A Modified Step Characteristic Method for Solving the S_N Transport Equation

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Outline

- Background and motivation
  - Positivity or robustness
  - Accuracy
  - Diffusion limit
- Modified step characteristic method (mSC)
  - Numerical formulation
  - A proof on the diffusion limit of SC (Wang 2019, NSE)
  - Numerical results
- Conclusion

Finite difference sweeping methods

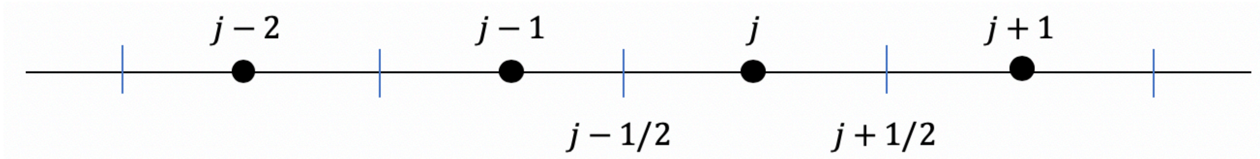
Linear methods

- Step difference (SD)
  - 1^{st}-order upwind
  - Positivity preserving
  - Intermediate diffusion limit, $\Delta x = \varepsilon^l h$, where $l = 1$
- Diamond difference (DD)
  - 2^{nd}-order;
  - Not positivity preserving
  - Thick diffusion limit in interior homogeneous regions, $l = 0$
- Step characteristic (SC)
  - Weighted DD
  - 2^{nd}-order, but less accurate than DD for diffusive problems
  - Positivity preserving
  - Intermediate diffusion limit, $l = 0$

Nonlinear methods

- LF-WENO methods (Wang 2019)
  - High-order
  - Very robust, but not positivity preserving. Can be made positive!
  - Between thick and intermediate, $l = 1/k$, where k is the order of spatial accuracy

SC



$$\frac{\mu_n}{h_j}\left(\psi_{n,j+1/2} - \psi_{n,j-1/2}\right) + \Sigma_{t,j}\left[\left(\frac{1-\alpha_{n,j}}{2}\right)\psi_{n,j-1/2} + \left(\frac{1+\alpha_{n,j}}{2}\right)\psi_{n,j+1/2}\right] =$$

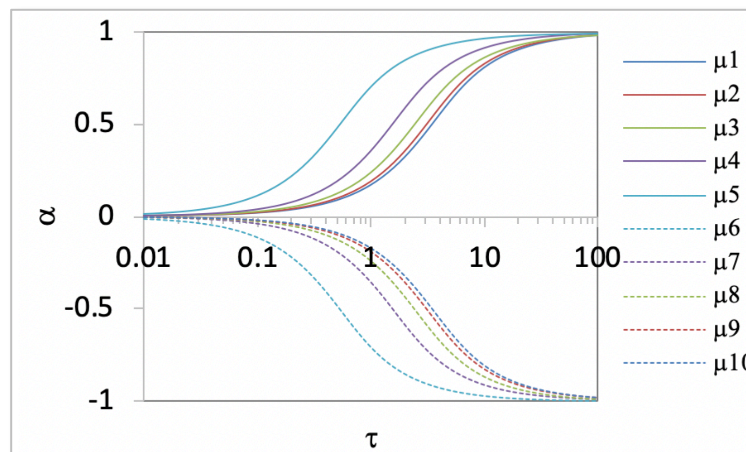
$$\frac{\Sigma_{s,j}}{2}\sum_{n'=1}^{N}\left[\left(\frac{1-\alpha_{n',j}}{2}\right)\psi_{n',j-\frac{1}{2}} + \left(\frac{1+\alpha_{n',j}}{2}\right)\psi_{n',j+1/2}\right]w_{n'} + \frac{Q_j}{2}$$

where

$$\alpha_{n,j} = \frac{1+e^{-\Sigma_{t,j}h_j/\mu_n}}{1-e^{-\Sigma_{t,j}h_j/\mu_n}} - \frac{2\mu_n}{\Sigma_{t,j}h_j} = \frac{1+e^{-\tau_j/\mu_n}}{1-e^{-\tau_j/\mu_n}} - \frac{2\mu_n}{\tau_j}$$

