Perfectly Matched Layers for Linear Transport

Herbert Egger (TU Darmstadt), Matthias Schlottbom
Department of Applied Mathematics

UNIVERSITY OF TWENTE.

Introduction

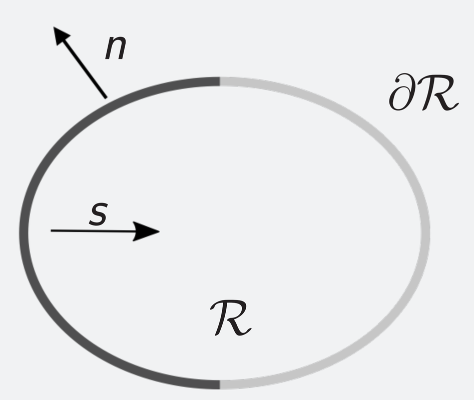
Linear Boltzmann equations are hyperbolic integro-partial differential equations describing the dynamics of a single-particle probability distribution in phase space. The dynamics is governed by streaming, damping and scattering. The two main challenges in the numerical approximation of solutions to linear Boltzmann equations are (i) the high dimensionality of the phase space, and (ii) the anisotropic structure of the solution. Item (i) refers to the seven space-velocity-time dimensions, making standard simulation methods extremely costly. Item (ii) stems from the interplay of transport and multiple scattering, such that it is impossible to find solutions analytically.
The linear Boltzmann equation is equivalent to a mixed variational problem that incorporates boundary conditions naturally [1, 2]. However, the natural inclusion of boundary conditions introduces a non-smooth coupling of spatial and velocity variables, which is inconvenient for practical implementations. To overcome this difficulty, we introduce an absorbing layer and consider a perturbed problem such that the resulting discretizations can be implemented easily and stored efficiently.

Remark 2. The question of proper boundary conditions for the P_N equations (and in fact moment models in general) is unsolved. In one space dimension various approaches exist, most prominently Marshak [15] or Mark [13, 14] boundary conditions. **(...)**
However, in two and three space dimensions, there is no agreement on the best choice of boundary conditions.

Figure 1: quoting: B. Seibold, M. Frank, StaRMAP - A second order staggered grid method for spherical harmonics moment equations of radiative transfer, ACM Trans. Math. Software, Vol. 41, No. 1, 2014.

Linear Transport Equation

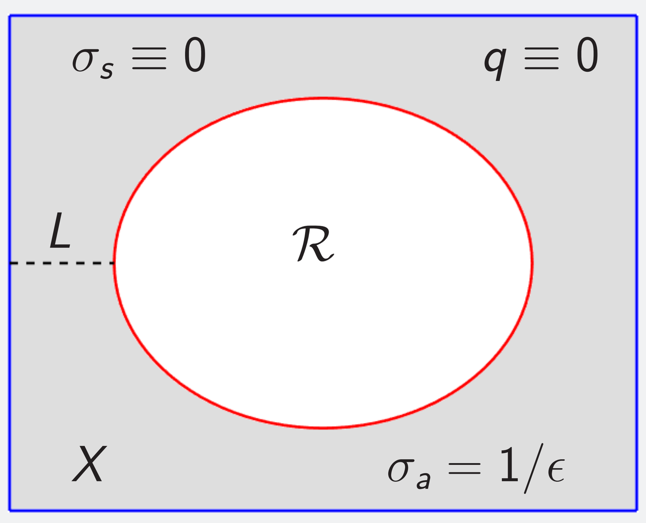
- $\phi(r,s)$ probability of finding a photon at point r with direction s
- $\mathcal{R} \subset \mathbb{R}^3$ bounded convex domain
- $\mathrm{supp}(q) \cup \mathrm{supp}(\sigma_s) \subset \mathcal{R}$
- $(K\phi)(r,s) = \int_S k(r,s'\cdot s)\phi(r,s')\,ds'$
- $\mathcal{C}\phi = (\sigma_a + \sigma_s)\phi - \sigma_s K\phi$

