Implicit Finite Volume Approximation of Nonlinear Advection-Diffusion Equations

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This work was supported by the U.S. National Science Foundation and the Taiwan Ministry of Science and Technology
Advection-Diffusion-Reaction Equations

\[ u_t + \nabla \cdot [f(u) - D(u) \nabla u] = g(u) \]

Within science and engineering, researchers often use models involving

1. **Advection**, \( u_t + \nabla \cdot f(u) = 0 \)
   - the *transport* of a substance
   - mathematically *hyperbolic*

2. **Diffusion**, \( u_t - \nabla \cdot D(u) \nabla u = 0 \)
   - the *spreading* of a substance to the average of its surroundings
   - mathematically *parabolic* (or elliptic)

3. **Reactions**, \( u_t = g(u) \) [Omit for this talk]
   - substances transform to other substances
   - mathematically an ordinary differential equation

These are systems of *advection-diffusion-reaction equations*.

**Main Difficulty:** The equations are often *advection dominated*.

The solution to the equations can develop steep fronts or even shock discontinuities.
Hyperbolic Equations

\[ u_t + \nabla \cdot f(u) = 0 \]

- **Mass conservative**
- **Linear transport in 1D is simple translation**
  \[ u_t + au_x = 0, \quad u(x,0) = u_0(x) \quad \implies \quad u(x,t) = u_0(x - at) \]
  A discontinuity in \( u_0 \) propagates as a **contact discontinuity**.
- **Nonlinear transport in 1D has variable speed**
  \[ u_t + f'(u)u_x = 0, \quad u(x,0) = u_0(x) \]
  If \( f(u) \) grows with \( u \), a **shock discontinuity** can form.

- **Solutions do not become smoother in time** (the operator is *not* compact), but solutions are **total variation diminishing**
  \[
  \text{TV}(u)(t) = \int |u_x(x,t)| \, dx \leq \text{TV}(u_0) = \int |u'_0(x)| \, dx
  \]
  The solution does not **oscillate**.
- **Hyperbolic scaling**: Space and time scale as \( t \sim x \)
  \[ u(x,t) = U(\xi(x,t)) \quad \implies \quad u_t = U' \xi_t \sim u_x = U' \xi_x \quad \implies \quad dt \sim dx \]
Parabolic Equations

\[ u_t - \nabla \cdot [D(u)\nabla u] = 0 \]

- Mass conservative
- Solutions smooth in time (the operator is compact on Sobolev spaces)
- Solutions are continuous. Initial discontinuities disappear immediately.
- The maximum principle: $u$ is the average of nearby values. The solution does not oscillate.
- Parabolic scaling: Space and time scale as $t \sim x^2$

\[
\begin{align*}
  u(x, t) &= U(\xi(x, t)) \\
  \implies u_t &= U'(\xi_t) \sim u_{xx} = U'\xi_{xx} + U''(\xi_x)^2 \\
  \implies dt &\sim dx^2
\end{align*}
\]
1. The finite volume framework. Approximation requires
   • Reconstruction of the solution at points from average values
   • A time stepping method
2. Reconstruction: WENO with adaptive order (WENO-AO)
   • High order accurate when the solution is smooth
   • Reduce accuracy near shocks/steep fronts to suppress oscillations
3. Time stepping: method of lines
   • Implicit L-stable Runge-Kutta to handle stiffness (i.e., diffusion)
   • A new adaptive Runge-Kutta (high order Runge-Kutta combined with backward Euler) to further suppress oscillations
4. Numerical performance of iWENO-AO
5. Self-Adaptive Theta (SATh) scheme (a “better backward Euler”)
   • Discontinuity Aware Quadrature (DAQ)
   • Theoretical Properties
6. Numerical performance of SATh-LF
7. Summary and conclusions
1. The Finite Volume Framework
Derivation of the Governing Equations

Mass Conservation

- \( u \) is mass of a substance per unit volume (i.e., its density)
- \( v \) is the velocity of the substance
- \( E \) is a volume element
- \( \int_E u(x, t) \, dx \) is the total mass in \( E \)

The change in mass is

\[
\frac{d}{dt} \int_E u(x, t) \, dx \quad \overset{?}{=} \quad \int_E u_t(x, t) \, dx
\]

Changes are due to flow through \( \partial E \):

\[
- \int_{\partial E} v(x, t) \cdot \nu \, d\sigma(x) = - \int_E \nabla \cdot v(x, t) \, dx
\]

by the Divergence Theorem. Equating, we have

\[
\int_E [u_t(x, t) + \nabla \cdot v(x, t)] \, dx = 0 \quad \iff \quad u_t + \nabla \cdot v = 0
\]

since this is true for every measurable \( E \)

Empirical Constitutive Relation. How are \( u \) and \( v \) related? Assume

\[
v = f(u) - D(u) \nabla u
\]

- Transport: motion due to the amount of material present \( u \)
- Diffusion: motion due to gradients in \( u \)
The Equation in Finite Volume Form

**Finite volumes (mesh elements)**

- Fix a computational mesh of polytopal elements $E$ in $\mathbb{R}^d$
- The average of $u$ over element $E$ is

$$\bar{u}_E(t) = \frac{1}{|E|} \int_E u(x,t) \, dx$$

where $|E|$ is the $d$ dimensional volume of $E$

**The finite volume equation.** Mass conservation over mesh element $E$:

$$\bar{u}_{E,t} + \frac{1}{|E|} \int_{\partial E} \left( f(u) - D\nabla u \right) \cdot \nu_E \, d\sigma(x) = 0$$
A numerical flux function for the advective term is needed

- to stabilize the computations (by adding numerical diffusion)
- to account for potential discontinuities in the solution

**Lax-Friedrichs numerical flux**

\[
\hat{f}_E(u^-, u^+) = \frac{1}{2} \left[ (f(u^-) + f(u^+)) \cdot \nu_E - \alpha_{LF}(u^+ - u^-) \right]
\]

- \(u^-\) and \(u^+\) are left and right limits of the solution at the interface \(\partial E\)
- \(\alpha_{LF} = \max_u \left| \frac{\partial f}{\partial u} \right|\)
- if \(u\) is continuous, we have consistency with the original flux

\[
\hat{f}_E(u^-, u^+) = f(u) \cdot \nu_E
\]

**The averaged equation.** Thus the advection-diffusion equation is

\[
\bar{u}_{E,t} + \frac{1}{|E|} \int_{\partial E} \hat{F}(u^-, u^+, \nabla u \cdot \nu_E) \, d\sigma(x) = 0
\]

where \(\hat{F}_E(u^-, u^+, \nabla u \cdot \nu_E) = \hat{f}_E(u^-, u^+) - D \nabla u \cdot \nu_E\)
Semidiscrete Approximation

**Approximate integration.**

- Let the facets of \( \partial E \) be denoted \( e_1, e_2, \ldots \)
- On each \( e_j \), use a quadrature rule with points \( x_{j,k} \) and weights \( |e_j| \omega_{j,k} \)
- Denote

\[
u_{j,k}^\pm(t) = u_{j,k}(x_{j,k}, t) \approx u(x_{j,k}, t) \\
u_{j,k}(t) \approx u(x_{j,k}, t)
\]

