A Bound-Preserving Fourth Order Compact Finite Difference Scheme for Scalar Convection Diffusion Equations

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Overview

Stability: Compressible Euler Equations in Gas Dynamics

$$\begin{pmatrix} \rho \\ m \\ E \end{pmatrix}_t + \begin{pmatrix} m \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}_x = 0,$$

with

$$m = \rho u, \quad E = \frac{1}{2}\rho u^2 + \rho e, \quad p = (\gamma - 1)\rho e.$$

The speed of sound is given by $c = \sqrt{\gamma p/\rho}$ and the three eigenvalues of the Jacobian are $u, u \pm c$.

If either $\rho < 0$ or $p < 0$, then the sound speed is imaginary and the system is no longer hyperbolic. Thus the initial value problem is ill-posed. This is why it is computationally unstable.

Bound Preserving for Scalar Conservation Laws

Consider the initial value problem

$$u_t + \nabla \cdot \mathbf{F}(u) = 0, u(\mathbf{x}, 0) = u^0(\mathbf{x}), \mathbf{x} \in \mathbb{R}^n$$

for which the unique entropy solution $u(x, t)$ satisfies

$$\min_{\mathbf{x}} u(\mathbf{x}, t_0) \leq u(\mathbf{x}, t) \leq \max_{\mathbf{x}} u(\mathbf{x}, t_0), \quad \forall t \geq t_0. \qquad \text{Maximum Principle}$$

In particular,

$$\min_{\mathbf{x}} u_0(\mathbf{x}) = m \leq u(\mathbf{x}, t) \leq M = \max_{\mathbf{x}} u_0(\mathbf{x}). \qquad \text{Bound Preserving}$$

It is also a desired property for numerical solutions due to

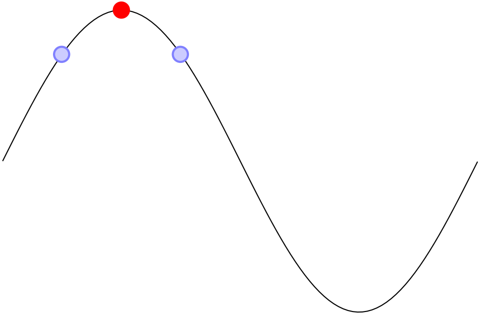
1. Physical meaning: vehicle density (traffic flow), mass percentage (pollutant transport), probability distribution (Boltzmann equation) and etc.
2. Stability for systems: positivity of density and pressure (gas dynamics), water height (shallow water equations), particle density for describing electrical discharges (a convection-dominated system) and etc.

For numerical schemes, this is a completely DIFFERENT problem from discrete maximum principle in solving elliptic equations.

Scalar Equations

- IVP: $u_t + f(u)_x = 0, u(x,0) = u^0(x)$.
- Maximum Principle (Bound Preserving): $u(x,t) \in [m, M]$ where $m = \min u_0(x), M = \min u_0(x)$.
- For finite difference, any scheme satisfying $\min_j u_j^n \leq u_j^{n+1} \leq \max_j u_j^n$ can be at most first order accurate.

Harten's Counter Example: consider $u_t + u_x = 0, \quad u(x,0) = \sin x$. Put the grids in a way such that $x = \frac{\pi}{2}$ is in the middle of two grid points.



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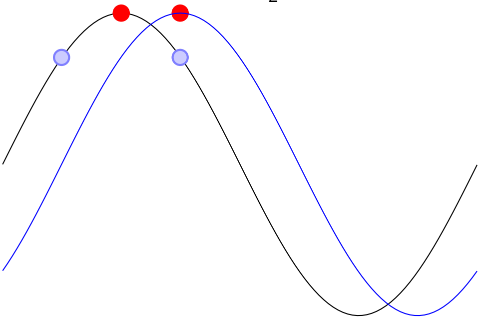

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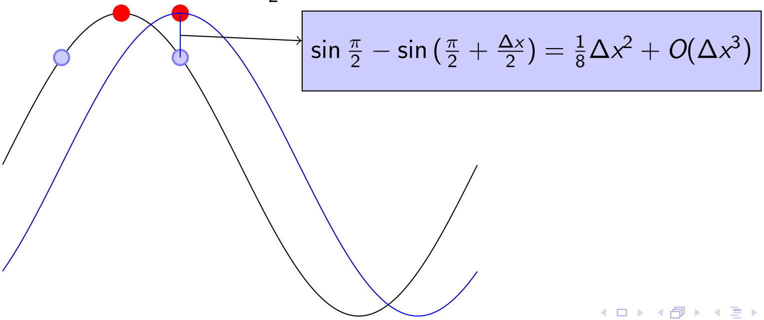


