AM213B Numerical Methods for the Solution of Differential Equations

Lecture 15
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List of topics in this lecture

- Numerical solution of conservation laws: importance of the conservation form both for PDEs and for numerical methods, Lax-Wendroff Theorem
- Numerical methods in conservation form, finite volume discretization, numerical flux, FTCS method, Lax-Friedrichs method, upwind method
- Entropy fix for the upwind method

Review

Modified PDE for first order methods:

$$w_t = -a w_x + \sigma w_{xx}$$

Behavior of a single mode:

$$w(x,t) = \underbrace{e^{\sqrt{-1}\xi(x-at)}}_{\substack{\text{convection,}\\ \text{traveling wave}\\ \text{with velocity } a}} \cdot \underbrace{e^{-\sigma\xi^2 t}}_{\substack{\text{dissipation,}\\ \text{exponential decay}\\ \text{of amplitude}}}$$

Behavior of a cluster of modes:

$$w(x,t) = \int e^{\sqrt{-1}\xi(x-at)} \cdot e^{-\sigma\xi^2 t} \alpha(\xi) d\xi$$

Discontinuities and corners are smoothed out.

Modified PDE for second order methods:

$$w_t = -a w_x + \mu w_{xxx}$$

Behavior of a single mode:

$$w(x,t) = \exp[\sqrt{-1}(\xi x - \underbrace{\omega(\xi)}_{\substack{\text{Angular}\\ \text{frequency}}} t)] = \exp[\sqrt{-1}\xi(x - \underbrace{\frac{\omega(\xi)}{\xi}}_{\substack{\text{Phase}\\ \text{velocity}}} t)]$$

where

angular frequency: $\omega(\xi) = a\xi + \mu\xi^3$,

phase velocity: $v_p(\xi) = \dfrac{\omega(\xi)}{\xi} = a + \mu\xi^2$

Different wave numbers travel with different velocities. This is called dispersion.

Behavior of a cluster of modes near $\xi = \xi_0$:

$$w(x,t) = \int_{\substack{\text{near}\\ \xi=\xi_0}} \exp\left[\sqrt{-1}\left(\xi x - \omega(\xi)t\right)\right]\alpha(\xi)d\xi$$

$$\approx \underbrace{\exp\left[\sqrt{-1}\,\xi_0\left(x - \frac{\omega(\xi_0)}{\xi_0}t\right)\right]}_{\substack{\text{Fast varying in space,}\\ \text{traveling with}\\ \text{phase velocity}}} \cdot \underbrace{\phi\left(x - \omega'(\xi_0)t\right)}_{\substack{\text{Envelope of the wave,}\\ \text{slow varying in space,}\\ \text{traveling with}\\ \text{group velocity}}}$$

where

envelope: $$\phi(z) \equiv \int_{\substack{\text{near}\\ \xi=\xi_0}} \exp\left\{\sqrt{-1}(\xi - \xi_0)z\right\}\alpha(\xi)d\xi$$

group velocity: $v_g(\xi) = \omega'(\xi) = a + 3\mu\xi^2$

<u>End of review</u>

So far we discussed numerical solution of linear hyperbolic PDEs.

Next, we look at numerical solution of non-linear hyperbolic PDEs

Numerical solution of conservation laws

<u>Two forms of a hyperbolic PDE</u>

Conservation form $u_t + F(u)_x = 0$

Differential form: $u_t + F'(u)u_x = 0$

<u>Meaning of conservation form:</u>

Integrating over $[a, b]$, we have

$$\frac{d}{dt}\int_a^b u(x,t)dx = \underbrace{F\left(u(a,t)\right)}_{\text{in-flux}} - \underbrace{F\left(u(b,t)\right)}_{\text{out-flux}}$$

Quantity u is conserved:

Rate of change of u = (in-flux) – (out-flux)

$F(u(x, t))$: flux (amount of flow per time) at position x, time t.

