Asymptotic-Preserving operator splitting for moment methods in kinetic transport

Jeff Haack
University of Wisconsin

Collaborators: Cory Hauck (ORNL), Rob Lowrie (LANL)

March 3, 2010

Transport Equations

$$\partial_t F + v \cdot \nabla_x F = C(f)$$

- $F = F(x, v, t)$: Distribution function
- v: direction of particle motion

Can use F to get macroscopic quantities of interest by taking moments

- $\langle \cdot \rangle = \int (\cdot) dv$
- $\langle F \rangle = \rho$, density
- $\langle vF \rangle = \rho u$, momentum
- etc...

Main problem for solving: collision operator is hard.

Transport Equations with background collisions

Assume a distribution of particles with single speed which scatter off a background with slab geometry.

$$\partial_t F + \mu \partial_x F = -\sigma(x) \left(F - \frac{1}{2} \langle F \rangle \right).$$

- $\mu \in [-1, 1]$: Cosine of the angle between particle motion and x-axis
- $\sigma = \sigma(x)$: scattering cross section
- $\langle \cdot \rangle = \int_{-1}^{1} \cdot \, d\mu$

Next, we look at what happens in highly collisional regimes

Diffusion limit

Make a *diffusive scaling* $t = O(\varepsilon^2), x = O(\varepsilon)$

$$\partial_t F + \frac{\mu}{\varepsilon}\partial_x F = -\frac{\sigma(x)}{\varepsilon^2}\left(F - \frac{1}{2}\langle F\rangle\right).$$

For $\varepsilon << 1$, we have

$$\left(F - \frac{1}{2}\langle F\rangle\right) = O(\varepsilon)$$

Which implies $F = F(x,t) + O(\varepsilon) := \rho + O(\varepsilon)$.
Some more work results in $\langle \mu F\rangle = -\frac{1}{3\sigma}\rho_x$, which gives

$$\rho_t - \partial_x \frac{1}{3\sigma(x)}\rho_x = O(\varepsilon),$$

which is a diffusion equation.

Solution methods

$$\partial_t F + \frac{1}{\varepsilon}\mu\partial_x F = -\frac{\sigma}{\varepsilon^2}\left(F - \frac{1}{2}\langle F\rangle\right).$$

- Problem: How to handle μ - especially in the integral on the RHS?
- Discrete ordinates - use a quadrature in μ space
- Problem - ray effects
- The macroscopic quantities we want are moments anyway!

Moment Methods

$$\partial_t F + \frac{1}{\varepsilon}\mu\partial_x F = -\frac{\sigma}{\varepsilon^2}\left(F - \frac{1}{2}\langle F\rangle\right).$$

Moment methods multiply the equation by a set of moment functions $\mathbf{m}(v)$ and integrate, resulting in a system of equations

$$\partial_t\langle \mathbf{m}F\rangle + \partial_x\frac{1}{\varepsilon}\langle\mu\mathbf{m}F\rangle = -\frac{\sigma}{\varepsilon^2}\langle(\mathbf{m}F - \frac{1}{2}\langle\mathbf{m}F\rangle)\rangle$$

P_N Methods

- P_N expands F in μ using Legendre Polynomials on $[-1,1]$.

$$F(x,\mu,t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} u_n(x,t) p_n(\mu)$$

- Use orthogonality of p_n to get a system of equations for u_n
- Useful fact: $\mu p_n = \frac{n}{2n+1} p_{n-1} + \frac{n+1}{2n+1} p_{n+1}$

The P_N approximation

$$\partial_t u_n + \frac{1}{\varepsilon}\left(\frac{n}{2n+1}\partial_x u_{n-1} + \frac{n+1}{2n+1}\partial_x u_{n+1}\right) = -\frac{\sigma}{\varepsilon^2} u_n(1-\delta_{0,n})$$

P_N consists of taking the first N equations

Closure: We will always have u_{N+1}

- Set $u_{N+1} = 0$ $\left(F = \sum_{n=0}^{N} \frac{2n+1}{2} u_n p_n\right)$
- Other approaches exist

