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MONOTONICITY & POSITIVITY

We know that solutions of advection-diffusion equations possess a positivity property

$$u(x,0) \geq 0 \implies u(x,t) \geq 0 \text{ for all } t>0$$

We know centered advection and other dispersive schemes generate oscillations and violate positivity.

Can we construct schemes that don't?

START WITH SPATIAL DISCRETIZATION

An ODE system is <u>positive</u> (2)

(non-negativity preserving) if

$$w'(t) = F(t, w(t)) \quad \ldots\ldots (*)$$

$$w(0) \geq 0 \implies w(t) \geq 0 \text{ for all } t > 0$$

<u>Theorem</u>: If F is Lipschitz $(*)$ is positive <u>iff</u>

$$\boxed{\forall v \in \mathbb{R}^m,\ v \geq 0,\ v_i = 0 \implies F_i(t, v) \geq 0}$$

If $F = Aw$

$$\implies \boxed{a_{ij} \geq 0 \quad \forall i \neq j}$$

An even stronger property is obeying a <u>maximum principle</u>

$$\boxed{\min_j w_j(0) \le w_i(t) \le \max_j w_j(0)}$$

This is fobidding <u>global</u> overshoots and undershoots, but still allows oscillations to occur.

A yet stronger property is to disallow local oscillations (over and under shoots). To do this precisely, we look at a quantity

Total variation (discrete)

$$|v|_{TV} = h \sum_{j=1}^{m} |v_{j-1} - v_j| \quad \text{(periodic)}$$

A scheme or ODE system is said to be

$$\boxed{\text{TVD} = \text{total variation diminishing}}$$

if $|w(t)|_{TV}$ is a non-increasing function of time.

This prevents local oscillations

Consider a general linear scheme to solve $u_t + a u_x = 0$

$$w_j'(t) = \frac{a}{h} \sum_{k=-r}^{r} \gamma_k \, w_{j+k}$$

For this to be <u>positive</u> we need

$$a\gamma_k \geq 0 \quad \text{for all } k \neq 0$$

So first order upwind <u>is</u> positive, and the central or upwind biased ones are <u>not</u>. This is a general conclusion: known as the <u>Godunov order barrier</u>

A linear positive or monotone advection scheme can be at most first-order accurate

The upwind scheme is in fact the best of all positive linear schemes

This implies:

We need <u>non-linear</u> schemes to do advection with high accuracy and high robustness!

This is what makes CFD hard!

Before we discuss nonlinear advection, let's look at diffusion

$$u_t = d\, u_{xx}$$

$$w_j'(t) = \frac{d}{h^2} \sum_{k=-r}^{r} \gamma_k\, w_{j+k}(t)$$

$$\Rightarrow \quad d\,\gamma_k \geq 0$$

So centered second-order scheme is positive, and an order barrier exists here also:

$$\boxed{\text{order} \leq 2 \quad \text{for positive linear diffusion}}$$

And now advection-diffusion

$$\begin{cases} u_t + (a(x,t)\,u)_x = (d(x,t)\,u_x)_x \\ d(x,t) \geq 0 \end{cases}$$

If we discretize with centered second-order differences for positivity we require

$$\boxed{P_e = \max_{x,t} \frac{|a(x,t)|\,h}{d(x,t)} \leq 2}$$

and if we use upwinding for the advection there is no restriction

NON-OSCILLATORY MOL SCHEMES

$$u_t + a\, u_x = 0$$

$$\begin{cases} w_j' = \frac{1}{h}\left[f_{j-1/2} - f_{j+1/2} \right] \\ f_{j+1/2}(w) = a\, w_{j+1/2} \end{cases}$$

Finite volume discretiz.