**The semidiscrete finite volume approximation.**

\[
\bar{u}_{E,t} + \sum_j \frac{|e_j|}{|E|} \sum_k \omega_{j,k} \hat{F}_E(u_{j,k}^-, u_{j,k}^+, \nabla u \cdot \nu_E)_{j,k} = 0
\]

- Fix time levels \( 0 = t^0 < t^1 < t^2 < \ldots \)
- We approximate \( \bar{u}_E^n \approx \bar{u}_E(t^n) \) for each \( n > 0 \)

**Remaining Issues.**

- **Reconstruct** \( u_{j,k}^\pm \) and \( (\nabla u \cdot \nu_E)_{j,k} \) from the discrete averages \( \bar{u}_E^n \)
- Define a fully discrete time evolution scheme
2. Reconstruction: Weighted Essentially Non-Oscillatory with Adaptive Order (WENO-AO)

For simplicity, reconstruct in 1D and assume uniform meshes of spacing $\Delta x = h$
**Classic ENO3 Reconstructions in 1D**

(Harten, Engquist, Osher & Chakravarthy 1987)

**Idea:** Find a polynomial that reconstructs $u(x)$ from its average values. Shocks are isolated, so compute using several stencils.

Find $P_i^3(x)$ of degree 2 so mass is conserved on each 3 element stencil

$$\frac{1}{h} \int_{E_j} P_i^3(x) \, dx = \bar{u}^n_{E_j} \quad (E_j \text{ in the stencil}) \quad \Rightarrow \quad u(x) = P_i^3(x) + O(h^3)$$

Use the “essentially non-oscillatory” polynomial not crossing the shock.

$$u(x) \approx R(x) = P_i^3(x)$$

for some chosen $i$, $O(h^3)$

**Problems**

- Wasted stencil computations.
- Get a wide stencil.
**Idea:** Take a weighted average of smaller stencil polynomials that give the larger stencil polynomial.

$$u(x^*) \approx R(x^*) = \tilde{\alpha}P_{-1}^2(x^*) + \tilde{\beta}P_1^2(x^*) \approx \begin{cases} P_{-1}^2(x^*) & \text{if shock right, } O(h^2) \\ P_0^3(x^*) & \text{if no shock, } O(h^3) \\ P_1^2(x^*) & \text{if shock left, } O(h^2) \end{cases}$$

**Problems**
- The weights are difficult to find (not exist?!) and may be negative.
- Requires rectangular meshes in 2D/3D.
**WENO with Adaptive Order in 1D, WENO-AO(3,2)**

(Levy, Puppo & Russo 2000; Balsara, Garain & Shu 2016; Arbogast, Huang & Zhao 2018)

**Idea:** Use large and small stencil polynomials of different degrees.

For any $x$, take arbitrary (positive) $\alpha, \beta, \gamma$ so that $\alpha + \beta + \gamma = 1$

\[ u(x) \approx R(x) = \frac{\tilde{\gamma}}{\gamma} \left[ P_0^3(x) - \alpha P_{-1}^2(x) - \beta P_1^2(x) \right] + \tilde{\alpha} P_{-1}^2(x) + \tilde{\beta} P_1^2(x) \]

\[ \approx \begin{cases} P_{-1}^2(x) & \text{if shock right, } \tilde{\alpha} \approx 1, \tilde{\beta} \approx 0, \tilde{\gamma} \approx 0, \mathcal{O}(h^2) \\ P_0^3(x) & \text{if no shock, } \tilde{\alpha} \approx \alpha, \tilde{\beta} \approx \beta, \tilde{\gamma} \approx \gamma, \mathcal{O}(h^3) \\ P_1^2(x) & \text{if shock left, } \tilde{\alpha} \approx 0, \tilde{\beta} \approx 1, \tilde{\gamma} \approx 0, \mathcal{O}(h^2) \end{cases} \]

**Advantage**

- Freedom from rectangular geometry (so extension to 2-D/3-D).
Weighting Procedure — Smoothness Indicator

**Smoothness indicator** (Jiang & Shu 1996)

The smoothness (roughness) of $P^s(x)$ on $E$ is measured as

$$\sigma_{P^s} = \sum_{\ell=1}^{s-1} \int_E h^{2\ell-1} \left( \frac{d^\ell}{dx^\ell} P^s(x) \right)^2 dx$$

- If $u$ is smooth, $\sigma_{P^s} = Dh^2 + \mathcal{O}(h^3)$ ($D \approx u'$)
- If $u$ has a discontinuity, $\sigma_{P^s} = \mathcal{O}(1)$

**Folklore.** If $u$ has a discontinuity, $\sigma_{P^s} = \Theta(1)$ as $h \to 0$ (i.e., $0 < c_* \leq \sigma_{P^s} \leq c_* < \infty$).

**Theorem** (Arbogast, Huang & Zhao 2018)

If $u$ has a discontinuity, $\sigma_{P^s}$ may tend to zero as $h \to 0$. If the discontinuity is bounded away from the grid points, then $\sigma_{P^s} = \Theta(1)$.

**Assumption.** We will henceforth assume that the discontinuity is bounded away from the grid points, so $\sigma_{P^s} = \Theta(1)$. 
Weighting Procedure — Nonlinear Weights

(Jiang & Shu 1996)

Scaled nonlinear weights. For weight \( \delta \) for polynomial \( P(x) \)

\[
\tilde{\delta} = \frac{\delta}{(\epsilon_h + \sigma_P)^\eta}
\]

Classically, \( \epsilon_h \approx 10^{-6} \), but \( \epsilon_h = \epsilon_0 h^2 \) should be taken.

(Normalized) Nonlinear weights. So that \( \sum_i \tilde{\delta}_i = 1 \),

\[
\tilde{\delta}_i = \frac{\tilde{\delta}_i}{\sum_j \tilde{\delta}_j} = \frac{\delta_i}{\delta_i + \sum_{j \neq i} \delta_j \left( \frac{\epsilon_h + \sigma_{P_j}}{\epsilon_h + \sigma_{P_i}} \right)^\eta}
\]

Lemma. (Aràndiga, Baeza, Belda & Mulet 2011)

\[
\tilde{\delta} = \begin{cases} 
\delta + \mathcal{O}(h^{s-1}) & \text{if } u \text{ is smooth (} s \text{ is size of smaller stencil)} \\
\Theta(h^{2\eta}) & \text{if } u \text{ is discontinuous and } \epsilon_h = \epsilon_0 h^2
\end{cases}
\]
General WENO-AO($r, s$)
(Levy, Puppo & Russo 2000; Balsara, Garain & Shu 2016)

**Idea:** Use small stencils of $s$ elements and the union (large stencil) of size $r$, with corresponding polynomials.

Take *arbitrary* (positive) $\gamma$ and $\alpha_i$, $\gamma + \sum_i \alpha_i = 1$

\[
u(x) \approx R(x) = \frac{\tilde{\gamma}}{\gamma} \left[ P^r_0(x) - \sum_i \alpha_i P^s_i(x) \right] + \sum_i \tilde{\alpha}_i P^s_i(x)
\]

where

\[
\tilde{\gamma} = \frac{\gamma}{(\epsilon_h + \sigma P^r_0) \eta} \quad \tilde{\alpha}_i = \frac{\alpha_i}{(\epsilon_h + \sigma P^s_i) \eta}
\]

\[
\hat{\gamma} = \frac{\tilde{\gamma}}{\gamma + \sum_i \tilde{\alpha}_i} \quad \hat{\alpha}_i = \frac{\tilde{\alpha}_i}{\gamma + \sum_i \tilde{\alpha}_i}
\]

