A conservative spectral method for the Boltzmann equation with anisotropic scattering and the grazing collisions limit

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Outline of talk

1. Spectral method for Boltzmann-type collision operators with anisotropic scattering
   - Parallelization

2. Grazing collisions and the Landau equation

The Boltzmann equation

Boltzmann equation:

$$\frac{Df}{Dt}(\mathbf{x}, \mathbf{v}, t) = Q(f, f)(\mathbf{v}), \quad \mathbf{v} \in \mathbb{R}^3,$$

$Q(f, f)$ is the collision operator:

$$Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{u}|, \hat{\mathbf{u}} \cdot \sigma)(f(\mathbf{v}'_*)f(\mathbf{v}') - f(\mathbf{v}_*)f(\mathbf{v}))d\sigma d\mathbf{v}_*$$

Numerical methods

- Direct Simulation Monte Carlo
  - Bird, Nanbu, ...
  - conservation, positivity, overcomes dimensionality
  - noise, transients, time dependent problems, tails, low speed flows, etc.
- Deterministic methods (spectral, DVM....)
  - Advantages: no noise, accuracy in $\mathbf{v}$
  - Disadvantages: Positivity, conservation, **dimensionality**

  Previous spectral works
  - Bobylev (75), Bobylev-Rjasanow (97, 99, 00), Ibragimov-Rjasanow (02), Pareschi-Russo (00), Mouhot-Pareschi (04), Pareschi-Russo-Toscani (00) (Landau), Pareschi-Toscani-Villani (03) (Grazing collisions consistency)
  - Weak form: **Gamba-Tharkabhushanam** (09, 10) - conservation, inelastic

Spectral formulation of collision operator

- Weak (Maxwell) form of collision operator:

$$\int Q(f,f)\,\phi(\mathbf{v})\,d\mathbf{v} = \int f(\mathbf{v})f(\mathbf{v}_*)[\phi(\mathbf{v}')-\phi(\mathbf{v})]\,B(|\mathbf{u}|,\cos\theta)\,d\sigma d\mathbf{v}_* d\mathbf{v}\,,$$

- Let

$$\phi(\mathbf{v}) = e^{-i\zeta\cdot\mathbf{v}}/(\sqrt{2\pi})^3,$$

then we have that the Fourier transform of the collision integral is

$$\begin{aligned}
\widehat{Q}(\zeta) &= \int_{\mathbb{R}^3} \mathcal{F}\{f(\mathbf{v})f(\mathbf{v}-\mathbf{u})\}(\zeta)G(\zeta,\mathbf{u})d\mathbf{u} \\
&= \int_{\mathbf{u}\in\mathbb{R}^3} G(\mathbf{u},\zeta)\frac{1}{(\sqrt{2\pi})^3}\int_{\xi\in\mathbb{R}^3}\hat{f}(\zeta-\xi)\hat{f}(\xi)e^{-i\xi\cdot\mathbf{u}}d\xi d\mathbf{u} \\
&= \boxed{\frac{1}{(\sqrt{2\pi})^3}\int_{\xi\in\mathbb{R}^3}\hat{f}(\zeta-\xi)\hat{f}(\xi)\hat{G}(\xi,\zeta)d\xi}
\end{aligned}$$

Spectral formulation of collision operator

The convolution weights $G(\zeta, \mathbf{u})$, $\hat{G}(\xi, \zeta)$ are given by

$$G(\zeta, \mathbf{u}) = \int_{\sigma \in S^2} B(|u|, \cos\theta)(e^{-i\frac{\zeta}{2}\cdot(\mathbf{u}'-\mathbf{u})} - 1)d\sigma.$$

$$\hat{G}(\xi, \zeta) = \int_{\mathbf{u}\in\mathbb{R}^3} e^{-i\xi\cdot\mathbf{u}} \int_{\sigma \in S^2} B(|u|, \cos\theta)(e^{-i\frac{\zeta}{2}\cdot(\mathbf{u}'-\mathbf{u})} - 1)d\sigma d\mathbf{u}.$$