Upwinding (positive)

$$f_{j+1/2} = \max(a,0)\, w_j + \min(a,0)\, w_{j+1}$$

If $a > 0$

$$f_{j+1/2} = a\, w_j$$

For second-order centered (13)

$$f_{j+1/2} = a\left[w_j + \frac{1}{2}(w_{j+1} - w_j) \right]$$

for third-order upwind biased

$$f_{j+1/2} = a\left[w_j + \left(\frac{1}{3} + \frac{\theta_j}{6}\right)(w_{j+1} - w_j) \right]$$

Or more generally, for a

flux limiter $\Psi(\theta)$

$$\begin{cases} f_{j+1/2} = a\left[w_j + \Psi(\theta_j)(w_{j+1} - w_j) \right], & a \geq 0 \\ f_{j+1/2} = a\left[w_{j+1} + \Psi\left(\frac{1}{\theta_j}\right)(w_j - w_{j+1}) \right], & a < 0 \end{cases}$$

where θ measures the local smoothness of w:

$$\boxed{\theta_j = \frac{w_j - w_{j-1}}{w_{j+1} - w_j}}$$ (slope ratio)

Flux limiter function $\psi(\theta)$

$$\begin{cases} \psi(\theta) = \frac{1}{2} & \text{centerd} \\ \psi(\theta) = \frac{1}{3} + \frac{\theta_j}{6} & \text{upwind biased} \\ \psi(\theta) = 0 & \text{for upwind} \end{cases}$$

needs to be chosen to balance accuracy with robustness

To guarantee positivity for the spatial discretization we require:

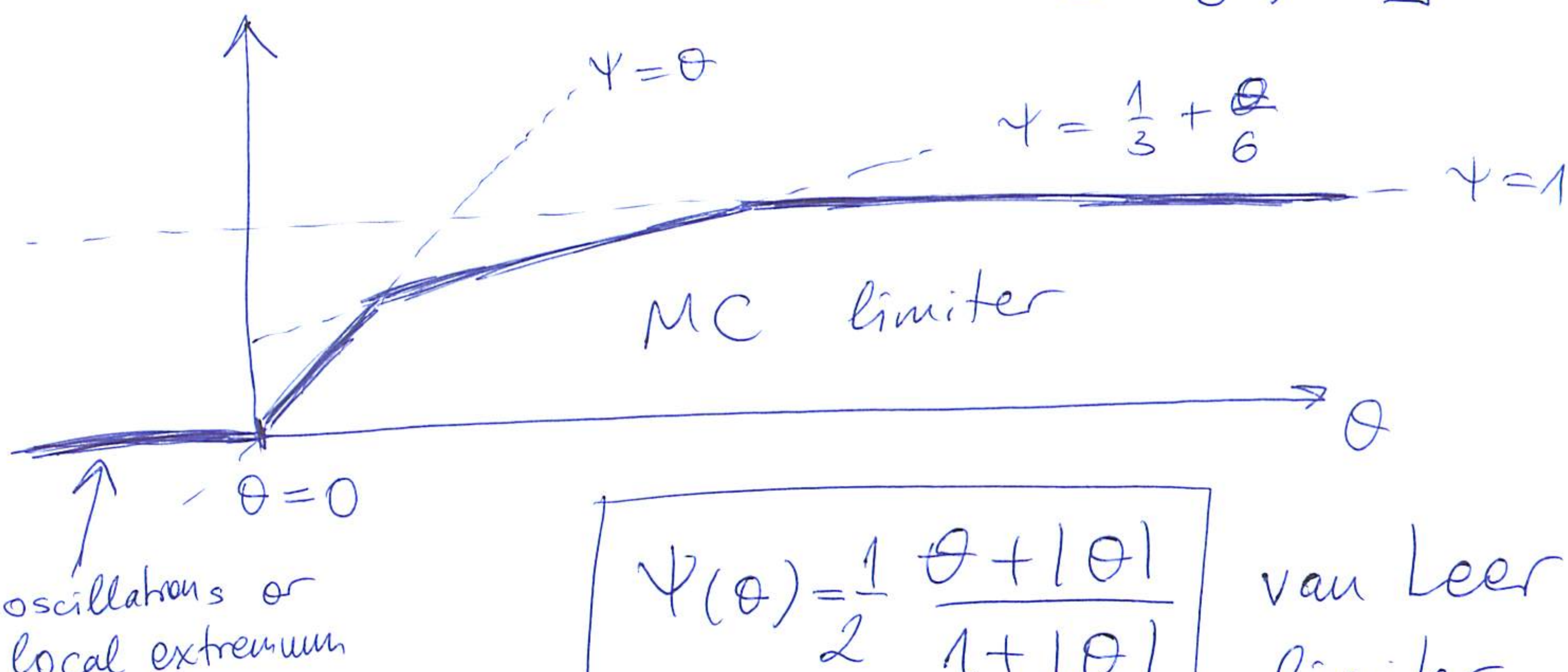
$$1 - \Psi(\theta_{j-1}) + \frac{1}{\theta_j}\Psi(\theta_j) \geq 0 \quad \forall j$$

