Galaxy formation – Burns, Greif, Bromm, and Klessen –- Texas Advanced Computing Center-- www.tacc.utexas.edu/research/gallery

PHYS 8750
Numerical Fluid Dynamics

PHYS 8750

CLASS #16
FLUX CORRECTED TRANSPORT

Class #15 (Chapter 5.1)

Finite Volume Method

Outline

1. Review of FV method

1.1 fundamental concept of finite volume method

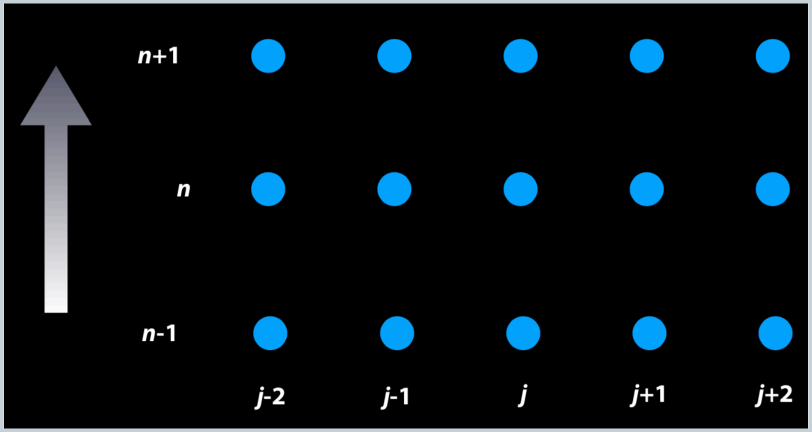
1.2 Flux form (high-order vs low-order) for different schemes.

2. Flux corrected transport methods

3. Examples (coding)

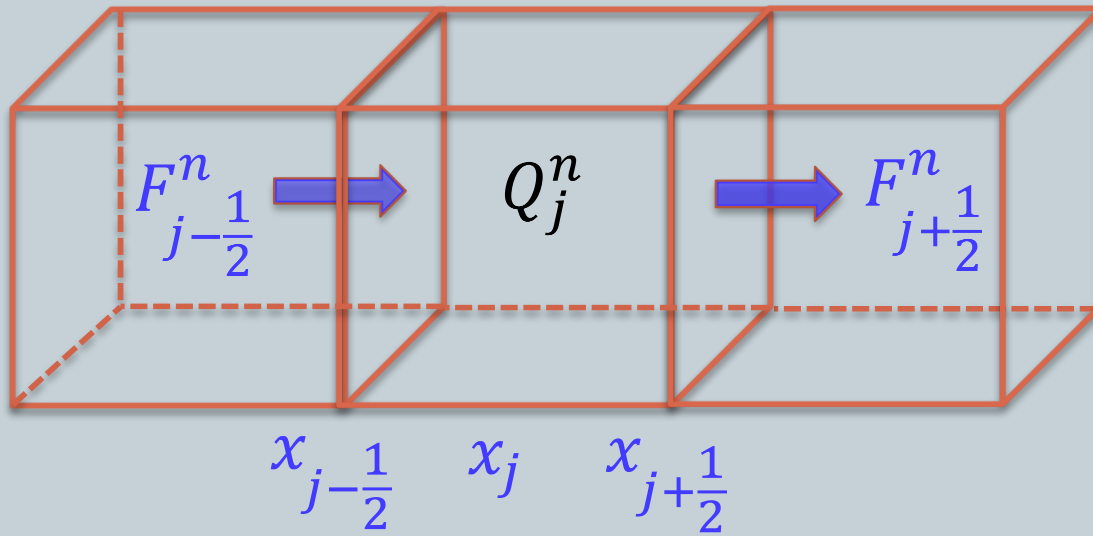
Finite Volume Principle

Finite Difference



Values and derivatives are evaluated at discrete grid points.