Importance of putting a PDE in the conservation form

Example: (uncertainty associated with the differential form)

Consider the PDE below in the differential form.

$$u_t + u u_x = 0, \qquad u(x,0) = \begin{cases} 1, & x \le 0 \\ 0, & x > 0 \end{cases}$$

Putting it in one conservation form:

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0$$

Solution: $u(x,t) = \begin{cases} 1, & x - \gamma t < 0 \\ 0, & x - \gamma t > 0 \end{cases}$

Shock velocity is determined by the Rankine-Hugoniot condition.

$$\gamma = \frac{[F(u)]}{[u]} = \frac{F(u_R) - F(u_L)}{u_R - u_L} = \frac{1}{2} \cdot \frac{1-0}{1-0} = \frac{1}{2}$$

Putting it in a different conservation form:

$$u^2 u_t + u^3 u_x = 0$$

$$\Longrightarrow \quad \left(\frac{u^3}{3}\right)_t + \left(\frac{u^4}{4}\right)_x = 0$$

Let $w = u^3$. The conservation form for w is

$$w_t + \left(\frac{3}{4} w^{4/3}\right)_x = 0$$

Solution: $w(x,t) = \begin{cases} 1, & x - \gamma_2 t < 0 \\ 0, & x - \gamma_2 t > 0 \end{cases}$

Shock velocity is determined by the Rankine-Hugoniot condition.

$$\gamma_2 = \frac{[F(w)]}{[w]} = \frac{3}{4} \cdot \frac{1-0}{1-0} = \frac{3}{4}$$ which is different from $\gamma = 1/2$ above.

Using $u = w^{1/3}$, we write out the solution for $u(x, t)$.

$$u(x,t)=\begin{cases}1, & x-\gamma_2 t<0\\ 0, & x-\gamma_2 t>0\end{cases}$$

Conclusion: solution is well defined only when the conservation form is specified.

Importance of building numerical methods in the conservation form

Example: (a non-conservative method may converge to a wrong solution)

Consider the hyperbolic PDE

$$u_t+F(u)_x=0 \qquad \text{==>} \qquad \underbrace{u_t=-F'(u)u_x}_{\text{Non-conservation form}}$$

We extend the upwind method using the differential form (non-conservative).

Numerical method:

$$\underbrace{u_i^{n+1}=u_i^n-\frac{\Delta t}{\Delta x}F'(u_i^n)\cdot\begin{cases}(u_i^n-u_{i-1}^n), & F'(u_i^n)\ge 0\\ (u_{i+1}^n-u_i^n), & F'(u_i^n)<0\end{cases}}_{\text{Non-conservation form}}$$

Try the method on the initial value problem

$$u_t+\left(\frac{1}{2}u^2\right)_x=0, \qquad u(x,0)=\begin{cases}1, & x\le 0\\ 0, & x>0\end{cases} \qquad \text{(IVP-2)}$$

Exact solution:

$$u(x,t)=\begin{cases}1, & x\le t/2\\ 0, & x>t/2\end{cases}$$ a shock wave with velocity = 1/2

Numerical solution:

$$u_i^0=\begin{cases}1, & i\le 0\\ 0, & i\ge 1\end{cases}$$

$$u_i^1=u_i^0-\frac{\Delta t}{\Delta x}\underbrace{F'(u_i^0)}_{\substack{>0 \text{ for } i\le 0\\ =0 \text{ for } i\ge 1}}\underbrace{(u_i^0-u_{i-1}^0)}_{=0 \text{ for } i\le 0}=u_i^0$$

Numerical solution is a stationary shock, which is NOT a weak solution of (IVP-2)!

The velocity of shock wave in numerical solution is wrong.

Note: In this simple example, it does not even involve switching directions.

Conclusion: It is important to do everything in conservation form.

Numerical methods in conservation form

<u>New view of spatial discretization:</u>

We view each grid point as the center of a cell.

cell $i = [x_{i-1/2}, x_{i+1/2}]$

x_i = center of cell i

$x_{i+1/2}$ = boundary between cell i and cell $(i+1)$.

Draw cells i, $(i-1)$, and $(i+1)$, and boundaries $x_{i-1/2}$ and $x_{i+1/2}$.

<u>PDE in conservation form</u>:

$$\frac{d}{dt}\int_a^b u(x,t)\,dx = \underbrace{F\big(u(a,t)\big)}_{\text{in-flux}} - \underbrace{F\big(u(b,t)\big)}_{\text{out-flux}}$$

Integrate from t_n to t_{n+1}.

$$\underbrace{\int_a^b u(x,t_{n+1})\,dx}_{\text{amount of } u \text{ at } t_{n+1}} - \underbrace{\int_a^b u(x,t_n)\,dx}_{\text{amount of } u \text{ at } t_n} = \underbrace{\int_{t_n}^{t_{n+1}} F\big(u(a,t)\big)dt}_{\text{in-flow}} - \underbrace{\int_{t_n}^{t_{n+1}} F\big(u(b,t)\big)dt}_{\text{out-flow}}$$

Apply this view to cell i, we write out a new type of numerical methods.