**Question.** Does it really work?

- When $\nu$ is smooth, is $R$ accurate to $O(h^r)$?
- When $\nu$ has a discontinuity on some (but not all) stencils, is $R \, O(h^s)$?
Convergence Results for WENO-AO\((r, s)\)
(Cravero, Puppo, Semplice & Visconti 2018; Arbogast, Huang & Zhao 2018)

\[
u(x) \approx R(x) = \frac{\tilde{\gamma}}{\gamma} [P_0^r(x) - \sum_i \alpha_i P_i^s(x)] + \sum_i \tilde{\alpha}_i P_i^s(x)
\]

Recall \(\epsilon_0\) and \(\eta\):

\[
\tilde{\delta} = \frac{\delta}{(\epsilon_0 h^2 + \sigma) \eta}
\]

**Theorem.** Let \(\eta \geq 1\), \(\epsilon_0 > 0\), and \(r > s \geq 2\). Then WENO-AO\((r, s)\) has order of accuracy

- \(O(h^r)\) if \(u\) is smooth on the larger stencil \(S^r\) and
  \[r \leq 2s - 1\]
- \(O(h^s)\) if \(u\) is smooth except for a jump discontinuity in some (but not all) stencils, the grids are bounded away from the discontinuity, and
  \[\eta \geq s/2\]
There is a recursive, multilevel version WENO-AO($r_\ell, r_{\ell-1}, \ldots, r_0 = s$).

- $h = 0.1 \times 2^{-n}$
- $u(x) = x^3 + \sin(x) + H(x_\ast - x)$ ($H$ is the Heaviside function)
- Shock location $x_\ast = -4h, -3h, -2h, -h$
- $u$ is smooth only on stencils $S^9, S^7, S^5, S^3$, respectively
- set $\eta$ based on the Theorem and $\epsilon_0 = 1$

### Error and convergence rate of WENO-AO($9, 7, 5, 3$) at $x = 0$

The convergence rate is indeed from the largest smooth stencil

<table>
<thead>
<tr>
<th>$n$</th>
<th>$x_\ast = -4h$</th>
<th>$x_\ast = -3h$</th>
<th>$x_\ast = -2h$</th>
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<td>error</td>
<td>order</td>
<td>error</td>
<td>order</td>
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<tr>
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<td>9.00</td>
<td>2.26E-23</td>
<td>7.00</td>
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</table>

Expected order: $9$, $7$, $5$, $3$
Numerical Test — Choice of Parameter $\eta$

- $h = 2^{-n}$
- $u(x) = H(-x)$ ($H$ is the Heaviside function)
- $S^5 = \{[-\frac{3h}{2}, -\frac{h}{2}], [-\frac{h}{2}, \frac{h}{2}], [\frac{h}{2}, 3h], [\frac{3h}{2}, \frac{5h}{2}], [\frac{5h}{2}, 7h]\}$
- $\bar{u}_i = 1, 1/2, 0, 0, 0$, respectively

**WENO-AO(5,3) error and convergence rate at $x = h/2$**

The convergence rates are indeed $\Theta(h^{2\eta})$

<table>
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<tr>
<th>$n$</th>
<th>$\eta = 1$</th>
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<th>$\eta = 2$</th>
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<td>2.00</td>
<td>3.36E-8</td>
<td>3.00</td>
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</tbody>
</table>

Expected order 2 3 4 6

**Remark:** The good stencil polynomials are exact, so the rate is not limited to $O(h^3)$. 
\[
\bar{u}_{i,t} + \frac{1}{h} \left[ \hat{F}(u_{i+1/2}^-, u_{i+1/2}^+, u'_{i+1/2}) - \hat{F}(u_{i-1/2}^-, u_{i-1/2}^+, u'_{i-1/2}) \right] = 0
\]

**WENO-AO(3,2) for point values**

\[
\begin{align*}
\bar{u}_{i-1} & & u_{i-1/2} & & u_{i} & & u_{i+1/2} & & \bar{u}_{i+1} \\
x_{i-3/2} & & x_{i-1} & & x_{i} & & x_{i+1/2} & & x_{i+3/2} \\
S_{L}^{2} & & S_{C}^{3} & & S_{R}^{2}
\end{align*}
\]

\[
u(x) \approx R(x) = \frac{\bar{\gamma}}{\gamma} \left[ P_{C}^{3}(x) - \alpha P_{L}^{2}(x) - \beta P_{R}^{2}(x) \right] + \tilde{\alpha} P_{L}^{2}(x) + \tilde{\beta} P_{R}^{2}(x)
\]

\[
u_{i-1/2}^{+} = R(x_{i-1/2}) \quad \text{and} \quad \nu_{i+1/2}^{-} = R(x_{i+1/2})
\]

**WENO-AO(4,3) for derivatives**

\[
\begin{align*}
\bar{u}_{i-1} & & u_{i-1/2} & & u_{i} & & u_{i+1/2} & & u_{i+1} & & \bar{u}_{i+2} \\
x_{i-3/2} & & x_{i-1} & & x_{i} & & x_{i+1/2} & & x_{i+3/2} & & x_{i+5/2} \\
S_{L}^{3} & & S_{C}^{4} & & S_{R}^{3}
\end{align*}
\]

\[
u'(x) \approx R'(x) = \frac{\bar{\gamma}}{\gamma} \left[ P_{C}^{4'}(x) - \alpha P_{L}^{3'}(x) - \beta P_{R}^{3'}(x) \right] + \tilde{\alpha} P_{L}^{3'}(x) + \tilde{\beta} P_{R}^{3'}(x)
\]

(maintains symmetry of the diffusion operator)
3. Time Stepping: Method of Lines

Use implicit Runge-Kutta methods
so $\Delta t \sim \Delta x$
The Courant-Fredrichs-Lewy (CFL) Timestep

- $\Delta t_{\text{CFL}}$ is the time for fluid to move a distance $\Delta x$

\[
\max |f'(u)| \Delta t_{\text{CFL}} = \Delta x
\]

- The CFL number is

\[
\text{CFL} = \frac{\Delta t}{\Delta t_{\text{CFL}}} \begin{cases} 
\leq 1 & \text{fluid moves one cell per time step} \\
> 1 & \text{fluid moves many cells per time step}
\end{cases}
\]

- For explicit methods, stability requires
  - CFL $\leq 1$
  - With diffusion, $\Delta t \sim \Delta x^2$ (parabolic scaling, i.e., stiffness)

**Conclusion.** We must do something!

- Operator splitting: split diffusion from advection (IMEX methods)
- Monolithic: Use fully implicit methods [we use this]