Finite Volume



Flux Form

$$\boxed{Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}\left(F^n_{j+1/2} - F^n_{j-1/2}\right)}$$

FV methods seek to obtain an appropriate flux term "*F*", to approximate an averaged flux at the cell interfaces occurring between certain time steps.

$$F^n_{j+1/2} \approx \frac{1}{\Delta t}\int_{t_1}^{t_2} f\left(t, x_{j+1/2}\right)dt \quad \& \quad F^n_{j-1/2} \approx \frac{1}{\Delta t}\int_{t_1}^{t_2} f\left(t, x_{j-1/2}\right)dt$$

Physical Meaning

Flux Form

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

- Q_j^{n+1}, Q_j^n: cell (volume) average ψ at current and next time steps.
- $F_{j+1/2}^n$,$F_{j-1/2}^n$: time average flux at right and left surface

Change of averaged ψ in a certain volume equals to the flux coming in minus the flux coming out (net flux coming in) of the surface that encloses the volume.

Example (continuity or mass conservation):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

Forward Time/Upstream Method

- Different schemes use different flux forms for the finite volume methods.
- Key issue: identify the most efficient/appropriate flux terms.

Upstream solution for constant coefficient advection equation:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = c\,\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x}$$

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}\left(cQ_j^n - Q_{j-1}^n\right)$$

Flux form

$$F_{j+1/2}^n = cQ_j^n,\ F_{j-1/2}^n = cQ_{j-1}^n$$

Lax-Wendroff

Upstream solution for constant coefficient advection equation:

$$\phi_j^{n+1} = \phi_j^n - \frac{c\Delta t}{2\Delta x}\left(\phi_{j+1}^n - \phi_{j-1}^n\right) + \frac{1}{2}\left(\frac{c\Delta t}{\Delta x}\right)^2 \left(\phi_{j-1}^n - 2\phi_j^n + \phi_{j+1}^n\right)$$

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

Flux form

$$F_{j+1/2}^n = \frac{1}{2}c\left(Q_{j+1}^n + Q_j^n\right) - \frac{1}{2}\frac{\Delta t}{\Delta x}c^2\left(Q_{j+1}^n - Q_j^n\right)$$

$$F_{j-1/2}^n = \frac{1}{2}c\left(Q_{j-1}^n + Q_j^n\right) - \frac{1}{2}\frac{\Delta t}{\Delta x}c^2\left(Q_j^n - Q_{j-1}^n\right)$$

Goals of FVM

- First-order scheme (forward time/upstream) keeps good performance on TVD and monotonicity. But it is highly diffusive and first-order accurate.
- Pure second (higher) order methods cannot be monotone; any linear monotone scheme is at best first-order accurate. Less errors.
- We week to use flux limiters to control the inclusion of high-order terms, creating nonlinear schemes with greater than first order accuracy, while preserving TVD criteria.

Flux-Limited Methods

Different schemes can define different flux forms (from low to high orders), flux limited & flux corrected methods combine the best features of low order and high order methods:

Flux Limited

$$F_{j+\frac{1}{2}} = F^{L}_{j+\frac{1}{2}} + \gamma_{j+\frac{1}{2}}\left(F^{H}_{j+\frac{1}{2}} - F^{L}_{j+\frac{1}{2}}\right)$$

$$F_{j-\frac{1}{2}} = F^{L}_{j-\frac{1}{2}} + \gamma_{j-\frac{1}{2}}\left(F^{H}_{j-\frac{1}{2}} - F^{L}_{j-\frac{1}{2}}\right)$$

$$if\ \gamma = 0, totally\ low - order\ flux, highly\ diffusive$$

$$if\ \gamma = 1, totally\ high - order\ flux, doesnot\ necessarily\ satisfy\ TVD$$

$$if\ 0 < \gamma < 1, mix\ of\ low\ and\ \ high - order\ fluxes$$

Flux-Corrected Transport

- **General Idea:**

Flux Form

$$\phi_j^{n+1} = \phi_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

1. Compute low-order fluxes $F^1_{j+\frac{1}{2}}$ using a monotone scheme
2. Compute high-order fluxes $F^h_{j+\frac{1}{2}}$ using a high-order scheme
3. Transported & diffused (td) solution:

$$\phi_j^{td} = \phi_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^1 - F_{j-1/2}^1\right)$$