Bound-Preserving Schemes

1. First order monotone schemes.
2. FD/FV schemes satisfying $\min_j u_j^n \le u_j^{n+1} \le \max_j u_j^n$: can have any formal order of accuracy in the monotone region but are only first order accurate around the extrema. E.g.,
   - Conventional total-variation-diminishing (TVD) schemes.
   - High Resolution schemes such as the MUSCL scheme.
3. FV schemes satisfying $\min_x u^n(x) \le u^{n+1}(x) \le \max_x u^n(x)$:
   - R. Sanders, 1988: a third order finite volume scheme for 1D.
   - X.Z. and Shu, 2009: higher order (up to 6th) extension of Sanders' scheme.
   - Liu and Osher, 1996: a third order FV scheme for 1D (can be proven bound-preserving only for linear equations).
   - Noelle, 1998; Kurganov and Petrova, 2001: 2D generalization of *Liu and Osher*.
   - All schemes in this category use the exact time evolution.

Bound-Preserving Schemes

Practical/popular high order schemes are NOT bound-preserving.
It was unknown previously how to construct a high order bound-preserving scheme for 2D nonlinear equations.

Conservative Eulerian Schemes

Conservative Schemes: The scheme must have the following form:

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x_j} \left[\hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} \right].$$

Global Conservation: $\sum_j \overline{u}_j^{n+1} \Delta x_j = \sum_j \overline{u}_j^n \Delta x_j$.

We insist on using conservative schemes:

1. Lax-Wendroff Theorem: If converging (as mesh sizes go to zero), the converged solution of a conservative scheme is a weak solution.
2. The shock location will be wrong if the conservation is violated.
3. If a scheme is conservative and positivity preserving, then we have L1-stability: $\sum_j |\overline{u}_j^{n+1}| \Delta x_j = \sum_j \overline{u}_j^{n+1} \Delta x_j = \sum_j \overline{u}_j^n \Delta x_j = \sum_j |\overline{u}_j^n| \Delta x_j$.
    - In Euler equations, if density and pressure are positive, then we have L1-stability for density and total energy.
    - Crude replacement of negative values by positive ones is simply unacceptable and unstable because it destroys the local conservation.

Objective

We want to construct a scheme which is

1. genuinely high order accurate (at least third order)
2. conservative
3. positivity/bound preserving
4. Practical concern: cost effective, multi-dimensions, unstructured meshes, parallelizability and etc.

Why high order schemes?

- For smooth solutions, the computational cost of higher order schemes is smaller to reach the same accuracy.
- Near shocks, the error in L^∞ norm of any scheme will at most half order. For a lot of problems: accuracy is still high order away from discontinuities.

Motivation: nonlinear stability is one of the main reasons why high order schemes have not been widely used for more real world problems.

Time Discretization: SSP Runge-Kutta or Multi-Step Method

High order strong stability preserving (SSP) Runge-Kutta or multi-step method is a convex combination of several forward Euler schemes. E.g., the 5 stages 4th order SSP Runge-Kutta method for solving $u_t = F(u)$ is given by

$$
\begin{aligned}
u^{(1)} &= u^n + 0.391752226571890 \Delta t F(u^n) \\
u^{(2)} &= 0.444370493651235 u^n + 0.555629506348765 u^{(1)} \\
&\quad + 0.368410593050371 \Delta t F(u^{(1)}) \\
u^{(3)} &= 0.620101851488403 u^n + 0.379898148511597 u^{(2)} \\
&\quad + 0.251891774271694 \Delta t F(u^{(2)}) \\
u^{(4)} &= 0.178079954393132 u^n + 0.821920045606868 u^{(3)} \\
&\quad + 0.544974750228521 \Delta t F(u^{(3)}) \\
u^{n+1} &= 0.517231671970585 u^{(2)} + 0.096059710526147 u^{(3)} \\
&\quad + 0.063692468666290 \Delta t F(u^{(3)}) + 0.386708617503269 u^{(4)} \\
&\quad + 0.226007483236906 \Delta t F(u^{(4)})
\end{aligned}
$$

This method was numerically found to be optimal.

Time Discretization: SSP Runge-Kutta or Multi-Step Method

- If the forward Euler is bound-preserving, then so is the high order Runge-Kutta/Multi-Step.
- SSP time discretization has been often used to construct positivity preserving schemes.

