An angular multigrid method for modeling charged-particle transport in Flatland

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Charged-Particle Transport

Interest originated with radiation dose planning problem:

Given a known tumor within a patient, calculate a radiation beam configuration to irradiate the tumor while not harming nearby tissue.

Key assumption:

- Know tumor and healthy tissue locations and scattering properties

Constrained Optimization Problem

In general, the radiation dose planning problem takes the form of an optimization problem,

$$\min_{g:Lf=g} J(f),$$

where

- g describes the geometry and properties of the radiation beams
- f is the phase-space density of particles per unit volume
- $J(f)$ is a given cost function
- $Lf = g$ is the linear Boltzmann Transport Equation

While our ultimate goal is to solve this optimization problem, our focus for this talk is on the forward solver.

Linear Boltzmann Transport Equation

In general, $f = f(\mathbf{x}, \mathbf{v}, E, t)$, and $Lf = g$ takes the form

$$\frac{1}{c}\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \sigma_t(\mathbf{x}, E) f - \mathcal{K}_s f = 0$$

$$f(\mathbf{x}, \mathbf{v}, E, t_0) = f_0(\mathbf{x}, \mathbf{v}, E)$$

$$f(\mathbf{x}, \mathbf{v}, E, t) = g(\mathbf{x}, \mathbf{v}, E, t) \text{ for } \mathbf{x} \in \partial\Omega$$

where

- the phase-space density, f, is a function of particle location, $\mathbf{x}$, direction of travel, $\mathbf{v}$, energy, E, and time, t
- c is the particle speed
- σ_t is the probability of interaction per unit of distance traveled, $\sigma_t = \left(\overline{\lambda}\right)^{-1}$ for mean free path $\overline{\lambda} > 0$
- $\mathcal{K}_s$ is the scattering kernel

Our assumptions

$$\frac{1}{c}\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f + \sigma_t(\mathbf{x}, E)f - \mathcal{K}_s f = 0$$

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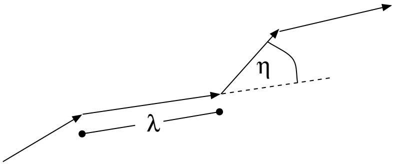
- time-independent case, $\frac{\partial f}{\partial t} = 0$
- E, c are constant (mono-energetic transport)
- $\mathcal{K}_s f = \left(\overline{\lambda}\right)^{-1} p * f$, for some convolution kernel, p
    - all interactions result in scattering

Flatland Model

Additionally, consider transport in only 2 spatial dimensions:

$$\mathbf{v} = (\cos(\theta), \sin(\theta))^T \text{ for } -\pi < \theta \leq \pi$$

Picture:



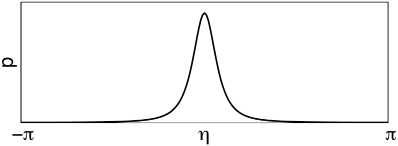
- Intercollision distances, λ, are independent, exponentially distributed with expectation $\overline{\lambda}$
- Scattering angles, η, are independent of each other and of λ

E.A. Abbott, *Flatland: a romance of many dimensions*, 1884

Choice of Scattering Kernel

Scattering for electron beams is highly forward peaked

- Let $p(\eta)$ be probability density for scattering with angle η
- $\mathcal{K}_s f = \left(\overline{\lambda}\right)^{-1} p * f = \left(\overline{\lambda}\right)^{-1} \int_{-\pi}^{\pi} p(\eta) f(\mathbf{x}, \theta - \eta) d\eta$



Compare to Neutron transport:

$$\mathcal{K}_s f = \sigma_s \int_{-\pi}^{\pi} f(\mathbf{x}, \theta - \eta) d\eta$$

for scattering cross-section σ_s.

The Fokker-Planck Limit

$$\cos(\theta)f_x + \sin(\theta)f_y = \frac{p * f - f}{\overline{\lambda}} = Qf$$

When $p(\eta)$ is small everywhere except near $\eta = 0$,

$$\begin{aligned} Qf &= \frac{1}{\overline{\lambda}}\left(\int_{-\pi}^{\pi} p(\eta)f(\theta-\eta)d\eta - f(\theta)\right) \\ &\approx \frac{1}{\overline{\lambda}}\left(\int_{-\pi}^{\pi} p(\eta)\left(f(\theta) - f_\theta(\theta)\eta + f_{\theta\theta}(\theta)\frac{\eta^2}{2}\right)d\eta - f(\theta)\right) \\ &= Df_{\theta\theta}(\theta) \end{aligned}$$

for $D = \frac{1}{2\overline{\lambda}}\int_{-\pi}^{\pi}\eta^2 p(\eta)d\eta$

In limit as $\overline{\lambda} \to 0$ and $\int_{-\pi}^{\pi}\eta^2 p(\eta)d\eta \to 0$, $Qf \rightharpoonup Df_{\theta\theta}$