4. Compute anti-diffusive fluxes

$$A_{j+\frac{1}{2}} = F^h_{j+\frac{1}{2}} - F^1_{j+\frac{1}{2}}$$

Flux-Corrected Transport

5. Correct $A_{j+1/2}$ by weighting it, so "antidiffusion" step does not generate new minima or maxima:

$$A^c_{j+\frac{1}{2}} = C_{j+\frac{1}{2}} A_{j+\frac{1}{2}}$$

6. Correct td solutions:

$$\phi_j^{\mathrm{n}+1} = \phi_j^{td} - \frac{\Delta t}{\Delta x}\left(A^c_{j+\frac{1}{2}} - A^c_{j-\frac{1}{2}}\right)$$

$$\phi_j^{td} = \phi_j^n - \frac{\Delta t}{\Delta x}\left(F^1_{j+1/2} - F^1_{j-1/2}\right)$$

$$A_{j+\frac{1}{2}} = F^h_{j+\frac{1}{2}} - F^1_{j+\frac{1}{2}}$$

Flux-Corrected Transport

$$\phi_j^{n+1} = \phi_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^1 - F_{j-1/2}^1\right) - \frac{\Delta t}{\Delta x}\left(C_{j+\frac{1}{2}} A_{j+\frac{1}{2}} - C_{j-\frac{1}{2}} A_{j-\frac{1}{2}}\right)$$

$$= \phi_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^1 - F_{j-1/2}^1\right) - \frac{\Delta t}{\Delta x}\left(C_{j+\frac{1}{2}}\left(F^h_{j+\frac{1}{2}} - F^1_{j+\frac{1}{2}}\right) - C_{j-\frac{1}{2}}\left(F^h_{j-\frac{1}{2}} - F^1_{j-\frac{1}{2}}\right)\right)$$

$$= \phi_j^n - \frac{\Delta t}{\Delta x}\left(\left[\underline{F^1_{j+\frac{1}{2}} + C_{j+\frac{1}{2}}\left(F^h_{j+\frac{1}{2}} - F^1_{j+\frac{1}{2}}\right)}\right] - \left[\underline{F^1_{j-\frac{1}{2}} + C_{j-\frac{1}{2}}\left(F^h_{j-\frac{1}{2}} - F^1_{j-\frac{1}{2}}\right)}\right]\right)$$

Corrected Flux at j+1/2

Corrected Flux at j-1/2

Flux Correction

- Boris and Book (1973)

$$\phi_j^{n+1} = \phi_j^{td} - \frac{\Delta t}{\Delta x}\left(A^c_{j+\frac{1}{2}} - A^c_{j-\frac{1}{2}}\right)$$

$$A^c_{j+\frac{1}{2}} = \mathrm{sgn}\left(A_{j+\frac{1}{2}}\right) max\left\{0, min\begin{bmatrix} \left|A_{j+\frac{1}{2}}\right| \\ \mathrm{sgn}\left(A_{j+\frac{1}{2}}\right)\left(\phi_{j+2}^{td} - \phi_{j+1}^{td}\right)\frac{\Delta x}{\Delta t} \\ \mathrm{sgn}\left(A_{j+\frac{1}{2}}\right)\left(\phi_{j}^{td} - \phi_{j-1}^{td}\right)\frac{\Delta x}{\Delta t} \end{bmatrix}\right\}$$