Since θ_{j-1} and θ_j are independent we narrow down $\Psi(\theta)$ with

$$\begin{cases} 0 \leq \Psi(\theta) \leq 1 \\ 0 \leq \frac{1}{\theta}\Psi(\theta) \leq \mu \quad \left[\text{often } \frac{\Psi(\theta)}{\theta} = \Psi\left(\frac{1}{\theta}\right)\right] \\ \mu \geq 0 \text{ , usually } \mu = 1 \end{cases}$$

Example limiters

$$\Psi(\theta) = \max\left[0, \min\left(1, \frac{1}{3}+\frac{\theta}{6}, \theta\right)\right]$$

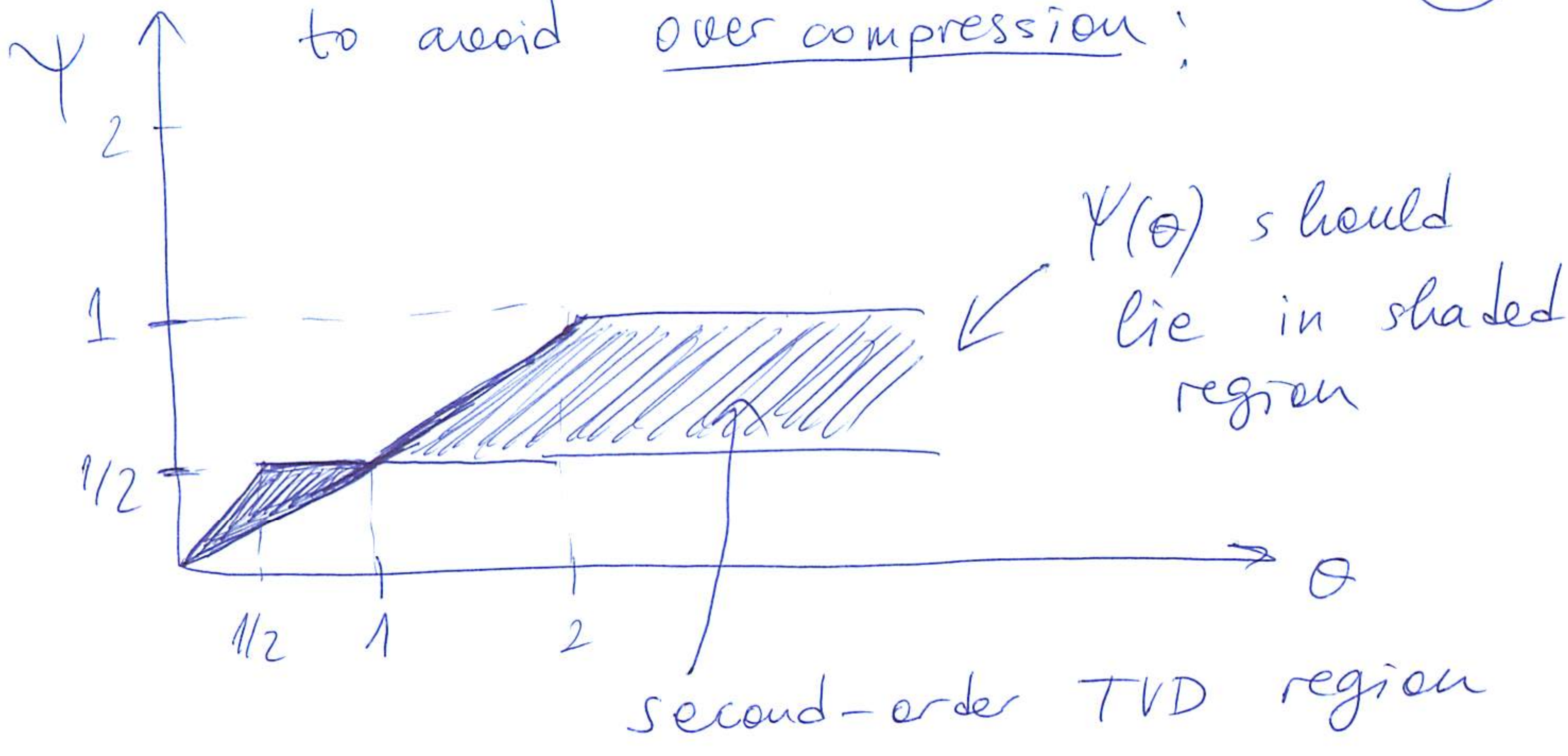


$$\boxed{\Psi(\theta) = \frac{1}{2}\,\frac{\theta+|\theta|}{1+|\theta|}}$$ van Leer limiter

This one does not give second-order accuracy even for smooth functions

For second-order methods, we want: (17)