C. Börgers, J. Comput. Phys. 1997, **133**:323-339

Mixed Elliptic-Hyperbolic Operator

$$\cos(\theta) f_x + \sin(\theta) f_y = \frac{p * f - f}{\bar{\lambda}} = Qf$$

Operator has mixed character

- Left-hand side has hyperbolic character in x and y
- Right-hand side, Qf, is always negative definite
  - $Qf \rightharpoonup Df_{\theta\theta}$ in appropriate limit

Goal: develop a fast solver for this equation

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Large body of literature on accurate discretization for Boltzmann Transport

We start with the simplest possible one

Discretization in Angle

Define Fourier coefficients,

$$\hat{p}_n = \int_{-\pi}^{\pi} e^{-in\eta} p(\eta)\, d\eta, \text{ and } \hat{f}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-in\tau} f(\tau)\, d\tau,$$

so that

$$Qf(\theta) = \sum_{n=-\infty}^{\infty} \frac{\hat{p}_n - 1}{\bar{\lambda}} \hat{f}_n \exp(in\theta).$$

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Define $\Delta\theta = \frac{2\pi}{n_\theta}$, and $\Gamma_{n_\theta} = \{\theta_l = l\Delta\theta \mid -\frac{n_\theta}{2} + 1 \le l \le \frac{n_\theta}{2}\}$. Discretize $f(\mathbf{x}, \theta)$ in angle by writing $\mathbf{f} = f(\mathbf{x}, \theta_l)$ for $\theta_l \in \Gamma_{n_\theta}$, giving

$$\left(Q^{\Delta\theta}\mathbf{f}\right)_l = \frac{1}{n_\theta} \sum_{n=-n_\theta/2+1}^{n_\theta/2} \sum_{m=-n_\theta/2+1}^{n_\theta/2} \frac{\hat{p}_n - 1}{\bar{\theta}} \cos(n(\theta_l - \theta_m)) f(\theta_m)\,.$$

Discretization in Space

For each θ_l, equation in x and y is simply advection:

$$\cos(\theta_l) f_x + \sin(\theta_l) f_y = (Q^{\Delta\theta}\mathbf{f})_l$$

To accurately capture these effects, use upstream finite differences for each of f_x and f_y:

$$\varphi'(s) = \frac{\varphi(s) - \varphi(s - \Delta s)}{\Delta s} + O(\Delta s),$$
$$\varphi'(s) = \frac{1.5\varphi(s) - 2\varphi(s - \Delta s) + 0.5\varphi(s - 2\Delta s)}{\Delta s} + O(\Delta s^2).$$

Choose sign of Δs based on signs of $(\cos(\theta_l), \sin(\theta_l))$.

An Angular Relaxation Scheme

Consider block ordering of equations by Γ_{n_θ}:

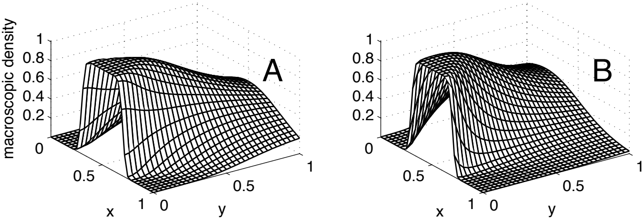
$$\begin{bmatrix} D_{-\frac{n_\theta}{2}+1} + Q_0 & Q_1 & \dots & Q_{-1} \\ Q_{-1} & D_{-\frac{n_\theta}{2}+2} + Q_0 & \dots & Q_{-2} \\ & \ddots & \ddots & \vdots \\ Q_1 & \dots & Q_{-1} & D_{\frac{n_\theta}{2}} + Q_0 \end{bmatrix} \begin{bmatrix} f_{-\frac{n_\theta}{2}+1} \\ f_{-\frac{n_\theta}{2}+2} \\ \vdots \\ f_{\frac{n_\theta}{2}} \end{bmatrix}$$

For each l, can order f_l so that $D_l + Q_0$ is lower triangular

- Block Jacobi solves can be done exactly
- Choose Red-Black (or Black-Red) ordering for efficiency of the resulting multigrid algorithm

Performance of Relaxation

Test Problem with smooth broad beam, not grid-aligned:



	$n_\theta = 32$	$n_\theta = 64$	$n_\theta = 128$	$n_\theta = 256$	$n_\theta = 512$
$n_s = 32$	0.304	0.662	0.953	0.977	0.988
$n_s = 64$	0.299	0.652	0.943	0.971	0.984
$n_s = 128$	0.294	0.642	0.930	0.963	0.977
$n_s = 256$	0.290	0.633	0.917	0.951	0.969
$n_s = 512$	0.286	0.624	0.903	0.938	0.958

Coarsening in Angle

Performance of relaxation seems independent of n_s

Idea: Coarsen only in θ.