For $B = |u|^\lambda/4\pi$ (isotropic), this can be reduced to

$$\hat{G}(\xi, \zeta) = \int_0^\infty r^{\lambda+2}[\mathrm{sinc}(\frac{r|\zeta|}{2})\mathrm{sinc}(r|\xi - \frac{\zeta}{2}|) - \mathrm{sinc}(r|\xi|)]dr$$

no time dependence

Difficulties in simulating the Boltzmann equation

$$Q(f,f)(v) = \int_{\mathbb{R}^3}\int_{S^2} B(|\mathbf{u}|, \hat{\mathbf{u}}\cdot\sigma)(f(\mathbf{v}'_*)f(\mathbf{v}') - f(\mathbf{v}_*)f(\mathbf{v}))d\sigma d\mathbf{v}_*$$

Issues:

- **Dimensionality**: requires $O(N^6)$ operations for a single evaluation of weighted convolution

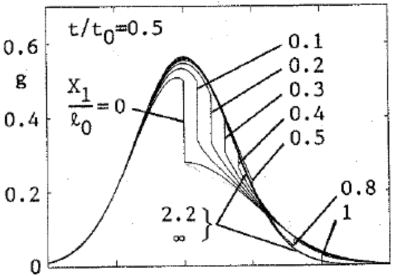
Computation is embarassingly parallel!

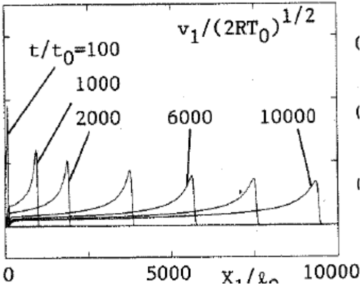
Test problem: 1280 spatial points, 24^3 velocity mesh points
Time listed: wall time using Stampede (NSF XSEDE resource) for one timestep ($\sim$244 billion operations)

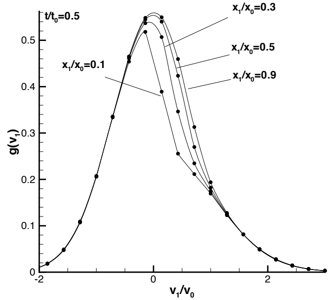
nodes	cores	time (s)
1	16	456.313
2	32	235.315
4	64	120.762
8	128	61.345
16	256	30.943
32	512	15.252
64	1024	7.813
128	2048	4.042

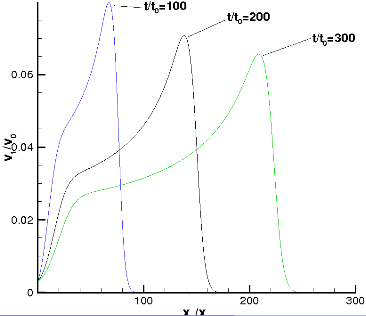
[H. submitted 2013, also arXiv]

Sudden Heating problem









Difficulties in simulating the Boltzmann equation

$$Q(f,f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{u}|, \hat{\mathbf{u}} \cdot \sigma)(f(\mathbf{v}'_*)f(\mathbf{v}') - f(\mathbf{v}_*)f(\mathbf{v}))d\sigma d\mathbf{v}_*$$

Issues:

- **Dimensionality**: requires $O(N^6)$ operations for a single evaluation of weighted convolution
- **Conservation**: collision invariants need to be preserved.

$$\int_{\mathbf{v} \in \mathbb{R}^3} Q(f,f) \begin{pmatrix} 1 \\ \mathbf{v} \\ |v|^2 \end{pmatrix} = 0.$$

Solve the constrained minimization problem in $O(N^3)$ (Gamba, Tharkabhushanam)

$$\left\{ \min \frac{1}{2} \|\tilde{\mathbf{Q}} - \mathbf{Q}\|_2^2 \mid \mathbf{CQ} = \mathbf{0} \right\}$$