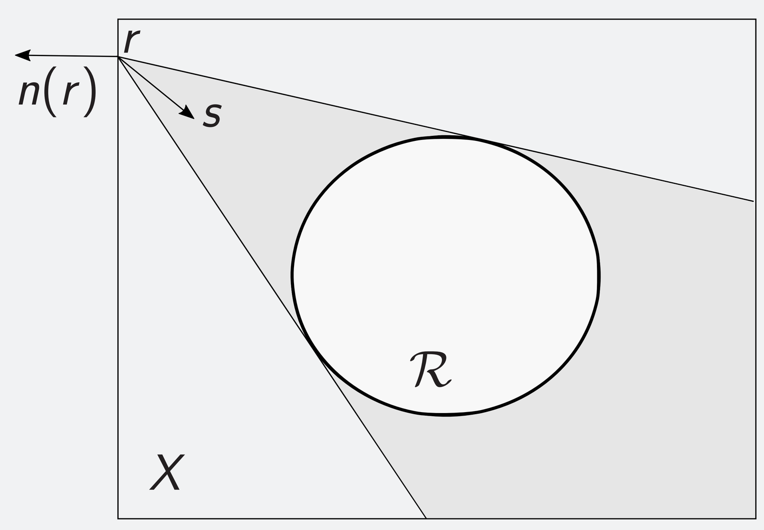


$$s\cdot\nabla\phi + \mathcal{C}\phi = q \quad \text{in } \mathcal{R}\times\mathcal{S}$$
$$\phi = 0 \quad \text{on } \Gamma_- = \{(r,s)\in\partial\mathcal{R}\times\mathcal{S} : s\cdot n(r) < 0\}$$

Theorem: Let $q \in L^p(\mathcal{R}\times\mathcal{S})$. The transport problems has a unique solution $\phi \in L^p(\mathcal{R}\times\mathcal{S})$ with $s\cdot\nabla\phi \in L^p(\mathcal{R}\times\mathcal{S})$, and $\phi_{|\Gamma_+} \in L^p(\Gamma_+; |s\cdot n|)$.

Perfectly Matched Layers





$$s\cdot\nabla\phi_\epsilon + (\sigma_a+\sigma_s)\phi_\epsilon = \sigma_s K\phi_\epsilon + q \quad \text{in } X\times\mathcal{S}$$
$$\phi_\epsilon(r,s) = \rho(r,s)\phi_\epsilon(r,-s) \quad \text{on } \Gamma_-^L$$

Theorem: The modified problem has a unique solution $\phi_\epsilon \in L^p(X\times\mathcal{S})$ with $s\cdot\nabla\phi_\epsilon \in L^p(X\times\mathcal{S})$ and $\phi_{\epsilon|\Gamma_+^L} \in L^p(\Gamma_+^L; |s\cdot n|)$.

Lemma: For $\rho = 0$ we have $\phi_{\epsilon|\mathcal{R}\times\mathcal{S}} = \phi_{|\mathcal{R}\times\mathcal{S}}$ and
$$\int_{\Gamma_+^L} |\phi_\epsilon|^2 |s\cdot n|\,d\Gamma \le e^{-2L/\epsilon}\int_{\Gamma_+} |\phi|^2|s\cdot n|\,d\Gamma.$$
$\exists \alpha = \alpha(X,\mathcal{R}) > 0$ such that $\phi(r,s) = 0$ for $(r,s)\in\Gamma_+^L$ with $|s\cdot n| \le \alpha$.

References

[1] Herbert Egger and Matthias Schlottbom.
A mixed variational framework for the radiative transfer equation.
Math. Mod. Meth. Appl. Sci., 22:1150014, 2012.

[2] Herbert Egger and Matthias Schlottbom.
A class of Galerkin Schemes for Time-Dependent Radiative Transfer.
SIAM J. Numer. Anal., 54(6):3577–3599, 2016.

[3] Herbert Egger and Matthias Schlottbom.
An L^p theory for stationary radiative transfer.
Appl. Anal., 93(6):1283–1296, 2014.

Mixed variational framework

Even-odd parities
$$\phi^\pm(s) = \frac{1}{2}(\phi(s) \pm \phi(-s))$$

Transport problem with reflection b.c. is equivalent to the system
$$s\cdot\nabla\phi_\epsilon^- + \mathcal{C}_\epsilon\phi_\epsilon^+ = q^+ \quad \text{in } X\times\mathcal{S}$$
$$s\cdot\nabla\phi_\epsilon^+ + \mathcal{C}_\epsilon\phi_\epsilon^- = q^- \quad \text{in } X\times\mathcal{S}$$
$$(1-\rho)\phi_\epsilon^+ + (1+\rho)\phi_\epsilon^- = 0 \quad \text{on } \Gamma_-^L$$