Asymptotics

- To determine the behavior as $\varepsilon \to 0$, take asymptotic expansions of the coefficients

$$u_n = u_n^{(0)} + \varepsilon u_n^{(1)} + \dots$$

- It can be proved that $u_n = O(\varepsilon^n)$
- Let $u_n \to \varepsilon^n u_n$

$$\partial_t u_n + \frac{1}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} + \frac{n+1}{2n+1}\partial_x u_{n+1} = -\frac{\sigma}{\varepsilon^2} u_n(1-\delta_{0,n})$$

Diffusion Limit

$$\partial_t u_0 + \partial_x u_1 = 0$$
$$\partial_t u_1 + \frac{1}{\varepsilon^2}\frac{1}{3}\partial_x u_0 + \frac{2}{3}\partial_x u_2 = -\frac{\sigma}{\varepsilon^2} u_1$$
$$\cdots$$

As $\varepsilon \longrightarrow 0$, at $O\left(\frac{1}{\varepsilon^2}\right)$ we have

$$u_1^{(0)} = -\frac{1}{3\sigma}\partial_x u_0^{(0)}$$

At $O(1)$ we then have

$$\partial_t u_0^{(0)} - \partial_x\left(\frac{1}{3\sigma}\partial_x u_0^{(0)}\right) = 0$$

Numerical difficulties

$$\partial_t u_n + \frac{1}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} + \frac{n+1}{2n+1}\partial_x u_{n+1} = -\frac{\sigma}{\varepsilon^2} u_n(1-\delta_{0,n})$$

- Linear hyperbolic problem — use a standard solver
- Wave speeds of $\lambda = O\left(\frac{1}{\varepsilon}\right)$
  Small time step needed for stability - *stiffness*
- Numerical dissipation for hyperbolic solvers:
  $O(\Delta x \lambda) = O\left(\frac{\Delta x}{\varepsilon}\right)$
  Small mesh size needed to offset *excessive numerical dissipation*
- **Goal: create a numerical method that avoids these two restrictions, independently of ε.**

First attempt

$$\partial_t u_n + \frac{1}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} + \frac{n+1}{2n+1}\partial_x u_{n+1} = -\frac{\sigma}{\varepsilon^2}u_n(1-\delta_{0,n})$$

The equations themselves suggest a numerical splitting of

Stiff:

$$\partial_t u_n + \frac{1}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} = -\frac{\sigma}{\varepsilon^2}u_n(1-\delta_{0,n})$$

Non-stiff:

$$\partial_t u_n + \frac{n+1}{2n+1}\partial_x u_{n+1} = 0$$

Non-stiff system has zero eigenvalues

First attempt

$$\partial_t u_n + \frac{1-\varepsilon^2+\varepsilon^2}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} + \frac{n+1}{2n+1}\partial_x u_{n+1} = -\frac{\sigma}{\varepsilon^2}u_n(1-\delta_{0,n})$$

Then we have

Stiff:

$$\partial_t u_n + \frac{1-\varepsilon^2}{\varepsilon^2}\frac{n}{2n+1}\partial_x u_{n-1} = -\frac{\sigma}{\varepsilon^2}u_n(1-\delta_{0,n})$$

Non-stiff:

$$\partial_t u_n + \frac{n+1}{2n+1}\partial_x u_{n+1} + \frac{n}{2n+1}\partial_x u_{n-1} = 0$$

Example: N=3 - stiff step

$$\frac{u_0^* - u_0^n}{\Delta t} = 0$$

$$\frac{u_1^* - u_1^n}{\Delta t} = -\frac{1-\varepsilon^2}{\varepsilon^2}\frac{1}{3}d_x u_0^* + \frac{\sigma}{\varepsilon^2}u_1^*$$

$$\frac{u_2^* - u_2^n}{\Delta t} = -\frac{1-\varepsilon^2}{\varepsilon^2}\frac{2}{5}d_x u_1^* + \frac{\sigma}{\varepsilon^2}u_2^*$$

$$\frac{u_3^* - u_3^n}{\Delta t} = -\frac{1-\varepsilon^2}{\varepsilon^2}\frac{3}{7}d_x u_2^* + \frac{\sigma}{\varepsilon^2}u_3^*$$

Can be solved algebraically! Plug into non-stiff step.

