

# FV discretization of Conservation Law

Conservation (balance): In any volume  $V$ , per unit time  
 change of  $u$  in  $V$  = net amount crossing into  $V$  thru  $\partial V$   
 + net created within  $V$

Integral form of Conservation Law:

$$\frac{d}{dt} \int_V u dV = - \int_{\partial V} \vec{F} \cdot \vec{n} dA + \int_V S dV$$

$u$  = amount / vol

$\vec{F}$  = flux = amount / area / time

$\vec{n}$  = outgoing unit normal to  $\partial V$

$S$  = source = amount / vol / time

most general (only integrals need to exist, no smoothness required)

Divergence Theorem:  $\int_{\partial V} \vec{F} \cdot \vec{n} dA = \int_V \nabla \cdot \vec{F} dV$ , assuming  $\nabla \cdot \vec{F}$  integrable  
 "Green domain"

$$\text{divergence: } \nabla \cdot \vec{F} = \text{div}(\vec{F}) = \sum_i \frac{\partial F_i}{\partial x_i} \equiv \left( \frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n} \right) \cdot (\vec{F}_1, \dots, \vec{F}_n)$$

$$\text{component form of Div Thm: } \int_V \frac{\partial \varphi}{\partial x_i} dV = \int_{\partial V} \varphi n_i dA, i=1, \dots, n$$

Differential Form of Conservation Law:  $\frac{\partial u}{\partial t} + \nabla \cdot \vec{F} = S$  "at each point" of  $\Omega$   
 assuming  $\frac{\partial u}{\partial t}, \frac{\partial F_i}{\partial x_i}$  integrable

$$\text{By Div Thm, } \frac{d}{dt} \int_V u dV + \int_V \nabla \cdot \vec{F} dV = \int_V S dV \text{ for any } V \subset \Omega$$

$$\Leftrightarrow \int_V \left\{ \frac{\partial u}{\partial t} + \nabla \cdot \vec{F} - S \right\} dV = 0 \quad \forall V \subset \Omega$$

$$\Rightarrow u_t + \nabla \cdot \vec{F} = S \text{ "almost everywhere" in } \Omega$$

Discretization: discretize region  $\Omega$  into control volumes  $\{V_i\}_{i=1:M}$   
 time into timesteps  $\{t_n\}_{n=0:N}$

integrate PDE over each  $V_i$  and over  $[t_n, t_{n+1}]$ :

$$\int_{t_n}^{t_{n+1}} \frac{d}{dt} \int_{V_i} u dV dt + \int_{t_n}^{t_{n+1}} \underbrace{\int_{\partial V_i} \vec{F} \cdot \vec{n} dA}_{} dt = \int_{t_n}^{t_{n+1}} \int_{V_i} S dV dt \quad \text{discrete conservation}$$

$\sum_{\text{faces}} \int_{\text{face}} \vec{F} \cdot \vec{n} dA = \sum_{\text{faces}} (\vec{A}\vec{F}) \cdot \vec{n} = \text{sum of flow rates across faces of } V_i$



Set  $U_i^n = \frac{1}{\Delta V_i} \int_{V_i} u(x, t_n) dV = \text{mean value of } u \text{ over } V_i \text{ at time } t_n$

$(\vec{A}\vec{F})_{\text{face}}^{n+\theta} = \frac{1}{\Delta t_n} \int_{t_n}^{t_{n+1}} (\vec{A}\vec{F})_{\text{face}} dt = \text{mean flow rate across face during time step}$

$S_i^{n+\theta} = \frac{1}{\Delta t_n} \int_{t_n}^{t_{n+1}} \frac{1}{\Delta V_i} \int_{V_i} S dV dt = \text{mean source over } V_i \text{ and over } \Delta t_n$

$$\Rightarrow \Delta V_i [U_i^{n+1} - U_i^n] + \Delta t_n \sum_{\text{faces}} (\vec{A}\vec{F})_{\text{face}}^{n+\theta} \cdot \vec{n} = \Delta t_n \Delta V_i \cdot S_i^{n+\theta} \quad \text{exact discrete conservation}$$

$0 \leq \theta \leq 1$ : implicitness parameter to be chosen

$\theta$ -scheme:

$$U_i^{n+1} = U_i^n + \frac{\Delta t_n}{\Delta V_i} \sum_{\text{faces}} -(\vec{A}\vec{F})_{\text{face}}^{n+\theta} \cdot \vec{n} + \Delta t_n S_i^{n+\theta}, \quad i=1:M, n=0, 1, \dots, N$$

holds in any dimension,

$\theta=0$ : explicit scheme, Forward Euler in time,  $O(\Delta t)$

$0 < \theta \leq 1$ : implicit scheme, need to solve system for  $U_1, \dots, U_M$

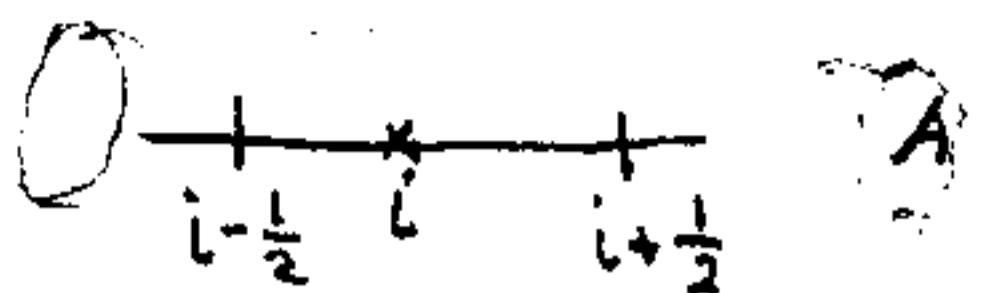
$$F^{n+\theta} = (1-\theta) F^n + \theta F^{n+1}, \quad S^{n+\theta} = (1-\theta) S^n + \theta S^{n+1}, \quad t_{n+1} = (1-\theta)t_n + \theta t_{n+1}$$