$\tau_j = \Sigma_{t,j}h_j$, cell optical thickness

$h_j =$ mesh size of cell j



M-matrix and stability

$$\frac{\mu_n}{h_j}\left(\psi_{n,j+1/2}-\psi_{n,j-1/2}\right)+\Sigma_{t,j}\left[\left(\frac{1-\alpha_{n,j}}{2}\right)\psi_{n,j-1/2}+\left(\frac{1+\alpha_{n,j}}{2}\right)\psi_{n,j+1/2}\right]=\frac{\Sigma_{s,j}}{2}\sum_{n'=1}^{N}\phi_{n',j}w_{n'}+\frac{Q_j}{2},$$

$j=1,\ldots m,$ for $\mu_n>0$

In matrix form: $\mathbf{A\Psi}=\mathbf{S}$

where A is lower diagonal matrix

$$\mathbf{A}=\begin{bmatrix}\vdots & \vdots & \ddots & \vdots & \vdots\\ \cdots & -\frac{\mu_n}{h_j}+\Sigma_{t,j}\left(\frac{1-\alpha_{n,j}}{2}\right) & \frac{\mu_n}{h_j}+\Sigma_{t,j}\left(\frac{1+\alpha_{n,j}}{2}\right) & \cdots & \cdots\\ \vdots & \vdots & \vdots & \ddots & \vdots\end{bmatrix}$$

For A is a M-matrix, we need to have $-\frac{\mu_n}{h_j}+\Sigma_{t,j}\left(\frac{1-\alpha_{n,j}}{2}\right)\le 0$, and therefore

SD $\left(\alpha_{n,j}=1\right)$: A is unconditionally M-matrix

DD $\left(\alpha_{n,j}=0\right)$: $h_j\le\frac{2\mu_n}{\Sigma_{t,j}}$, or $\tau_j\le 2\mu_n$

>1

SC: $h_j\le\frac{2\mu_n}{\Sigma_{t,j}(1-\alpha_{n,j})}$, or $\tau_j\le\frac{2\mu_n}{(1-\alpha_{n,j})}=\frac{1}{\left[1-\frac{1}{\frac{\mu_n}{\tau_j}\left(e^{\tau_j/\mu_n}-1\right)}\right]}\tau_j,$

and therefore A is unconditionally M-matrix

Diffusion limit of S$_N$ – a recap

$$\mu_n \frac{d}{dx}\psi_n + \Sigma_t \psi_n = \frac{\Sigma_s}{2}\sum_{n'=1}^{N} \psi_{n'} w_{n'} + \frac{Q}{2}$$

Scaling $\boldsymbol{\Sigma_t \to \frac{\Sigma_t}{\varepsilon}}$, $\boldsymbol{\Sigma_a \to \varepsilon \Sigma_a}$, $\boldsymbol{Q \to \varepsilon Q}$

$$\mu_n \frac{d}{dx}\psi_n + \frac{\Sigma_t}{\varepsilon}\psi_n = \frac{1}{2}\left(\frac{\Sigma_t}{\varepsilon} - \varepsilon \Sigma_a\right)\sum_{n'=1}^{N} \psi_{n'} w_{n'} + \frac{\varepsilon Q}{2}$$

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

Where ϕ satisfies the following diffusion equation

$$-\frac{d}{dx}\frac{1}{3\Sigma_t}\frac{d}{dx}\phi + \Sigma_a \phi = Q$$

Diffusion limit of SC (Wang, 2019)

$$\alpha_{n,j} = \frac{1 + e^{-\left(\frac{\Sigma_{tj}}{\varepsilon}\right)(\varepsilon^l h_j)/\mu_n}}{1 - e^{-\left(\frac{\Sigma_{tj}}{\varepsilon}\right)(\varepsilon^l h_j)/\mu_n}} - \frac{2\mu_n}{\left(\frac{\Sigma_{tj}}{\varepsilon}\right)\left(\varepsilon^l h_j\right)} = \frac{1 + e^{-(\Sigma_{tj} h_j/\mu_n)\varepsilon^{l-1}}}{1 - e^{-(\Sigma_{tj} h_j/\mu_n)\varepsilon^{l-1}}} - \frac{2\mu_n}{\left(\Sigma_{tj} h_j\right)\varepsilon^{l-1}}$$

Proof (by contradiction).