Example: N=3 - nonstiff step

$$\frac{u_0^{n+1} - u_0^*}{\Delta t} + \partial_x u_1^* = 0$$
$$\frac{u_1^{n+1} - u_1^*}{\Delta t} + \frac{2}{3}\partial_x u_2^* + \frac{1}{3}\partial_x u_0 = 0$$
$$\frac{u_2^{n+1} - u_2^*}{\Delta t} + \frac{3}{5}\partial_x u_3^* + \frac{2}{5}\partial_x u_1 = 0$$
$$\frac{u_3^{n+1} - u_3^*}{\Delta t} + \frac{3}{7}\partial_x u_2 = 0$$

Can be solved algebraically! Plug into non-stiff step.

Asymptotics

For simplicity, let's look at P_1. Consider $\varepsilon << 1$. Then from the stiff step we have

$$u_0^* = u_0^n$$
$$-\sigma u_1^* = \frac{1}{3} d_x u_0^n,$$

which is the discrete analogue of the diffusion limit! Plugging into non-stiff, we have

$$\frac{u_0^{n+1} - u_0^n}{\Delta t} + \partial_x u_1^* = 0$$
$$\frac{u_0^{n+1} - u_0^n}{\Delta t} - \partial_x \frac{1}{3\sigma} d_x u_0^n = 0$$

Neutron Transport — Streaming

$\varepsilon = 2$

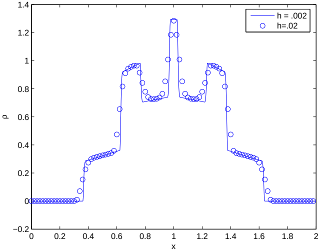
$t = 1$

$N = 3$

$\sigma = 1$

Initial condition:

$$u_0(x,0) = \begin{cases} 2, & .8 \le x \le 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Neutron Transport — Collisional

$\varepsilon = 10^{-4}$

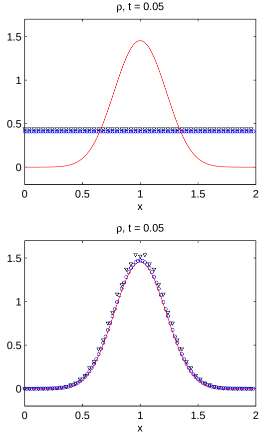
$t = .05$

$N = 1$

$\sigma = 1$

Initial condition:

$$u_0(x,0) = \begin{cases} 2, & .8 \leq x \leq 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Radiative Transfer

$$\partial_t I + \frac{1}{\varepsilon}\mu\partial_x I = -\frac{\sigma}{\varepsilon^2}(I - \frac{1}{2}T^4)$$
$$\partial_t T = -\frac{\sigma}{\varepsilon^2}(T^4 - \langle I \rangle)$$

- $I(x,\mu,t)$: Specific Intensity
- T: Material temperature
- σ: opacity ($\sigma = \frac{1}{T^3}$ in following examples)

Radiative Transfer

Do the same process, and have the same equations as for Neutron Transport, except

$$\partial_t u_0 + \partial_x u_1 = -\frac{\sigma(T)}{\varepsilon^2}(u_0 - T^4)$$

Diffusion Limit:

$$\partial_t T^4 = \partial_x \left(\frac{T^3}{3} \partial_x T^4 \right)$$

Marshak Wave — Thin Medium

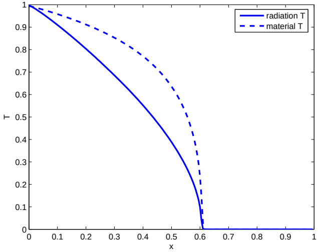
$\varepsilon = 1$

$t = 1$

$N = 37$

$\sigma = \frac{1}{T^3}$

Boundary: $T = 1, u_0 = 1$



Marshak Wave — Thick Medium

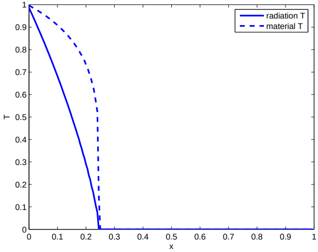
$\varepsilon = 10^{-8}$

$t = .2$

$N = 37$

$\sigma = \frac{1}{T^3}$

Boundary: $T = 1, u_0 = 1$



Marshak Waves — Thick Medium

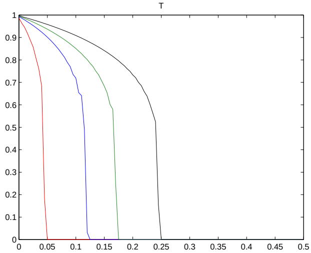
$\varepsilon = 10^{-8}$

$t = .01, .05, .1, .2$

$N = 37$

$\sigma = \frac{1}{T^3}$

Boundary: $T = 1, u_0 = 1$



Neutron Transport — Discontinuous Cross Section

$\varepsilon = 2$

$t = .1$

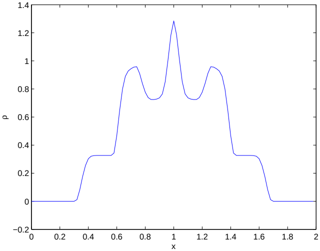
$N = 3$

σ:

$$\begin{cases} 0.02, & x \in [0.35, 0.65] \cup [1.35, 1.65] \\ 1.0, & \text{otherwise} \end{cases}$$

Initial condition:

$$u_0(x, 0) = \begin{cases} 2, & .8 \leq x \leq 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Neutron Transport — Discontinuous Cross Section

$\varepsilon = .04$

$t = .1$

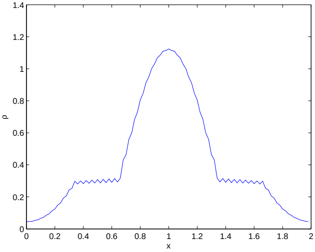
$N = 3$

σ:

$$\begin{cases} 0.02, & x \in [0.35, 0.65] \cup [1.35, 1.65] \\ 1.0, & \text{otherwise} \end{cases}$$

Initial condition:

$$u_0(x,0) = \begin{cases} 2, & .8 \le x \le 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Neutron Transport — Discontinuous Cross Section

$\varepsilon = 10^{-5}$

$t = .1$

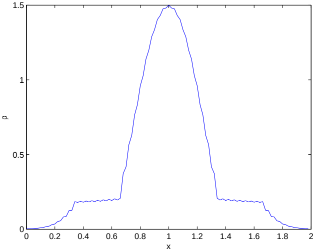
$N = 3$

σ:

$$\begin{cases} 0.02, & x \in [0.35, 0.65] \cup [1.35, 1.65] \\ 1.0, & \text{otherwise} \end{cases}$$

Initial condition:

$$u_0(x, 0) = \begin{cases} 2, & .8 \leq x \leq 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Neutron Transport — Vanishing Cross Section

$\varepsilon = 10^{-3}$

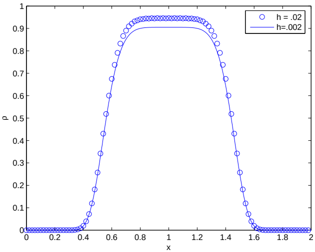
$t = .1$

$N = 3$

$\sigma = 100(x-1)^4$

Initial condition:

$$u_0(x,0) = \begin{cases} 2, & .8 \le x \le 1.2 \\ 0, & \text{otherwise} \end{cases}$$



Neutron Transport — Small σ

$\varepsilon = .1$

$t = .1$

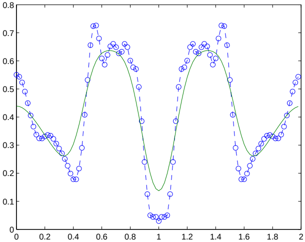
$N = 3$

$\sigma = .02$

Initial condition:

$$u_0(x,0) = \begin{cases} 2, & .8 \le x \le 1.2 \\ 0, & \text{otherwise} \end{cases}$$

First order scheme!