Anisotropic scattering

- Potentials interactions (e.g. Coulomb) include an angular component. Write $B = |\mathbf{u}|^\lambda b(\cos\theta)$.
- In this case, the untransformed weight $G(\mathbf{u},\zeta)$ is given by

$$G(\mathbf{u},\zeta) = |\mathbf{u}|^\lambda \left(\int_{S^{d-1}} b(\hat{\mathbf{u}}\cdot\sigma)(e^{i\frac{\zeta}{2}\cdot\mathbf{u}} e^{-i\frac{\zeta|\mathbf{u}|}{2}\cdot\sigma} - 1) d\sigma \right)$$

$$= 2\pi|\mathbf{u}|^\lambda \int_0^\pi b(\cos\theta)\sin\theta \left(e^{i\frac{(1-\cos\theta)\zeta}{2}\cdot\mathbf{u}} J_0\left(\frac{|\mathbf{u}|\sin\theta|\zeta^\perp|}{2} \right) - 1 \right) d\theta,$$

$\zeta^\perp = \zeta - (\zeta\cdot\mathbf{u}/|u|)\mathbf{u}/|u|$.

$$\widehat{G}(\zeta,\xi) = 4\pi^2 \int_0^L r^{\lambda+2} \int_0^\pi \int_0^\pi b(\cos\theta)\sin\theta\sin\phi J_0\left(r|\xi^\perp|\sin\phi\right) \times$$

$$\left[\cos\left(r(\xi - \frac{\zeta}{2}(1-\cos\theta))\cdot\frac{\zeta}{|\zeta|}\cos\phi \right) J_0\left(\frac{1}{2} r|\zeta|\sin\phi\sin\theta \right) - \cos\left(r\xi\cdot\frac{\zeta}{|\zeta|}\cos\phi \right) \right] d\theta d\phi dr$$

The Coulombic (grazing) limit

- It is well known that when the underlying potential is Coulombic, long distance grazing collisions dominate the collision term (Landau '36).

$$Q_L = \nabla_{\mathbf{v}} \cdot \left(\int |u|^{\lambda+2} (\delta_{ij} - \frac{u_i u_j}{|\mathbf{u}|^2})(f(\mathbf{v}_*)\nabla_v f(\mathbf{v}) - f(\mathbf{v})\nabla_v f(\mathbf{v}_*)) \right) d\mathbf{v}_*$$

- Similar weak formulation gives

$$\boxed{G_L(\mathbf{u}, \zeta) = |u|^\lambda \left(4i(\zeta \cdot \mathbf{u}) - |u|^2 |\zeta^\perp|^2 \right)}$$

- Pareschi, Toscani, and Villani (2003): convergence to Landau for collocation.
- However, no computations were done in this limiting regime to our knowledge.

Approximating Boltzmann by Landau

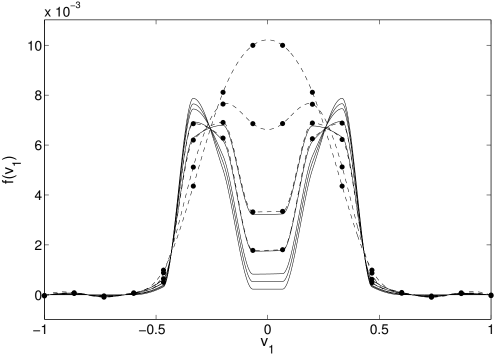
Using Screened Coulomb:

$$B = |\mathbf{u}|^{-3} \frac{C}{\sin^4(\theta/2)} 1_{\theta \geq \varepsilon},$$

$\varepsilon \sim r_0/\lambda_D^3$.
Isotropic initial condition:

$$f(\mathbf{v}, 0) = \frac{1}{100} e^{\left(-10\left(\frac{|\mathbf{v}|-1.5}{1.5}\right)^2\right)}$$

$\varepsilon = 10^{-4}, N = 16$



Solid lines: Landau solution. Dashed lines: Boltzmann solution.
$t = 0, 1, 2, 5, 10.$

Scattering kernel

Make the following assumptions on the scattering kernel. Let $\varepsilon > 0$ be the small parameter associated with the grazing collision limit. A family of kernels b_ε are grazing if (Villani, Bobylev):

- $\Lambda_\varepsilon = 2\pi \int_0^\pi b_\varepsilon(\cos\theta)\sin^2(\theta/2)\sin\theta d\theta \to \Lambda_0 < \infty$
- $\forall\theta_0 > 0, \qquad b_\varepsilon(\cos\theta) \to 0 \qquad$ uniformly on $\theta \geq \theta_0$
- This corresponds to $\int_0^\pi b_\varepsilon(\cos\theta)\sin\theta\ \theta^k d\theta \to 0, \quad k > 2$

