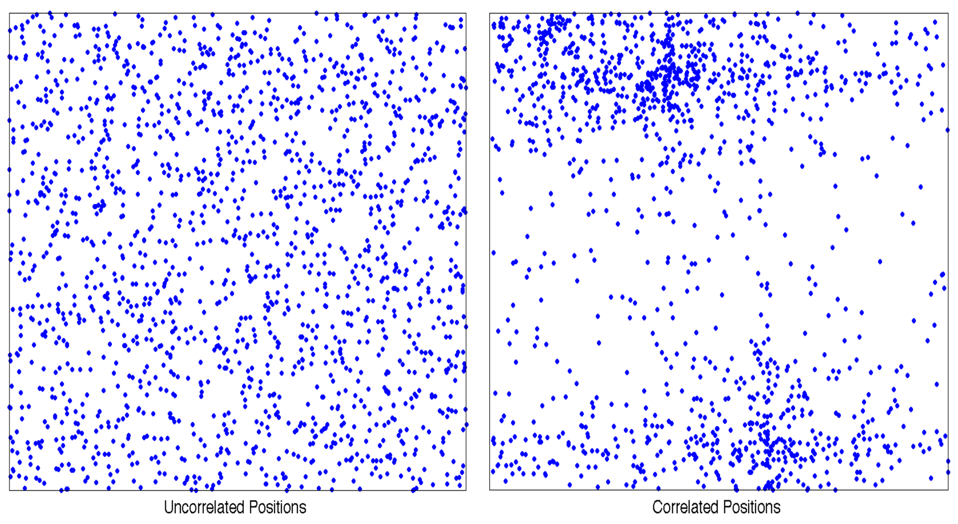
Numerical schemes for a non-classical linear Boltzmann equation for transport through spatially correlated media

Kai Krycki, Richard Vasques

Center for Computational Engineering Sciences
RWTH Aachen University

Introduction

Standard radiative transfer models assume that the positions of the scattering centers are uncorrelated, which means that the underlying distribution of scattering centers in space is Poisson-like.



This results in an exponential decay of the path-length distribution $p(s)$ due to the Beer-Lambert law. However, this disagrees with recent observations indicating that the path-length distribution decays algebraically, that is, non-exponentially. It has been suggested [1] that this is rooted in spatial correlations of the scattering centers. This issue is not modeled by the classical linear Boltzmann equation for radiative transfer.

A non-classical linear Boltzmann equation

Larsen [2, 3] introduced the following Boltzmann-like equation to model the transport of particles through a correlated background medium:

$$\partial_s \Psi + \mathbf{\Omega}\nabla_x \Psi + \Sigma_t(s)\Psi = 0,$$
$$\Psi(0,\mathbf{x},\mathbf{\Omega}) = (S\Psi)(\mathbf{x},\mathbf{\Omega}) + Q(\mathbf{x},\mathbf{\Omega}),$$

with

$$(S\Psi)(\mathbf{x},\mathbf{\Omega}) = c\iint \sigma(\mathbf{\Omega},\mathbf{\Omega}')\Sigma_t(s')\Psi(s',\mathbf{x},\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'\mathrm{d}s'$$

where

- $\Psi(s,\mathbf{x},\mathbf{\Omega})$ is the angular flux at point $\mathbf{x}$ into direction $\mathbf{\Omega}$,
- $s \in (0,\infty)$ is the path-length traveled by the particle since its previous interaction (birth or scattering),
- $\mathbf{x} \in \mathbb{R}^N$ is the position in space,
- $\mathbf{\Omega} \in S^{N-1}$ is the direction of travel,
- $\Sigma_t(s)$ is the collision frequency,
- $c \in [0,1]$ is the scattering ratio,
- $\sigma(\mathbf{\Omega},\mathbf{\Omega}')$ is the scattering kernel,
- $Q(\mathbf{x},\mathbf{\Omega})$ is an external source.

The additional variable s makes this equation "non-classical". It can also be seen as the time elapsed since the previous interaction and can hence be treated as a pseudo-time variable. The probability density p can be defined in terms of the collision frequency Σ_t and vice versa:

$$p(s) = \Sigma_t(s)\exp\left(\int_0^\infty \Sigma_t(\tau)d\tau\right).$$

For later use, we define the first and second moments of the path-length distribution as

$$\langle s\rangle := \int_0^\infty sp(s)ds, \quad \langle s^2\rangle := \int_0^\infty s^2 p(s)ds.$$

It has been shown in [4] that a unique and non-negative solution exists under reasonable assumptions. For Σ_t constant this equation reduces to the classical radiative transfer equation [2].