to avoid over compression:



For smooth problems $\theta = 1$ and

$\Psi(\theta) \simeq \frac{1}{2}$ (second-order centered)

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Linear methods:

$\varphi \equiv 2\psi$ (different convention!)

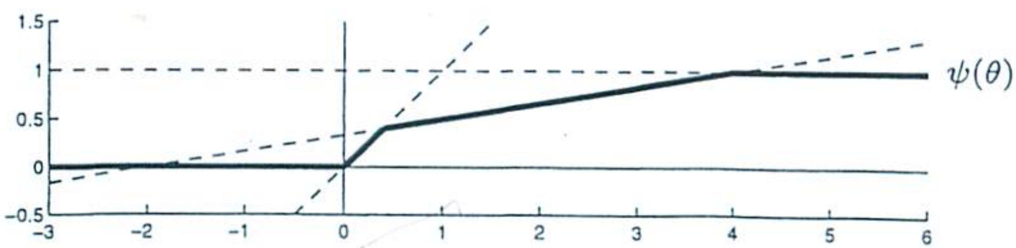
$$
\begin{aligned}
\text{upwind}: &\quad \phi(\theta) = 0, \\
\text{Lax–Wendroff}: &\quad \phi(\theta) = 1, \\
\text{Beam–Warming}: &\quad \phi(\theta) = \theta, \\
\text{Fromm}: &\quad \phi(\theta) = \frac{1}{2}(1+\theta).
\end{aligned}
$$

High-resolution limiters:

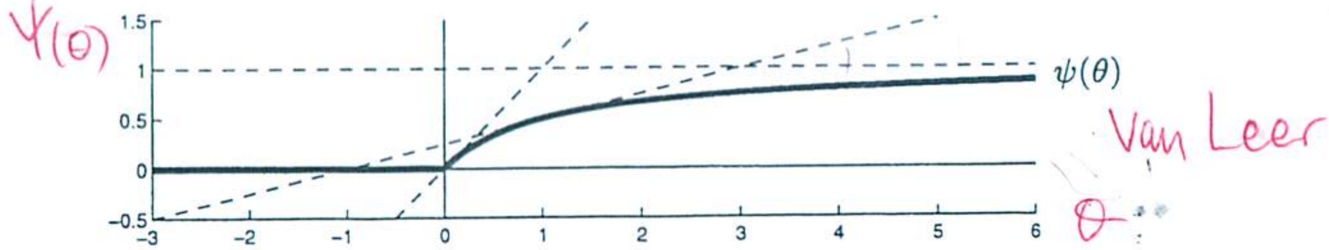
3rd upwind: $\varphi(\theta) = \frac{2}{3} + \frac{\theta}{3}$