A closer look at P_1

Assume σ constant, $\varepsilon < 1$ ($\phi = 1$)
P_1 Equations:

$$\partial_t \rho + \partial_x m = 0$$
$$\partial_t m + \frac{1}{3}\partial_x \rho = -\frac{\sigma}{\varepsilon^2} m - \frac{1-\varepsilon^2}{\varepsilon^2}\partial_x \frac{1}{3}\rho$$

Stiff part:

$$\frac{\rho^* - \rho^n}{\Delta t} = 0$$
$$\frac{m^* - m^n}{\Delta t} = -\frac{\sigma}{\varepsilon^2} m^* - \frac{1-\varepsilon^2}{3\varepsilon^2}\frac{{\rho^*}_{j+1} - {\rho^*}_{j-1}}{2\Delta x}$$

A closer look at P_1

$$\rho_j^* = \rho_j^n$$
$$m_j^* = \gamma(m_j^n - \frac{\Delta t}{2\Delta x}\frac{1-\varepsilon^2}{\varepsilon^2}({\rho^*}_{j+1} - {\rho^*}_{j-1}))$$
$$\gamma = \frac{\varepsilon^2}{\varepsilon^2 + \sigma\Delta t}$$

Non-stiff:

$$\frac{\rho_j^{n+1} - \rho_j^*}{\Delta t} + \frac{m_{j+1}^* - m_{j-1}^*}{2\Delta x} - \frac{1}{\sqrt{3}}\frac{\rho_{j+1}^* - 2\rho_j^* + \rho_{j-1}^*}{2\Delta x} = 0$$
$$\frac{m_j^{n+1} - m_j^*}{\Delta t} + \frac{1}{3}\frac{\rho_{j+1}^* - \rho_{j-1}^*}{2\Delta x} - \frac{1}{\sqrt{3}}\frac{m_{j+1}^* - 2m_j^* + m_{j-1}^*}{2\Delta x} = 0$$

Combined stepping scheme

$$\frac{\rho_j^{n+1}-\rho_j^n}{\Delta t}+\gamma\frac{m_{j+1}^n-m_{j-1}^n}{2\Delta x}-\frac{\gamma\Delta t}{4\Delta x^2}\frac{1-\varepsilon^2}{\varepsilon^2}\frac{\rho_{j+2}^n-2\rho_j^n+\rho_{j-2}^n}{3}$$
$$-\frac{1}{\sqrt{3}}\frac{\rho_{j+1}^n-2\rho_j^n+\rho_{j-1}^n}{2\Delta x}=0$$

$$\frac{m_j^{n+1}-m_j^n}{\Delta t}+\frac{1}{3}\frac{\rho_{j+1}^n-\rho_{j-1}^n}{2\Delta x}-\frac{\gamma}{\sqrt{3}}\frac{m_{j+1}^n-2m_j^n+m_{j-1}^n}{2\Delta x}$$
$$+\frac{1}{3\sqrt{3}}\frac{\gamma\Delta t}{4\Delta x^2}\frac{1-\varepsilon^2}{\varepsilon^2}(\rho_{j+2}^n-2\rho_{j+1}^n+2\rho_{j-1}^n-\rho_{j-2}^n)$$
$$=\frac{(\gamma-1)m_j^n}{\Delta t}-\frac{\gamma}{2\Delta x}\frac{1-\varepsilon^2}{\varepsilon^2}\frac{\rho_{j+1}^n-\rho_{j-1}^n}{3}$$

Modified equation for this scheme

The modified equation is

$$\rho_t + \gamma m_x = \frac{1-\varepsilon^2}{3\sigma}(1-\gamma)\rho_{xx} + \frac{\Delta x}{2\sqrt{3}}\rho_{xx}$$

$$m_t + \frac{\gamma}{\varepsilon^2}\frac{1}{3}\rho_x = -\frac{\gamma}{\varepsilon^2}m + \frac{\gamma \Delta x}{2\sqrt{3}}m_{xx} - (1-\gamma)\frac{\Delta x}{6\sqrt{3}}(1-\varepsilon^2)\rho_{xxx} + \left(\frac{\gamma-1}{3}\right)\rho_x$$

