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

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Issues in Solving the Boltzmann Equation for Aerospace Applications

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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:

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

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

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

\[
\int Q(f, f) \phi(v) dv = \int f(v)f(v_*)[\phi(v')-\phi(v)] B(|u|, \cos \theta) d\sigma dv_* dv,
\]

- Let

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

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

\[
\hat{Q}(\zeta) = \int \mathcal{F}\{f(v)f(v-u)\}(\zeta) G(\zeta, u) du
\]

\[
= \int_{u \in \mathbb{R}^3} G(u, \zeta) \frac{1}{(\sqrt{2\pi})^3} \int_{\xi \in \mathbb{R}^3} \hat{f}(\zeta - \xi) \hat{f}(\xi) e^{-i\xi \cdot u} d\xi du
\]

\[
= \frac{1}{(\sqrt{2\pi})^3} \int_{\xi \in \mathbb{R}^3} \hat{f}(\zeta - \xi) \hat{f}(\xi) \hat{G}(\xi, \zeta) d\xi
\]
The convolution weights $G(\zeta, u)$, $\hat{G}(\xi, \zeta)$ are given by

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

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

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

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

no time dependence
Difficulties in simulating the Boltzmann equation

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

Issues:

- **Dimensionality**: requires \( O(N^6) \) operations for a single evaluation of weighted convolution
Computation is embarrassingly parallel!

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

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[H. submitted 2013, also arXiv]
Sudden Heating problem

- For $t/t_0 = 0.5$
  - $x_1/x_0 = 0.1, 0.2, 0.3, 0.4, 0.5$
- For $t/t_0 = 100$
  - $v_1/(2RT_0)^{1/2} = 1000, 2000, 6000, 10000$

$g(v_1)$ vs $v_1/v_0$ for $x_1/x_0 = 0.1, 0.3, 0.5, 0.9$

$g(v_1)$ vs $v_1/v_0$ for $t/t_0 = 100, 200, 300$
Difficulties in simulating the Boltzmann equation

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

Issues:

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

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

Solve the constrained minimization problem in \( O(N^3) \) (Gamba, Tharkabushanam)

\[ \left\{ \min \frac{1}{2} \| \tilde{Q} - Q \|_2^2 \mid CQ = 0 \right\} \]
Anisotropic scattering

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

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

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

$\zeta \perp = \zeta - (\zeta \cdot u / |u|) u / |u|$.

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

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

$$- \cos \left( r \xi \cdot \frac{\zeta}{|\zeta|} \cos \phi \right) \right] d\theta d\phi dr.$$
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).

\[ Q_L = \nabla_v \cdot \left( \int |u|^\lambda+2 (\delta_{ij} - \frac{u_i u_j}{|u|^2}) (f(v_*) \nabla_v f(v) - f(v) \nabla_v f(v_*)) \right) dv_* \]

- Similar weak formulation gives

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


- However, no computations were done in this limiting regime to our knowledge.
Approximating Boltzmann by Landau

Using Screened Coulomb:

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

\[ \varepsilon \sim r_0/\lambda^3_D. \]

Isotropic initial condition:

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

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

\[ t = 0, 1, 2, 5, 10. \]
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 $b_\varepsilon$ are grazing if (Villani, Bobylev):

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

Some examples

**Coulomb:**

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

**$\varepsilon$-linear:**

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

Note for $\varepsilon$-linear:

$$\int_0^\pi b_\varepsilon(\cos \theta) \sin \theta (\theta^2) d\theta \approx \frac{C\varepsilon}{\theta} \bigg|_{\varepsilon}^\pi = C(1 - \frac{\varepsilon}{\pi})$$
Convergence of Boltzmann to Landau

\[ \hat{Q}_\varepsilon(\zeta) = \int_{\mathbb{R}^3} \mathcal{F}\{f_\varepsilon(v)f_\varepsilon(v-u)\}(\zeta)G_\varepsilon(\zeta, u)du \]