Some examples

$$\text{Coulomb: } b_\varepsilon(\cos\theta)\sin\theta = C\frac{\sin\theta}{\sin^4(\theta/2)\log\sin(\varepsilon/2)}1_{\theta\geq\varepsilon}$$

$$\varepsilon\text{-linear: } b_\varepsilon(\cos\theta)\sin\theta = \frac{8\varepsilon}{\pi\theta^4}1_{\theta\geq\varepsilon},$$

Note for ε-linear:

$$\int_0^\pi b_\varepsilon(\cos\theta)\sin\theta(\theta^2)d\theta \approx \frac{C\varepsilon}{\theta}\Big|_\varepsilon^\pi = C(1-\frac{\varepsilon}{\pi})$$

Convergence of Boltzmann to Landau

$$\widehat{Q}_\varepsilon(\zeta) \;=\; \int_{\mathbb{R}^3} \mathcal{F}\{f_\varepsilon(\mathbf{v})f_\varepsilon(\mathbf{v}-\mathbf{u})\}(\zeta)G_\varepsilon(\zeta,\mathbf{u})d\mathbf{u}$$

Theorem

(H., Gamba.) Assume that f_ε satisfies

$$|\mathcal{F}\{f_\varepsilon(\mathbf{v})f_\varepsilon(\mathbf{v}-\mathbf{u})\}(\zeta)| \le \frac{A(\zeta)}{1+|u|^3}, \tag{1}$$

with A uniformly bounded in ζ, and that $b(\cos\theta)$ is the screened Rutherford cross section. Then the rate of convergence of the Boltzmann collision operator with grazing collisions to the Landau collision operator is given by

$$\left|\widehat{Q}_L[f_\varepsilon](\zeta) - \widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta)\right| \;\le\; O\left(\frac{1}{|\log\sin(\varepsilon/2)|}\right) \to 0 \quad \text{as } \varepsilon \to 0. \tag{2}$$

sketch of proof

$$G_\varepsilon(\mathbf{u},\zeta) = |\mathbf{u}|^\lambda \left(\int_{S^{d-1}} b_\varepsilon(\cos\theta)(e^{i\frac{\zeta}{2}\cdot\mathbf{u}} e^{-i\frac{\zeta|\mathbf{u}|}{2}\cdot\sigma} - 1) d\sigma \right)$$

$$= |\mathbf{u}|^\lambda \int_0^\pi \int_0^{2\pi} b_\varepsilon(\cos\theta)\sin\theta$$

$$\times \left(e^{\frac{i}{2}((1-\cos\theta)\zeta\cdot\mathbf{u} + |u|\zeta\cdot j\sin\theta\sin\phi + |u|\zeta\cdot k\sin\theta\cos\phi)} - 1 \right) d\phi d\theta,$$

First two terms of the expansion:

$$= \frac{2|u|^{-3}}{-\log\sin(\varepsilon/2)} \int_\varepsilon^\pi \frac{\cos(\theta/2)}{\sin(\theta/2)} i(\mathbf{u}\cdot\zeta) - \frac{1}{2}\sin(\theta/2)\cos(\theta/2)(\mathbf{u}\cdot\zeta)^2 d\theta$$

$$= |u|^{-3}\left(4i(\mathbf{u}\cdot\zeta) - |u|^2|\zeta^\perp|^2\right)$$

$$- |u|^{-3}\left(\frac{1}{2}(\mathbf{u}\cdot\zeta)^2 + \frac{1}{4}|\zeta^\perp|^2|u|^2\right)\frac{(1+\cos\varepsilon)}{\log\sin(\varepsilon/2)}.$$

sketch of proof

$$\widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta) = \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v)f_\varepsilon(v-u)\}(\zeta)R(\zeta,\mathbf{u})du \qquad (3)$$