- Relaxation damps all errors in x and y
- Elliptic character means Jacobi smooths in θ

Angular coupling has a constant stencil, so try to use simple grid-transfers

- Linear interpolation
- Full-weighting restriction
- Rediscretization for coarse-grid operators

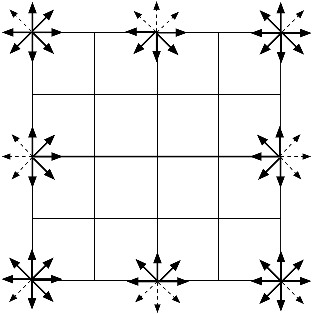
J. Morel and T. Manteuffel, Nuclear Science and Engineering, 1991, **107**:330-342

S. Vandewalle and G. Horton, Computing, 1995, **54**:317-330

Complication: Boundary Conditions

Boundary values are prescribed only at inflow boundaries

Natural choice: if $(\cos(\theta_l), \sin(\theta_l))$ points into domain at $(x, y) \in \partial\Omega$, prescribe $f(x, y, \theta_l)$
Difficulty: What to do at $\theta = -\frac{\pi}{2}, 0, \frac{\pi}{2}, \pi$?



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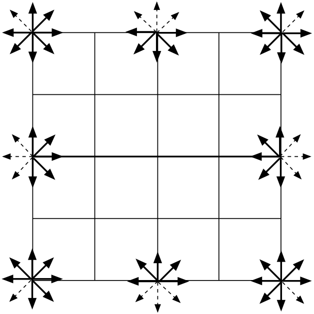

Possible Solutions:

1. Carefully define transfer operators for θ_l near transitions from inflow to outflow
2. Redefine “inflow” and “outflow” so that simple transfer operators don’t mix them

Numerical Results

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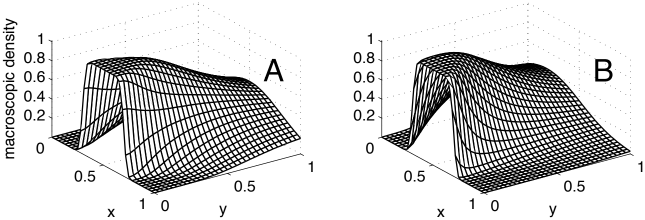

Effective convergence factors for V(0,1) cycles

	$n_\theta = 32$	$n_\theta = 64$	$n_\theta = 128$	$n_\theta = 256$	$n_\theta = 512$
$n_s = 32$	0.698	0.702	0.701	0.706	0.714
$n_s = 64$	0.701	0.707	0.705	0.706	0.712
$n_s = 128$	0.703	0.708	0.714	0.706	0.710
$n_s = 256$	0.706	0.708	0.715	0.708	0.711
$n_s = 512$	0.708	0.709	0.726	0.712	0.711

Numerical Results

Dependence on mean free path for $n_s = n_\theta = 128$:

$\overline{\lambda}$	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$\left(\overline{\rho}_{1,24}\right)^{1/4}$	0.704	0.704	0.706	0.713	0.716	0.717	0.717

Performance for 3-point Fokker-Planck Discretization:

	$n_\theta = 32$	$n_\theta = 64$	$n_\theta = 128$	$n_\theta = 256$	$n_\theta = 512$
$n_s = 32$	0.699	0.699	0.702	0.709	0.718
$n_s = 64$	0.702	0.702	0.703	0.708	0.716
$n_s = 128$	0.704	0.704	0.705	0.708	0.714
$n_s = 256$	0.705	0.707	0.707	0.708	0.713
$n_s = 512$	0.708	0.709	0.724	0.709	0.713

Summary

- Simplified, “Flatland” model of Boltzmann Transport Equation
- Collision operator is elliptic, model is mixed elliptic-hyperbolic
- Angular multigrid method based on downstream relaxation
- Efficient and scalable solution algorithm

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Future Directions

- Three space dimensions, scattering in S^2
- Local grid refinement in space and angle
- Other discretization techniques