [1]



Finite volumes [2]

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

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

still exact!!!

Re-arranging and dividing by Δx:

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

$\frac{1}{\Delta x} \int_{C_i} u(x,t^{n+1})\,dx \approx U_i^{n+1}$ (at time level t^{n+1})

$\frac{1}{\Delta x} \int_{C_i} u(x,t^n)\,dx \approx U_i^{n}$ (at time level t^{n})

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

"in conservative form"

approximation

Finite volumes [3]

Note (!)

"exact"

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

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

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

suppose $= 0$

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

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

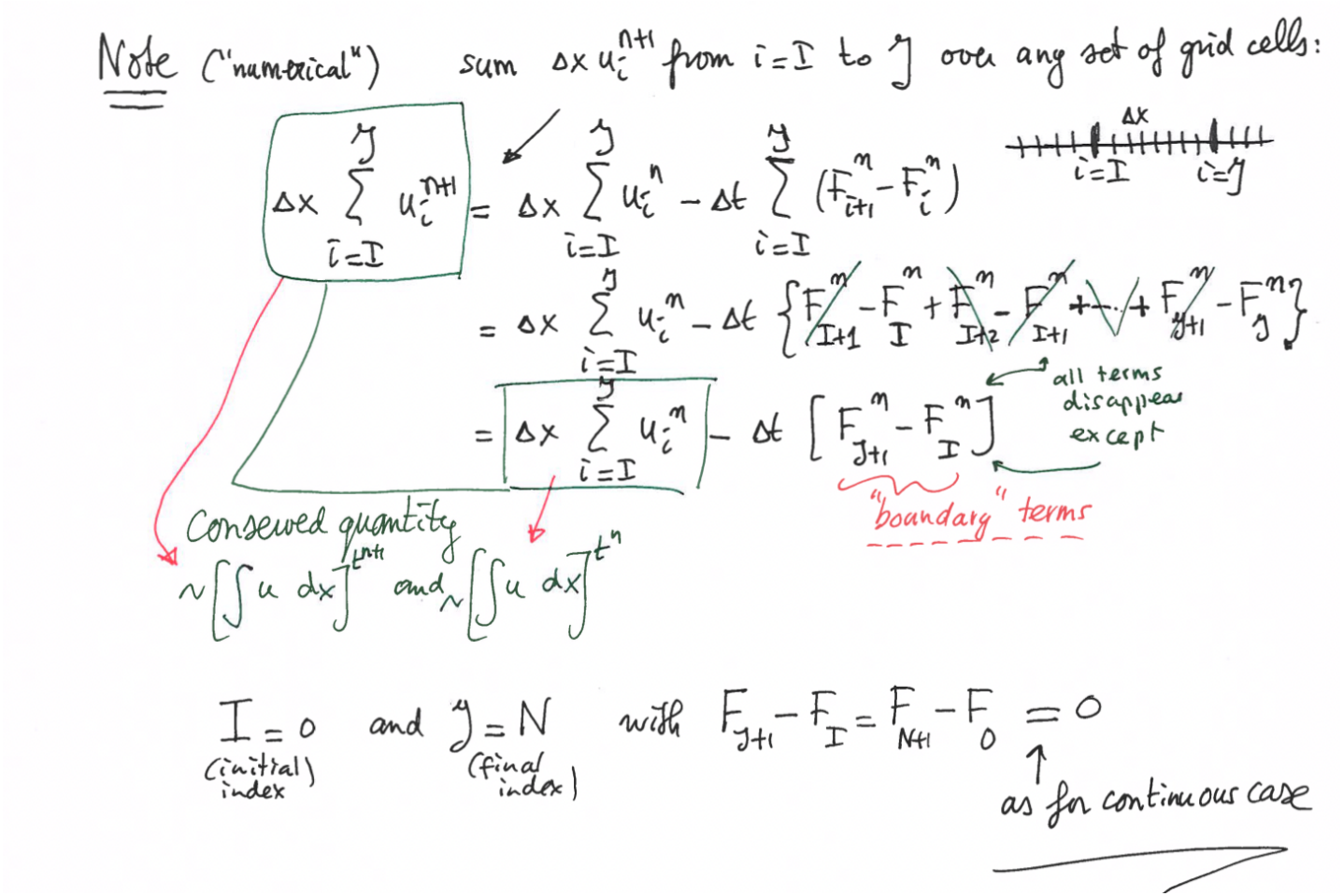
$$\Leftrightarrow \int_{-\infty}^{\infty} u(x,t)\,dx = \int_{-\infty}^{\infty} u(x,0)\,dx$$

initial condition

$\forall\, t \geq 0$

"conservation of mass"