Diffusive scaling

In an optically thick medium we introduce a diffusive scaling:

$$Q \to \varepsilon Q, \quad \Sigma_t(s) \to \frac{1}{\varepsilon}\Sigma_t(s/\varepsilon), \quad c \to 1-\kappa\varepsilon^2,$$

where $\kappa > 0$. Applying a formal Hilbert expansion in the parameter ε and letting $\varepsilon \to 0$, one derives the following non-classical diffusion approximation $[2-4]$:

$$-\frac{1}{3}\left(\frac{\langle s^2\rangle}{2} + \frac{\bar{\mu}_0}{1-\bar{\mu}_0}\right)\nabla^2\Phi_0 + \kappa\Phi_0 = \langle s\rangle Q(\mathbf{x}),$$

with $\Phi_0 = \Phi_0(\mathbf{x})$ and $\bar{\mu}_0$ being the mean scattering cosine. This is an approximation of the scalar radiation flux up to first order. Note that this diffusion limit is not valid any more as soon as $p(s) \geq C/s^3$, because in this case $\langle s^2\rangle = \infty$.

Moment models

We approximate the solution of the scaled system using the method of moments. Defining the first two angular moments as

$$E(s,\mathbf{x}) = \int \Psi(s,\mathbf{x},\mathbf{\Omega})d\mathbf{\Omega}, \quad F(s,\mathbf{x}) = \int \mathbf{\Omega}\Psi(s,\mathbf{x},\mathbf{\Omega})d\mathbf{\Omega},$$

we can write the scaled system as

$$\partial_s E + \varepsilon\nabla F = 0, \qquad \partial_s F + \varepsilon\nabla\chi(E,F)E = 0;$$
$$E(0,\mathbf{x}) = (1-\kappa\varepsilon^2)\int_0^\infty p(s)E(s,\mathbf{x})ds + \varepsilon^2\langle s\rangle Q(\mathbf{x}), \quad F(0,\mathbf{x}) = 0.$$

where $\chi(E,F)E$ is a model for the second angular moment. For the Eddington factor χ we choose the P1 and M1 closures

$$\textbf{(P1)}\ \chi(E,F) = \frac{1}{3}, \qquad \textbf{(M1)}\ \chi(E,F) = \frac{3+4(F/E)^2}{5+2\sqrt{4-3(F/E)^2}}.$$

Both closures are the first representatives of a full hierarchy of moment closures, called the P_N or M_N closures, respectively. They all yield a coupled **hyperbolic system of first order differential equations**.

Numerical schemes

In [5] we use HLL as a guideline to derive discretization schemes

$$\frac{E_i^{n+1}-E_i^n}{\Delta s} + \varepsilon\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} - \varepsilon^2\frac{E_{i+1}^n - 2E_i^n + E_{i-1}^n}{2\Delta x} = 0,$$
$$\frac{F_i^{n+1}-F_i^n}{\Delta s} + \varepsilon\frac{P_{i+1}^n - P_{i-1}^n}{2\Delta x} - \varepsilon^2\frac{F_{i+1}^n - 2F_i^n + F_{i-1}^n}{2\Delta x} = 0,$$
$$E_i^0 = (1-\kappa\varepsilon^2)\sum_{n=0}^{\infty}\omega_n p_n E_i^n \Delta s + \varepsilon^2\langle s\rangle Q_i, \qquad F_i^0 = 0,$$

where $P = \chi(E,F)E$. The ε^2- factor in front of the numerical diffusion term makes the schemes **asymptotic preserving** (see next text box). Furthermore, the schemes have the following properties:

- The numerical scheme preserves the convex set of **admissible and realizable** states.
- The scheme is L^2**-stable** for the linear P1 model.
- Source iteration **converges slowly** in the optically thick case ($\varepsilon << 1$), since its contraction rate is $1-\kappa\varepsilon^2$.
- Suitable **initialization** can be derived from the P1 model.