Flux Correction

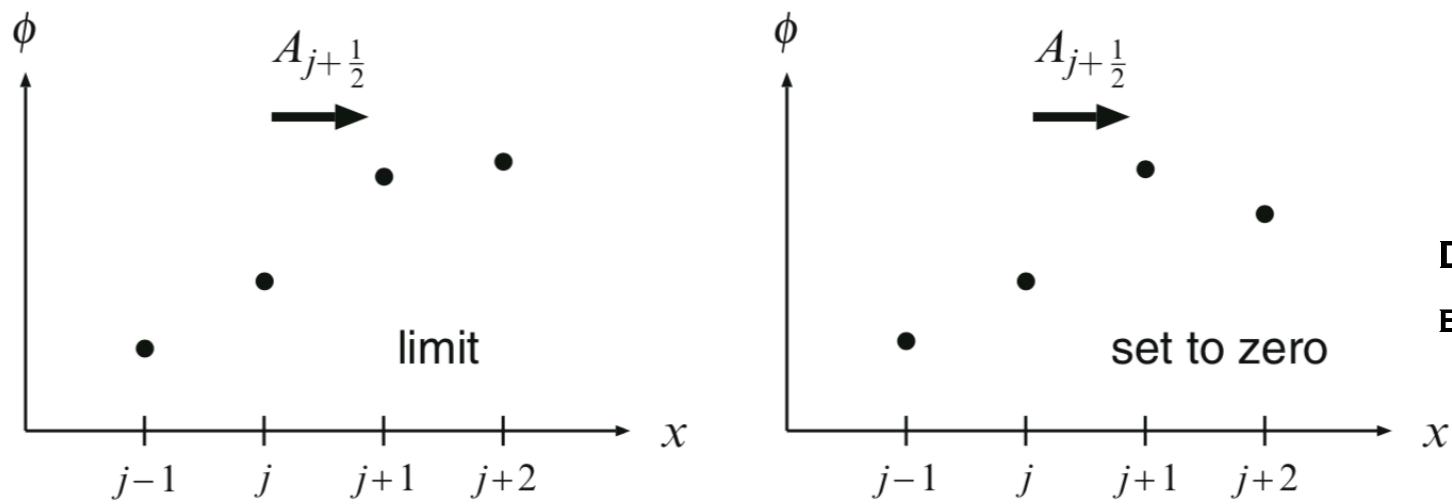
Assume $\mathrm{sgn}\left(A_{j+\frac{1}{2}}\right) > 0$, higher-order scheme transports more fluxes

$$\underbrace{A^{c}_{j+\frac{1}{2}} = max}_{\text{Won't be negative and do anti-correction}} \left\{ 0, \underbrace{min \begin{bmatrix} A_{j+\frac{1}{2}} \\ \left(\phi^{td}_{j+2} - \phi^{td}_{j+1}\right)\frac{\Delta x}{\Delta t} \\ \left(\phi^{td}_{j} - \phi^{td}_{j-1}\right)\frac{\Delta x}{\Delta t} \end{bmatrix}}_{\text{Won't create new minima or maxima: retain the monotonity of low-order scheme}} \right\}$$

Won't be negative and do anti-correction

Won't create new minima or maxima: retain the monotonity of low-order scheme

Flux Correction Principle



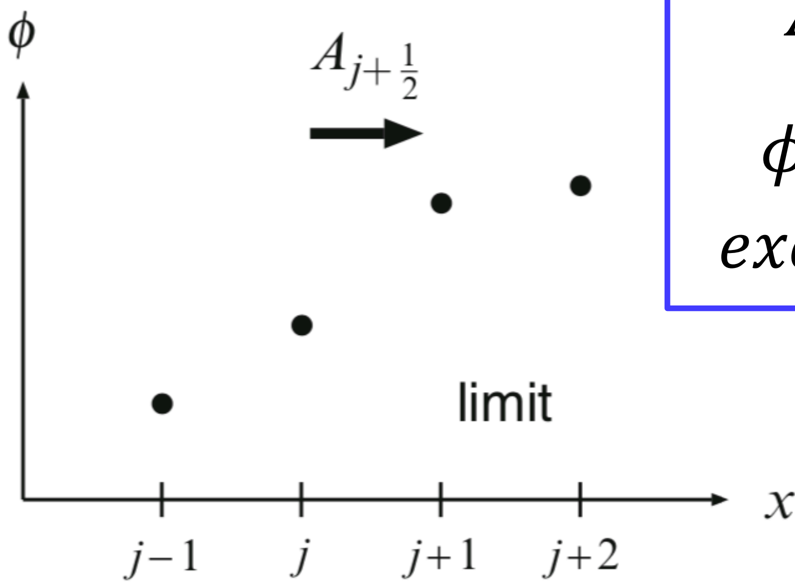
DURRAN'S BOOK

Fig. 5.9 Two possible configurations in which an antidiffusive flux, indicated by the *heavy arrow*, may be modified by a flux limiter