First Order Monotone Schemes

Let $\lambda = \frac{\Delta t}{\Delta x}$, a monotone scheme for $u_t + f(u)_x = 0$ is given by

$$
\begin{aligned}
u_j^{n+1} &= u_j^n - \lambda \left[\widehat{f}(u_j^n, u_{j+1}^n) - \widehat{f}(u_{j-1}^n, u_j^n) \right] \\
&= H(u_{j-1}^n, u_j^n, u_{j+1}^n).
\end{aligned}
$$

where the numerical flux $\widehat{f}(\uparrow, \downarrow)$ is monotonically increasing w.r.t. the first variable and decreasing w.r.t. the second variable. E.g., the Lax-Friedrichs flux

$$\widehat{f}(u, v) = \frac{1}{2}(f(u) + f(v) - \alpha(v - u)), \alpha = \max_u |f'(u)|.$$

If $m \leq u_j^n \leq M$ for all j, then

$$u_j^{n+1} = H(u_{j-1}^n, u_j^n, u_{j+1}^n) = H(\uparrow, \uparrow, \uparrow) \tag{1}$$

implies

$$m = H(m, m, m) \leq u_j^{n+1} \leq H(M, M, M) = M.$$

Fourth Order Compact Finite Difference

Standard centered finite difference:

$$u_i' = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2),\ u_i'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

Fourth order compact finite difference:

$$\frac{1}{6}u_{i+1}' + \frac{4}{6}u_i' + \frac{1}{6}u_{i-1}' = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^4)$$

$$\frac{1}{12}u_{i+1}'' + \frac{5}{6}u_i'' + \frac{1}{12}u_{i-1}'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^4)$$

A tridiagonal system needs to be solved:

$$\frac{1}{6}\begin{pmatrix} 4 & 1 & & & & 1 \\ 1 & 4 & 1 & & & \\ & 1 & 4 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 4 & 1 \\ 1 & & & & 1 & 4 \end{pmatrix} \begin{pmatrix} u_1' \\ u_2' \\ u_3' \\ \vdots \\ u_{N-1}' \\ u_N' \end{pmatrix} = \frac{1}{2\Delta x}\begin{pmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix},$$

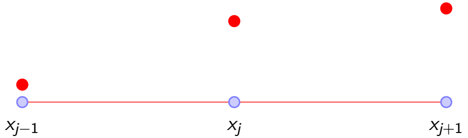
$$\textit{i.e.} \quad W\mathbf{u}' = D_x\mathbf{u}$$

The Weighting Operator for Convection

If we regard W as an operator mapping a vector to another vector, then

$$(Wu)_j = \frac{1}{6}u_{j+1} + \frac{4}{6}u_j + \frac{1}{6}u_{j-1},$$

which happens to be the Simpson's rule (or 3-point Gauss-Lobatto Rule) in quadrature.



Locally, for each interval $[x_{j-1}, x_{j+1}]$, there exists a cubic polynomial $p_j(x)$, obtained through interpolation at $x_{j-1}, x_j, x_{j+1}, x_{j+2}$ (or $x_{j-2}, x_{j-1}, x_j, x_{j+1}$)

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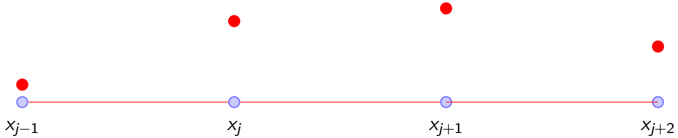

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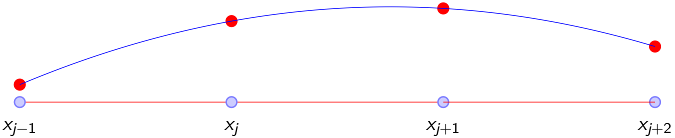

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The Fourth Order Compact Finite Difference Scheme for Convection

Let $\overline{u}_i = (Wu)_i = \frac{1}{6}u_{i-1} + \frac{4}{6}u_i + \frac{1}{6}u_{i+1}$. The fourth order compact finite difference for $u_t + f(u)_x = 0$ can be written as

$$\overline{u}_i^{n+1} = \overline{u}_i^n - \frac{\Delta t}{\Delta x}\frac{1}{2}[f(u_{i+1}^n) - f(u_{i-1}^n)] = \overline{u}_i^n - \frac{\Delta t}{\Delta x}(\hat{f}_{i+\frac{1}{2}}^n - \hat{f}_{i-\frac{1}{2}}^n),$$

$$\hat{f}_{i+\frac{1}{2}} = \frac{1}{2}(f(u_{i+1}) + f(u_i)).$$

The weak monotonicity holds under the CFL constraint $\lambda \max_u |f'(u)| \leq \frac{1}{3}$:

$$\begin{aligned}\overline{u}_i^{n+1} &= \frac{1}{6}u_{i-1}^n + \frac{4}{6}u_i^n + \frac{1}{6}u_{i+1}^n + \frac{1}{2}\lambda[f(u_{i+1}^n) - f(u_{i-1}^n)] \\ &= \frac{1}{6}[u_{i-1} - 3\lambda f(u_{i-1}^n)] + \frac{1}{6}[u_{i+1}^n + 3\lambda f(u_{i+1}^n)] + \frac{4}{6}u_i^n \\ &= H(u_{i-1}^n, u_i^n, u_{i+1}^n) = H(\uparrow, \uparrow, \uparrow).\end{aligned}$$