- If $l > 1$, then $\alpha_{n,j} \downarrow 0$ as $\varepsilon \downarrow 0$, and thus SC tends to DD, whereas DD has $l = 0$.
- If $l < 1$, then $\alpha_{n,j} \uparrow 1$ for $\mu_m > 0$, and $\alpha_{n,j} \downarrow -1$ for $\mu_n < 0$, as $\varepsilon \downarrow 0$. Thus, SC tends to SD, but SD has $l = 1$.
- So we should have $l = 1$ for SC, and then $\alpha_{n,j} = \frac{1+e^{-\left(\Sigma_{tj} h_j/\mu_n\right)}}{1-e^{-\left(\Sigma_{tj} h_j/\mu_n\right)}} - \frac{2\mu_n}{\left(\Sigma_{tj} h_j\right)}$.

Modified SC (mSC)

$$\alpha_{n,j} = \frac{1+e^{-\Sigma_{t,j} h_j \left(1-c_j^{\beta}\right)/\mu_n}}{1-e^{-\Sigma_{t,j} h_j \left(1-c_j^{\beta}\right)/\mu_n}} - \frac{2\mu_n}{\Sigma_{t,j} h_j \left(1-c_j^{\beta}\right)} = \frac{1+e^{-\tau_j \left(1-c_j^{\beta}\right)/\mu_n}}{1-e^{-\tau_j \left(1-c_j^{\beta}\right)/\mu_n}} - \frac{2\mu_n}{\tau_j \left(1-c_j^{\beta}\right)},$$

where

β is a positive number larger than 1 (e.g., $\beta = 3$)

$c_j \equiv \frac{\Sigma_{s,j}}{\Sigma_{t,j}}$

Note: $c \downarrow 0$: mSC $\rightarrow$ SC

$c \uparrow 1$: mSC $\rightarrow$ DD

Diffusion limit of mSC (Wang, 2019)

$$\alpha_{n,j} = \frac{1 + e^{-\left(\frac{\Sigma_{tj}}{\varepsilon}\right)(\varepsilon^l h_j)\left(1-c_j^\beta\right)/\mu_n}}{1 - e^{-\left(\frac{\Sigma_{tj}}{\varepsilon}\right)(\varepsilon^l h_j)\left(1-c_j^\beta\right)/\mu_n}} - \frac{2\mu_n}{\left(\frac{\Sigma_{tj}}{\varepsilon}\right)(\varepsilon^l h_j)\left(1-c_j^\beta\right)}$$

$$= \frac{1 + e^{-(\Sigma_{tj} h_j/\mu_n)\varepsilon^{l-1}\left(1-c_j^\beta\right)}}{1 - e^{-(\Sigma_{tj} h_j/\mu_n)\varepsilon^{l-1}\left(1-c_j^\beta\right)}} - \frac{2\mu_n}{(\Sigma_{tj} h_j)\varepsilon^{l-1}\left(1-c_j^\beta\right)}$$

Proof.