$$A^{c}_{j+\frac{1}{2}} = max\left\{0, min\left[\begin{array}{c} A_{j+\frac{1}{2}} \\ \left(\phi^{td}_{j+2} - \phi^{td}_{j+1}\right)\dfrac{\Delta x}{\Delta t} \\ \left(\phi^{td}_{j} - \phi^{td}_{j-1}\right)\dfrac{\Delta x}{\Delta t} \end{array}\right]\right\}$$

$A_{j+\frac{1}{2}}$: antidiffusion flux goes from ϕ_j *to* ϕ_{j+1}, correct it with constrains

Scenario 1



$$\phi^{td}_{j+2} - \phi^{td}_{j+1} > 0$$

$$A^{c}_{j+\frac{1}{2}} \sim min\left[A_{j+\frac{1}{2}}, (\phi^{td}_{j+2} - \phi^{td}_{j+1})\frac{\Delta x}{\Delta t}\right]$$

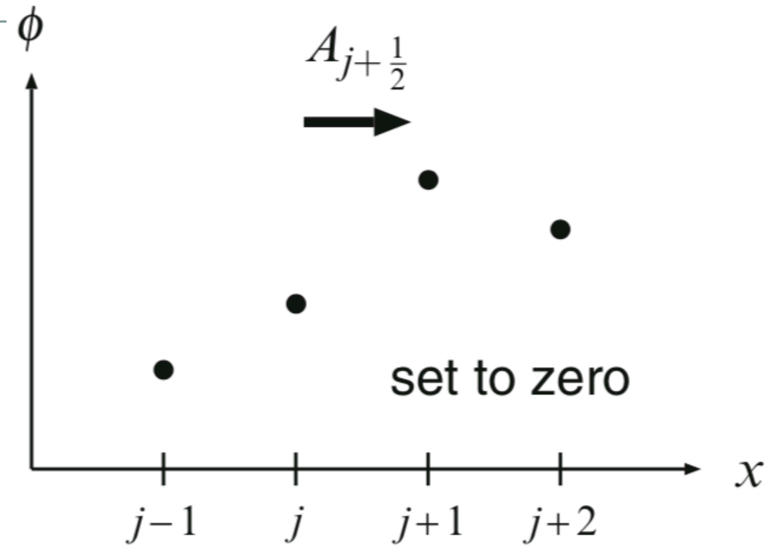
ϕ^{n+1}_{j+1} *will not increase too much to exceed* ϕ^{n+1}_{j+2} → keep monotonicity

$$\phi^{td}_{j} - \phi^{td}_{j-1} > 0$$

$$A^{c}_{j+\frac{1}{2}} \sim min\left[A_{j+\frac{1}{2}}, (\phi^{td}_{j} - \phi^{td}_{j-1})\frac{\Delta x}{\Delta t}\right]$$

ϕ^{n+1}_{j} *will not decrease too much to be less than* ϕ^{n+1}_{j-1} → keep monotonicity

Scenario 2



$$\phi_{j+2}^{td} - \phi_{j+1}^{td} < 0$$

$$min\left[A_{j+\frac{1}{2}}, \left(\phi_{j+2}^{td} - \phi_{j+1}^{td}\right)\frac{\Delta x}{\Delta t}\right] < 0,\ A_{j+\frac{1}{2}}^{c} = 0$$

No correction

ϕ_{j+1}^{n+1} will not increase to amplify the local maximum.

