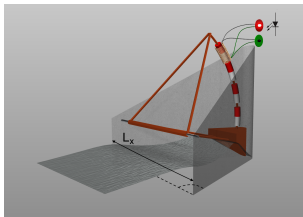


Numerical methods for fluid dynamics

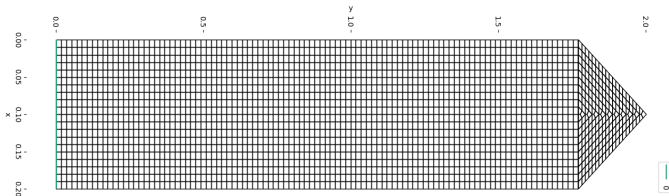
[Onno Bokhove,](#)

£: CDT Fluid Dynamics



Outline: assessment

- ▶ Attendance at practical sessions.
- ▶ Three numerical exercises (on finite difference, finite volume and finite element methods); to be handed in individually but you may work as a team.
- ▶ Example programs (for use at your own risk) will be provided in Python. Python use is recommended.



Finite differences: θ -method

- ▶ θ -method will be explained for heat equation w. Dirichlet BCs:

$$\partial_t u = \partial_{xx} u \quad (1)$$

$$u(x, 0) = u_0(x) \quad (2)$$

$$u(0, t) = u(1, t) = 0. \quad (3)$$

- ▶ Mesh points are $x_j = j\Delta x$; constant time step is used
 $t_n = n\Delta t$ for $j = 0, \dots, N_x$ and $n = 0, 1, \dots$
- ▶ Time step can also be varied, in which case Δt_n varies and t_n is sum of time steps taken.
- ▶ Approximate values of $u(x, t)$ on mesh points are denoted by
 $U_j^n \approx u(x_j, t_n)$.
- ▶ Initial values are $U_j^0 = u_0(x_j)$; in general exact (why could there be an issue here?).

Finite differences: approximations

- The next issue is to find a difference approximation of the PDE (1) in terms of the approximations U_j^n .
- Time derivative is approximated in a forward manner, expressed in terms of several difference operators Δ_{+t} and δ_t :

$$(\partial_t u)(x_j, t_n) \approx \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} \quad (4)$$

$$\equiv \frac{\Delta_{+t} u(x_j, t_n)}{\Delta t} \quad (5)$$

$$\equiv \frac{\delta_t u(x_j, t_{n+1/2})}{\Delta t} \quad (6)$$

$$\approx (\partial_t u)(x_j, t_{n+1/2}) \quad (7)$$

- *Exercise:* check approximations by performing suitable Taylor expansions of u around, e.g., $t^n = t_n$ or $t^{n+1/2} = t_{n+1/2}$.

Finite differences: Taylor expansions

- ▶ 2nd spatial derivative approximated symmetrically as

$$(\partial_{xx}u)(x_j, t_n) \approx \frac{u(x_{j-1}, t_n) - 2u(x_j, t_n) + u(x_{j+1}, t_n))}{\Delta x^2} \quad (8)$$

$$= \frac{\delta_x^2 u(x_j, t_n)}{\Delta x^2} = \frac{\delta_x(\delta_x u)|_{x_j}^{t_n}}{\Delta x^2} \quad (9)$$

with $\delta_x u(x, t) \equiv (u(x + \Delta x/2, t) - u(x - \Delta x/2, t))/\Delta x$.

- ▶ *Exercise:* check this approximation by using Taylor expansions of u around, e.g., t^n and x_j .
- ▶ This approximation also holds at t_{n+1}

$$(\partial_{xx}u)(x_j, t_{n+1}) \approx \frac{u(x_{j-1}, t_{n+1}) - 2u(x_j, t_{n+1}) + u(x_{j+1}, t_{n+1}))}{\Delta x^2} \\ = \frac{\delta_x^2 u(x_j, t_{n+1})}{\Delta x^2}. \quad (10)$$

Finite differences: θ scheme

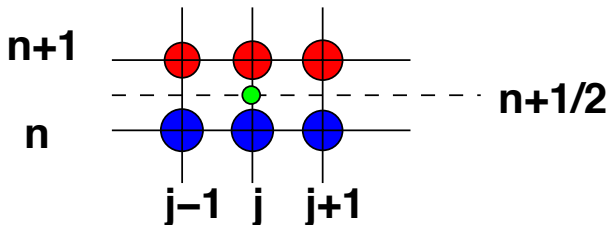
- By combining approximations with $\mu = \Delta t / \Delta x^2$, PDE (1) can be approximated on a 6-point stencil (see Fig.))