$$
\begin{aligned}
\text{minmod}: &\quad \phi(\theta) = \text{minmod}(1, \theta), \\
\text{superbee}: &\quad \phi(\theta) = \max(0, \min(1, 2\theta), \min(2, \theta)), \\
\text{MC}: &\quad \phi(\theta) = \max(0, \min((1+\theta)/2, 2, 2\theta)) \\
\text{van Leer}: &\quad \phi(\theta) = \frac{\theta + |\theta|}{1 + |\theta|}.
\end{aligned}
$$

$$\psi(\theta) = \max\left(0, \min\left(1, \tfrac{1}{3} + \tfrac{1}{6}\theta, \theta\right)\right). \qquad (1.7$$



This limiter function was introduced by Koren (1993) and can be seen to coincide with the original third-order upwind-biased function $\psi(\theta) = \frac{1}{3} + \frac{1}{6}\theta$ for $\frac{2}{5} \le \theta \le 4$.



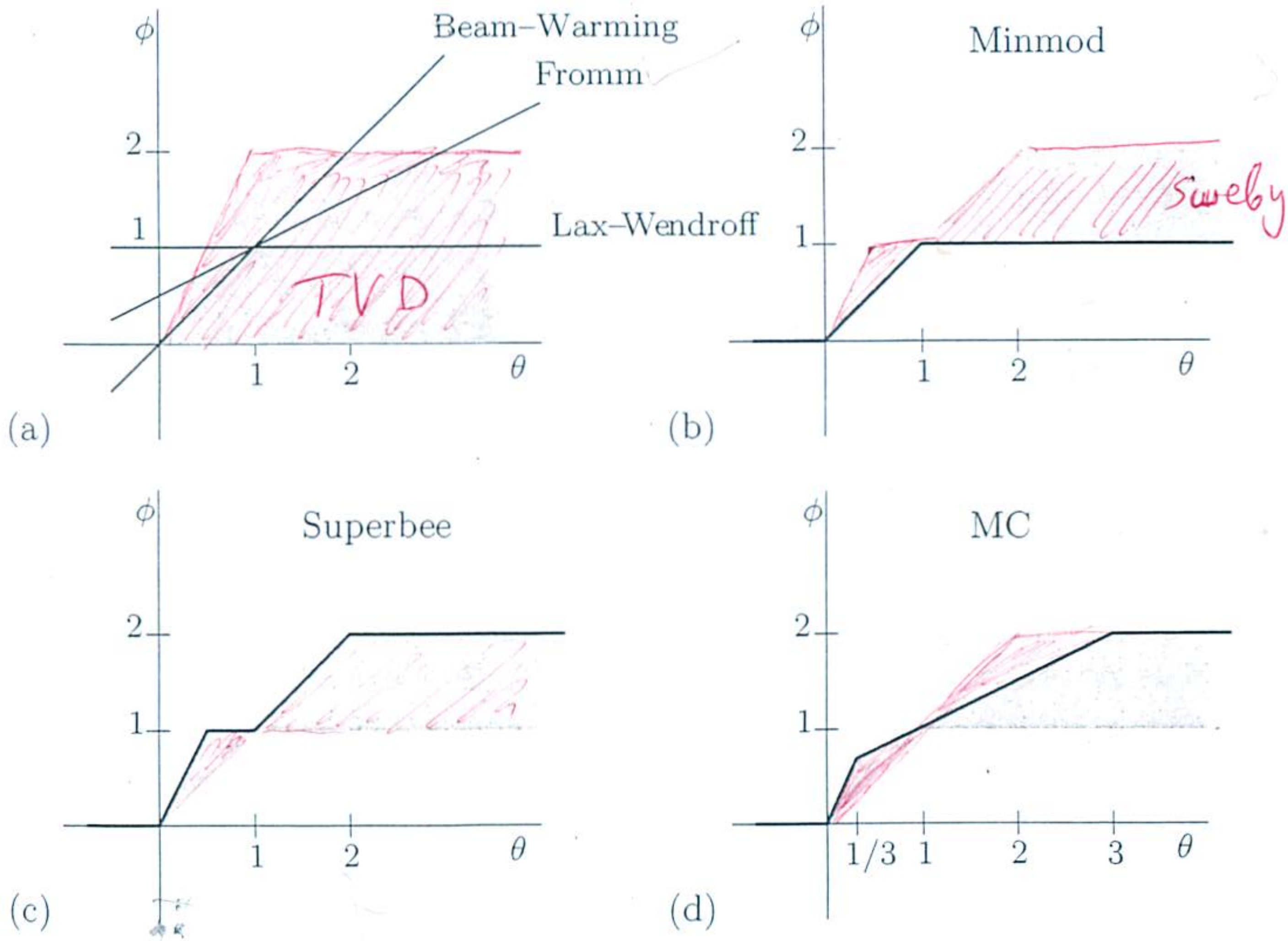


Fig. 6.6. Limiter functions $\phi(\theta)$. (a) The shaded regions shows where function values must lie for the method to be TVD. The second-order linear methods have functions $\phi(\theta)$ that leave this region. (b) The shaded region is the Sweby region of second-order TVD methods. The minmod limiter lies along the lower boundary. (c) The superbee limiter lies along the upper boundary. (d) The MC limiter is smooth at $\phi = 1$.

Variable - coefficients

(18)

$$u_t + [a(x,t)\,u]_x = 0$$

$$f_{j+1/2} = \max(a_{j+1/2}, 0)\, w^R_{j+1/2} + \min(a_{j+1/2}, 0)\, w^L_{j+1/2}$$

where

$$\begin{cases} w^R_{j+1/2} = w_j + \Psi(\theta_j)\,(w_{j+1} - w_j) \\ w^L_{j+1/2} = w_{j+1} + \Psi\left(\frac{1}{\theta_{j+1}}\right)(w_j - w_{j+1}) \end{cases}$$

Now a few words about how temporal discretization works with positive spatial discretizations (MOL): 9