Won't create new or amplify the existing local maxima and minima → correct with constraint and keep monotonicity

The Zalesak Corrector (1979)

1. As an optional preliminary step, set certain down-gradient antidiffusive fluxes to zero, such that

$$
\begin{aligned}
A_{j+\frac{1}{2}} = 0, \qquad & \text{if} \qquad A_{j+\frac{1}{2}}(\phi^{\mathrm{td}}_{j+1} - \phi^{\mathrm{td}}_{j}) < 0 \\
& \text{and either} \quad A_{j+\frac{1}{2}}(\phi^{\mathrm{td}}_{j+2} - \phi^{\mathrm{td}}_{j+1}) < 0 \\
& \text{or} \qquad A_{j+\frac{1}{2}}(\phi^{\mathrm{td}}_{j} - \phi^{\mathrm{td}}_{j-1}) < 0.
\end{aligned}
\tag{5.32}
$$

Zalesak refers to this as a cosmetic correction, and it is usually omitted. This cosmetic correction has, nevertheless, been used in the FCT computations shown in this chapter. It has no effect on the solution shown in Fig. 5.10a, makes a minor improvement in the solution shown in Fig. 5.10b, and makes a major improvement in the solution shown in Fig. 5.13b.

2. Evaluate the range of permissible values for ϕ_j^{n+1}:

$$
\begin{aligned}
\phi_j^{\max} &= \max\left(\phi^n_{j-1}, \phi^n_j, \phi^n_{j+1}, \phi^{\mathrm{td}}_{j-1}, \phi^{\mathrm{td}}_{j}, \phi^{\mathrm{td}}_{j+1}\right), \\
\phi_j^{\min} &= \min\left(\phi^n_{j-1}, \phi^n_j, \phi^n_{j+1}, \phi^{\mathrm{td}}_{j-1}, \phi^{\mathrm{td}}_{j}, \phi^{\mathrm{td}}_{j+1}\right).
\end{aligned}
$$

If the flow is nondivergent, the ϕ^{td} are not needed in the preceding formulae because the extrema predicted by the monotone scheme will be of lower amplitude than those at the beginning of the time step. If, however, the flow is divergent, then the local minima and maxima in the true solution may be increasing, and the increase predicted by the monotone scheme should be considered in determining $\phi^{\max}$ and $\phi^{\min}$.

3. Compute the sum of all antidiffusive fluxes into grid cell j,

$$
P_j^+ = \max\left(0, A_{j-\frac{1}{2}}\right) - \min\left(0, A_{j+\frac{1}{2}}\right).
$$

4. Compute the maximum net antidiffusive flux divergence that will preserve $\phi_j^{n+1} \le \phi_j^{\max}$,

$$
Q_j^+ = \left(\phi_j^{\max} - \phi_j^{\mathrm{td}}\right)\frac{\Delta x}{\Delta t}. \tag{5.33}
$$

5. Compute the required limitation on the net antidiffusive flux into grid cell j,

$$
R_j^+ = \begin{cases} \min\left(1, Q_j^+/P_j^+\right) & \text{if } P_j^+ > 0, \\ 0 & \text{if } P_j^+ = 0. \end{cases}
$$

6. Compute the corresponding quantities involving the net antidiffusive flux out of grid cell j,

$$
\begin{aligned}
P_j^- &= \max\left(0, A_{j+\frac{1}{2}}\right) - \min\left(0, A_{j-\frac{1}{2}}\right). \\
Q_j^- &= \left(\phi_j^{\mathrm{td}} - \phi_j^{\min}\right)\frac{\Delta x}{\Delta t}. \\
R_j^- &= \begin{cases} \min\left(1, Q_j^-/P_j^-\right) & \text{if } P_j^- > 0, \\ 0 & \text{if } P_j^- = 0. \end{cases}
\end{aligned}
\tag{5.34}
$$

7. Limit the antidiffusive flux so that it neither produces an overshoot in the grid cell into which it is directed nor generates an undershoot in the grid cell out of which it flows:

$$
C_{j+\frac{1}{2}} = \begin{cases} \min\left(R^+_{j+1}, R^-_j\right) & \text{if } A_{j+\frac{1}{2}} \ge 0, \\ \min\left(R^+_{j}, R^-_{j+1}\right) & \text{if } A_{j+\frac{1}{2}} < 0. \end{cases}
$$