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{\theta}{\Delta x^2} \delta_x^2 U_j^{n+1} + \frac{(1-\theta)}{\Delta x^2} \delta_x^2 U_j^n \quad (11a)$$

$$U_j^{n+1} = U_j^n + \mu \theta (U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}) + \mu(1-\theta)(U_{j-1}^n - 2U_j^n + U_{j+1}^n). \quad (11b)$$

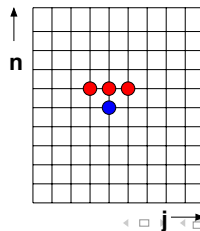
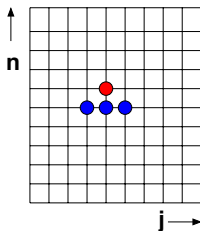
- Rewritten form with unknowns on the LHS and $0 \leq \theta \leq 1$

$$-\mu \theta U_{j-1}^{n+1} + (1 + 2\mu \theta) U_j^{n+1} - \mu \theta U_{j+1}^{n+1} = (1 - 2\mu(1-\theta)) U_j^n + \mu(1-\theta)(U_{j-1}^n + U_{j+1}^n). \quad (12)$$



Finite differences: EF, EB, CN schemes

- ▶ When $\theta = 0$ scheme is explicit, solved for U_j^{n+1} : *Euler forward* scheme uses stencil of 4 points with 1 point in future.
- ▶ When $\theta = 1$ scheme is fully implicit; *Euler backward* scheme. Uses a stencil of 4 points with 3 points in future, see Fig.
- ▶ When $\theta = 1/2$, a stencil of 6 points is used: this is the classical Crank-Nicolson scheme (Crank & Nicolson 1947).
- ▶ *Exercise θ -scheme*: suitable space-time grid point for a Taylor expansion?



Finite difference methods: homework

- ▶ Study Morton and Mayers (2005), Chapter 2, sections 2.2, 2.4, 2.5.
- ▶ Read Morton and Mayers (2005), Chapter 2 (intro), sections 2.1, 2.3.
- ▶ Sign up to GitHub and send login name.
- ▶ Run/study the two example codes and study the example task.
- ▶ Study and start exercise-I.

Finite difference methods: Fourier analysis

- ▶ To assess stability of scheme, Fourier analysis will be used. Substitute Fourier Ansatz $U_j^n = \lambda^n e^{ijk\Delta x}$ with imaginary number i satisfying $i^2 = -1$, amplification factor λ , and wavenumber k into discretization (11).
- ▶ In general λ is complex with real and imaginary parts such that $\lambda = \Re(\lambda) + i \Im(\lambda)$. Scheme is stable when $|\lambda| \leq 1$, which for complex λ implies that we need to take the modulus of λ .
- ▶ When $|\lambda| > 1$, approximation U_j^n will blow up over time since $|\lambda|^n$ becomes unbounded and the scheme is unstable.

$$-\theta\mu\lambda e^{-ik\Delta x} + (1 + 2\theta\mu)\lambda - \theta\mu\lambda e^{ik\Delta x} = 1 - 2(1 - \theta)\mu + (1 - \theta)\mu(e^{ik\Delta x} + e^{-ik\Delta x}) \quad (13)$$

$$\iff \lambda + \lambda\theta\mu(2 - e^{ik\Delta x} - e^{-ik\Delta x}) = 1 - (1 - \theta)\mu(2 - e^{ik\Delta x} - e^{-ik\Delta x}) \quad (14)$$

$$\iff \lambda = \frac{1 - 4(1 - \theta)\mu \sin^2(k\Delta x/2)}{1 + 4\theta\mu \sin^2(k\Delta x/2)}. \quad (15)$$

Finite difference methods: Fourier analysis

- Note that this scheme is a special, symmetric case for which λ is real. Since $0 \leq \theta \leq 1$ and $\mu > 0$, we note that $\lambda < 1$.
- Instability can then occur only when $\lambda < -1$, i.e., when

$$\begin{aligned} 1 - 4(1 - \theta)\mu \sin^2(k\Delta x/2) &< - (1 + 4\theta\mu \sin^2 k(\Delta x/2)) \\ \implies 4\mu(1 - 2\theta) \sin^2(k\Delta x/2) &> 2. \end{aligned} \quad (16)$$

- Instability occurs for $\mu(1 - 2\theta) > 1/2$ for case $k\Delta x/2 = \pi/2$. For $\theta \geq 1/2$ the θ -scheme unconditionally stable, while for $0 \leq \theta < 1/2$ scheme conditionally stable when

$$\mu = \frac{\Delta t}{(\Delta x)^2} < \frac{1}{[2(1 - 2\theta)]}. \quad (17)$$

- Note that we ignored the boundary conditions in deriving Fourier stability because we imposed the harmonic Ansatz for periodic boundaries. Other BCs, see Morton and Mayers 2005.

