Chapter 1. Review on ‘Introduction to CFD’

Chap. 1-1. Topics Covered

- **Classification of PDE**
  - Characteristics of 2nd-order linear PDE → Elliptic, Parabolic, and Hyperbolic PDE
- **Basic concept and linear stability**
  - Finite difference approximation of spatial and temporal derivatives
  - Truncation error and consistency → Fourier error analysis
  - Modified equation → numerical dissipation and numerical dispersion
  - General concept of stability → Von Neumann stability and Lax equivalence theorem
  - Domain of dependence/influence → CFD condition and stability
- **Discretization of Parabolic PDE**
  - Basic explicit/implicit schemes, and stability analysis
  - Splitting or factorized schemes for multi-D problems → ADI/AF-ADI in terms of delta/non-delta forms
  - Difference between delta and non-delta form for steady-state computations
- **Discretization of Elliptic PDE**
  - Relaxation methods depending on the choice of P with $A = P+B$ → Jacobi/G-S/ADI, and versions of over-relaxation
  - Similarity between relaxation method for elliptic PDE and time-marching method for parabolic PDE
  - Multigrid convergence acceleration → CGC strategy for linear elliptic PDE, V-/W-cycle

Chap. 1-2. Basic Theory of SCL

- ***Hyperbolic PDEs***
  - **Wave propagation problems with *limited D of Dep. and limited D. of Inf.***
    - Formation, propagation and interaction of linear and nonlinear waves
  - **Convection-dominated flows, compressible flows, convective flows admitting discontinuous solutions**
  - **Scalar conservation law**
    - Linear convection equation $\left(u_t + a u_x = 0\right)$
    - Burgers' equation $\left(u_t + u u_x = 0\right)$
  - **Euler Equations**
- ***General Form of SCL***

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0 \qquad \text{Eq.(*1)}$$

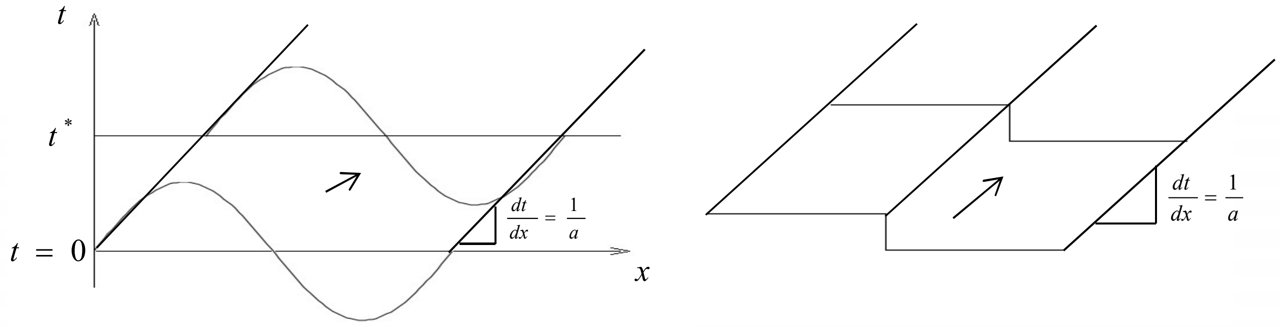
- u : conserved quantity, $f(u)$: convex flux function, $a(u) \equiv \dfrac{\partial f(u)}{\partial u}$: wave speed
- With I.C. of $u(x,0) = u_0(x)$, the exact soln. of Eq. (*1) is $u(x,t) = u_0\left(x - a(u)t\right)$.
- $u(x,t) = const$ along the 'charactersitic line' of $x - a(u)t = const$, with the wave speed of $\dfrac{dx}{dt} = a(u)$

Chap. 1-2. Basic Theory of SCL

- **Ex 1) Linear wave equation**
  - If $a(u) = a = const, f(u) = au$ and $u_t + au_x = 0$

    $\rightarrow\ u(x,t) = u_0(x - at)$ with $\dfrac{dx}{dt} = a = const$

    $\rightarrow$ Initial profile moves with the same speed of a, and the initial shape is preserved.