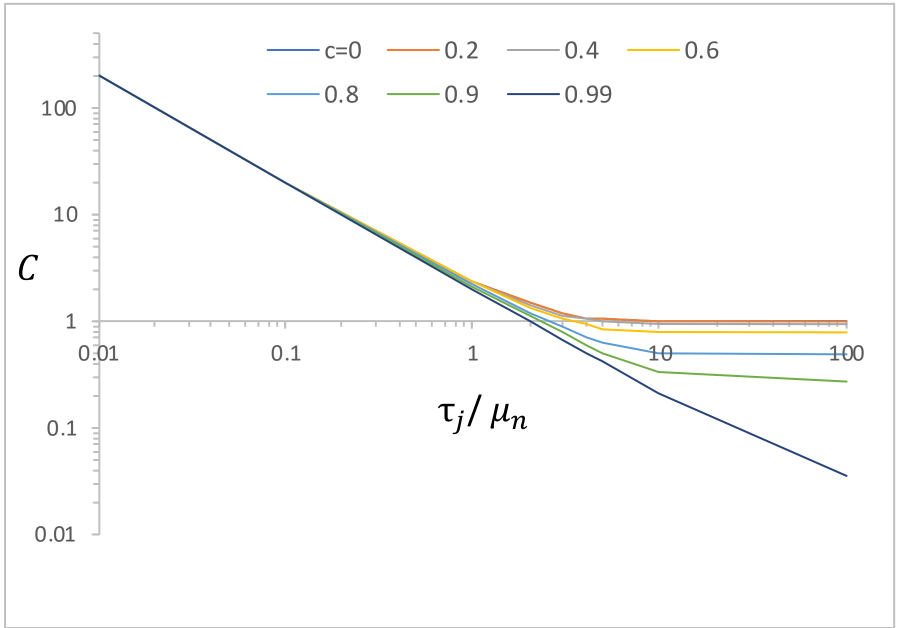
- $c_j = 1 - \varepsilon^2 \frac{\Sigma_{aj}}{\Sigma_{tj}}$.
- As $\varepsilon \downarrow 0$, the $\boldsymbol{\varepsilon^{l-1}\left(1-c_j^\beta\right)}$ term tends to zero, and thus $\alpha \downarrow 0$. As a result, the SC reverts to the DD scheme, and therefore it can attain the **thick diffusion limit** as DD does.

How about positivity?

$$\alpha_{n,j} = \frac{1 + e^{-\tau_j\left(1-c_j^{\beta}\right)/\mu_n}}{1 - e^{-\tau_j\left(1-c_j^{\beta}\right)/\mu_n}} - \frac{2\mu_n}{\tau_j\left(1 - c_j^{\beta}\right)}$$

For A is a M-matrix, we need to have

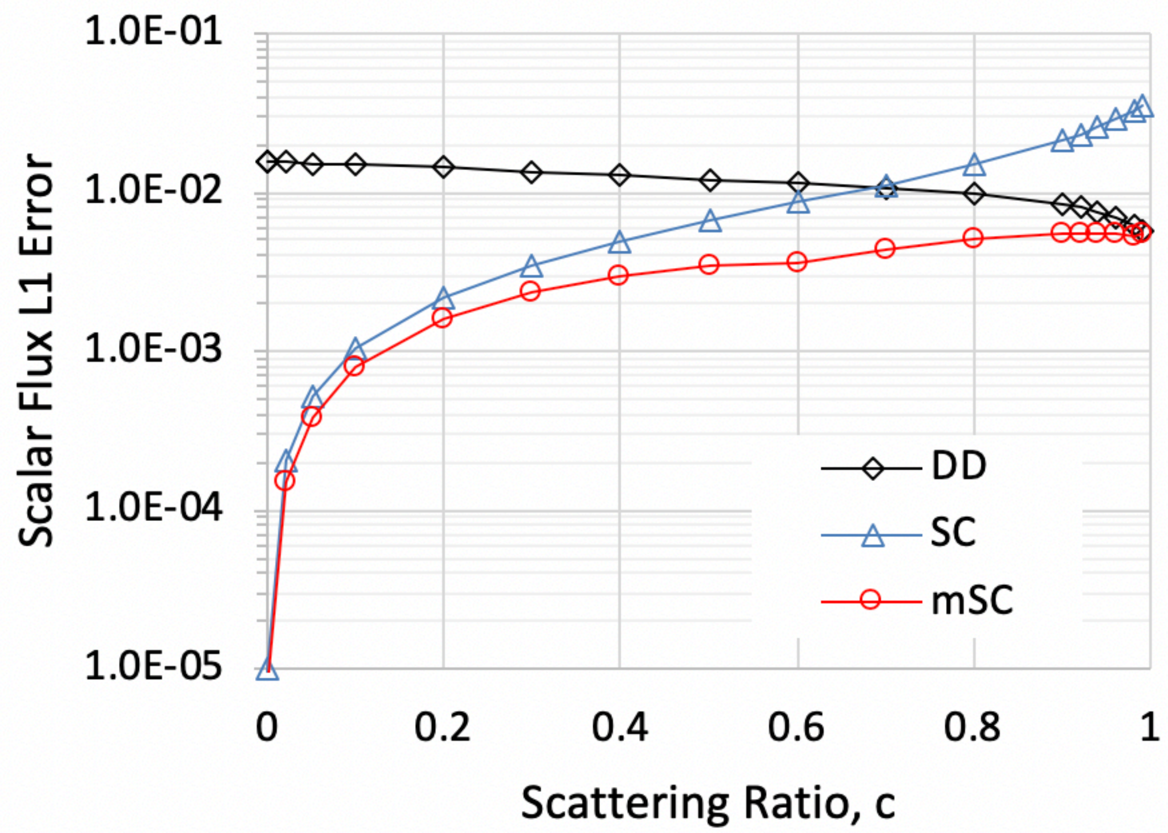
$$\tau_j \le \frac{2\mu_n}{(1-\alpha_{n,j})} = C\tau_j \text{ , where } C = \frac{1-c_j^{\beta}}{1-\frac{\tau_j\left(1-c_j^{\beta}\right)/\mu_n}{e^{\tau_j\left(1-c_j^{\beta}\right)/\mu_n}-1}}$$