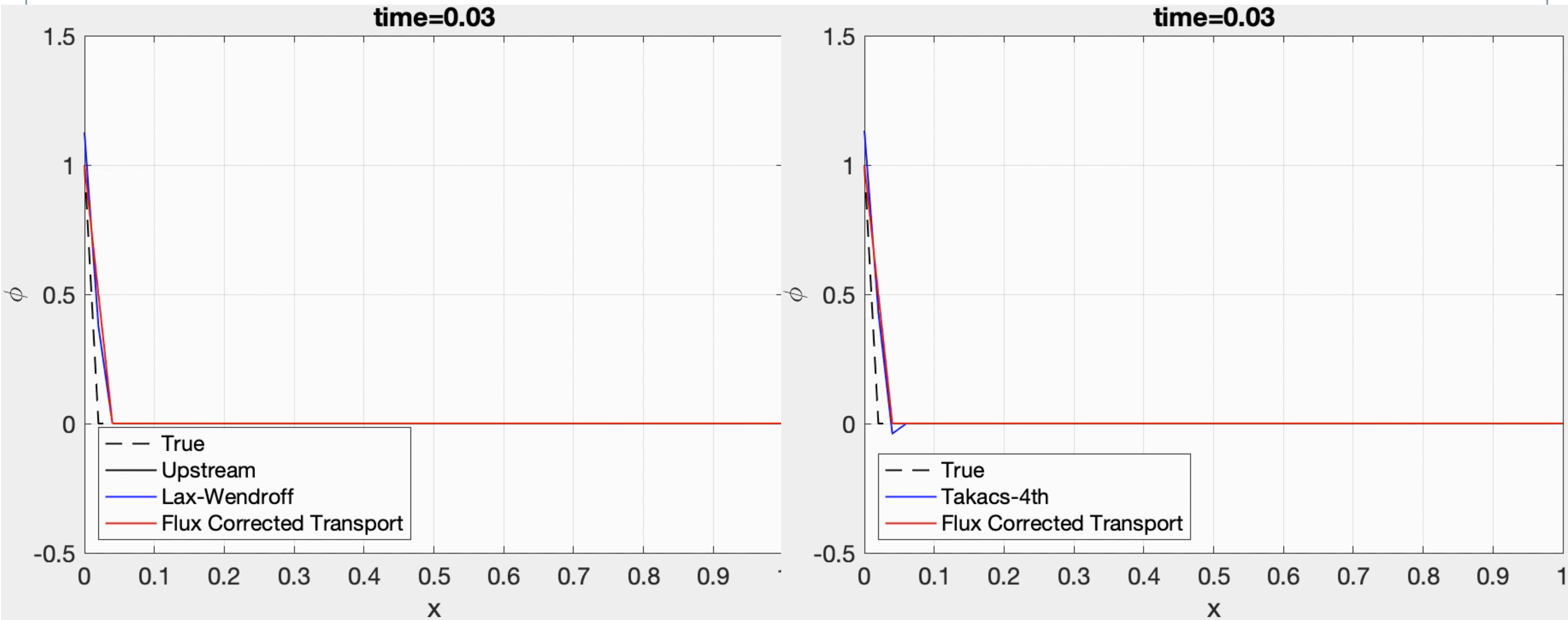
Two examples illustrating the performance of the Zalesak FCT algorithm on the constant-wind-speed one-dimensional advection equation are shown in Fig. 5.10. In these examples, the monotone flux is computed using the upstream method with

$$
F^{\mathrm{l}}_{j+\frac{1}{2}} = \frac{c}{2}(\phi_j + \phi_{j+1}) - \frac{|c|}{2}(\phi_{j+1} - \phi_j), \tag{5.35}
$$

