Solving the $S_N$ Neutron Transport Equation Using High Order Lax-Friedrichs WENO Fast Sweeping Methods

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Outline

• Background and motivation
  • Robustness
  • High order
  • Efficiency

• LF-WENO methods
  • Theory (Wang 2019)
  • Numerical properties (Wang 2019, NSE)
  • Diffusion limit

• Conclusion
Numerical methods for $S_N$

- **Finite difference sweeping methods**
  - SD: $1^{st}$-order upwind; positivity preserving
  - DD: $2^{nd}$-order; not positivity preserving
  - SC: weighted DD; $2^{nd}$-order; positivity preserving; less accurate than DD for diffusive problems

- **Short characteristic methods**
  - SC: constant source
  - LC: linear source & linear incoming flux; **positivity preserving**?
  - QC: Quadratic source & quadratic incoming flux; can be made to be positivity preserving (on-going work)

- **Galerkin methods: LD, FEM, DFEM**
  - High-order
  - FEM or DFEM can be very robust with stabilization; however may not as efficient as finite difference sweeping methods.
Motivation

• A sweeping based numerical method is more accurate than DD, and much more robust as well.

• A challenging task...

• Chen et al. in 2013 proposed Lax-Friedrichs fast sweeping methods for steady-state hyperbolic conservation laws.

• A perfect framework for the $S_N$ transport equation!
\( S_N \) in 2-D conservative form

\[
f(\psi)_x + g(\psi)_y + \Sigma_t \psi = s(\psi, x, y)
\]

where,

\[
f(\psi) = \mu \psi ,
\]

\[
g(\psi) = \eta \psi ,
\]

\[
s(\psi, x, y) = \frac{\Sigma_s}{4} \phi(x, y) + \frac{1}{4} Q(x, y)
\]
Finite difference discretization

\[
\begin{align*}
\hat{f}_{i+\frac{1}{2},j} - \hat{f}_{i-\frac{1}{2},j} & \quad \frac{\Delta x}{\Delta y} \quad + \quad \hat{g}_{i,j+\frac{1}{2}} - \hat{g}_{i,j-\frac{1}{2}} \quad \frac{\Delta y}{\Delta x} \\
+ \quad \Sigma t \psi_{i,j} & = s(\psi_{i,j}, x_i, y_j) \quad (1)
\end{align*}
\]

Where

\[
\hat{f}_{i\pm\frac{1}{2},j} \quad \text{and} \quad \hat{g}_{i,j\pm\frac{1}{2}} \quad \text{are numerical fluxes}
\]
High order WENO fluxes

For \((2K - 1)\)-th order WENO scheme, the \(K\) numerical fluxes are computed as

\[
\hat{f}_{i + \frac{1}{2}, j}^{(r)} = \sum_{k=0}^{K-1} c_{rk} f_{i-r+k, j}, \quad r = 0, \ldots, K - 1,
\]

which corresponds to \(K\) different stencils: \(S_r(i) = \{(x_{i-r}, y_j), \ldots, (x_{i-r+K-1}, y_j)\}, r = 0, \ldots, K - 1\). Each of these numerical fluxes is \(k\)-th order accurate.

The \((2K - 1)\)-th order WENO flux is a superposition of all these \(K\) numerical fluxes

\[
\hat{f}_{i + \frac{1}{2}, j} = \sum_{k=0}^{K-1} w_k \hat{f}_{i + \frac{1}{2}, j}^{(k)}
\]

The nonlinear weights \(w_k\) satisfy \(w_k \geq 0, \sum_{k=0}^{K-1} w_k = 1\), and are defined as

\[
w_k = \frac{\alpha_k}{\sum_{k=0}^{K-1} \alpha_k}, \quad \alpha_k = \frac{d_k}{(\epsilon + \beta_k)}.
\]
Third order WENO (WENO3)

For $K = 2$, the 2nd-order accurate numerical fluxes for $\mu > 0$ are given as

$$
\hat{f}_{i+\frac{1}{2},j}^{(0)} = \frac{1}{2} f_{i,j} + \frac{1}{2} f_{i+1,j}, \quad \hat{f}_{i+\frac{1}{2},j}^{(1)} = -\frac{1}{2} f_{i-1,j} + \frac{3}{2} f_{i,j} \tag{5}
$$