Finite difference methods: maximum principle

Theorem

M&M 2005: The θ -method (11) satisfies

$$U_{min} \leq U_j^n \leq U_{max}$$

$$U_{min} = \min(U_0^m, 0 \leq m \leq n; U_j^0, 0 \leq j \leq N_x; U_{N_x}^m, 0 \leq m \leq n)$$

$$U_{max} = \max(U_0^m, 0 \leq m \leq n; U_j^0, 0 \leq j \leq N_x; U_{N_x}^m, 0 \leq m \leq n)$$

given the conditions $0 \leq \theta \leq 1$ and $\mu(1 - \theta) \leq 1/2$.

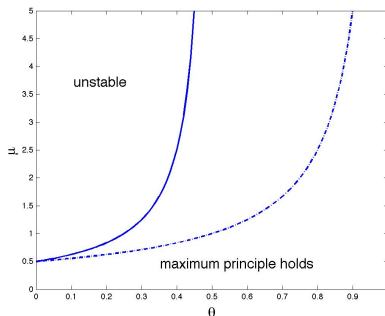
Finite difference methods: maximum principle

- ▶ Verification of conditions required for maximum principle to hold forms a practical test for stability of numerical finite difference schemes for diffusion and advection-diffusion equations.
- ▶ Maximum principle states that value of variable U_j^n bounded between boundary values and initial values. E.g., when u is seen as a temperature, temperature values can not go above or below temperatures imposed initially or at boundaries.

Finite difference methods: stability criteria

The Fourier stability condition (17) and condition for maximum principle, displayed in Fig.:

$$\mu = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{[2(1 - 2\theta)]} \quad \text{and} \quad \mu(1 - \theta) \leq \frac{1}{2}. \quad (18)$$



Finite difference methods: homework, week 2

- ▶ Study Morton and Mayers (2005), Chapter 2, sections 2.7, 2.11.
- ▶ Read Morton and Mayers (2005), Chapter 2, sections 2.8, 2.9, 2.10.
- ▶ Continue/finish exercise-I.
- ▶ Urgent: get *Firedrake* installed on your machines, asap, please!
- ▶ ... hints for Exercise-I

Finite volume or Godunov method

- ▶ Finite volume methods may be most natural for hyperbolic PDEs expressed as conservation laws.
- ▶ We only consider the 1D case here:

$$\partial_t u + \partial_x(f(u)) = 0 \quad \text{or} \quad (19)$$

$$\partial_t u_j + \partial_{x_j} f_{ij} = 0 \quad \text{with } j = 1 \quad (20)$$

with $u = (u_1, u_2, \dots, u_n)$ and $u = (f_1, f_2, \dots, f_n)$.

Finite volume: example conservation laws

Examples:

- Euler equations in 2D:

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(E + p) \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E + p) \end{pmatrix} = 0 \quad (21)$$

with u and v velocity components in x and y , p pressure and E total energy. EOS: $p = (\gamma - 1)(E - \frac{1}{2}\rho(u^2 + v^2))$.

- Shallow-water equations in 1D:

$$\partial_t h + \partial_x(hu) = 0, \partial_t(hu) + \partial_x(hu^2 + \frac{1}{2}gh^2) = 0 \quad (22)$$

with water depth $h(x, t)$ and depth-averaged velocity $u(x, t)$.

Finite volume: examples

Examples of conservative systems with extra terms:

- Width-averaged shallow-water or St. Venant equations:

$$\partial_t A + \partial_s(Au) = S \quad (23)$$

$$\partial_t(Au) + \partial_s(Au^2 + gAh) = gh\partial_s A - gA\partial_s b - F, \quad (24)$$

with source and friction terms $S = S(s, t)$,
 $F = gC_m Au|u|/R(A, s)^{4/3}$; along-river coordinate s ;
cross-section $A(s, t)$; water depth $h = h(A, s)$; depth-averaged
velocity $u(s, t)$; river slope $-\partial_s b$, and, accelation of gravity g .