**Theorem**

(H., Gamba.) Assume that \( f_\varepsilon \) satisfies

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

with \( A \) uniformly bounded in \( \zeta \), 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

\[ \left| \hat{Q}_L[f_\varepsilon](\zeta) - \hat{Q}_{b_\varepsilon}[f_\varepsilon](\zeta) \right| \leq O \left( \frac{1}{|\log \sin(\varepsilon/2)|} \right) \rightarrow 0 \quad \text{as} \ \varepsilon \rightarrow 0. \]
sketch of proof

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

\[ = |u|^\lambda \int_0^\pi \int_0^{2\pi} b_\varepsilon(\cos \theta) \sin \theta \]
\[ \times \left( e^{i \frac{\zeta}{2} \cdot (1 - \cos \theta) \cdot u + |u| \zeta \cdot j \sin \theta \sin \phi + |u| \zeta \cdot k \sin \theta \cos \phi} - 1 \right) d\phi d\theta, \]

First two terms of the expansion:

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

\[ = |u|^{-3} \left( 4i(u \cdot \zeta) - |u|^2 |\zeta^\perp|^2 \right) \]
\[ - |u|^{-3} \left( \frac{1}{2} (u \cdot \zeta)^2 + \frac{1}{4} |\zeta^\perp|^2 |u|^2 \right) \frac{(1 + \cos \varepsilon)}{\log \sin(\varepsilon/2)}. \]
sketch of proof

\[
\widehat{Q_{b\varepsilon}}[f_\varepsilon](\zeta) = \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(\nu)f_\varepsilon(\nu - u)\}(\zeta)R(\zeta, u)\,du
\]

\[
= \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(\nu)f_\varepsilon(\nu - u)\}(\zeta)
\times \left( \frac{|u|^{-3}}{|\log \sin(\varepsilon/2)|} \left( \frac{(u \cdot \zeta)^2}{2} + \frac{1}{4}|\zeta|^2|u|^2 \right) (1 + \cos \varepsilon) \right)
\]

\[
+ \frac{|u|^{-3}}{|\log \sin(\varepsilon/2)|} \sum_{n=3}^{\infty} G_{b_\varepsilon,n}(\zeta, u)\right)\,du.
\]
sketch of proof

\[ |R(\zeta, \mathbf{u})| \leq \frac{2|\zeta|^2}{|\mathbf{u}||\log \sin(\epsilon/2)|} (1 + \cos \epsilon) \]

\[ + \frac{2\pi|\zeta|^3}{|\log \sin(\epsilon/2)|} \left( \frac{|\zeta|^2}{|\mathbf{u}|} + \frac{2|\zeta|}{|\mathbf{u}|^2} + \frac{2\sqrt{2}\sin(2|\mathbf{u}||\zeta|)}{|\mathbf{u}|^3} \right). \tag{4} \]

All integrable at zero, and

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

gives integrability at \( \infty \)

\[ \widehat{Q}_{b_\epsilon}[f_\epsilon](\zeta) = \widehat{Q}_L[f_\epsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\epsilon(\mathbf{v})f_\epsilon(\mathbf{v} - \mathbf{u})\}(\zeta)R(\zeta, \mathbf{u})d\mathbf{u} \tag{5} \]

Note: this ansatz is satisfied by the Maxwellian distribution.
Numerical Results

Using $\varepsilon$-linear:

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

Isotropic initial condition:

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

Rate of convergence to equilibrium

\[ \log (H - H_{eq}) \]

\( t \)

Landau
Coulomb
\( \epsilon \)-Linear

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Conclusions, future work

- 'Extra' term in $b_ε$ - different time scale?
- Main issue for large scale calculation: **storage**
  - Weights $\hat{G}(ζ, ξ)$ require $O(N^6)$ storage. ($N = 40 \rightarrow \sim 250$ GB of memory)
  - "Flops are free" - can we compute weights on the fly?
  - work in progress (with J. Hu, I. Gamba): $O(M^2N^4 \log N)$ 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!