Thus $m \leq u_i^n \leq M$ implies $m = H(m, m, m) \leq \overline{u}_i^{n+1} \leq H(M, M, M) = M$.

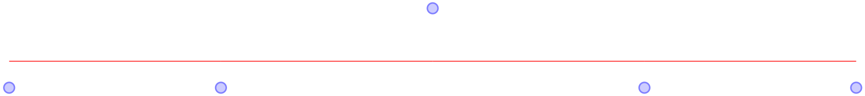
How to enforce bounds?

Consider enforcing the positivity (general lower/upper bounds can be similarly treated). Given point values u_i, if $\frac{1}{6}u_{i-1} + \frac{4}{6}u_i + \frac{1}{6}u_{i+1} \geq 0$ for any i, then the following hold:

- For any three consecutive points, at least one point value is non-negative.
- If $u_i < 0$, local average is non-negative: $\frac{1}{3}u_{i-1} + \frac{1}{3}u_i + \frac{1}{3}u_{i+1} \geq 0$. This means that it is possible to eliminate the undershoot without changing $\frac{1}{3}u_{i-1} + \frac{1}{3}u_i + \frac{1}{3}u_{i+1}$.
- If $u_i < 0$, then either $u_i + \frac{1}{2}u_{i+1} \geq 0$ or $u_i + \frac{1}{2}u_{i-1} \geq 0$.

So a simple local limiter can enforce the positivity (or general lower/upper bounds):

$$\begin{aligned} &\text{if} \quad u_{i+1} \geq u_{i-1}, \quad \text{set} \quad u_{i+1} \leftarrow u_{i+1} + u_i, u_i \leftarrow 0, \\ &\text{if} \quad u_{i+1} < u_{i-1}, \quad \text{set} \quad u_{i-1} \leftarrow u_{i-1} + u_i, u_i \leftarrow 0. \end{aligned}$$



2D Convection

Let $u_{i,j}$ denote point values on a 2D uniform grid. Define two weighting operators:

$$(W_x u)_{i,j} = \frac{1}{6} u_{i-1,j} + \frac{4}{6} u_{i,j} + \frac{1}{6} u_{i+1,j},$$

$$(W_y u)_{i,j} = \frac{1}{6} u_{i,j-1} + \frac{4}{6} u_{i,j} + \frac{1}{6} u_{i,j+1}.$$

Let $\overline{u}$ denote $W_x W_y u$. The fourth order compact finite difference for $u_t + f(u)_x + g(u)_y = 0$ can be written as

$$\overline{u}^{n+1}_{i,j} = \overline{u}^{n}_{i,j} + \frac{\Delta t}{\Delta x}\frac{1}{2} W_y [f(u^n_{i+1,j}) - f(u^n_{i-1,j})] + \frac{\Delta t}{\Delta y}\frac{1}{2} W_x [g(u^n_{i,j+1}) - f(u^n_{i,j-1})]$$

$\overline{u}^{n+1}_{i,j}$ has weak monotonicity thus $u^n_{i,j} \geq 0$ implies $\overline{u}^{n+1}_{i,j} \geq 0$.
A dimension by dimension fashion 2D limiter:

- Introduce a new variable $v = W_x u$. So $\overline{u} = W_y v$.
- Given $\overline{u} \geq 0$, apply 1D limiter in y-direction on v to enforce $v \geq 0$.
- Given $v \geq 0$, apply 1D limiter in x-direction on u to enforce $u \geq 0$.

Diffusion

$$\frac{1}{12}(u''_{i+1} + 10u''_i + u''_{i-1}) = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^4)$$

Let $\tilde{u}_i = (Wu)_i = \frac{1}{12}(u_{i-1} + 10u_i + u_{i+1})$. The fourth order compact finite difference for $u_t = g(u)_{xx}$ can be written as

$$\tilde{u}_i^{n+1} = \tilde{u}_i^n + \frac{\Delta t}{\Delta x^2}[g(u_{i+1}^n) - 2g(u_i^n) + g(u_{i-1}^n)],$$

Assuming $g'(u) \geq 0$. The weak monotonicity holds under the CFL constraint $\frac{\Delta t}{\Delta x^2} \max_u |f'(u)| \leq \frac{1}{6}$. The same 1D limiter can be used for enforcing bounds.