Choose $\Delta t \sim \Delta x$ for accuracy, not stability
Choice of Runge-Kutta Method

\[ \frac{du}{dt} = G(u) \]

**Strong-Stability Preserving (SSP) Runge-Kutta**
- Preserves stability of backward Euler
- Requires CFL-like constraint for stability \( (\Delta t \lesssim \Delta t_{CFL}) \)
- Becomes unstable for large \( \Delta t \)

**L-Stable Runge-Kutta**
- Not SSP, but unconditionally stable
- Robust for stiff problems (e.g., with diffusion)
  - Stable: For \( u' = au \ (a < 0) \), \( u^{n+1} = Q(\Delta t)u^n \) and \( |Q(\Delta t)| \leq 1 \).
  - L-Stable: Also \( |Q(\Delta t)| \to 0 \) as \( \Delta t \to \infty \) (i.e., stable if \( \Delta t \) too large)

**Radau IIA Runge-Kutta**: 3rd order method:

\[
\begin{align*}
  u^{n+1/3} &= u^n + \frac{\Delta t}{12} \left[ 5G(u^{n+1/3}) - G(u^{n+1}) \right] \\
  u^{n+1} &= u^n + \frac{\Delta t}{4} \left[ 3G(u^{n+1/3}) + G(u^{n+1}) \right]
\end{align*}
\]

Only two unknowns per mesh element (at times \( t^{n+1/3} \) and \( t^{n+1} \))
Numerical Test — Burgers’ and Buckley-Leverett Equations

Small $\Delta t$ Radau IIA and SSP-RK perform similarly

$\Delta t = 2\Delta x$

Large $\Delta t$ Radau IIA overshoots a bit, SSP-RK is unstable

$\Delta t = 0.5\Delta x$

$\Delta t = 5\Delta x$

$\Delta t = 2\Delta x$
Idea: Suppress the small oscillations near discontinuities by using

- Radau IIA Runge-Kutta when $u$ is smooth
- composite backward Euler (BE) when $u$ is discontinuous

Basically, we want

$$u^{n+1} \overset{?}{=} \tilde{w}^{\text{Radau}} u^{n+1, \text{Radau}} + \tilde{w}^{\text{BE}} u^{n+1, \text{BE}}$$

for some nonlinear weights $\tilde{w}^{\text{Radau}} + \tilde{w}^{\text{BE}} = 1$

Butcher Tableau: Gives the Runge-Kutta coefficients and time levels

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<thead>
<tr>
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Radau IIA

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<tr>
<td>$1$</td>
<td>$3/4\tilde{w}^{\text{Radau}} + 1/3\tilde{w}^{\text{BE}}$</td>
<td>$1/4\tilde{w}^{\text{Radau}} + 2/3\tilde{w}^{\text{BE}}$</td>
</tr>
<tr>
<td>$3/4$</td>
<td>$\tilde{w}^{\text{Radau}} + 1/3\tilde{w}^{\text{BE}}$</td>
<td>$1/4\tilde{w}^{\text{Radau}} + 2/3\tilde{w}^{\text{BE}}$</td>
</tr>
</tbody>
</table>

adaptive Runge-Kutta
Application to Advection-Diffusion Equation in 1D

\[
\bar{u}_{i,t} + \frac{1}{h} \left[ \hat{F}_{i+1/2} - \hat{F}_{i-1/2} \right] = 0
\]

- A conservative scheme requires unique fluxes at each grid point
- Apply the time-stepping to the flux at each grid point separately

\[
\bar{u}_{i}^{n+1/3} = \bar{u}_{i}^{n} - \frac{\Delta t_{n}}{\Delta x_{i}} \left[ \tilde{a}_{1}^{1/2} \hat{F}_{i+1/2}^{n+1/3} - \tilde{a}_{1}^{1/2} \hat{F}_{i-1/2}^{n+1/3} \right]
\]

\[
\bar{u}_{i}^{n+1} = \bar{u}_{i}^{n} - \frac{\Delta t_{n}}{\Delta x_{i}} \left[ \tilde{b}_{1}^{1/2} \hat{F}_{i+1/2}^{n+1/3} - \tilde{b}_{1}^{1/2} \hat{F}_{i-1/2}^{n+1/3} \right]
\]

where

\[
\hat{F}_{i}^{n+\theta} = \hat{F}(u_{i+1/2}^{n+\theta}, u_{i-1/2}^{n+\theta}, u_{i}^{n+\theta}), \quad \theta = 1/3, 1
\]

\[
\tilde{a}_{1}^{1/2} = \frac{5}{12} \tilde{w}_{i+1/2}^{\text{Radau}} + \frac{1}{3} \tilde{w}_{i+1/2}^{\text{BE}}
\]

\[
\tilde{a}_{2}^{1/2} = -\frac{1}{12} \tilde{w}_{i+1/2}^{\text{Radau}}
\]

\[
\tilde{b}_{1}^{1/2} = \frac{3}{4} \tilde{w}_{i+1/2}^{\text{Radau}} + \frac{1}{3} \tilde{w}_{i+1/2}^{\text{BE}}
\]

\[
\tilde{b}_{2}^{1/2} = \frac{1}{4} \tilde{w}_{i+1/2}^{\text{Radau}} + \frac{2}{3} \tilde{w}_{i+1/2}^{\text{BE}}
\]
Weighting Procedure

**Linear weighting**
- BE is locally $O(h^2)$ accurate, globally $O(h)$ (for a smooth problem!)
- BE weight is $w^{BE} = w_0^{BE} h^2$ (or $w_0^{BE} \Delta t^2$, since $\Delta t \sim h$)
- Radau weight is $w^{Radau} = 1 - w^{BE}$.

**Nonlinear weighting** ($\eta \geq 1$ and $\epsilon_h = \epsilon_0 h^2$)

\[
\hat{w}_{i \pm 1/2}^{Radau} = \frac{w^{Radau}_{i \pm 1/2}}{(\epsilon_h + \sigma_{Radau}^{i \pm 1/2})^\eta}, \quad \hat{w}_{i \pm 1/2}^{BE} = \frac{w^{BE}_{i \pm 1/2}}{(\epsilon_h + \sigma^{BE})^\eta},
\]

\[
\tilde{w}_{i \pm 1/2}^{Radau} = \frac{\hat{w}_{i \pm 1/2}^{Radau}}{\hat{w}_{i \pm 1/2}^{BE} + \hat{w}_{i \pm 1/2}^{Radau}}, \quad \tilde{w}_{i \pm 1/2}^{BE} = 1 - \tilde{w}_{i \pm 1/2}^{Radau}.
\]

**Smoothness indicators** (i.e., roughness)
- BE: $\sigma^{BE} = 0$ (BE can always be used)
- Radau: detect a shock in space

\[
\sigma_{i \pm 1/2}^{Radau} = (\bar{u}_{i \pm 1}^n - \bar{u}_i^n)^2 + (\bar{u}_{i \pm 1}^{n+1} - \bar{u}_i^{n+1})^2 + (\bar{u}_{i \pm 1}^{n+1/3} - \bar{u}_i^{n+1/3})^2.
\]
Consider the local time truncation error as a perturbation of Radau IIA. 