And the linear weights are given by

$$
d_0 = \frac{2}{3}, \quad d_1 = \frac{1}{3} \tag{6}
$$

Smoothness indicators are given by

$$
\beta_0 = \tau_0 (f_{i+1,j} - f_{i,j})^2, \quad \beta_1 = \tau_1 (f_{i,j} - f_{i-1,j})^2 \tag{7}
$$

where

$$
\tau_0 = a \times \max \left[ \text{abs} \left( \Sigma_{t_{i+1,j}} - \Sigma_{t_{i,j}} \right), \text{abs} \left( \Sigma_{s_{i+1,j}} - \Sigma_{s_{i,j}} \right) \right] \Delta x
$$

$$
\tau_1 = b \times \max \left[ \text{abs} \left( \Sigma_{t_{i,j}} - \Sigma_{t_{i-1,j}} \right), \text{abs} \left( \Sigma_{s_{i,j}} - \Sigma_{s_{i-1,j}} \right) \right] \Delta x
$$
Lax-Friedrichs sweeping framework

Define Lax–Friedrichs fluxes:

\[
\hat{f}_{i+\frac{1}{2},j} = \hat{f}_{i+\frac{1}{2},j} + \frac{\sigma \mu}{2} (\psi_{i+1,j} - \psi_{i,j}), \quad i = 1, \ldots, N_x \tag{8a}
\]

\[
\hat{g}_{i,j+\frac{1}{2}} = \hat{g}_{i,j+\frac{1}{2}} + \frac{\sigma \eta}{2} (\psi_{i,j+1} - \psi_{i,j}), \quad j = 1, \ldots, N_y \tag{8b}
\]

Then we have

\[
\hat{f}_{i+\frac{1}{2},j} = \hat{f}_{i+\frac{1}{2},j} - \frac{\sigma \mu}{2} (\psi_{i+1,j} - \psi_{i,j})
\]

\[
\hat{g}_{i,j+\frac{1}{2}} = \hat{g}_{i,j+\frac{1}{2}} - \frac{\sigma \eta}{2} (\psi_{i,j+1} - \psi_{i,j})
\]
\[
\psi_{i,j} = \frac{s(\psi_{i,j}, x_i, y_j) \Delta x - \left( f^\hat{i}_{j+\frac{1}{2}} - f^\hat{i}_{j-\frac{1}{2}} \right) - \sigma^\mu (\psi_{i+1,j} + \psi_{i-1,j}) - \left( \hat{g}_{i,j+\frac{1}{2}} - \hat{g}_{i,j-\frac{1}{2}} \right) - \sigma^\eta (\psi_{i,j+1} + \psi_{i,j-1})}{\sigma \left[ \mu + \eta \left( \frac{\Delta x}{\Delta y} \right) \right] \Delta x + \Sigma_t \Delta x}
\]

\[
\psi_{i,j} = \frac{\Delta y}{\Delta x}
\]

\[
f^\hat{i}_{j+\frac{1}{2}} = \frac{\delta \mu}{2} (\psi_{i+1,j} - \psi_{i,j}) - \frac{\delta \mu}{2} (\psi_{i,j} - \psi_{i-1,j})
\]

\[
\hat{g}_{i,j+\frac{1}{2}} = \frac{\delta \eta}{2} (\psi_{i,j+1} - \psi_{i,j}) + \frac{\delta \eta}{2} (\psi_{i,j} - \psi_{i,j-1})
\]

\[
\Delta x = \frac{\Delta y}{\Delta x}
\]

\[
\Delta y = \frac{\Delta x}{\Delta y}
\]
Computing algorithm

• Initialize $\psi_{i,j}$ and $S_{i,j}$
• While $\|e\| > \text{etol}$
  1. for $n = 1:\frac{N}{4}$
     for $i = 1: N_x$
     for $j = 1: N_y$
     • Calculate $f_{i\pm\frac{1}{2}j}^{(k)}$ and $g_{i\pm\frac{1}{2}j}^{(k)}$, $k = 1,2$ % Eq (5)
     • Calculate $\beta_0$, $\beta_1$ % Eq (7)
     • Calculate $\alpha_k$, $w_k$, $k = 1,2$ % Eq (4)
     • Calculate $f_{i\pm\frac{1}{2}j}$ and $f_{i\pm\frac{1}{2}j}$ % Eq (5)
     • Calculate $f_{i\pm\frac{1}{2}j}$ and $g_{i\pm\frac{1}{2}j}$ % Eq (8)
     • Calculate $\psi_{i,j}$
     • Calculate $S_{i,j}$
  2. for $n = \frac{N}{4} + 1: \frac{N}{2}$ % sweeping in angle ($\mu < 0, \eta > 0$)
     ...
  3. for $n = \frac{N}{2} + 1: \frac{3N}{4}$ % sweeping in angle ($\mu < 0, \eta < 0$)
     ...
  4. for $n = \frac{3N}{4} + 1: N$ % sweeping in angle ($\mu > 0, \eta < 0$)
Spatial convergence