Finite volume: examples

- Limit of kinematic river equation, conservative with extra source term:

$$\partial_t A + \partial_s \left(AR(A, s)^{2/3} \sqrt{-\partial_s b} / C_m \right) = S, \quad (25)$$

with Manning coefficient C_m , hydraulic radius $R(A, s)$ (wetted area A over wetted perimeter) and “volume” $S(s, t)$.

Finite volume: overview for Burgers-advection system

- ▶ Illustrate Godunov method or finite volume discretization for simple system of hyperbolic equations.
- ▶ Step by step discretization for system of uncoupled Burgers' and linear advection equations

$$u_t + (u^2/2)_x = 0 \quad (26)$$

$$v_t + a v_x = 0 \quad (27)$$

with $a > 0$ constant, $u = u(x, t)$ and $v = v(x, t)$ on $x \in [0, L]$, $(\cdot)_t = \partial_t$, etc.

- ▶ Boundary conditions required, not specified presently.
- ▶ Initial conditions $u(x, 0)$ and $v(x, 0)$ are given at $t = t_0 = 0$.

Finite volume method: studying

From Leveque's book *Finite volume methods*:

- ▶ Study §1.1 (conservation law) §3.1 (linear advection Eq.) till §3.1.1 & 3.2 (Burgers' Eq).
- ▶ Study §3.1, §3.3 (shock formation).

Godunov method example: Step-1

- ▶ Exposition of simple uncoupled system plus algorithm facilitates implementation for genuinely coupled fluid system, presented elsewhere.
- ▶ *Step 1:*
System (26) is written concisely in hyperbolic form (20)

$$u_t + (f(u))_x = 0, \quad (28)$$

after identification $u = (u, v)^T$ and flux $f(u) = (u^2/2, a v)^T$ (transpose $(\cdot)^T$).

Godunov method example: Step-3

- ▶ *Step 3: Integrate (28) in space-time element*
 $x_{k-1/2} < x < x_{k+1/2}$ and $t_n < t < t_{n+1}$, Fig. 22.
- ▶ Via coordinate transformation $x' = x - x_{k+1/2}$, $t' = t - t_n$, right-bottom corner becomes origin $(x', t')^T = (0, 0)^T$.
- ▶ After integration of (28) over space-time element:

$$U_k^{n+1} = U_k^n - \frac{1}{h_k} \int_{t_n}^{t_{n+1}} f_{k+1/2}(t) - f_{k-1/2}(t) dt, \quad (29)$$

with mean cell average U_k in cell k

$$U_k(t) = \frac{1}{h_k} \int_{x_{k-1/2}}^{x_{k+1/2}} u(x, t) dx. \quad (30)$$

- ▶ Flux is at the cell boundaries: $f_{k+1/2}(t) = f(u(x = x_{k+1/2}, t))$.
- ▶ $U_k(t)$ in (30) and $f_{k+1/2}(t)$ still functions of time t , and $U_k^n = U_k(t = t_n)$, etc.

Godunov method example: Step-3

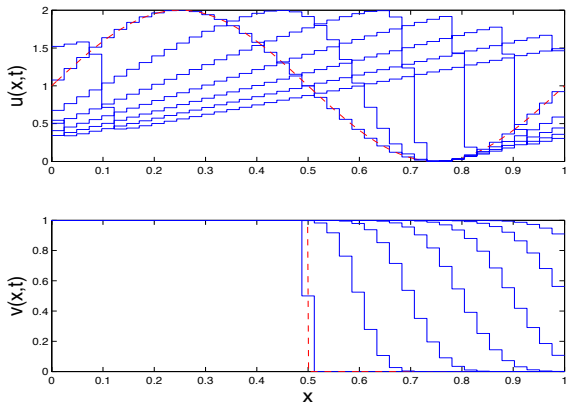
- ▶ Integral expression (29) exact provided that $u(x, t)$ known. Start at $n = 0$, calculate $U_k^0 = U_k(t = t_0)$ using (30).
- ▶ Graphically, U_k^0 is projection of initial data on piecewise constant profiles at time t_0 , cf. initial step profiles in Fig. 25.
- ▶ Determine $f_{k+1/2}(t)$ over $t_n < t < t_{n+1}$ in (29) to obtain

$$U_k^{n+1} = U_k^n - \frac{\Delta t}{h_k} \left(F_{k+1/2}(U_k^n, U_{k+1}^n) - F_{k-1/2}(U_{k-1}^n, U_k^n) \right) \quad (31)$$

with (approximate) numerical flux

$$F_{k+1/2}(U_k^n, U_{k+1}^n) \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f_{k+1/2}(t) dt. \quad (32)$$