Remarks

For approximating the 2D Laplacian, the fourth order compact finite difference scheme is also known as the 9-point discrete Laplacian (the second order centered difference is 5-point Laplacian). For solving heat equation, Crank-Nicolson time discretization and the 9-point Laplacian give an M-matrix, thus it can preserve bounds/positivity. However, such a result cannot be easily extended to nonlinear cases.

Convection-Diffusion

For the equation $u_t + f(u)_x = g(u)_{xx}$, define two weighting operators:

$$(W_1 u)_j = \frac{1}{6}(u_{j+1} + 4u_j + u_{j-1}),$$

$$(W_2 u)_j = \frac{1}{12}(u_{j+1} + 10u_j + u_{j-1}).$$

Let $\tilde{\bar{u}}_i = (W_1 W_2 u)_i = (W_2 W_1 u)_i$, then the scheme is

$$\tilde{\bar{u}}_j^{n+1} = \tilde{\bar{u}}_j^n - \lambda \frac{1}{2} W_2[f(u_{j+1}^n) - f(u_{j-1}^n)] + \mu W_1[g(u_{j+1}^n) - 2g(u_j^n) + g(u_{j-1}^n)]$$

$\tilde{\bar{u}}_j^{n+1}$ has weak monotonicity, thus $u_j^n \geq 0$ implies $\tilde{\bar{u}}_j^{n+1} \geq 0$.
The same 1D limiter can be applied twice to for enforcing the bound.

TVB limiter

- The result is still true if adding the TVB limiter in Bernardo Cockburn and Chi-Wang Shu. Nonlinearly stable compact schemes for shock calculations. SIAM Journal on Numerical Analysis, 31(3):607-627, 1994.
- Using both TVB limiter and the simple local bound-preserving limiter can eliminate overshoot/undershoot and oscillations without losing accuracy/conservation.

The stream function formulation of 2D incompressible Navier-Stokes equations:

$$\omega_t + (u\omega)_x + (v\omega)_y = \Delta\omega$$

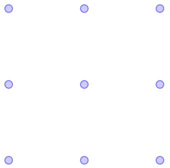
$$u = -\psi_y, v = \psi_x$$

$$\psi = \Delta\omega$$

The weak monotonicity holds. But to have $H(M, M, M) = M$, we need a discrete incompressible condition:

$$\frac{1}{\Delta x}\left[\frac{1}{6}u_{i+1,j-1} + \frac{4}{6}u_{i+1,j} + \frac{1}{6}u_{i+1,j+1} - \frac{1}{6}u_{i-1,j-1} - \frac{4}{6}u_{i-1,j} - \frac{1}{6}u_{i-1,j+1}\right]$$

$$+\frac{1}{\Delta y}\left[\frac{1}{6}v_{i+1,j+1} + \frac{4}{6}v_{i,j+1} + \frac{1}{6}v_{i-1,j+1} - \frac{1}{6}v_{i+1,j-1} - \frac{4}{6}v_{i,j-1} - \frac{1}{6}v_{i-1,j-1}\right] = 0$$



Inflow-outflow boundary conditions

For the equation $u_t + f(u)_x = 0$ on $[0,1]$ with initial value $u(x,0) = u^0(x)$ and inflow boundary condition $u(0,t) = g(t)$. We have the 4th-order compact finite difference

$$
\frac{d}{dt}\frac{1}{6}\begin{pmatrix} 1 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ & & 1 & 4 & 1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & 1 & 4 & 1 \\ & & & & & 1 & 4 & 1 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ u_3 \\ \vdots \\ u_N \\ u_{N+1} \end{pmatrix} = -\frac{1}{2\Delta x}\begin{pmatrix} -1 & 0 & 1 & & & & \\ & -1 & 0 & 1 & & & \\ & & -1 & 0 & 1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -1 & 0 & 1 \\ & & & & & -1 & 0 & 1 \end{pmatrix}\begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_N \\ f_{N+1} \end{pmatrix}
$$

Inflow-outflow boundary conditions

With forward euler time discretization the scheme is

$$\bar{u}_i^{n+1} = \bar{u}_i^n - \frac{\Delta t}{2\Delta x}(f_{i+1} - f_{i-1}), 1 \leq i \leq N.$$