<u>Formulation based on conservation</u>

$$\underbrace{\Delta x\, u_i^{n+1}}_{\substack{\text{amount of } u\\ \text{in cell } i \text{ at } t_{n+1}}} - \underbrace{\Delta x\, u_i^{n}}_{\substack{\text{amount of } u\\ \text{in cell } i \text{ at } t_{n}}} = \underbrace{\Delta t\, F_{i-1/2}}_{\substack{\text{flow into}\\ \text{cell } i}} - \underbrace{\Delta t\, F_{i+1/2}}_{\substack{\text{flow out}\\ \text{of cell } i}}$$

<u>New meaning of</u> u_i^n and $F_{i+1/2}$

$$u_i^n \approx \frac{1}{\Delta x}\int_{\text{cell } i} u(x,t_n)dx\,,$$ <u>average</u> of u in cell i at time t_n.

$$F_{i+1/2} \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} F\Big(u(x_{i+1/2},t)\Big)dt\,,$$ flux at $x_{i+1/2}$ <u>averaged</u> over time $[t_n, t_{n+1}]$,

$F_{i+1/2}$ is called the numerical flux at $x_{i+1/2}$, and is based on a few local cells:

$$F_{i+1/2} = F_{num}(u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i+2}^n)$$

This new type of methods is called <u>*finite volume method*</u> (FVM).

Dividing by Δx, we write the numerical method as

<u>Numerical method in conservation form:</u>

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

Remark:

A numerical method in conservation form is completely specified by the numerical flux

$$F_{i+1/2} = F_{num}\left(u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i+2}^n\right)$$

Here is the key advantage of conservation form.

Theorem (Lax-Wendroff Theorem):

Consider a numerical method in conservation form

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

Suppose the numerical flux satisfies two properties

- $F_{i+1/2} = F_{num}\left(u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i+2}^n\right)$ is a continuous function, and
- $F_{num}\left(u, u, u, u\right) = F\left(u\right)$

If the numerical solution converges, then it converges to a weak solution of

$u_t + F(u)_x = 0$.

Remarks:

- Numerical solution of a method in conservation form obeys the Rankine-Hugoniot condition, which ensures that the velocity of shock wave is correctly captured.
- Since the shock wave velocity is correctly captured, a numerical method in conservation form is also called a shock-capturing method.
- The conservation form does not guarantee the entropy condition. A numerical method in conservation form may capture a fake shock.

Numerical methods for solving conservation laws

Recall two key points:

- We build/study numerical methods in the conservation form

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

- For each method, we only need to specify the numerical flux

$$F_{i+1/2} = F_{num}(u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i+2}^n) \qquad \text{Or} \qquad F_{i+1/2} = F_{num}(u_i^n, u_{i+1}^n)$$

FTCS method: $u_i^{n+1} = u_i^n - \dfrac{\Delta t}{\Delta x}\left(\dfrac{F(u_{i+1}^n) - F(u_{i-1}^n)}{2}\right)$

We write it in the conservation form

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(\underbrace{\frac{F(u_{i+1}^n)+F(u_i^n)}{2}}_{F_{i+1/2}^{(\mathrm{FTCS})}} - \frac{F(u_i^n)+F(u_{i-1}^n)}{2} \right)$$

$$F_{i+1/2}^{(\mathrm{FTCS})} = \frac{1}{2}\left[F(u_{i+1}^n)+F(u_i^n) \right]$$

Modified PDE of FTCS for $u_t + a\, u_x = 0$:

$$w_t = -a w_x + \sigma w_{xx}$$

$$\sigma = \frac{-\Delta x}{2} a^2 r < 0 \qquad \text{negative dissipation!}$$

FTCS is unconditionally unstable.