Godunov method example: Step-3



Godunov method example: Step-4

- ▶ *Step 4:* Calculate numerical fluxes $F_{k+1/2}(U_k^n, U_{k+1}^n)$ in (32) at all nodes $x_{k+1/2}$ for $k = 0, 2, \dots, N$.
- ▶ There are various strategies to find (32), usually involving an approximation.
- ▶ Consider classical Godunov strategy based on the Riemann solution.
- ▶ Calculate $F_{k+1/2}(t)$ in (32) exactly over $t_n < t < t_{n+1}$ in (29), only feasible for piecewise constant approximation U_k^n at time t_n and starting with projected initial condition U_k^0 , instead of smoother initial condition.
- ▶ Solution of Riemann problem in new coordinates, i.e. with $u = u(x', t')$ and $f = f(u(x', t'))$, provides such exact solution.

Godunov method example: Riemann problem

- ▶ The Riemann problem is defined as

$$\frac{\partial u}{\partial t'} + \frac{\partial f}{\partial x'} = 0 \quad (33)$$

for special initial conditions

$$u(x', t' = 0) = \begin{cases} u_{left} = u_l = U_k^n & \text{for } x' < 0 \\ u_{right} = u_r = U_{k+1}^n & \text{for } x' \geq 0 \end{cases} \cdot \quad (34)$$

- ▶ Riemann solution such that $u(x', t')$ constant along characteristics $x' = x'_0 + C t'$ for some C depending on $u_{l,r}$.
- ▶ $f_{k+1/2}(t) = f_{k+1/2}(u(x_{k+1/2}, t))$ is constant; (32) can be integrated —note that $u(x' = 0, t') = u(x_{k+1/2}, t)$ due to coordinate change.

Godunov method example: Riemann problem

NB:

- ▶ While formula (29) exact, numerical approximation occurs because we continue from a piecewise constant profile with value U_k^n in cell k at a certain time t_n .
- ▶ At cell boundary $x_{k+1/2}$ between cells k and $k+1$, adjacent values are U_k^n and U_{k+1}^n .
- ▶ When other cell boundaries $x_{k-1/2}$ and $x_{k+3/2}$ are “far away” in sense that time step Δt is “small enough”, we are locally dealing with a Riemann problem around cell boundary $x_{k+1/2}$.
- ▶ Although Riemann solution no longer piecewise constant within each cell at end of time step, we continue only with information stored in the mean values U_k^{n+1} .
- ▶ This is the approximation made.

Godunov method example: Riemann problem

- The characteristic form of (26)–(27) is as follows

$$\frac{du}{dt} = 0 \quad \text{on} \quad \frac{dx}{dt} = u \quad (35)$$

$$\frac{dv}{dt} = 0 \quad \text{on} \quad \frac{dx}{dt} = a, \quad (36)$$

which has solution”

$$x = x_{01} + ut, \quad u = u_0(x_{01}) \quad \text{s. t.} \quad u(x, t) = u_0(x - u(x, t))$$

$$x = x_{02} + at, \quad v = v_0(x_{02}) \quad \text{s. t.} \quad v(x, t) = v_0(x - at).$$

- At $t = 0$ we see that $x = x_{01}$ or $x = x_{02}$ and these parameterise the domain for each equation.
- Instead of two PDEs, we have four ODEs.
- For constant a , solution of linear advection equation is a mere shift of original profile to left or right, depending on sign of a .

Godunov method: studying

From Leveque's book *Finite volume methods*:

- ▶ Study §3.5 (Riemann problem), §3.6 (shock speed).
- ▶ Study §13.2 (Godunov method), §13.5 (Godunov for scalar conservation laws); read Chap. 9.

Godunov method example: Riemann problem

The Riemann problem for the uncoupled system (26) special: consists of separate Riemann problems for two equations.

- Solution of Riemann problem for linear advection equation:

$$\frac{\partial v}{\partial t'} + \frac{\partial(a v)}{\partial x'} = 0 \quad (37)$$

with constant $a > 0$.