$\theta=\frac{1}{2}$ : Crank-Nicolson,  $O(\Delta t^2)$

$\theta=1$ : backward Euler, fully implicit,  $O(\Delta t)$

FV scheme in 1D

$$\Delta V_i = A \cdot \Delta x, \quad \text{faces} = A \times \{x_{i-\frac{1}{2}}\}, \quad A = \text{fixed area}$$



$$A \cdot \Delta x [U_i^{n+1} - U_i^n] + \Delta t [A F_{i+\frac{1}{2}}^{n+\theta} - A F_{i-\frac{1}{2}}^{n+\theta}] = \Delta t \cdot A \Delta x \cdot S_i^{n+\theta}$$

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x} [F_{i-\frac{1}{2}}^{n+\theta} - F_{i+\frac{1}{2}}^{n+\theta}] + \Delta t \cdot S_i^{n+\theta}, \quad i=1:M, n=0:N$$

exact discrete conservation on each control volume.

CFL for 1D diffusion for  $\theta$ -scheme

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x} \left\{ (1-\theta) [F_{i-\frac{1}{2}}^n - F_{i+\frac{1}{2}}^n] + \theta \cdot [F_{i-\frac{1}{2}}^{n+1} - F_{i+\frac{1}{2}}^{n+1}] \right\}, \quad F_{i-\frac{1}{2}} = -D \frac{U_i - U_{i-1}}{\Delta x}$$

$$\mu = \frac{D \Delta t}{\Delta x^2}$$

$$= U_i^n + \frac{\Delta t}{\Delta x} (1-\theta) \left\{ -D \frac{U_i - U_{i-1}}{\Delta x} + D \frac{U_{i+1} - U_i}{\Delta x} \right\} + \frac{\Delta t}{\Delta x} \theta \left\{ -D \frac{U_i^{n+1} - U_{i-1}^{n+1}}{\Delta x} + D \frac{U_{i+1}^{n+1} - U_i^{n+1}}{\Delta x} \right\}$$

$$\Rightarrow [1 + 2\mu\theta] U_i^{n+1} = [1 - 2\mu(1-\theta)] U_i^n + (1-\theta)\mu [U_{i-1}^n + U_{i+1}^n] + \theta\mu [U_{i-1}^{n+1} + U_{i+1}^{n+1}]$$

Positive Coefficient Rule to preserve positivity (monotonicity preserving scheme):

$$1 - 2\mu(1-\theta) \geq 0 \Rightarrow \boxed{\mu = \frac{D \Delta t}{\Delta x^2} \leq \frac{1}{2(1-\theta)}} : \text{CFL}$$

For  $\theta=0$ : CFL is  $\mu \leq \frac{1}{2}$  i.e.  $\Delta t \leq \frac{\Delta x^2}{2D} =: \Delta t_{\text{expl}}$ ; Explicit scheme

For  $\theta=\frac{1}{2}$ : CFL is  $\mu \leq 1$  i.e.  $\Delta t \leq \frac{\Delta x^2}{D} = 2 \cdot \Delta t_{\text{expl}}$ ; Crank-Nicolson

For  $\theta=1$ : CFL  $\mu < \infty$ , no restriction on  $\Delta t$  for stability; Fully implicit  
need to restrict  $\Delta t$  only for accuracy  
only Backward Euler is unconditionally positivity preserving!

Any  $\theta \neq 1$  needs  $\Delta t \leq \Delta t_{\text{stable}} = \frac{\Delta x^2}{2D(1-\theta)}$

Time-scales: Each physical process has (one or more) physical time-scales  $\Delta t_{\text{phys}}$  needed to capture the physical changes.

Computationally, there are two time-scales

$$\Delta t_{\text{stable}} = \max \Delta t \text{ for stability of scheme}$$

$$\Delta t_{\text{accuracy}} = \max \Delta t \text{ for accuracy in numerical solution}$$

If  $\Delta t_{\text{expl}} \approx \Delta t_{\text{accr}} (\approx \Delta t_{\text{phys}})$  then use explicit scheme.

If  $\Delta t_{\text{expl}} \ll \Delta t_{\text{accr}} (\ll \Delta t_{\text{phys}})$  then use a more stable scheme allowing  $\Delta t_{\text{accr}}$

This happens for simple diffusion processes often  
and most Numerical Analysis books say to use implicit schemes...

However, it may not happen in tough problems...  
e.g. phase change problems, rapidly varying nonlinear coeffs, ...

Implicit timestep is always more expensive than explicit ( $\gtrsim 10$  times or more)  
nothing cheaper than Explicit Euler, for ODEs and PDEs!

For implicit to beat explicit, at same accuracy, would need  $\Delta t_{\text{impl}} \gg \Delta t_{\text{expl}}$   
solving systems is computationally expensive, no to mention coding hassle...  
and very hard to parallelize!

Parallelization of explicit scheme is a viable alternative!