$$\begin{cases} w' = Aw \\ a_{i,j} \geq 0 \quad \text{for } i \neq j \text{ (positive)} \\ a_{ii} \geq -\alpha \quad , \alpha > 0 \quad , \text{e.g. } \alpha = \frac{2d}{h^2} \end{cases}$$

If we use <u>forward Euler</u>

$$w_{n+1} = (I + \tau A) w_n$$

$\Rightarrow 1 + \tau a_{ii} \geq 0 \quad \forall i$ for positivity

$\Rightarrow \alpha \tau \leq 1$ (alike stability)

Conditional positivity

Now consider BE: (10)

$$w_{n+1} = (I - \tau A)^{-1} w_n$$

and assume $Re(\lambda) \le 0$ $\Rightarrow$

$$(I - \tau A)^{-1} \geq 0 \quad \text{(component wise)}$$

with <u>no restriction</u> on timestep.

So <u>Backward Euler is positive</u>

Similar analysis shows:

Crank-Nicolson (implicit trapezoidal)	is positive <u>iff</u>	$\alpha\tau \le 2$
Predictor-corrector (explicit trapezoidal)		$\alpha\tau \le 1$

Monotonicity

Monotone ODE system
$$\begin{cases} w'(t) = A\,w(t) \\ a_{ij} \geq 0 \quad \text{for } i \neq j \\ a_{ii} \geq -\alpha, \quad \alpha > 0 \\ A \text{ has no eigenvalue on positive real axes} \end{cases}$$

Take a linear <u>one-step</u> method

$$w^{n+1} = \underbrace{R(\tau A)}_{\text{stability function}} w^n$$

(see old lectures)

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<u>Theorem</u>

$$\begin{cases} R(\tau A) \geq 0 \quad \underline{\text{iff}} \\ \alpha\tau \leq \gamma_R \end{cases}$$

where γ_R is the largest γ for which $R(\cancel{x})$ <u>and</u> all of its derivatives are positive on $[-\gamma, 0]$

So here γ_R is a monotonicity <u>limit on the timestep</u>, similar to stability limits but distinct.