Contact

Dipl.-Math. Kai Krycki
Email: `krycki@mathcces.rwth-aachen.de`

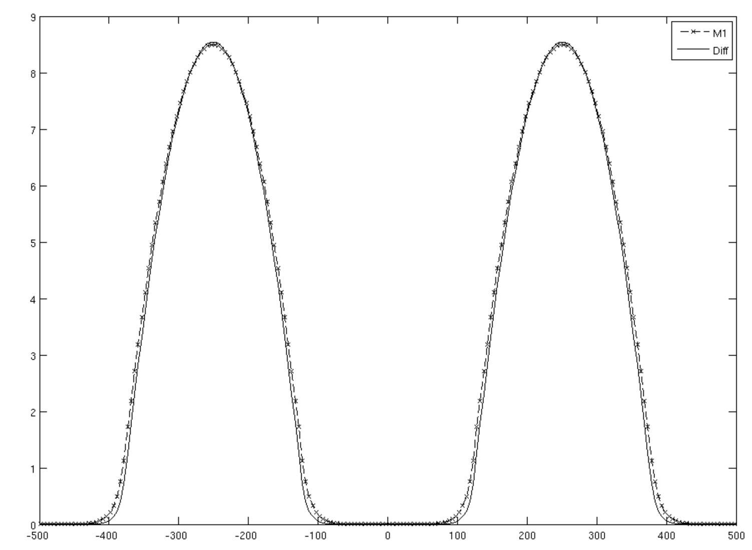
Dr. Richard Vasques
Email: `vasques@mathcces.rwth-aachen.de`

Asymptotic limit

In the asymptotic limit $\varepsilon \to 0$ both the continuous moment models and the discretization have the correct diffusion limit:

- The P1 and M1 model are **asymptotic preserving** on a continuous level.
- The numerical schemes are **asymptotic preserving** for explicit and implicit pseudo-time discretization.

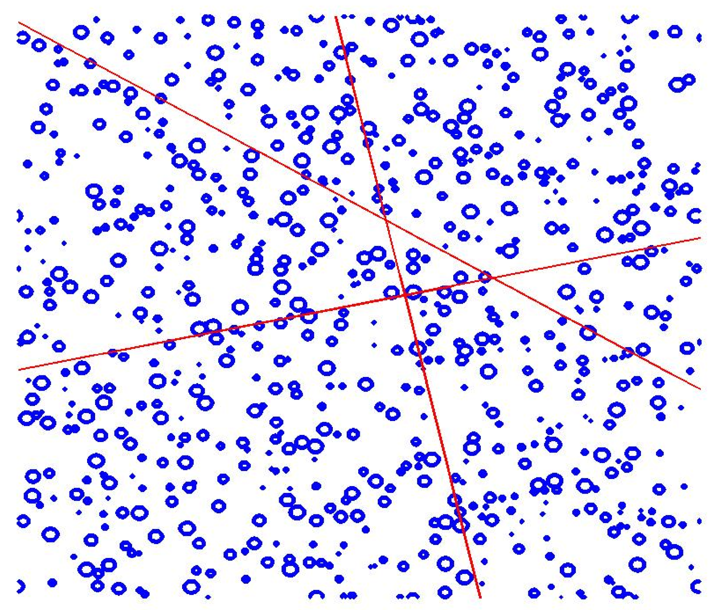
The only difference from the HLL scheme is the additional factor ε^2 in front of the numerical diffusion term; HLL alone yields a factor of ε. The moment models are asymptotic preserving without any adaptations.



M1 solution against diffusion, $\varepsilon = 0.02$

Work in progress

The key for an application of this new model is the knowledge of the collision frequency $\Sigma_t(s)$, which can be calculated from the **path-length distribution** $p(s)$. Therefore, in an ongoing project, we study the impact of spatial correlations between scatterers on the path-length distribution function in the **Boltzmann-Grad limit** through the use of Monte Carlo simulations. Furthermore, different scatterer-size distributions are also taken into account.



Path-lengths in a random medium

We expect that the limit exists for general correlated media and that the limiting distribution becomes independent of space and direction as long as the statistics of the medium is homogeneous.

References

[1] A.B. Kostinski, J. Optical Society of America, A. 18, no.8, 1929–1933, (2001).

[2] E. W. Larsen, Joint Int. Meeting on Math. Comp. & Supercomp. in Nucl. App., Monterey, California, on CD-ROM, Am. Nuc. Soc., LaGrange Park, IL (2007).

[3] E. W. Larsen, R. Vasques, JQRST, Vol. 112 (4), pp. 619–631 (2011).

[4] M. Frank, T. Goudon, Kinet. Relat. Models 3, 395–407 (2010).

[5] K. Krycki, C. Berthon, M. Frank, R. Turpault, accepted for publication in MMA (2013).

LaTeX TikZposter