**Perturbed Radau weights**

\[
\begin{align*}
\tilde{a}_{i\pm 1/2}^1 &= \frac{5}{12} - \frac{1}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{b}_{i\pm 1/2}^1 &= \frac{3}{4} - \frac{5}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{a}_{i\pm 1/2}^2 &= -\frac{1}{12} + \frac{1}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{b}_{i\pm 1/2}^2 &= \frac{1}{4} + \frac{5}{12} \tilde{w}_{i\pm 1/2}
\end{align*}
\]

**Theorem.** The adaptive Runge-Kutta scheme remains globally $O(h^3)$ accurate when $\omega$ is smooth. [Because $\omega^{BE} = O(h^2)$]
### Numerical Test — Smooth Burgers’ Equation

\[ u_t + \left( \frac{u^2}{2} \right)_x = 0, \quad x \in (0, 2) \]

\[ u(x, 0) = \frac{1}{2} \left( 1 - \frac{1}{2} \sin(\pi x) \right) \]

Error and convergence order at \( T = 1 \) (no shocks)

<table>
<thead>
<tr>
<th>( m )</th>
<th>( L^1_h ) error</th>
<th>( L^1_h ) order</th>
<th>( L^\infty_h ) error</th>
<th>( L^\infty_h ) order</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta t = h )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>640</td>
<td>3.21E-06</td>
<td>2.93</td>
<td>4.28E-05</td>
<td>2.87</td>
</tr>
<tr>
<td>1280</td>
<td>4.05E-07</td>
<td>2.99</td>
<td>5.47E-06</td>
<td>2.97</td>
</tr>
<tr>
<td>2560</td>
<td>5.07E-08</td>
<td>3.00</td>
<td>6.87E-07</td>
<td>2.99</td>
</tr>
<tr>
<td>( \Delta t = 10h )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1280</td>
<td>1.86E-04</td>
<td>2.29</td>
<td>2.81E-03</td>
<td>1.92</td>
</tr>
<tr>
<td>2560</td>
<td>2.86E-05</td>
<td>2.70</td>
<td>4.84E-04</td>
<td>2.54</td>
</tr>
<tr>
<td>5120</td>
<td>3.78E-06</td>
<td>2.92</td>
<td>6.57E-05</td>
<td>2.88</td>
</tr>
<tr>
<td>( \Delta t = 50h )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5120</td>
<td>3.09E-04</td>
<td>2.06</td>
<td>4.39E-03</td>
<td>1.67</td>
</tr>
<tr>
<td>10240</td>
<td>5.12E-05</td>
<td>2.59</td>
<td>8.45E-04</td>
<td>2.38</td>
</tr>
<tr>
<td>20480</td>
<td>7.13E-06</td>
<td>2.85</td>
<td>1.23E-04</td>
<td>2.78</td>
</tr>
<tr>
<td>Expected</td>
<td>3</td>
<td></td>
<td>3</td>
<td></td>
</tr>
</tbody>
</table>
Analysis of Errors in Time — Discontinuous Case

Consider the local time truncation error (LTE) as a perturbation of BE.

**Perturbed BE weights**

\[
\begin{align*}
\tilde{a}^1_{i\pm 1/2} &= \frac{1}{3} + \frac{1}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{b}^1_{i\pm 1/2} &= \frac{1}{3} + \frac{5}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{a}^2_{i\pm 1/2} &= -\frac{1}{12} \tilde{w}_{i\pm 1/2} \\
\tilde{b}^2_{i\pm 1/2} &= \frac{2}{3} - \frac{5}{12} \tilde{w}_{i\pm 1/2}
\end{align*}
\]

**Conclusion.** The LTE is formally the same as BE (i.e., \(O(h)\)). However:

- BE should be \(O(h^{1/2})\) accurate with a discontinuity (LTE = \(O(h^{3/2})\)).
- In practice, BE is \(O(h)\) accurate (LTE = \(O(h^2)\)).

Numerical results show \(O(h)\) accuracy. Further investigation is underway.
Remarks.

- The Radau overshoot is stable and does not grow.
- The adaptive scheme removes the oscillation and improves on BE.
- Away from the shock, the adaptive scheme is $O(h^3)$ accurate.
- The SSP Runge-Kutta method is unstable at $\Delta t = 5h$. 
### Numerical Test — Burgers’ Equation with Shock

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \quad x \in (0, 2)$$

$$u(x, 0) = 1 - H(x - 1/2) \quad (H \text{ is the Heaviside function})$$

**Error and convergence order at** $T = 1$ (initial shock)

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\Delta t = 2h$ $L^1_h$ error</th>
<th>$\Delta t = 10h$ $L^1_h$ error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>order</td>
<td>order</td>
</tr>
<tr>
<td><strong>BE</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>160</td>
<td>1.04E-02 0.98</td>
<td>2.73E-02 0.98</td>
</tr>
<tr>
<td>320</td>
<td>5.22E-03 0.99</td>
<td>1.37E-02 0.99</td>
</tr>
<tr>
<td>640</td>
<td>2.62E-03 1.00</td>
<td>6.86E-03 1.00</td>
</tr>
<tr>
<td><strong>Radau</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>160</td>
<td>7.27E-03 1.00</td>
<td>1.70E-02 1.00</td>
</tr>
<tr>
<td>320</td>
<td>3.64E-03 1.00</td>
<td>8.47E-03 1.00</td>
</tr>
<tr>
<td>640</td>
<td>1.82E-03 1.00</td>
<td>4.23E-03 1.00</td>
</tr>
<tr>
<td><strong>Radau + BE</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>160</td>
<td>1.03E-02 0.98</td>
<td>2.71E-02 0.97</td>
</tr>
<tr>
<td>320</td>
<td>5.19E-03 0.99</td>
<td>1.36E-02 0.99</td>
</tr>
<tr>
<td>640</td>
<td>2.60E-03 0.99</td>
<td>6.83E-03 1.00</td>
</tr>
</tbody>
</table>

**Expected?** 1

---

**The Babuška Forum, May 29, 2020**

**CSM: Center for Subsurface Modeling**
### Numerical Test — Smooth Burgers’ with Diffusion

**Error and convergence order at** $T = 1$ **with** $\Delta t = 10.5h$

<table>
<thead>
<tr>
<th>$m$</th>
<th>$L_h^1$ Error</th>
<th>Order</th>
<th>$L_h^\infty$ Error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$D = 1E-01$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>320</td>
<td>1.36E-04</td>
<td>2.56</td>
<td>1.19E-04</td>
<td>2.56</td>
</tr>
<tr>
<td>640</td>
<td>1.93E-05</td>
<td>2.82</td>
<td>1.67E-05</td>
<td>2.82</td>
</tr>
<tr>
<td>1280</td>
<td>2.50E-06</td>
<td>2.95</td>
<td>2.17E-06</td>
<td>2.95</td>
</tr>
<tr>
<td></td>
<td>$D = 1E-02$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>320</td>
<td>5.36E-08</td>
<td>2.97</td>
<td>6.15E-08</td>
<td>2.97</td>
</tr>
<tr>
<td>640</td>
<td>6.72E-09</td>
<td>2.99</td>
<td>7.72E-09</td>
<td>2.99</td>
</tr>
<tr>
<td>1280</td>
<td>8.47E-10</td>
<td>2.99</td>
<td>9.73E-10</td>
<td>2.99</td>
</tr>
<tr>
<td></td>
<td>$D = 1E-04$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>320</td>
<td>1.86E-12</td>
<td>2.96</td>
<td>4.20E-12</td>
<td>2.95</td>
</tr>
<tr>
<td>640</td>
<td>2.36E-13</td>
<td>2.98</td>
<td>5.33E-13</td>
<td>2.98</td>
</tr>
<tr>
<td>1280</td>
<td>2.96E-14</td>
<td>2.99</td>
<td>6.71E-14</td>
<td>2.99</td>
</tr>
</tbody>
</table>