Find ϕ_ϵ such that for all sufficiently smooth ψ
$$2\langle\frac{1-\rho}{1+\rho}\phi_\epsilon^+, \psi^+|s\cdot n|\rangle_{\Gamma_-^L} + (s\cdot\nabla\phi_\epsilon^+,\psi^-) - (\phi_\epsilon^-, s\cdot\nabla\psi^+) + (\mathcal{C}_\epsilon\phi_\epsilon,\psi) = (q,\psi)$$

Observations
- odd part $\phi_\epsilon^- \in L^2(X\times\mathcal{S}) =: \mathbb{V}$
- even part $\phi_\epsilon^+ \in \mathbb{W}$ has more regularity: $s\cdot\nabla\phi_\epsilon^+ \in L^2$, regular trace
- boundary conditions are incorporated naturally

$$\rho(r,s) = \frac{|s\cdot n| - 1}{|s\cdot n| + 1} \quad \Longrightarrow \quad 2\langle\frac{1-\rho}{1+\rho}\phi^+, \psi^+|s\cdot n|\rangle_{\Gamma_-^L} = \langle\phi^+,\psi^+\rangle_{\partial X\times\mathcal{S}}$$

Theorem: Let $\|\psi\|_{\mathcal{C}_\epsilon}^2 = (\mathcal{C}_\epsilon\psi,\psi)$. The mixed variational problem has a unique solution $\phi_\epsilon \in \mathbb{W}^+ \oplus \mathbb{V}^-$, and the error $e_\epsilon = \phi_\epsilon - \phi$ satisfies the estimate
$$\|s\cdot\nabla e_\epsilon^+\|_{\mathcal{C}_\epsilon^{-1}} + \|e_\epsilon\|_{\mathcal{C}_\epsilon} + \|e_{\epsilon|\Gamma_+^L}\|_{L^2(\Gamma_+^L)} \le C\|\phi_{|\Gamma_+^L}\|_{L^2(\Gamma_+^L)}.$$

Galerkin approximations

- $\mathbb{W}_h^+ \subset \mathbb{W}^+$ and $\mathbb{V}_h^- \subset \mathbb{V}^-$ finite dimensional spaces
- $s\cdot\nabla\mathbb{W}_h^+ \subset \mathbb{V}_h^-$

Find $\phi_{\epsilon,h} \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$ such that for all $\psi_h \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$
$$\langle\phi_{\epsilon,h}^+, \psi_h^+\rangle_{\Gamma^L} + (s\cdot\nabla\phi_{\epsilon,h}^+, \psi_h^-) - (\phi_{\epsilon,h}^-, s\cdot\nabla\psi_h^+) + (\mathcal{C}_\epsilon\phi_{\epsilon,h},\psi_h) = (q,\psi_h)$$

- Galerkin problem is well-posed
- Quasi-best approximation error estimate in energy norm for $\phi_\epsilon - \phi_{\epsilon,h}$
- Error estimate for $\phi - \phi_{\epsilon,h}$ via triangle inequality

Tensor products and P_N approximation

- $\mathbb{S}_N^+ = \mathrm{span}\{Y_{2l}^m : 0 \le l \le N, -l \le m \le l\}$ spherical harmonics
- $\mathbb{X}_h^+ = \mathrm{span}\{\varphi_j : j \in J^+\} = P_1(T_h) \cap H^1(X)$
- Approximation space $\mathbb{W}_h^+ = \mathbb{S}_N^+ \otimes \mathbb{X}_h^+$, i.e.,

$$\phi_{\epsilon,h}^+(r,s) = \sum_{2l=0}^{N}\sum_{m=-l}^{l}\sum_{j\in J^+} a_{2l,m}^j\varphi_j(r)Y_{2l}^m(s) \in \mathbb{S}_N^+ \otimes \mathbb{X}_h^+$$

- $\dim\mathbb{X}_h^+ \sim h^{-d}$, $\dim\mathbb{S}_N^+ \sim N^{d-1}$

$$\langle\phi_{\epsilon,h}^+, \psi_h^+\rangle_{\Gamma^L} = \sum_{l,m,i}\sum_{k,n,j}\left(a_{2l,m}^i b_{2k,n}^j \int_{\partial X}\varphi_i\varphi_j\int_S Y_{2l}^m Y_{2k}^n\right) = \mathbf{a}^\mathsf{T}\mathbf{M}\mathbf{b}$$

- Storage complexity for $\mathbf{M} = O(h^{-d})$.