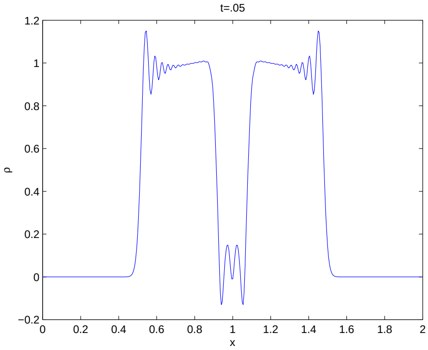
Which is an $O(\Delta t, \Delta x)$ approximation of the so-called *regularized equations*

$$\rho_t + \gamma m_x = \frac{1-\varepsilon^2}{3\sigma}(1-\gamma)\rho_{xx}$$

$$m_t + \frac{\gamma}{\varepsilon^2}\frac{1}{3}\rho_x = -\frac{\gamma}{\varepsilon^2}m$$

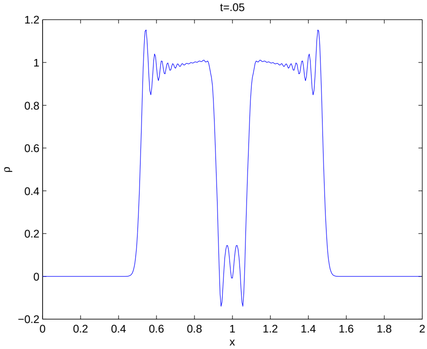
Dispersion term

If we eliminate the dispersion term, we get the following result



Staggered difference

The limiting second derivative has a wide stencil. Replacing with a standard stencil,



Numerical Dissipation

The numerical dissipation terms that pop out of the hyperbolic solver for the split equations are

$$\frac{1}{\sqrt{3}} \frac{\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n}{2\Delta x}$$

$$\frac{\gamma}{\sqrt{3}} \frac{m_{j+1}^n - 2m_j^n + m_{j-1}^n}{2\Delta x}$$

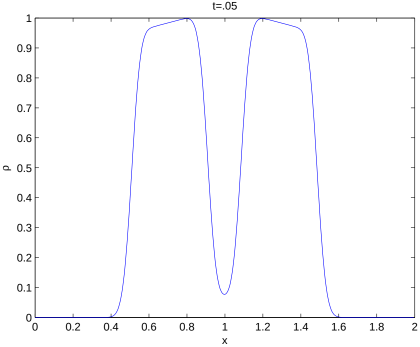
However, if we discretized the modified equations, we would have dissipation terms of the form

$$\frac{\gamma}{\varepsilon\sqrt{3}} \frac{\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n}{2\Delta x}$$

$$\frac{\gamma}{\varepsilon\sqrt{3}} \frac{m_{j+1}^n - 2m_j^n + m_{j-1}^n}{2\Delta x}$$

We have **too little** numerical dissipation now, instead of too much

With additional dissipation, keeping the staggered diffusion term and dispersion,



Conclusion

Moral of the story:

Try to derive the regularized equations **before** discretizing in space

Future Work

- Dissipation fix for general N - can it come from the splitting?
- Further investigation of variable cross section - difficult to maintain conservation
- CFL condition problem - parity form?
- Extension to higher dimensions

References

- J. Haack, C. Hauck, *Oscillatory behavior of Asymptotic-Preserving splitting methods for a linear model of diffusive relaxation*, Los Alamost Report LA-UR-08-0571, Kinetic and Related Models, , 573–590, 2008.
- C. Hauck and R. Lowrie, *Temporal regularization of the P_N equations*, Multiscale Model. Simul., 1, 1497–1524, 2009.
- S. Jin, L. Pareschi, G. Toscani. *Diffusive relaxation schemes for multiscale discrete-velocity kinetic equations.* SIAM J. Numer. Anal., 35, 2405–2439, 1998.
- S. Jin. *Efficient asymptotic-preserving (AP) schemes for some multiscale kinetic equations.* SIAM J. Sci. Comput., 21, 441–454, 1999.