**Expected** $3$

### Remarks.

- Convergence is maintained as $D \to 0$
4. Numerical Performance of iWENO-AO
Numerical Test — Convergence for Burgers’ equation in 2D

\[ \frac{\partial u}{\partial t} + \frac{u^2}{2} \frac{\partial}{\partial x} \frac{\partial}{\partial y} - D \frac{\partial^2 u}{\partial x^2} = 0 \]

We use randomly perturbed meshes of quadrilaterals in 2D.

Error and convergence order for smooth solution at \( t = 1 \) using \( \Delta t = 5h \) and quadrilateral meshes

<table>
<thead>
<tr>
<th>( m )</th>
<th>( L^1_{\Delta x} ) error order</th>
<th>( L^\infty_{\Delta x} ) error order</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D = 0.1 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>3.254E-03 — —</td>
<td>1.570E-03 — —</td>
</tr>
<tr>
<td>40</td>
<td>4.908E-04 2.73</td>
<td>2.172E-04 2.85</td>
</tr>
<tr>
<td>80</td>
<td>6.687E-05 2.88</td>
<td>2.910E-05 2.90</td>
</tr>
<tr>
<td>160</td>
<td>8.742E-06 2.94</td>
<td>3.764E-06 2.95</td>
</tr>
<tr>
<td>( D = 0.0001 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>2.023E-08 — —</td>
<td>5.617E-08 — —</td>
</tr>
<tr>
<td>40</td>
<td>5.705E-09 1.83</td>
<td>2.487E-08 1.18</td>
</tr>
<tr>
<td>80</td>
<td>1.058E-09 2.43</td>
<td>5.766E-09 2.11</td>
</tr>
<tr>
<td>160</td>
<td>1.330E-10 2.99</td>
<td>6.748E-10 3.10</td>
</tr>
<tr>
<td>Expected</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>
Numerical Test — Porous Medium Equation in 1D

\[ u_t = (u^m)_{xx} = ((mu^{m-1})u_x)_x \]

**Barenblatt solution**

\[ B_m(x, t) = t^{-k} \left[ \max \left( 0, 1 - \frac{k(m-1)}{2m} \frac{|x|^2}{t^{2k}} \right) \right]^{1/(m-1)} \quad k = \frac{1}{m + 1}, \quad m > 1 \]

This solution has compact support \([-\alpha_m(t), \alpha_m(t)]\), where

\[ \alpha_m(t) = \sqrt{\frac{2m}{k(m-1)}} t^k \]

Non-uniform mesh of 120 elements at \( t = 2 \) (from \( t = 1 \)), \( \Delta t = h \)
Quarter 5 spot pattern of petroleum wells

Permeability on Quadrilateral Mesh

Undershoot wave: $-3.14E-4$

$t = 5$ days $t = 50$ days $t = 455$ days
$t = 1$ day $t = 10$ days $t = 15$ days

Some small undershoots, but essentially non-oscillatory
General Remarks on iWENO-AO

**Extensions.** Easily extends to:
- higher order schemes;
- 3D on general computational meshes;
- systems of equations.

**Efficiency.**
- Uses 2 unknowns per mesh element per system component, independent of the space dimension! (For third order Radau IIA)
- Can use very long time steps, and $\Delta t \sim h$, not $h^2$.
- Reconstruction boosts parallel computing (less data transfer, more local computation)

**Numerical Accuracy.**
- Formal accuracy is $O(h^3 + \Delta t^3)$ for smooth solutions.
- Essentially non oscillatory.
- The scheme is unconditionally von Neumann (Fourier) L-stable for smooth solutions to the linear problem.

**Physical Accuracy.**
- Locally mass conservative at $t^{n+1/3}$ and $t^{n+1}$.
- Handles both advection and diffusion (even $D = 0$).
5. A Self-Adaptive Theta Scheme (SATh)

Replace backward Euler in the adaptive time stepping
Notation:

\[
\begin{align*}
\Delta t & \quad t^n \quad t^{n+1} \\
\Delta x_i & \quad x_{i-3/2} \quad x_{i-1} \quad x_{i-1/2} \quad x_i \quad x_{i+1/2} \quad x_{i+1} \quad x_{i+3/2}
\end{align*}
\]

Basic equation 1. The governing equation directly controls \( \bar{u}_{i+}^{n+1} \).

\[
\bar{u}_{i+1}^{n+1} = \bar{u}_i^n - \frac{1}{\Delta x_i} \int_{t^n}^{t^{n+1}} \left[ f(u_{i+1/2}(t)) - f(u_{i-1/2}(t)) \right] dt
\]

Problem. A shock in space is also a shock in time! Using only \( \bar{u}_i^n \) and \( \bar{u}_{i+1}^{n+1} \) (and nearest neighbors), we cannot tell where the shock is in time.

Requirement. We need information over the entire time interval!
The space-time cell average of $u$ is

$$\bar{u}_i^{n+1} = \frac{1}{\Delta t \Delta x_i} \int_{t^n}^{t^{n+1}} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t) \, dx \, dt$$

**Fact.** The governing equation directly controls $\bar{u}_i^{n+1}$!
**Basic equation 2.** We use a test function \( w(t) = \left( t^{n+1} - t \right) / \Delta t \) to see

\[
\int_{t^n}^{t^{n+1}} \bar{u}_i(t) w(t) \, dt = \bar{u}_i(t) w(t) \bigg|_{t^n}^{t^{n+1}} - \int_{t^n}^{t^{n+1}} \bar{u}_i(t) w'(t) \, dt
\]

\[
= -\bar{u}_i^n + \bar{u}_i^{n+1}
\]

Then

\[
\int_{t^n}^{t^{n+1}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left( u_t + f(u) x \right) w(t) \, dx \, dt = 0
\]

\[\Rightarrow\]

\[
\bar{u}_i^{n+1} = \bar{u}_i^n - \frac{1}{\Delta t \Delta x_i} \int_{t^n}^{t^{n+1}} \left( f(u_{i+1/2}) - f(u_{i-1/2}) \right) (t^{n+1} - t) \, dt
\]
5.1. Discontinuity Aware Quadrature (DAQ)
**Problem description.** Accurately approximate

\[ \int_0^{\Delta t} g(v(t)) \, w(t) \, dt \]

- \( g \) and \( w \) are smooth
- \( v(t) \) is smooth except for a discontinuity at \( 0 \leq \tau \leq \Delta t \)