Finite volumes [4]



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

for $u_t + \left(F(u)\right)_x = 0$

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 $F(u) = c.u$ (linear advection): $F'(u) = c$

$\downarrow$

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

Wave equation [1]

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

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

chain rule:
$$\begin{cases} \frac{\partial}{\partial x} = \underbrace{\frac{\partial \xi}{\partial x}}_{=1} \cdot \frac{\partial}{\partial \xi} + \underbrace{\frac{\partial \eta}{\partial x}}_{=1} \cdot \frac{\partial}{\partial \eta} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial t} = \underbrace{\frac{\partial \xi}{\partial t}}_{=-c} \cdot \frac{\partial}{\partial \xi} + \underbrace{\frac{\partial \eta}{\partial t}}_{=+c} \cdot \frac{\partial}{\partial \eta} = -c \cdot \frac{\partial}{\partial \xi} + c \cdot \frac{\partial}{\partial \eta} \end{cases}$$

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

substitute $\Rightarrow$ in wave equation

$$\boxed{\frac{\partial^2 u}{\partial \xi \partial \eta} = 0}$$

integrating twice

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

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)

integrating from 0 to x $\Rightarrow$

$$\begin{cases} F(x) = \frac{1}{2} f(x) + \frac{1}{2c} \int_0^x g(s)\,ds - \frac{1}{2}(G(0) - F(0)) \\ G(x) = \frac{1}{2} f(x) - \frac{1}{2c} \int_0^x g(s)\,ds + \frac{1}{2}(G(0) - F(0)) \end{cases}$$

$\Leftarrow$ from general solution

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

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 $c > 0$

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

CTCS

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

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

substitute in PDE $\Rightarrow$

$$u_i^{n+1} = \sigma^2 u_{i+1}^n + 2(1-\sigma^2) u_i^n + \sigma^2 u_{i-1}^n - u_i^{n-1}$$

$i = \cdots$

$n = \cdots$

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

Wave equation [4]

re-write in matrix-vector form: $\vec{u}^{n+1} = B\vec{u}^{n} - \vec{u}^{n-1} + \vec{b}^{n}$

$$B = \begin{pmatrix} 2(1-\sigma^2) & \sigma^2 & & 0 \\ \sigma^2 & 2(1-\sigma^2) & \sigma^2 & \\ & \ddots & \ddots & \ddots \\ 0 & & \sigma^2 & 2(1-\sigma^2) \end{pmatrix}$$

$$\vec{u}^{n} = \begin{pmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_{N-1}^n \end{pmatrix}$$

$$\vec{b}^{n} = \begin{pmatrix} \sigma^2 \alpha_n \\ 0 \\ \vdots \\ 0 \\ \sigma^2 \beta_n \end{pmatrix}$$

$= \alpha(t^n)$, $= \beta(t^n)$

This is a three-level scheme. How to get started?

* we know $\vec{u}^0$, since $u_i^0 = f(x_i) = f_i$
* we also need $\vec{u}^1$ with $u_i^1 = u(x_i, \Delta t)$, i.e. at time $t^1 = \Delta t$
* note that $u_t(x,0) = g(x)$ prescribes derivatives at time $t=0$: $u_t(x_i,0) = g(x_i) = g_i$

$$\rightsquigarrow \quad g(x_i) = \frac{\partial u}{\partial t}(x_i,0) \approx \frac{u(x_i,\Delta t) - u(x_i,0)}{\Delta t} \approx \frac{u_i^1 - f_i}{\Delta t} \quad \text{and} \quad u_i^1 \approx f_i + \Delta t\, g_i \ \text{(Euler-Forward)}$$

however, this is only first-order accurate

the remaining part of the scheme is $O((\Delta t)^2)$

Wave equation [5]