Since u_0 is known, to solve the previous linear system, we need to find a good approximation of u_{N+1}. A cubic polynomial $p_j(x)$, obtained through enforcing its integral equals $\bar{u}_i$ over interval $[x_{i-1}, x_{i+1}]$ for $i = N-3, N-2, N-1, N$. We get

$$u_{N+1} = -\frac{2}{3}\bar{u}_{N-3} + \frac{17}{6}\bar{u}_{N-2} + \frac{14}{3}\bar{u}_{N-1} + \frac{7}{2}\bar{u}_N.$$

A filter

$$u_{N+1} = \max(\min(u_{N+1}, ubound), lbound)$$

should be used to make $u_{N+1} \in [m, M]$. Next we can compute $u_i, 1 \leq i \leq N$. Apply the previous bound-preserving limiter to u_i to make sure $u_i \in [m, M]$. Then we can update the value of $\bar{u}_i, 1 \leq i \leq N$ and compute the solution at next level.

Dirichlet boundary conditions

Consider $u_t + f(u)_x = g(u)_{xx}$ on $[0, L]$ with initial value $u(x,0) = u^0(x)$ and Dirichlet boundary condition $u(0,t) = L(t), u(L,t) = R(t)$. Define $W := W_1 W_2 = W_2 W_1$, we will have

$$\frac{d}{dt}(WU) + W_2 D_x f + W_2 F = W_1 D_{xx} g + W_1 G. \tag{2}$$

and

$$-W_2 F + W_1 G = \begin{pmatrix} -\frac{1}{18} u_{t,0} + \frac{1}{12} f_{x,0} + \frac{5}{12\Delta x} f_0 + \frac{2}{3\Delta x^2} g_0 \\ -\frac{1}{72} u_{t,0} + \frac{1}{24\Delta x} f_0 + \frac{1}{6\Delta x^2} g_0 \\ 0 \\ \vdots \\ 0 \\ -\frac{1}{72} u_{t,N+1} - \frac{1}{24\Delta x} f_{N+1} + \frac{1}{6\Delta x^2} g_{N+1} \\ -\frac{1}{18} u_{t,N+1} + \frac{1}{12} f_{x,N+1} - \frac{5}{12\Delta x} f_{N+1} + \frac{2}{3\Delta x^2} g_{N+1} \end{pmatrix} \tag{3}$$

Dirichlet boundary conditions

We need to approximate $f(u)_{x,0}$ and $f(u)_{x,N+1}$. But to have weak monotonicity, only 3rd-order approximation can be made.

$$f(u)_{x,0} = \frac{1}{\Delta x}(-\frac{11}{6}f_0 + 3f_1 - \frac{3}{2}f_2 + \frac{1}{3}f_3)$$

and

$$f(u)_{x,N+1} = \frac{1}{\Delta x}(-\frac{1}{3}f_{N-2} + \frac{3}{2}f_{N-1} - 3f_N + \frac{11}{6}f_{N+1}).$$

Then we plug these approximations in and rearrange (2). Finally we have the space discretization

$$\frac{d}{dt}\widetilde{W}\tilde{u} = -\widetilde{D}_x\tilde{f} + \widetilde{D}_{xx}\tilde{g}.$$

$$\widetilde{W}=\frac{1}{72}\begin{pmatrix} \frac{24}{5} & \frac{246}{5} & \frac{84}{5} & \frac{6}{5} & & & & \\ 1 & 14 & 42 & 14 & 1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 1 & 14 & 42 & 14 & 1 \\ & & & & \frac{6}{5} & \frac{84}{5} & \frac{246}{5} & \frac{24}{5} \end{pmatrix}_{N\times(N+2)}, \tilde{u}=\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \\ u_{N+1} \end{pmatrix}_{(N+2)\times 1}, \quad (4)$$

$$\widetilde{D}_x=\frac{1}{24\Delta x}\begin{pmatrix} -\frac{38}{5} & -\frac{42}{5} & \frac{78}{5} & \frac{2}{5} & & & & \\ -1 & -10 & 0 & 10 & 1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & -1 & -10 & 0 & 10 & 1 \\ & & & & -\frac{2}{5} & -\frac{78}{5} & \frac{42}{5} & \frac{38}{5} \end{pmatrix}_{N\times(N+2)}, \tilde{f}=\begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_N \\ f_{N+1} \end{pmatrix}_{(N+2)\times 1}, \quad (5)$$

$$\widetilde{D}_{xx}=\frac{1}{6\Delta x^2}\begin{pmatrix} \frac{24}{5} & -\frac{42}{5} & \frac{12}{5} & \frac{6}{5} & & & & \\ 1 & 2 & -6 & 2 & 1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 1 & 2 & -6 & 2 & 1 \\ & & & & \frac{6}{5} & \frac{12}{5} & -\frac{42}{5} & \frac{24}{5} \end{pmatrix}_{N\times(N+2)}, \tilde{g}=\begin{pmatrix} g_0 \\ g_1 \\ \vdots \\ g_N \\ g_{N+1} \end{pmatrix}_{(N+2)\times 1} \quad (6)$$

Weak monotonicity and consistency hold. The previous limiter can be applied to preserve the bound. 2D case can be treated similarly.