Use only the data

\[ v^0 = v(0) \quad v^1 = v(\Delta t) \quad \tilde{v} = \frac{1}{\Delta t} \int_0^{\Delta t} v(t) \, dt \]
Idealize the picture.

\[ \tilde{v} = \frac{1}{\Delta t} \left[ \tau v^0 + (1 - \tau)v^1 \right] \implies \tau = \frac{v^1 - \tilde{v}}{v^1 - v^0} \Delta t \]

**DAQ approximation.**

\[
\int_0^{\Delta t} g(v(t)) w(t) \, dt \approx g(v^0) \int_0^{\tau} w(t) \, dt + g(v^1) \int_{\tau}^{\Delta t} w(t) \, dt
\]

**Application.** Let \( \theta = 1 - \frac{\tau}{\Delta t} = \frac{\tilde{v} - v^0}{v^1 - v^0} \)

\[
w = 1 \quad \int_0^{\Delta t} g(v(t)) \, dt \approx \left[ g(v^0) + \theta \left( (g(v^1) - g(v^0)) \right) \right] \Delta t
\]

\[
w = \frac{t^1 - t}{\Delta t} \quad \int_0^{\Delta t} g(v(t)) w(t) \, dt \approx \frac{1}{2} \left[ g(v^0) + \theta^2 \left( (g(v^1) - g(v^0)) \right) \right] \Delta t
\]
5.2. Application to Finite Volume Schemes
**An Upstream-Weighted Scheme SATh-up**

**Monotone flux.** Suppose that \( f'(u) > 0 \).

- Use one-point upstream weighting to stabilize the scheme
- Let \( \bar{f}_i^n = f(\bar{u}_i^n) \)

**The upstream-weighted scheme. (SATh-up)**

\[
\bar{u}_i^{n+1} = \bar{u}_i^n - \frac{\Delta t}{\Delta x_i} \left[ \bar{f}_i^n + \theta_i (\bar{f}_i^{n+1} - \bar{f}_i^n) - \bar{f}_{i-1}^n - \theta_{i-1} (\bar{f}_{i-1}^{n+1} - \bar{f}_{i-1}^n) \right]
\]

\[
\tilde{u}_i^{n+1} = \bar{u}_i^n - \frac{\Delta t}{2\Delta x_i} \left[ \bar{f}_i^n + \theta_i^2 (\bar{f}_i^{n+1} - \bar{f}_i^n) - \bar{f}_{i-1}^n - \theta_{i-1}^2 (\bar{f}_{i-1}^{n+1} - \bar{f}_{i-1}^n) \right]
\]

where

\[
\theta_i = \begin{cases} 
\max \left( \frac{1}{2}, \frac{\tilde{u}_i^{n+1} - \bar{u}_i^n}{\bar{u}_i^{n+1} - \bar{u}_i^n} \right) & \text{if } |\bar{u}_i^{n+1} - \bar{u}_i^n| > \epsilon \\
\theta^* & \text{if } |\bar{u}_i^{n+1} - \bar{u}_i^n| \leq \epsilon
\end{cases}
\]

- \( \epsilon \geq 0 \) is very small (even zero)
- \( \theta^* = 1 \) (backward Euler) or possibly \( \theta^* = 1/2 \) (Crank-Nicolson)

This is a **self-adaptive** theta method!

**Remark.** A Lax-Friedrichs stabilized SATh-LF scheme is similar.
Test Example: Propagation of a Contact Discontinuity

\[ u_t + u_x = 0 \quad \text{for} \ 0 < x < 1 \]

\[ \Delta x = 1/100, \ \Delta t = 1/20 \ (\text{CFL} = 5), \ t = 0.5 \ (10 \ \text{steps}) \]

<table>
<thead>
<tr>
<th>( m )</th>
<th>( L^1_{\Delta x} ) error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.95E-1</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>1.53E-1</td>
<td>0.35</td>
</tr>
<tr>
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<td>1.10E-1</td>
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<td>80</td>
<td>7.56E-2</td>
<td>0.54</td>
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<tr>
<td>160</td>
<td>5.17E-2</td>
<td>0.55</td>
</tr>
<tr>
<td>320</td>
<td>3.54E-2</td>
<td>0.55</td>
</tr>
</tbody>
</table>

- Crank-Nicholson
- backward Euler, CFL/2
- SATh-LF scheme \( \bar{u} \)
- SATh-LF scheme \( \tilde{u} \)
- SATh-LF scheme \( \theta \)
5.3. Theoretical Properties of SATh
**Accuracy of DAQ**

**Theorem.** Let $g(v)$ be a smooth function and $v(t)$ satisfy the conditions for an isolated discontinuity at $\tau \in (0, \Delta t)$. If $\tau^*$ is the approximation to $\tau$, then

$$|\tau - \tau^*| \leq C \Delta t^2$$

$$\left| \int_0^{\Delta t} g(v(t)) w(t) \, dt - \text{DAQ}(gw) \right| \leq C \Delta t^2$$

where $C$ depends only on the $L^\infty$ norms of $g'$, $w$, $v'_L$, and $v'_R$.

**Consequence.** The local truncation error is $O(\Delta t^2)$.

The scheme should be $O(\Delta x + \Delta t)$.
Stability of the Upstream-Weighted Scheme

**Theorem.** Assume that

- $f(0) = 0$ and $f'(u) > 0$ for $u \neq 0$
- the problem has a boundary condition imposed on the left

The upstream weighted scheme (SATh-up) is unconditionally stable for the nonlinear problem if

$$\theta_i \geq \frac{1}{2}$$
**Theorem.** For the upstream weighted scheme (SATh-up), assume
- \( f = f(u) \) only, \( f'(u) > 0 \) and \( \epsilon = 0 \) (in defining \( \theta_i \))
- the problem has a boundary condition on the left (so \( \bar{u}^n_0 \) is given)

If the IC and BC of the flow is monotonically decreasing,

\[
\bar{u}^n_{i-1} \geq \bar{u}^n_i \quad \text{and} \quad \bar{u}^n_0 \leq \bar{u}^n_0 + 1 \quad \text{then} \quad \bar{u}^n_i \leq \bar{u}^n_i + 1 \leq \bar{u}^n_i - 1
\]

If the IC and BC of the flow is monotonically increasing,

\[
\bar{u}^n_{i-1} \leq \bar{u}^n_i \quad \text{and} \quad \bar{u}^n_0 \geq \bar{u}^n_0 + 1 \quad \text{then} \quad \bar{u}^n_i \geq \bar{u}^n_i + 1 \geq \bar{u}^n_i - 1
\]

Moreover,
- If \( \tilde{u}^{n+1}_0 \) lies between \( \bar{u}^n_0 \) and \( \bar{u}^n_0 + 1 \), then \( 1/2 \leq \theta_i \leq 1 \)
- If \( \theta^* = 1 \) (in defining \( \theta_i \)), then \( \tilde{u}^{n+1}_i \) lies between \( \bar{u}^n_i \) and \( \bar{u}^{n+1}_i \)