Lax-Friedrichs method:

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \underbrace{\frac{\Delta t}{\Delta x}}_{\#\#\#}\left(F_{i+1/2}^{(\mathrm{FTCS})} - F_{i-1/2}^{(\mathrm{FTCS})} \right)$$

We write $(u_{i+1}^n + u_{i-1}^n)/2$ as

$$\frac{u_{i+1}^n + u_{i-1}^n}{2} = u_i^n + \frac{1}{2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n) = u_i^n - \underbrace{\frac{\Delta t}{\Delta x}}_{\#\#\#}\left(-\frac{\Delta x}{2\Delta t} \right)\underbrace{\left((u_{i+1}^n - u_i^n) - (u_i^n - u_{i-1}^n) \right)}_{\text{Dissipation/Viscosity}}$$

Factor ### is formed to match that in the L-F above.

Combining the two, we write the L-F in the conservation form

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1/2}^{(\mathrm{L\text{-}F})} - F_{i-1/2}^{(\mathrm{L\text{-}F})} \right)$$

where the numerical flux of Lax-Friedrichs is

$$F_{i+1/2}^{(\mathrm{L\text{-}F})} = F_{i+1/2}^{(\mathrm{FTCS})} - \frac{\Delta x}{2\Delta t}(u_{i+1}^n - u_i^n) = \underbrace{\frac{1}{2}\left[F(u_{i+1}^n) + F(u_i^n) \right]}_{\text{Flux of FTCS}} - \underbrace{\frac{\Delta x}{2\Delta t}(u_{i+1}^n - u_i^n)}_{\text{Added viscosity term}}$$

Modified PDE of Lax-Friedrichs method for $u_t + a\, u_x = 0$:

$$w_t = -a w_x + \sigma w_{xx}$$

$$\sigma = \underbrace{\frac{\Delta x}{2r}}_{\substack{\text{contribution}\\ \text{from added}\\ \text{viscosity}}} - \underbrace{\frac{\Delta x}{2} a^2 r}_{\substack{\text{contribution}\\ \text{of FTCS}}} \geq 0 \quad \text{for} \quad |ar| \leq 1$$

Lax-Friedrichs method is stable for $|ar| \leq 1$.

Remarks:

- (Flux of Lax-Friedrichs) = (Flux of FTCS)+ (Added viscosity term)

  Note: when we add viscosity, it appears as (–) in numerical flux.

- Lax-Friedrichs works because it has sufficient added viscosity to counter the negative dissipation of FTCS.

Upwind method:

Case 1: $F'(u_i^n) \geq 0$ for all (i, n), everything is propagating from left to right

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(F(u_i^n) - F(u_{i-1}^n)\right), \qquad F_{num}(u_i^n, u_{i+1}^n) = F(u_i^n)$$

Case 2: $F'(u_i^n) \leq 0$ for all (i, n), everything is propagating from right to left

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(F(u_{i+1}^n) - F(u_i^n)\right), \qquad F_{num}(u_i^n, u_{i+1}^n) = F(u_{i+1}^n)$$

The general case:

Let $\alpha(u_i^n, u_{i+1}^n)$ denote the propagation velocity of discontinuity $[u_i^n, u_{i+1}^n]$.

We calculate $\alpha(u_i^n, u_{i+1}^n)$ based on the Rankine-Hugoniot relation

$$\alpha(u_i^n, u_{i+1}^n) = \begin{cases} \dfrac{F(u_{i+1}^n) - F(u_i^n)}{u_{i+1}^n - u_i^n}, & u_i^n \neq u_{i+1}^n \\ F'(u_i^n), & u_i^n = u_{i+1}^n \end{cases}$$

We use $\alpha(u_i^n, u_{i+1}^n)$ to switch between $F(u_i^n)$ and $F(u_{i+1}^n)$.

$$F_{num}(u_i^n, u_{i+1}^n) = \begin{cases} F(u_i^n), & \alpha(u_i^n, u_{i+1}^n) \geq 0 \\ F(u_{i+1}^n), & \alpha(u_i^n, u_{i+1}^n) < 0 \end{cases}$$

Remarks:

- If $[u_i^n, u_{i+1}^n]$ is a shock wave, $\alpha(u_i^n, u_{i+1}^n)$ captures the correct velocity.
- $\alpha(u_i^n, u_{i+1}^n)$ does not distinguish between a real shock and a fake shock.
- There is no ambiguity at $\alpha(u_i^n, u_{i+1}^n) = 0$

