

**LLNL RIPS Project Proposal: Negative Flux Correcting Schemes
for the Boltzmann Transport Equation**

Faculty Mentor: Thomas Cecil
Sponsor Liaison: Barna Bihari

In the one dimensional case where the problem is time independent, monoenergetic, and has slab geometry, the Boltzmann Equation takes the form

$$\mu \frac{\partial \psi}{\partial x} + \sigma \psi = f, \quad a < x < b, \quad \mu > 0. \quad (1)$$

The diamond difference discretization of this problem is constructed by first dividing the computational domain (a, b) into I intervals or cells whose mid-points are the points $\{x_i\}$. We have $x_i \equiv 1/2(x_{i+1/2} + x_{i-1/2})$, and we denote $\Delta x_i \equiv x_{i+1/2} - x_{i-1/2}$, $\psi_{i+1/2} \equiv \psi(x_{i+1/2})$. Suppressing the μ dependence and replacing the partial derivative by a two point approximation we have the balance equation

$$\mu \frac{\psi_{i+1/2} - \psi_{i-1/2}}{\Delta x_i} + \sigma_i \psi_i = f_i. \quad (2)$$

To relate the value ψ_i to the values $\psi_{i\pm 1/2}$ we use the diamond difference relation:

$$\psi_i = \frac{1}{2}(\psi_{i+1/2} + \psi_{i-1/2}). \quad (3)$$

If $\mu > 0$ the particles are moving from left to right so we assume that $\psi_{i-1/2}$ is known (the case when $\mu < 0$ is similar). We can then substitute (3) into (2) to find

$$\psi_i = \frac{1}{\sigma_i + \frac{2\mu}{\Delta x_i}} \left(\frac{2\mu}{\Delta x_i} \psi_{i-1/2} + f_i \right). \quad (4)$$

To find $\psi_{i+1/2}$ we use (3) and the now known values $\psi_{i-1/2}, \psi_i$.

The problem that can occur during the above procedure is that we may find that $\psi_{i+1/2} < 0$, this does not make physical sense. One correction to this negative flux problem is to reset $\psi_{i+1/2} = 0$, discard the diamond difference relation (3), and solve for ψ_i in (2) to get

$$\psi_i = \frac{1}{\sigma_i} \left(\frac{\mu}{\Delta x_i} \psi_{i-1/2} + f_i \right) > 0. \quad (5)$$

While this correction ensures positive ψ , it degrades the second order accuracy of the solution.

The goal of the RIPS students would be to find an improved negative flux fixup scheme that would not have the drawbacks of the currently used techniques. One option is to consider relaxing the equality in (3), and instead treating the relation as a quadratic programming minimization problem

$$\min h = \frac{1}{2} \left(\psi_i - \frac{1}{2} (\psi_{i+1/2} + \psi_{i-1/2}) \right)^2, \quad (6)$$

subject to (2) and $\psi_{i+1/2} \geq 0$. The minimum value of h will be when $h' = 0$. This reduces to $h = 0$ as in (3) if $\psi_{i+1/2} \geq 0$. However, if $\psi_{i+1/2} < 0$ when $h' = 0$, then we will have to choose a different minimum value that ensures $\psi_{i+1/2} \geq 0$.

To increase accuracy the students could also examine TVD or W/ENO schemes. The discrete form of (1) could be nonlinear

$$\mu G(\Psi)\Psi + \Sigma\Psi = F, \quad (7)$$

and perhaps an iteration of the form

$$\Psi^{n+1} = (\mu G(\Psi^n)\Psi^n + \Sigma)^{-1}F, \quad (8)$$

could be used to find the solution while ensuring that only positive fluxes are used in the computation through stencil point or stencil weight modification. In these cases the nonlinear nature of the discretization would need investigation and perhaps a least squares procedure would be applicable.

For any of these methods a scattering term could be added, and the time dependent evolution could be studied as well.