$\boxed{\text{Theorem: Any } \underline{\text{unconditionally positive}} \text{ method } (\gamma_R = \infty) \text{ has order } 1}$ <u>yet</u> another order barrier

So one cannot do better than Backward Euler if we want to take very large time steps and preserve non-negativity!

Often we can construct spatial discretizations such that forward Euler is monotone under a condition $\alpha \tau \leq 1$ ($\gamma_R = 1$).

This knowledge can then be used to construct higher-order methods that preserve this property

Regarding the <u>TVD property</u>, consider a general scheme (with diffusion)

$$\begin{cases} w_j^{n+1} = w_j^n + \tau \alpha_j(w_n)(w_{j-1}^n - w_j^n) \\ \qquad - \tau \beta_j(w_n)(w_j^n - w_{j+1}^n) \end{cases}$$

A sufficient condition for this scheme to be TVD (oscillation-free!):

$$\begin{cases} \alpha_j \geq 0 \\ \beta_j \geq 0 \\ \tau(\alpha_{j+1} + \beta_j) \leq 1 \end{cases} \qquad \text{for all } j \text{ and } w \in \mathbb{R}^m$$

Note: **TVD** is a desirable property but it is not sufficient. One must still look at **stability**! (and of course accuracy)

Example $a>0$ pure advection with slope-limiting:

$$\alpha_j = \frac{a}{h}\left(1 - \Psi(\theta_{j-1}) + \frac{1}{\theta_j}\Psi(\theta_j)\right)$$

$$0 \le \alpha_j \le \frac{a}{h}(1+\mu) \Rightarrow$$

If $\boxed{\frac{\tau a}{h} \le \frac{1}{1+\mu}}$ Forward Euler is TVD (usually $\mu=1$)

Nonlinear Positivity

$$w' = F(t, w)$$

Assume: forward Euler is positive:

$$\begin{cases} v + \tau F(\tau, v) \geq 0 \\ \text{if } v \geq 0 \text{ and } \alpha\tau \leq 1 \end{cases}$$

then one can prove that diagonally-implicit RK methods where the final update is a convex combination of forward and backward Euler steps is also positive if $\boxed{\alpha\tau \leq S}$

wher $S = O(1)$ depends on method

Such RK methods are called <u>Strong-Stability Preserving</u> (SSP) methods (Osher & Shu 1988)

(generalizes to <u>TVD</u> or in fact any convex functional)

<u>E.g.</u>

<u>Explicit Trapezoidal</u> Rule (RK2)

$$\begin{cases} w^{*} = w^{n} + \tau F^{n} & \text{(first Euler)} \\ w^{**} = w^{*} + \tau F^{*} & \text{(second Euler)} \\ w^{n+1} = \frac{1}{2}\left(w^{n} + w^{**}\right) & \text{(convex combo)} \\ \quad = w^{n} + \frac{1}{2}\left(\tau F^{n} + \tau F^{*}\right) \end{cases}$$

RK3 $\left\{\begin{matrix} \text{TVD} \\ \text{SSP} \end{matrix}\right\}$ scheme (explicit)

$$\begin{cases} w^{*} = w^{n} + \tau F^{n} & \text{(first Euler)} \\ w^{**} = \frac{3}{4} w^{n} + \frac{1}{4}\Big[\underbrace{w^{*} + \tau F^{*}}_{\text{second Euler}}\Big] & \text{(convex combo)} \\ w^{n+1} = \frac{1}{3} w^{n} + \frac{2}{3}\Big[\underbrace{w^{**} + \tau F^{**}}_{\text{third Euler}}\Big] & \text{(convex combo)} \end{cases}$$

this scheme is SSP, and its stability function includes a portion of the imaginary axes. Also third-order.
<u>Great for advection!</u>