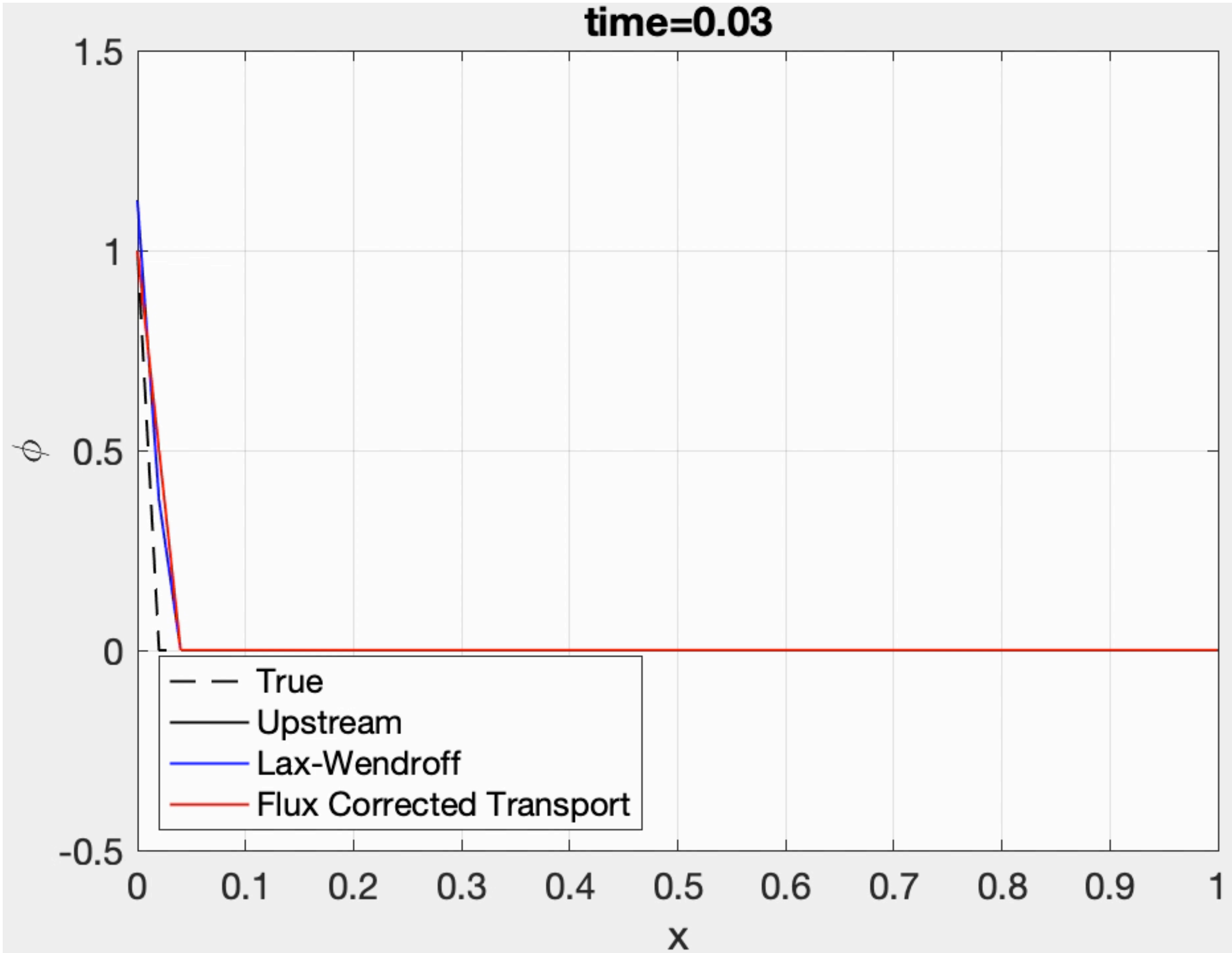
and the high-order flux is computed using the flux form of the Lax–Wendroff method such that

$$
F^{\mathrm{h}}_{j+\frac{1}{2}} = \frac{c}{2}(\phi_j + \phi_{j+1}) - \frac{c^2\Delta t}{2\Delta x}(\phi_{j+1} - \phi_j). \tag{5.36}
$$

Comparison w/wo FCT



FCT can efficiently remove ripples (avoid generating local new maxima/minima or make them extreme) and correct the high-order scheme.



Weighted high-order flux by a factor of $\Delta x/\Delta t$ even gives better results? Homework?