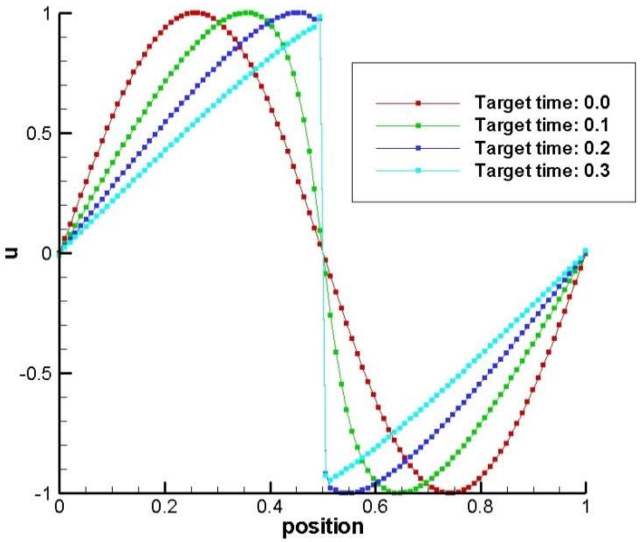


- **Ex 2) Nonlinear wave equation**
  - If $a(u) = u \neq const, f(u) = \dfrac{u^2}{2}$ and $u_t + uu_x = 0$

    $\rightarrow u(x,t) = u_0(x - ut)$ with $\dfrac{dx}{dt} = u \neq const$

    $\rightarrow$ Initial profile moves with the local speed of u, and a 'discontinuous' solution can be developed even with a 'smooth' initial profile.

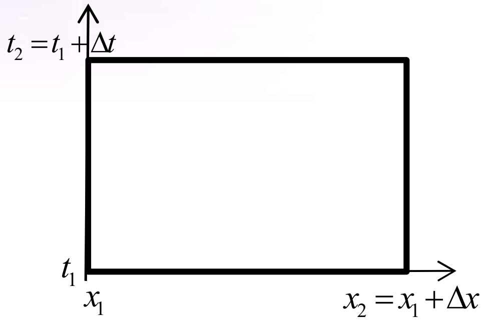
- **Ex 2) Nonlinear wave equation (cont'd)**
  - Problem of differentiability at discontinuity
    - A sinusoidal initial profile leading to a discontinuous saw-tooth profile



- **Behavior of the exact solution**
  - Assuming convex flux function ($f''(u) = a'(u) \geq 0$), extrema of the exact solution are determined by the initial condition, and after forming a discontinuity, they are decaying to $O(t^{-1/2})$ to create wider expansion region.
    - This is true to the case of intersection of discontinuities to create a single discontinuity.
    - In case of non-convex flux function for real gas flows or two-phase flows in porous media, intersection of discontinuities creates multiple discontinuities along with a new monotonic wave profile bounded by the multiple discontinuities.

Chap. 1-2. Basic Theory of SCL

- ***Integration of SCL → Conservative Finite Volume Discretization***



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

$$\rightarrow \int_{t_1}^{t_2} \int_{x_1}^{x_2} \left(\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} \right) dx dt = 0$$

$$\int_{x_1}^{x_2} u(x,t_2) dx - \int_{x_1}^{x_2} u(x,t_1) dx = \int_{t_1}^{t_2} f(u(x_1,t)) dt - \int_{t_1}^{t_2} f(u(x_2,t)) dt \qquad \text{Eq.(*2)}$$

$\rightarrow$ Conservation of u in (x,t) stating that

change of u over (x_1, x_2) during Δt = net flux across the boundary of x_1, x_2 during Δt

Introduce a finite volume computational cell with $(x_1, x_2) = (x_{j-1/2}, x_{j+1/2})$ and $(t_1, t_2) = (t^n, t^{n+1})$,

and define an approximate quantity averaged over $\Delta x = x_{j+1/2} - x_{j-1/2}$ and $\Delta t = t^{n+1} - t^n$

• cell-averaged value: $\frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t^n) dx \equiv u_j^n$, • cell-interface numerical flux: $\frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} f(u(x_{j+1/2},t)) dt \equiv F_{j+1/2}$

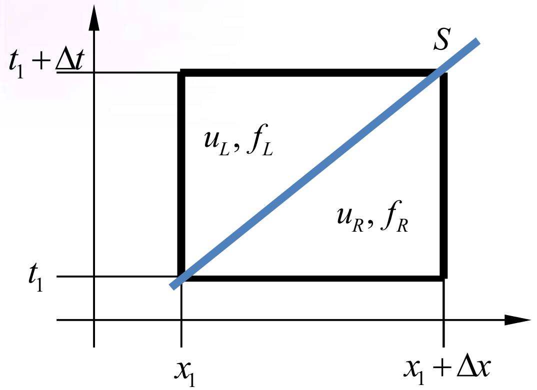
Then, Eq.(*2) can be discretized, called conservative finite volume discretization, as

$$\Delta x \left(u_j^{n+1} - u_j^n \right) = \Delta t \left(F_{j-1/2} - F_{j+1/2} \right) \rightarrow u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} \left(F_{j+1/2} - F_{j-1/2} \right) \qquad \text{Eq.(*3)}$$

By applying the integral form of SCL (or using Eq.(*3)), problem of differentiability is avoided.