$$= \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v)f_\varepsilon(v-u)\}(\zeta)$$
$$\times \left(\frac{|u|^{-3}}{|\log\sin(\varepsilon/2)|} \left(\frac{(\mathbf{u}\cdot\zeta)^2}{2} + \frac{1}{4}|\zeta^\perp|^2|u|^2 \right)(1+\cos\varepsilon) \right.$$
$$\left. + \frac{|u|^{-3}}{|\log\sin(\varepsilon/2)|} \sum_{n=3}^{\infty} G_{b_\varepsilon,n}(\zeta,\mathbf{u}) \right) du.$$

sketch of proof

$$|R(\zeta,\mathbf{u})| \leq \frac{2|\zeta|^2}{|u||\log\sin(\varepsilon/2)|}(1+\cos\varepsilon) + \frac{2\pi|\zeta|^3}{|\log\sin(\varepsilon/2)|}\left(\frac{|\zeta|^2}{|u|} + \frac{2|\zeta|}{|u|^2} + \frac{2\sqrt{2}\sin(2|u||\zeta|)}{|u|^3}\right). \tag{4}$$

All integrable at zero, and

$$|\mathcal{F}\{f_\varepsilon(\mathbf{v})f_\varepsilon(\mathbf{v}-\mathbf{u})\}(\zeta)| \leq \frac{A(\zeta)}{1+|u|^3},$$

gives integrability at ∞

$$\widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta) = \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v)f_\varepsilon(v-u)\}(\zeta)R(\zeta,\mathbf{u})d\mathbf{u} \tag{5}$$

Note: this ansatz is satisfied by the Maxwellian distribution.

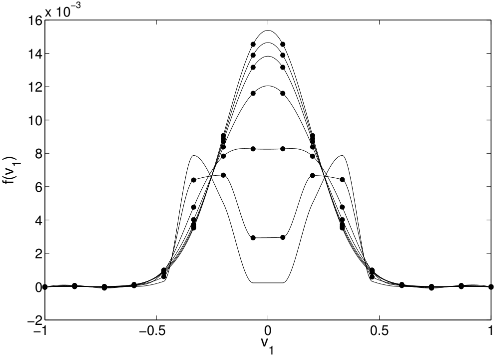
Numerical Results

Using ε-linear:

$$b_\varepsilon(\cos\theta)\sin\theta = \frac{8\varepsilon}{\pi\theta^4}1_{\theta\geq\varepsilon},$$

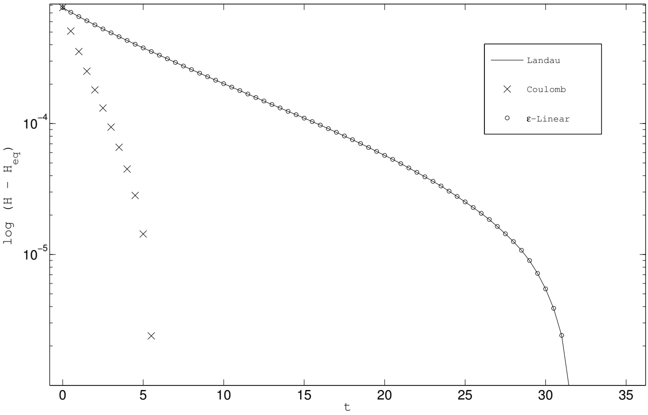
Isotropic initial condition:

$$f(\mathbf{v},0) = \frac{1}{100}e^{\left(-10\left(\frac{|\mathbf{v}|-1.5}{1.5}\right)^2\right)}$$



Solid line: solution to Landau. Dots: solution of Boltzmann with ε-linear scattering kernel.

Rate of convergence to equilibrium



Conclusions, future work

- 'Extra' term in b_ε - different time scale?
- Main issue for large scale calculation: **storage**
  - Weights $\widehat{G}(\zeta, \xi)$ require $O(N^6)$ storage. ($N = 40 \to \sim$250 GB of memory)
  - "Flops are free" - can we compute weights on the fly?
  - work in progress (with J. Hu, I. Gamba): $O(M^2 N^4 \log N)$ algorithm requires no precomputation, but inefficient for moderate N
- Other anisotropic scattering potentials
- Multispecies/multi-energy level (with T. Magin and A. Munafo)
- Parallel computing: MIC vs GPU?

Thank you!