Taylor: $$\frac{u(x_i,\Delta t)-u(x_i,0)}{\Delta t} = \frac{\partial u}{\partial t}(x_i,0) + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i,0) + O((\Delta t)^2)$$
$$= \frac{\partial u}{\partial t}(x_i,0) + \frac{c^2\Delta t}{2}\frac{\partial^2 u}{\partial x^2}(x_i,0) + O((\Delta t)^2)$$

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

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

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

Wave equation [6]

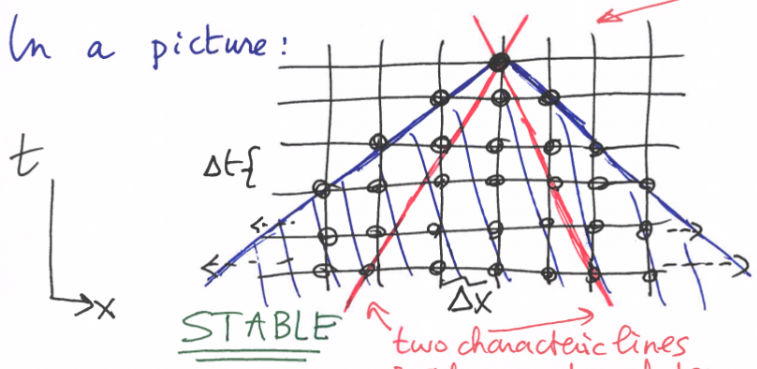
Stability ("CFL-condition" for the wave equation)

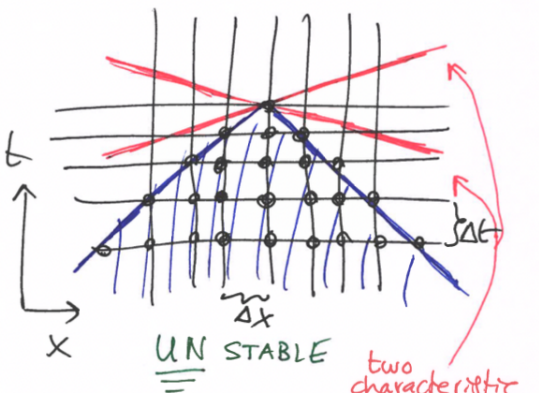
↕

"characteristics starting from grid point (x_i, t^n) must remain in the numerical domain of dependence for all $0 \le t \le t^n$"

→ here: triangle $\{(x,t) \mid 0 \le t \le t^n,\ x_i - t^n + t \le x \le x_i + t^n - t\}$

In a picture:





Characteristic lines are lines with slope $\pm c$

$\Rightarrow$ CFL-condition: $\frac{c\,\Delta t}{\Delta x} \le 1$ (necessary, not sufficient)

Wave equation [7]

Von Neumann - stability:

$$\Rightarrow G^2 + (4\sigma^2 \sin^2(\tfrac{1}{2}\theta\Delta x) - 2)G + 1 = 0$$

here: quadratic equation for the amplification factor G

$$G = \alpha \pm \sqrt{\alpha^2 - 1} \quad \text{with} \quad \alpha = 1 - 2\sigma^2 \sin^2(\tfrac{1}{2}\theta\Delta x)$$

↑ two amplification factors G_1 and G_2

If CFL-condition $\sigma = \frac{c\Delta t}{\Delta x} \leq 1$ holds, then $|\alpha| \leq 1 \Rightarrow |G_1| = 1, |G_2| = 1$ (stable numerical scheme)

If $\sigma > 1$, then $\alpha < -1$ for values of $\theta \Rightarrow$ G_1 and $G_2 \in \mathbb{R}$, one of the two: < -1 (stability)

In this case: CFL-condition $\Leftrightarrow$ von Neumann condition

Wave equation [8]

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

CTCS

$\Delta x = \Delta y = h$

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

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

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
- next week: tutorial 14:00-16:45 exercises 1-6 + C1A!
- Lecture 7: exact and nonstandard finite differences
(Wednesday November 4)
- splitting methods
(see also guest lecture 1 and C2)
- explicit-implicit methods (optional)
- exponential integrators (optional)