**Corollary.** The Total Variation

\[
\text{TV}(\bar{u}^n) = \sum_{i=1}^{\infty} |\bar{u}^n_{i-1} - \bar{u}^n_i|
\]

is bounded (TVB) and diminishes (TVD) under appropriate hypotheses.
6. Numerical Performance of SATh-LF
Burgers Equation, Riemann Shock

\[ u_t + \left(\frac{u^2}{2}\right)_x = 0 \quad \text{for} \ 0 < x < 1 \]

\[ \Delta x = 1/80, \ \Delta t = 1/16 \ (\text{CFL} = 5), \ t = 1.0 \]

\begin{array}{|c|c|c|}
\hline
m & L^1_{\Delta x} \text{ error} & \text{order} \\
\hline
10 & 1.76E-1 & - \\
20 & 9.74E-2 & 0.86 \\
40 & 4.97E-2 & 0.97 \\
80 & 2.49E-2 & 1.00 \\
160 & 1.24E-2 & 1.00 \\
320 & 6.22E-3 & 1.00 \\
\hline
\end{array}

- Crank-Nicholson
- backward Euler, CFL/2
- SATh-LF scheme \( \bar{u} \)
- SATh-LF scheme \( \tilde{u} \)
- SATh-LF scheme \( \theta \)
Burgers Equation, Riemann Rarefaction

\[ u_t + \left( \frac{u^2}{2} \right)_x = 0 \quad \text{for } 0 < x < 1 \]

\[ \Delta x = 1/80, \ \Delta t = 1/16 \ (\text{CFL } = 5), \ t = 0.25 \]

- Crank-Nicholson
- backward Euler, CFL/2
- SATh-LF scheme \( \bar{u} \)
- SATh-LF scheme \( \tilde{u} \)
- SATh-LF scheme \( \theta \)

<table>
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<tr>
<th>( m )</th>
<th>( L^1_{\Delta x} ) error</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>7.88E-2</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>4.66E-2</td>
<td>0.76</td>
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<td>2.72E-2</td>
<td>0.78</td>
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<td>160</td>
<td>1.56E-2</td>
<td>0.80</td>
</tr>
<tr>
<td>320</td>
<td>8.86E-3</td>
<td>0.82</td>
</tr>
<tr>
<td>640</td>
<td>4.96E-3</td>
<td>0.84</td>
</tr>
</tbody>
</table>
Burgers Equation, Shock formation

\[ u_t + \left( \frac{u^2}{2} \right)_x = 0 \quad \text{for } 0 < x < 1 \]

\[ \Delta x = 1/160, \Delta t = 1/24 \quad (\text{CFL} = 4) \]

\[ t = 0 \]

\[ t = 0.6 \]

\[ t = 1.2 \]

\[ TV \]

- \text{Crank-Nicholson}
- \text{backward Euler, CFL/2}
- SATh-LF scheme \( \bar{u} \)
- SATh-LF scheme \( \hat{u} \)
- SATh-LF scheme \( \theta \)
Buckley-Leverett Equation, Rarefaction and Shock

\[ u_t + \left( \frac{u^2}{u^2 + (1-u)^2} \right)_x = 0 \quad \text{for } 0 < x < 1 \]

\[ \alpha_{LF} = 2, \quad t = 0.5 \]

\[ \Delta x = 1/40, \text{CFL} = 2 \]

\[ \Delta x = 1/80, \text{CFL} = 5 \]

- Crank-Nicholson
- backward Euler, CFL/2
- SATh-LF scheme \( \bar{u} \)
- SATh-LF scheme \( \tilde{u} \)
- SATh-LF scheme \( \theta \)
A Non Monotone Flux Function, Step Down

\[ u_t + f(u)_x = 0 \quad \text{for } 0 < x < 1 \]

\[ \alpha_{LF} = 1 \]

\[ t = 0.75, \Delta x = 1/160, \text{CFL } = 1 \]

\[ t = 0.75, \Delta x = 1/160, \text{CFL } = 8 \]

\[ \Delta x = 1/80, \text{CFL } = 8 \]

Crank-Nicholson
backward Euler, CFL/2
forward Euler

SATh-LF scheme \( \bar{u} \)
SATh-LF scheme \( \tilde{u} \)
SATh-LF scheme \( \theta \)
Burgers Equation in 2D

\[ u_t + \left( \frac{u^2}{2} \right)_x + \left( \frac{u^2}{2} \right)_y = 0 \quad \text{for } 0 < x < 1, 0 < y < 1 \]

\[ \Delta x = \Delta y = 1/40, \Delta t = 1/10 \ (\text{CFL} = 4), \ \alpha_{LF} = 1 \]

\[ t = 0.2 \]

\[ t = 0.5 \]

\[ t = 1.0 \]

\[ t = 1.0, \text{ profile} \]

---

backward Euler, CFL/2

---

SATh-LF scheme \( \bar{u} \)
Buckley-Leverett Equation in 2D

\[ u_t + \left( \frac{u^2}{u^2 + (1-u)^2} \right)_x + \left( \frac{u^2}{u^2 + (1-u)^2} \right)_y = 0 \quad \text{for } 0 < x, y < 1 \]

\[ \Delta x = \Delta y = 1/40, \ \Delta t = 1/10 \ (CFL = 8), \ \alpha_{LF} = 2 \]

\[ t = 0.2 \]

\[ t = 0.5 \]

\[ t = 1.0 \]

\[ t = 1.0, \ \text{profile} \]

---

**backward Euler, CFL/2**  
**SATh-LF scheme \( \bar{u} \)**
7. Summary and Conclusions
\[ u_t + \nabla \cdot [f(u) - D(u)\nabla u] = 0 \]

**Finite volume framework**

- **Space:** use (implicit) WENO-AO reconstructions
- **Time:** use an adaptive, L-stable implicit, Runge-Kutta method

1. Locally conservative and captures the physics (advection, diffusion)
2. Only a few unknowns per mesh element per component (in n-D)

**WENO-AO spatial reconstruction**

1. High order accuracy when \( u \) is smooth, low order when discontinuous
2. Captures steep fronts ("essentially" non oscillatory)
3. Easy to extend to general 2D and 3D meshes

**Adaptive Runge-Kutta time stepping**

1. L-stable implicit Runge-Kutta (SSP not suitable)
2. \( \Delta t \sim \Delta x \), chosen for accuracy, not stability
3. Adapt between Radau IIA and composite backward Euler
4. Radau accuracy when \( u \) is smooth, BE when discontinuous
Self Adaptive Theta scheme. A “better backward Euler”

1. The differential equation controls both $\tilde{u}_i^{n+1}$ and $\bar{u}_i^{n+1}$
2. These are used to define Discontinuity Aware Quadrature (DAQ)
   - Accurate locally to $O(\Delta t^2)$, even with discontinuities
3. DAQ gives SATh schemes for conservation laws
   \[
   \theta_i = \max \left( \frac{1}{2}, \frac{\tilde{u}_i^{n+1} - \bar{u}_i^n}{\bar{u}_i^{n+1} - \bar{u}_i^n} \right)
   \]

The upstream scheme:
- is stable for monotone fluxes
- satisfies maximum principle for monotone flows and is TVB/TVD
4. Early stage of development:
- less diffusive than backward Euler
- the general SATh-LF seems to have all the good properties of BE
- shows promise!