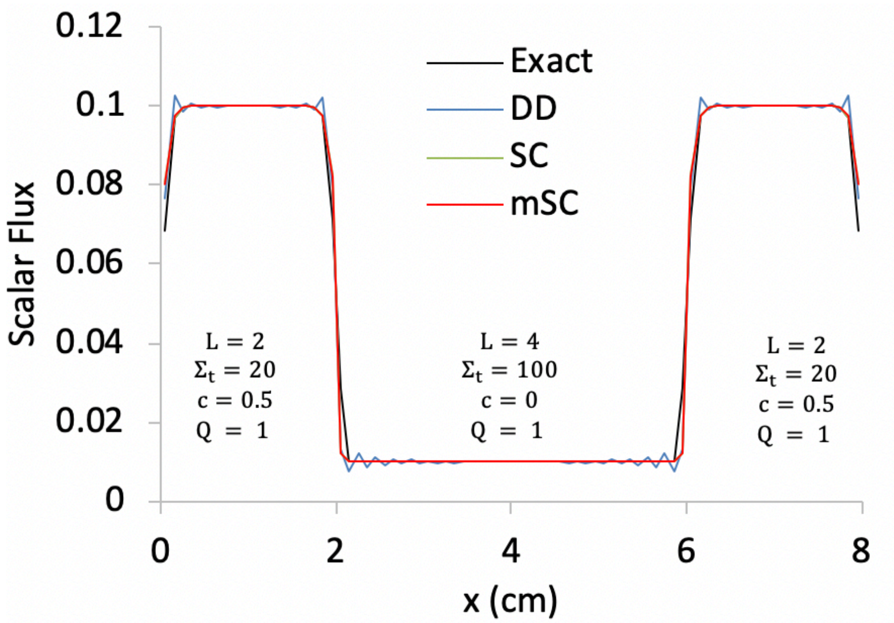
Numerical results – accuracy

$L = 1$ cm $\quad h = 0.1$ cm $\quad \Sigma_t = 5\ \text{cm}^{-1} \quad Q = 1\ \text{cm}^{-1}$