$\alpha(u_i^n, u_{i+1}^n) = 0 \quad ==> \quad F(u_i^n) = F(u_{i+1}^n)$

We write the numerical flux in a unified form

$$F_{num}(u_i^n, u_{i+1}^n) = \frac{1}{2}\left(F(u_{i+1}^n) + F(u_i^n)\right) - \frac{1}{2}\text{sign}\left(\alpha(u_i^n, u_{i+1}^n)\right)\left(F(u_{i+1}^n) - F(u_i^n)\right)$$

$$= \frac{1}{2}\left(F(u_{i+1}^n) + F(u_i^n)\right) - \frac{1}{2}\underbrace{\text{sign}\left(\alpha(u_i^n, u_{i+1}^n)\right)\alpha(u_i^n, u_{i+1}^n)}_{|\alpha(u_i^n, u_{i+1}^n)|}(u_{i+1}^n - u_i^n)$$

<u>Numerical flux of upwind method:</u>

$$F_{i+1/2}^{(\text{Up})} = \underbrace{\frac{1}{2}\left(F(u_{i+1}^n) + F(u_i^n)\right)}_{\text{Flux of FTCS}} - \underbrace{\frac{1}{2}\left|\alpha(u_i^n, u_{i+1}^n)\right|(u_{i+1}^n - u_i^n)}_{\text{Added viscosity term}}$$

Modified PDE of upwind method for $u_t + a\, u_x = 0, \quad a > 0$

$$w_t = -a w_x + \sigma w_{xx}$$

$$\sigma^{(\text{Up})} = \underbrace{\frac{\Delta x}{2} a}_{\substack{\text{contribution}\\ \text{from added}\\ \text{viscosity}}} - \underbrace{\frac{\Delta x}{2} a^2 r}_{\substack{\text{contribution}\\ \text{of FTCS}}} \geq 0 \quad \text{for } \; ar \leq 1$$

Upwind method is stable for $ar \leq 1$ (when $a > 0$).

We compare the dissipation of upwind with that of Lax-Friedrichs.

$$\sigma^{(\text{L-F})} = \underbrace{\frac{\Delta x}{2r}}_{\substack{\text{contribution}\\ \text{from added}\\ \text{viscosity}}} - \underbrace{\frac{\Delta x}{2} a^2 r}_{\substack{\text{contribution}\\ \text{of FTCS}}} \geq 0 \quad \text{for } \; |ar| \leq 1$$

Lax-Friedrichs has more added viscosity (which is unnecessary).

The version of upwind method above has the conservation form.

==> It obeys the Rankine-Hugoniot condition.

But it does not obey the <u>entropy condition</u>.

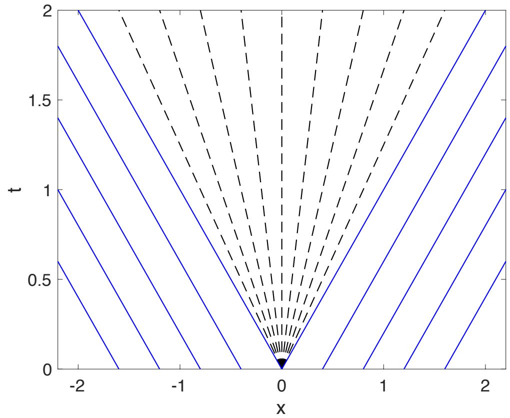
<u>Example:</u> (upwind method may capture a fake shock)

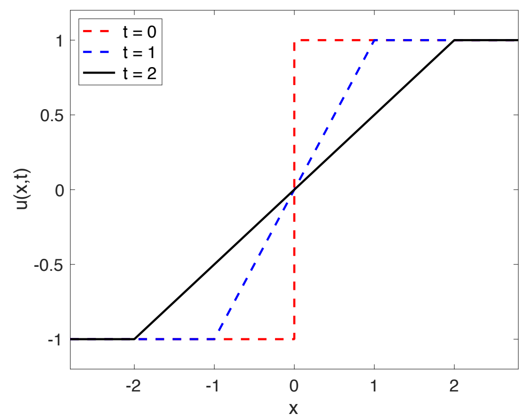
We apply the upwind method to the initial value problem

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0, \qquad u(x,0) = \begin{cases} -1, & x \leq 0 \\ 1, & x > 0 \end{cases} \qquad \text{(IVP-3)}$$

<u>Exact solution:</u>

$$u(x,t)=\begin{cases} -1\,, & x\le -t \\ x/t\,, & -t<x\le t \\ 1\,, & x>t \end{cases} \qquad \text{a rarefaction wave}$$