- For 2-cm slab with Vacuum BC, $\Sigma_t = 1 \text{ cm}^{-1}$, $c = 0.6$, $Q = 1 \text{ cm}^{-1}$, the flux L1 error is described by $y = 0.19x^{2.00}$.
- For 2 x 2-cm square with Vacuum BC, $\Sigma_t = 1 \text{ cm}^{-1}$, $c = 0.6$, $Q = 1 \text{ cm}^{-2}$, the flux L1 error is described by $y = 0.32x^{2.01}$.
Manufactured solution

\[ \psi(x, y, \mu_k, \eta_k) = x^3 y^3 (2 - x)^3 (2 - y)^3 \]

\[ Q_k(x, y) = 4 \left[ (24x^2 - 48x^3 + 30x^4 - 6x^5)y^3 (2 - y)^3 \mu_k + x^3 (2 - x)^3 (24y^2 - 48y^3 + 30y^4 - 6y^5)\eta_k \right] - \Sigma_a \phi(x, y) \]
Sweeping convergence rate

\[ \Sigma_t = 1 \text{ cm}^{-1} \text{ and } c = 0.6 \]

\[ \Sigma_t = 5 \text{ cm}^{-1} \text{ and } c = 0.6 \]
### Computational complexity

<table>
<thead>
<tr>
<th>Mesh</th>
<th># of grid points ((m))</th>
<th>DD</th>
<th>LF-WENO3</th>
<th>LF-WENO3</th>
<th>LF-WENO3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td># of iterations ((n))</td>
<td>Complexity ((m \times n))</td>
<td># of iterations</td>
<td>Complexity</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\sigma = 1.0)</td>
<td>(\sigma = 0.85)</td>
<td>(\sigma = 0.85)</td>
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<td>20 \times 20</td>
<td>20^2</td>
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<td>17200</td>
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<td>40 \times 40</td>
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<td>337</td>
<td>8627200</td>
</tr>
</tbody>
</table>

* Computational complexity: the number of grid points \(x\) the number of iterations
Positivity?

Note that LF-WENO3 can be rendered to be positivity preserving using the linear scaling limiter proposed by Zhang and Shu (2010).
Diffusion limit of $S_N$

$$\mu_m \frac{d}{dx} \psi_m + \Sigma_t \psi_m = \frac{\Sigma_s}{2} \phi + \frac{Q}{2}$$

Scaling \hspace{1cm} \Sigma_t \to \frac{\Sigma_t}{\varepsilon}, \hspace{1cm} \Sigma_a \to \varepsilon \Sigma_a, \hspace{1cm} Q \to \varepsilon Q,$$

We have $\psi_m = \frac{\phi}{2} + O(\varepsilon)$, for $\varepsilon \to 0$

Where $\phi$ satisfies the following diffusion equation

$$- \frac{d}{dx} \frac{1}{3\Sigma_t} \frac{d}{dx} \phi + \Sigma_a \phi = Q$$
Diffusion limit – smooth solution

\[ \Sigma_t = \frac{1}{\varepsilon}, \quad \Sigma_s = \frac{1}{\varepsilon} - 0.8\varepsilon, \quad Q = \varepsilon \]

\[ L = 1, \quad h = 0.1 \]

(a) \( \varepsilon = 0.01 \).

(b) \( \varepsilon = 0.001 \).
Diffusion limit – nonsmooth solution with boundary layer

\[ \varepsilon = 0.01 \]
Diffusion limit – 2D

$L \times L = 2 \times 2, \quad h_x = h_y = 0.2$

$$\Sigma_t = \frac{1}{\epsilon}, \quad \Sigma_s = \frac{1}{\epsilon} - 0.8\epsilon, \quad Q = \epsilon$$

(a) $\Delta x = h.$

(b) $\Delta x = 0.22h.$
A theoretical result on diffusion limit (Wang 2019, NSE): $\Delta x = \varepsilon^l h = \varepsilon^{1/k} h$

Larsen et al. 1987:

$l = 0$: Thick diffusion limit
$l = 1$: Intermediate diffusion limit
Conclusions

• LF-WENO3 is a sweeping scheme based on the Lax–Friedrichs fluxes with the WENO reconstruction.

• It can achieve better accuracy than DD, and more importantly it possesses good positivity-preserving property.

• In addition, LF-WENO3 can achieve almost linear computational complexity with underrelaxation.

• Finally, LF-WENO3 has the diffusion limit of $l = 1/3$, which lies between the thick diffusion regime ($l = 0$) and the intermediate regime ($l = 1$).
References


Thank You!