Chap. 1-2. Basic Theory of SCL

- **Integral conservative form and the condition for correct shock speed**



From Eq. (*3),

$$(u_L - u_R)\Delta x = (f_L - f_R)\Delta t$$

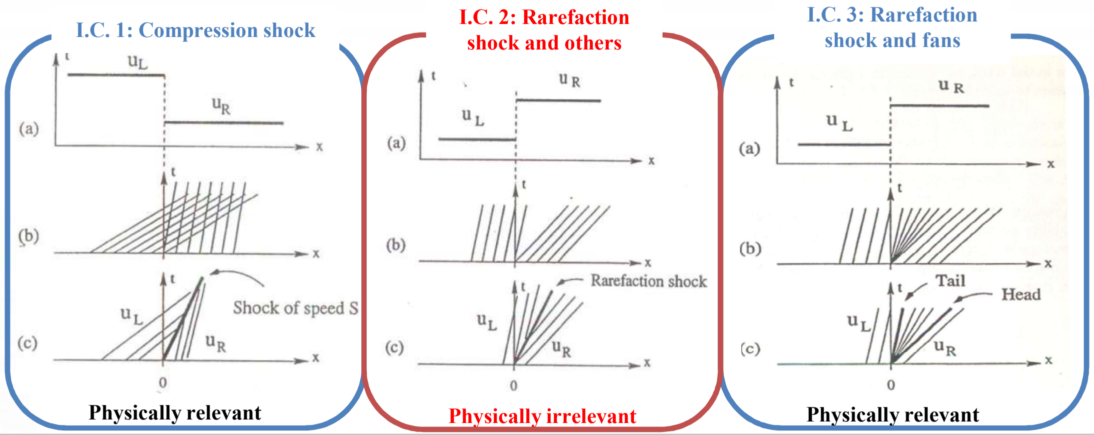
$$(f_R - f_L) = \frac{\Delta x}{\Delta t}(u_R - u_L) = S(u_R - u_L) \text{ with } S = \text{shock speed}$$

or $[f] = S[u]$ $\rightarrow$ Rankine-Hugoniout relation for SCL

• Note that S is the shock speed averaged over $\Delta x,\ \Delta t$.

- **Integral form and the problem of non-uniqueness**
  - Ex) Correct behavior of discontinuities under various initial conditions

$$S = \frac{[f]}{[u]} = \frac{\frac{1}{2}\left(u_L^2 - u_R^2\right)}{u_L - u_R} = \frac{1}{2}\left(u_L + u_R\right) \quad \text{for Burgers equation}$$



Chap. 1-2. Basic Theory of SCL

- **Flow physics from the 2nd law of thermodynamics states that expansion shock is not allowed. → entropy condition**
  - Characteristics across discontinuity should converge. → For the right-moving shock with $u_L > u_R,\ u_L > S = [f]/[u] > u_R$. Thus, case III is the physically correct solution.
  - More generally, the entropy condition by Oleinik can be considered to include non-convex cases.
    $(f(u) - f(u_L))/(u - u_L) > S = [f]/[u] > (f(u_R) - f(u))/(u_R - u)$
  - Ex) Consider a SCL with $u_0(x) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x > 0 \end{cases}$

    What would be the expected entropy solution for convex and non-convex flux functions?
- **How to implement ?**
  - Solve a vanishing viscosity form $u_t + au_x = \varepsilon u_{xx}$ with some(?) $\varepsilon > 0$
  - Design a numerical flux such that it contains a proper form of numerical viscosity
  - Entropy function and entropy flux → entropy inequality
    - Motivated by the entropy inequality of the Euler equations $(\rho s)_t + (\rho us)_x \geq 0$,
      Consider the entropy inequality of SCL as $U(u)_t + F(u)_x \geq 0$
      with $U(u)$: entropy function, $F(u)$: entropy flux.
      Then, by requiring $\frac{dF}{du} = \frac{df}{du}\frac{dU}{du}$ and $\frac{d^2U}{du^2} \leq 0$, $U(u)$ and $F(u)$ satisfying the entropy inequality can be obtained.