<u>Numerical solution:</u>

$$u_i^0=\begin{cases} -1\,, & i\le 0 \\ 1\,, & i\ge 1 \end{cases}$$

$$(u_i^0,\, u_{i+1}^0)=\begin{cases} (-1,\,-1)\,, & i\le -1 \\ (-1,\,+1)\,, & i=0 \\ (+1,\,+1) & i\ge 1 \end{cases}$$

$$\alpha(u_i^0,u_{i+1}^0)=\begin{cases} F'(u_i^0)\,, & i\le -1 \\ \dfrac{F(u_{i+1}^0)-F(u_i^0)}{u_{i+1}^0-u_i^0}\,, & i=0 \\ F'(u_i^0) & i\ge 1 \end{cases} = \begin{cases} -1\,, & i\le -1 \\ 0\,, & i=0 \\ 1 & i\ge 1 \end{cases}$$

$$F_{i+1/2}^{(\mathrm{Up})}=\underbrace{\frac{1}{2}\Big(F(u_{i+1}^0)+F(u_i^0)\Big)}_{=\frac{1}{2}\text{ for all } i}-\underbrace{\frac{1}{2}\left|\alpha(u_i^0,u_{i+1}^0)\right|}_{=0\text{ at } i=0}\underbrace{(u_{i+1}^0-u_i^0)}_{=0\text{ for } i\neq 0}$$

==> $\quad F_{i+1/2}^{(\mathrm{Up})}=\dfrac{1}{2}$ for all i

==> $\quad u_i^1=u_i^0$

==> Numerical solution is a stationary shock, which is

- a weak solution (satisfying the Rankine-Hugoniot condition);
- a fake shock (violating the entropy condition).

We need to modify the upwind method to satisfy the entropy condition.

An ad hoc entropy fix for the upwind method (by Ami Harten)

Start with the numerical flux of upwind method.

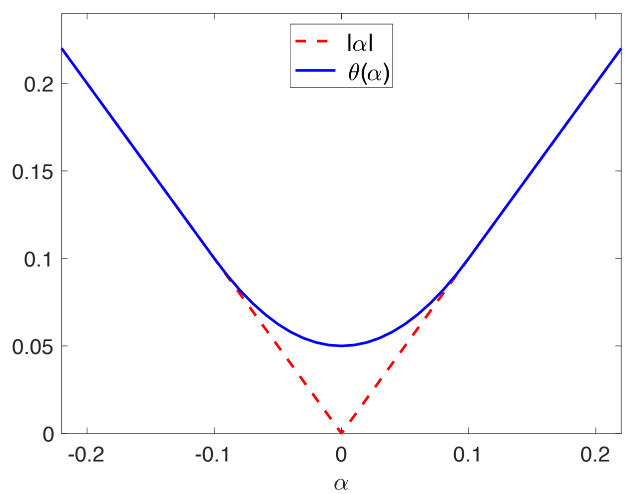
$$F_{i+1/2}^{(\mathrm{Up})} = \underbrace{\frac{1}{2}\left(F(u_{i+1}^n) + F(u_i^n)\right)}_{\text{Flux of FTCS}} - \underbrace{\frac{1}{2}\left|\alpha(u_i^n, u_{i+1}^n)\right|(u_{i+1}^n - u_i^n)}_{\text{Added viscosity term}}$$

In the numerical flux, the added viscosity disappear when $\alpha(u_i^n, u_{i+1}^n) = 0$.

We replace $|\alpha|$ with function $\theta(\alpha)$, defined below.

$$\theta(\alpha) \equiv \begin{cases} |\alpha|, & |\alpha| \geq \varepsilon \\ \dfrac{1}{2\varepsilon}(\alpha^2 + \varepsilon^2), & |\alpha| < \varepsilon \end{cases}$$

Note: Function $\theta(\alpha)$ is essentially the same as $|\alpha|$. It rounds out the corner at $\alpha = 0$ and makes the function strictly positive (so we always have some positive viscosity).



The new numerical flux of upwind method is

$$F_{i+1/2}^{(\mathrm{Up})}(\mathrm{new}) = \underbrace{\frac{1}{2}\left(F(u_{i+1}^n) + F(u_i^n)\right)}_{\text{Flux of FTCS}} - \underbrace{\frac{1}{2}\theta\left(\alpha(u_i^n, u_{i+1}^n)\right)(u_{i+1}^n - u_i^n)}_{\text{Added viscosity term}}$$