Checkerboard example

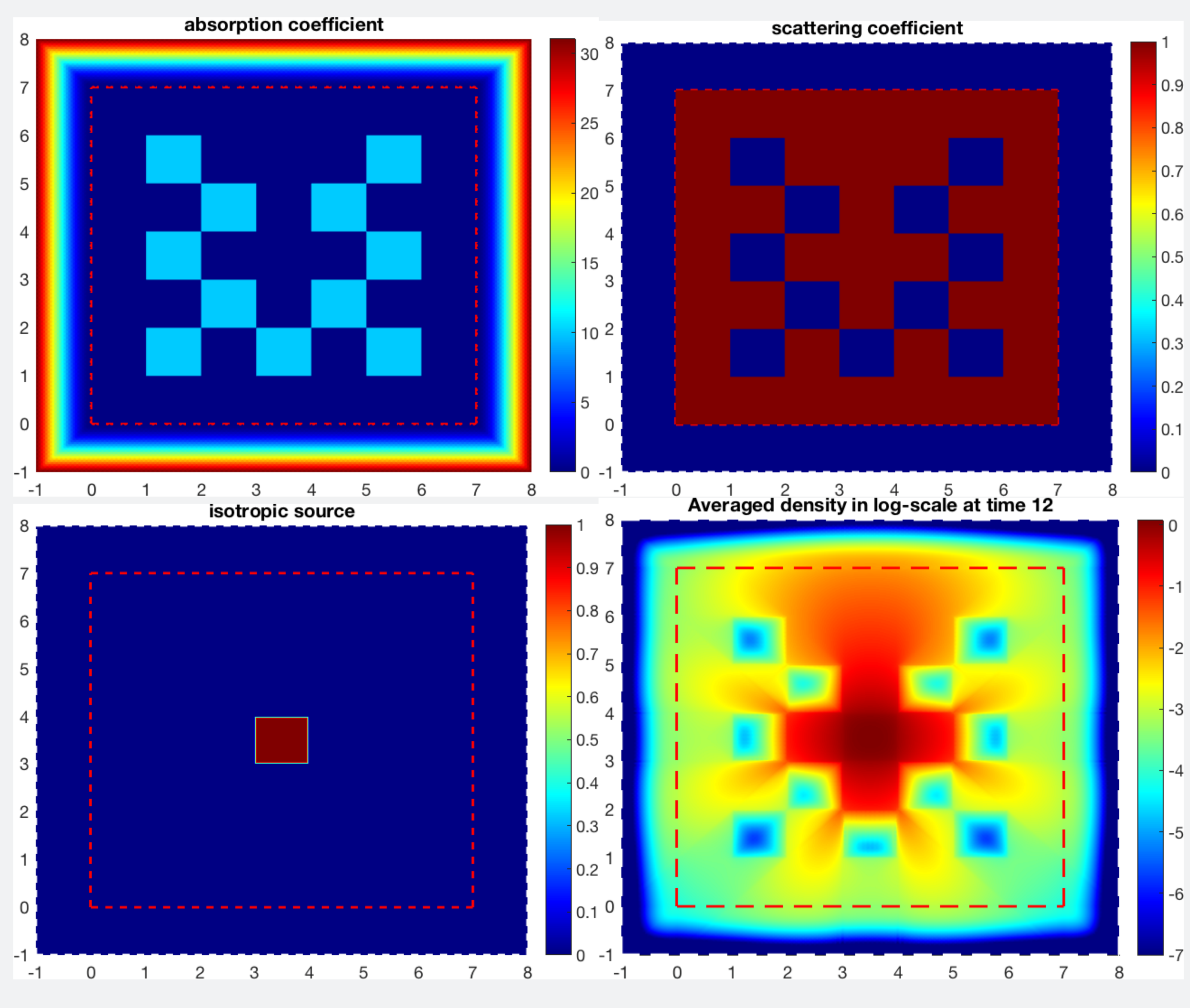


Figure 2: # vertices: 47,089. Angular dof: 2,704. total dof: 191,023,950.

http://wwwhome.ewi.utwente.nl/~schlottbomm/ m.schlottbom@utwente.nl