- NB: piecewise constant initial conditions

$$v(x', t' = 0) = \begin{cases} v_{left} = v_l = V_k^n & \text{for } x' < 0 \\ v_{right} = v_r = V_{k+1}^n & \text{for } x' \geq 0 \end{cases} \cdot \quad (38)$$

- For $a > 0$ all characteristics are $x' = x_0 + a t'$. Solution $v(x' = 0, t') = v(x_{k+1/2}, t) = v_l^n$ with $f(v(x_{k+1/2}, t)) = a v_l^n$ within a sufficiently small time interval.

Godunov method example: CFL condition

- ▶ Application of maximum principle to (39) yields, by imposing that all coefficients 1, $(1 - \Delta t a/h_k)$ and $a\Delta t/h_k$ of V_k^{n+1} , V_k^n , V_{k-1}^n are larger than zero (and $a > 0$):

$$V_k^{n+1} = (1 - \frac{\Delta t}{h_k} a) V_k^n + \frac{\Delta t}{h_k} a V_{k-1}^n \quad (40)$$

$$\Rightarrow 1 - \frac{\Delta t}{h_k} a > 0 \iff \Delta t < \frac{h_k}{a}. \quad (41)$$

- ▶ The well-known Courant-Friedrichs-Lewy or CFL condition.
- ▶ When $a < 0$, the upwind discretization should be:

$$V_k^{n+1} = V_k^n + \frac{\Delta t}{h_k} |a| (V_{k+1}^n - V_k^n). \quad (42)$$

- ▶ For general a , the CFL condition thus reads $\Delta t < h_k/|a|$, which also makes sense dimensionally since a is a “wind” speed.

Godunov method example: CFL condition

Graphically, upwinding for linear advection equation:

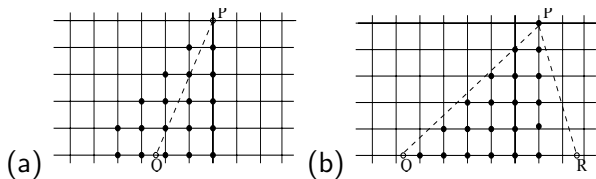


Figure: Consider the linear advection equation $u_t + a u_x = 0$ with $a > 0$.
(a) The solution $u(x, t) = u^0(x - at)$ has a characteristic tracing through point P back to point Q satisfying the CFL condition $\Delta t < \Delta x/|a|$. (b) The CFL condition is violated when $\Delta t > \Delta x/|a|$ as the information transported along the characteristic falls outside the discretization stencil. It shows the dependence of the numerical solution on the initial data.

Godunov method example: Riemann problem

- Burgers' equation allows discontinuous or shock solutions, where $u(x, t)$ obtains different limiting values.
- Discontinuity resides at position $x = x_b(t)$ and moves with shock speed $s \equiv dx_b/dt$.
- Integrate Burgers' equation in (26) around $x_b(t)$, and let $\epsilon \rightarrow 0$, to obtain

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \int_{x_b - \epsilon}^{x_b + \epsilon} \frac{\partial u(x, t)}{\partial t} dx + \int_{x_b - \epsilon}^{x_b + \epsilon} \frac{\partial (u^2/2)}{\partial x} dx = 0 \\ \Leftrightarrow & \frac{\partial}{\partial t} \lim_{\epsilon \rightarrow 0} \int_{x_b(t) - \epsilon}^{x_b(t) + \epsilon} u(x, t) dx - \frac{dx_b(t)}{dt} \lim_{\epsilon \rightarrow 0} u(x, t) \Big|_{x_b(t) - \epsilon}^{x_b(t) + \epsilon} + [u^2/2] = 0 \quad (43) \\ \Leftrightarrow & -\frac{dx_b(t)}{dt} [u] + [u^2/2] = 0 \Leftrightarrow s = \frac{dx_b(t)}{dt} = \frac{[u^2/2]}{[u]} = \frac{1}{2} (u_l + u_r) \end{aligned}$$

with $[u] = u_r - u_l$, $[u^2/2] = (u_r^2 - u_l^2)/2$, $u_r = u(x, t)|_{x \downarrow x_b}$ and $u_l = u(x, t)|_{x \uparrow x_b}$.

- In literature, approximate numerical fluxes are found such as Roe solvers and kinetic fluxes.

Godunov method example: Riemann problem Burgers

- ▶ *Exercise-Burgers:* (i) Derive the Riemann solution for the Riemann problem of the Burgers' equation.
- ▶ *Exercise-Burgers:* (ii) Complete the Godunov method for the Burgers' equation using this Riemann solution.

Godunov method example: Riemann problem

Homework Exercise-II.