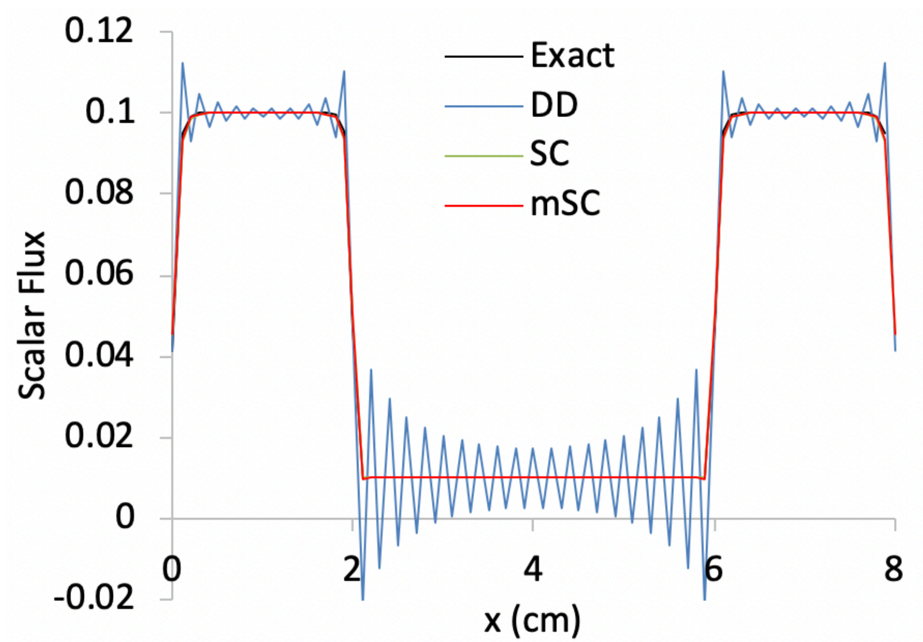
BC: Vacuum



Numerical Result – robustness



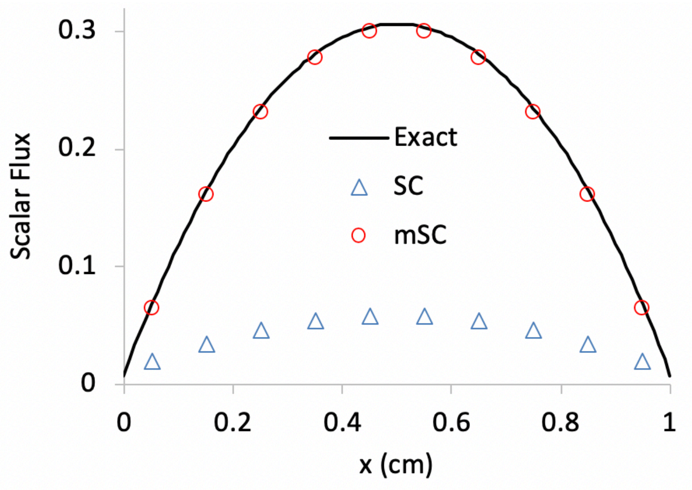
a. Cell-average flux.



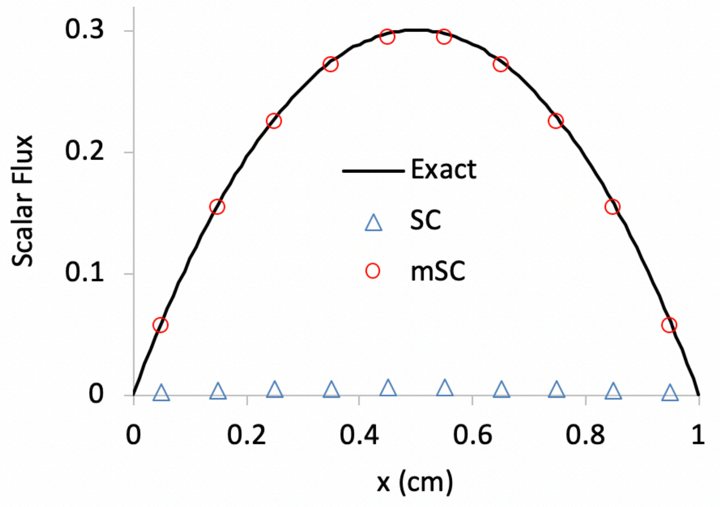
b. Cell-edge flux.

Numerical Result – diffusion limit

$$L = 1, \qquad h = 0.1,$$
$$\Sigma_t = \frac{1}{\varepsilon}, \qquad \Sigma_s = \frac{1}{\varepsilon} - 0.8\varepsilon,$$
$$Q = \varepsilon,$$



a. $\varepsilon = 0.01$.



b. $\varepsilon = 0.001$.

Conclusions

- We proposed a modified step characteristic method, called mSC, which can improve the accuracy of the original SC scheme.
- The idea is that we have introduced a scaling factor, $1 - c^{\beta}$ in the weighting α term of SC.
- The numerical results have demonstrated that the new mSC scheme can preserve great robustness of the original SC, and is much more accurate than SC and DD as well.
- More importantly it can attain the thick diffusion limit, which is of significant computational interest for thick diffusive problems such as radiative transfer.

References

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Thank You!