6th and 8th Order Scheme

6th order first derivative approximation with the weak monotonicity:

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_i + \alpha f'_{i+1} + \beta f'_{i+2} = b\frac{f_{i+2} - f_{i-2}}{4\Delta x} + a\frac{f_{i+1} - f_{i-1}}{2\Delta},$$

$$\beta = \frac{1}{12}(-1 + 3\alpha),\ a = \frac{2}{9}(8 - 3\alpha),\ b = \frac{1}{18}(-17 + 57\alpha),\ \alpha > \frac{1}{3}.$$

If we let $\alpha = \frac{4}{9}$, $\beta = \frac{1}{36}$, $a = \frac{40}{27}$, $b = \frac{25}{54}$, we acctually have the 8th order with the weak monotonicity.

6th-order second derivative approximation with the weak monotonicity:

$$\beta f''_{i-2} + \alpha f''_{i-1} + f'_i + \alpha f''_{i+1} + \beta f''_{i+2} = b\frac{f_{i+2} - 2f_i + f_{i-2}}{4\Delta x^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta^2},$$

$$a = \frac{-78\alpha + 48}{31},\ b = \frac{291\alpha - 36}{62},\ \alpha > 0.$$

If we let $\alpha = \frac{344}{1179}$, we acctually have the 8th order scheme with the weak monotonicity.

Non-uniform Grids

Consider a mapping for the physical non-uniform grid points x_j on the interval $[a, b]$ to uniform reference grid points ξ_j on the same interval $[a, b]$. Let $\xi(x)$ denote such a map and $\frac{d\xi(x)}{dx} \neq 0$. Then a convection diffusion equation in the form of

$$u_t + f(u)_x = g(u)_{xx}$$

can be written as:

$$\frac{\partial}{\partial t}\hat{u} + \left(\frac{d\xi}{dx} - \frac{d^2\xi}{dx^2}\right)\frac{\partial}{\partial \xi}f(\hat{u}) = \left(\frac{d\xi}{dx}\right)^2\frac{\partial^2}{\partial \xi^2}g(\hat{u}).$$

Therefore, it is equivalent to solve the following equation

$$u_t + c(x)f(u)_x = d(x)g(u)_{xx}, \quad d(x) > 0.$$

Accuracy Test

SSP 4th-order multistep for 2D linear convection:

Mesh	L^∞ error	order	L^1 error	order
20×20	5.81E-5	-	3.68E-5	-
40×40	3.52E-6	4.05	2.25E-6	4.03
80×80	2.17E-7	4.02	1.38E-7	4.03
160×160	1.35E-8	4.01	8.57E-9	4.01

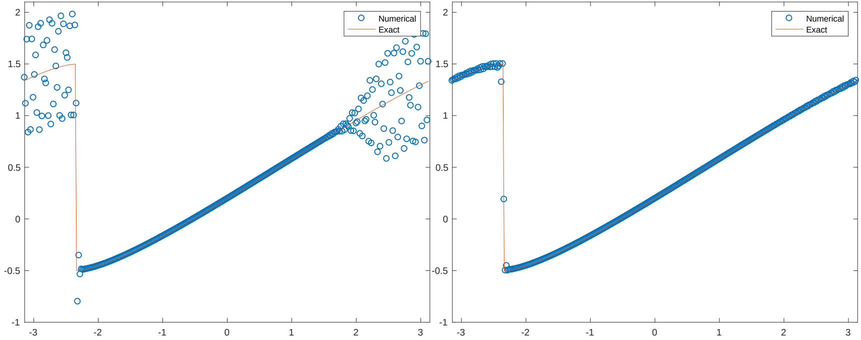
SSP RK4 for 1D linear convection:

Mesh	L^∞ error	order	L^1 error	order
40	2.72E-5	-	1.67E-5	-
80	1.77E-6	3.95	1.08E-6	3.94
160	2.52E-7	2.81	8.37E-8	3.69
320	1.17E-7	1.11	1.20E-8	2.81

SSP 4th-order multistep for 1D convection-diffusion equation:

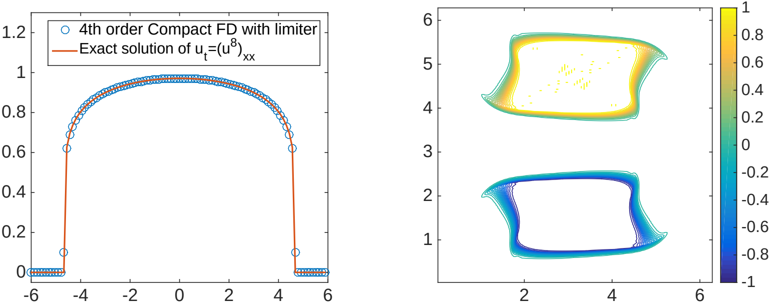
Mesh	L^∞ error	order	L^1 error	order
40	1.55E-6	-	9.92E-7	-
80	9.72E-8	4.00	6.19E-8	4.00
160	6.07E-9	4.00	3.87E-9	4.00
320	3.76E-10	4.01	2.40E-10	4.01

1D burgers equation when the exact solution has a shock



Left: numerical solutions without bound-preserving limiter.

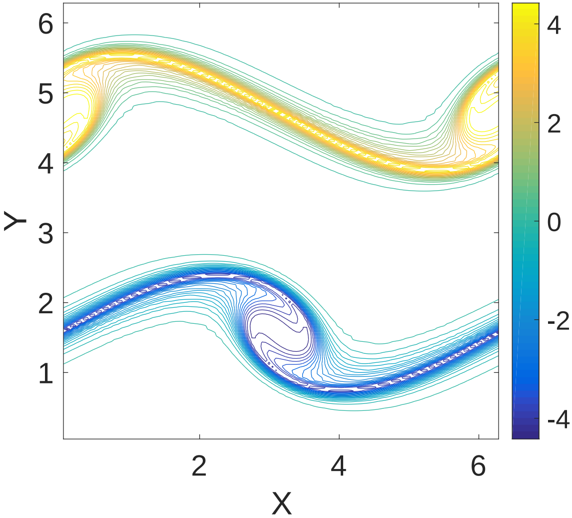
Right: numerical solutions with bound-preserving limiter.



Left: degenerate nonlinear parabolic equation $u_t = (u^8)_{xx}$, the numerical solution is strictly nonnegative.

Right: the vortex patch test for 2D incompressible NS equation with Reynolds number 3000, the solution is strictly bounded by 1 and -1.

2D Incompressible flow with Reynolds number 3000: double shear layer



The solution is strictly in the bound.

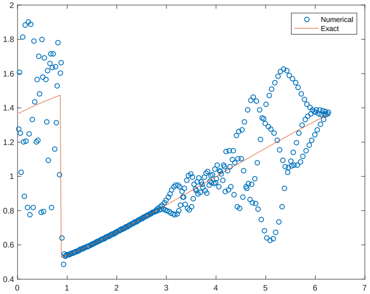
8th order scheme for linear convection equation:

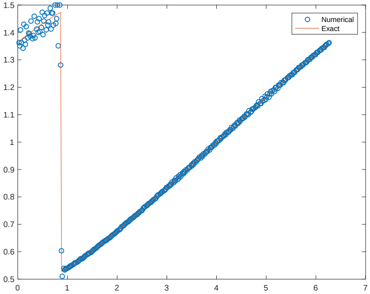
Mesh	L^∞ error	order	L^1 error	order
20	3.14E-6	-	1.99E-6	-
40	7.13E-8	5.46	4.55E-8	5.45
80	2.71E-10	8.04	1.73E-10	8.04
160	1.43E-12	7.57	7.24E-12	7.90

8th order scheme for burgers equation:

Mesh	L^∞ error	order	L^1 error	order
20	1.18E-3	-	3.37E-4	-
40	2.57E-5	5.52	2.23E-6	7.24
80	5.23E-8	8.94	2.97E-9	9.56
160	1.77E-10	8.21	9.90E-12	8.23

Inflow-outflow Boundary condition:





Burgers equation $u_t + (\frac{1}{2}u^2)_{xx} = 0$, when the solution is positive .
Left: numerical solution without bound-preserving limiter
Right: numerical solution with bound-preserving limiter. The solution is strictly bounded by 0.5 and 1.5.

SSP 4th-order multistep for 1D convection diffusion equation with Dirichlet boundary condition:

Mesh	L^∞ error	order	L^1 error	order
40	3.79E-5	-	2.03E-5	-
80	3.16E-6	3.58	1.16E-6	4.13
160	3.79E-7	3.06	1.26E-7	3.20
320	4.81E-8	2.98	1.86E-8	2.75
640	1.26E-9	5.25	4.72E-10	5.31

Generalization to Systems?

Try to use the idea of FV?

The End