Chap. 1-2. Basic Theory of SCL

- **Conservation law and weak solution**
  - Consider $u_t + \left(\frac{u^2}{2}\right)_x = 0$ vs. $\left(u^2\right)_t + \left(\frac{2}{3}u^3\right)_x = 0$

    $$S_u = \frac{[f]}{[u]} = \frac{1}{2}(u_L + u_R) \text{ vs. } S_{u^2} = \frac{\left[f\left(u^2\right)\right]}{\left[u^2\right]} = \frac{1}{2}(u_L + u_R) + \frac{1}{6}\frac{(u_L - u_R)^2}{u_L + u_R}$$

    - Mathematically both equations are the same in smooth region, but not, in discontinuous region
    - Note that $U(u) = -u^2$ and $F(u) = -\frac{2}{3}u^3$ are actually the entropy function and entropy flux, respectively.

- ***Conservative Scheme***
  - **Applying the integral form of SCL over $(\Delta x, \Delta t)$**

    $$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2} - F_{j-1/2}\right) \qquad \text{Eq. (*3)}$$

  - **For 1-D case with $\Omega = \text{JMAX} \times \Delta x$**

    $$\sum_{j=1}^{JMAX}(\text{Eq. (*3)}) \text{ gives } \sum_{j=1}^{JMAX} u_j^{n+1} - \sum_{j=1}^{JMAX} u_j^n + \frac{\Delta t}{\Delta x}\left(F_{JMAX+1/2}^n - F_{1/2}^n\right) = 0,$$

    if each cell-interface flux is *uniquely* and *consistently* determined from cell-averaged values

    $\rightarrow$ Change of u in the computational domain during Δt

    = Net flux across the computational boundary during Δt

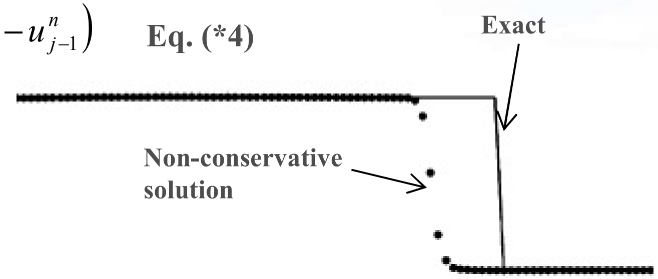
    $\rightarrow$ Discrete realization of the integral conservation law over the computational domain

Chap. 1-2. Basic Theory of SCL

- Ex) Non-conservative scheme and shock speed
  - For Burgers eqn. of $u_t + uu_x = 0$ with I.C. of $u_0(x) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x \geq 0 \end{cases}$
  - A non-conservative upwind scheme : $u_j^{n+1} = u_j^n - \dfrac{\Delta t}{\Delta x} u_j^n \left(u_j^n - u_{j-1}^n\right)$ **Eq. (*4)**

    with $u_j^0 = \begin{cases} 1 & \text{if } j < 0 \\ 0 & \text{if } j \geq 0 \end{cases}$
  - From Eq. (*4), $u_j^n = u_j^0$ for all n and j $\rightarrow$ S=0

    But from the R-H condition of SCL, $S = \dfrac{1}{2}(1+0) = 0.5$



- ***Consistency***
  - **General form of conservative scheme**

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}\left(u_{j-p}^n, u_{j-p+1}^n, \ldots, u_{j+q}^n\right) - F_{j-1/2}\left(u_{j-p-1}^n, u_{j-p}^n, \ldots, u_{j+q-1}^n\right)\right)$$ **Eq. (*5)**

  - Eq. (*5) is called consistent with SCL if $F_{j+1/2}$ goes to the true flux *f(u)* in the constant flow.

    $F(\bar{u}, \bar{u}, \ldots, \bar{u}) = f(\bar{u})$
  - A stronger condition to satisfy the consistency is the Lipschitz continuity of $F_{j+1/2}$, or that there is some $K > 0$ such that

    $\left|F\left(u_{j-p}, u_{j-p+1}, \ldots, u_{j+q}\right) - f(u)\right| \leq K \max_{-p \leq i \leq q} \left|u_{j+i} - u\right|$