Spectral computation of low probability tails for the homogeneous Boltzmann equation

John Zweck[(1)], Yanping Chen[(1)], Matthew Goeckner[(1)], and Yannan Shen[(2)]

[(1)]The University of Texas at Dallas, [(2)]The University of Kansas; email: zweck@utdallas.edu

Problem Setting

- **Motivation:** Accurate simulation of low-probability, high-energy processes in non-equilibrium plasmas.
- Reaction rates depend on overlap between electron velocity pdf and electron-ion impact cross sections.
- **Goal:** Accurate computation of low-probability tails of electron velocity pdf, $f = f(t, \boldsymbol{v})$:

$$\frac{\partial f}{\partial t} = Q(f, f), \qquad \text{Boltzmann equation}$$

for Boltzmann collision operator

$$Q(\boldsymbol{v}) = \int_{\mathbb{R}^3}\int_{S^2} [f(\boldsymbol{v}')f(\boldsymbol{w}') - f(\boldsymbol{v})f(\boldsymbol{v}+\boldsymbol{g})]\, g^\lambda d\Theta d\boldsymbol{g},$$

  - $\lambda = 0$: Isotropic Maxwell collisions
  - $\lambda = 1$: Isotropic hard-sphere collisions

Gamba's Spectral Method [1]

Truncated Collision Operator

$$Q^{\text{tr}}(\boldsymbol{v}) = \int_{|\boldsymbol{g}|\le g_{\text{tr}}}\int_{S^2} [f(\boldsymbol{v}')f(\boldsymbol{w}') - f(\boldsymbol{v})f(\boldsymbol{v}+\boldsymbol{g})]\, g^\lambda d\Theta d\boldsymbol{g}$$

- Ignores collisions for which $g = |\mathbf{v} - \mathbf{w}| > g_{\text{tr}}$.

$$\widehat{Q}^{\text{tr}}(\boldsymbol{\zeta}) = \int_{\mathbb{R}^3} \widehat{f}(\boldsymbol{\zeta}-\boldsymbol{\xi})\widehat{f}(\boldsymbol{\xi})\widehat{G}^{\text{tr}}(\boldsymbol{\xi},\boldsymbol{\zeta})\, d\boldsymbol{\xi}.$$

$$\widehat{G}^{\text{tr}}(\boldsymbol{\xi},\boldsymbol{\zeta}) = \int_{|\boldsymbol{g}|\le g_{\text{tr}}} G(\boldsymbol{g},\boldsymbol{\zeta})e^{-i\,\boldsymbol{\xi}\cdot\boldsymbol{g}}\, d\boldsymbol{g}.$$

$$G(\boldsymbol{g},\boldsymbol{\zeta}) = g^\lambda \left[e^{\frac{i}{2}\boldsymbol{\zeta}\cdot\boldsymbol{g}}\ \text{sinc}\,(g\zeta/2) - 1\right],$$

- Computational cost $\le \mathcal{O}(N^6)$.
- If $\text{supp}(f) \subseteq [-L, L]^3$, then $Q = Q^{\text{tr}}$ if $g_{\text{tr}} \ge 2\sqrt{3}L$.
- **Error:** $\mathcal{E}_{\text{tot}} \le |Q - Q^{\text{tr}}| + |Q^{\text{tr}} - Q^{\text{NC}}|$, where Q^{NC} is numerical approximation of Q^{tr} with N points.
- **How to choose g_{tr}?**
  1. As $g_{\text{tr}} \searrow 0$: $|Q - Q^{\text{tr}}| \uparrow$
  2. As $g_{\text{tr}} \nearrow \infty$: $|Q^{\text{tr}} - Q^{\text{NC}}| \uparrow$ as $\widehat{G}^{\text{tr}}$ oscillates.

Error estimate for Q^{tr} [2]

Theorem. *Suppose that $f(\boldsymbol{v}) \le c\, e^{-kv^2}$, where $v = |\boldsymbol{v}|$. Then, the truncation error, $\mathcal{E}_{\text{tr}} = |Q - Q^{\text{tr}}|$, satisfies*

$$\mathcal{E}_{\text{tr}}(\mathbf{v}) \le \mathcal{E}^{\text{UB}}_{\text{tr}}(g_{\text{tr}}, v) := c\exp(-kv^2)\,\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v),$$

where

$$\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) = \frac{\pi c}{kv}\int_{g_{\text{tr}}}^{\infty} e^{-k(v-g)^2}\,(1 - e^{-4kvg})\, g^{1+\lambda}\, dg.$$

Corollary. *If $\lambda \in [0, 1]$ and if k and g_{tr} are both large enough,*

$$\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) \approx \begin{cases} c(\frac{\pi}{k})^{3/2}v^\lambda & \text{if } g_{\text{tr}} < v,\\ \frac{\pi c}{2k^2}[(\pi k)^{1/2} + (1+\lambda)g_{\text{tr}}^{-1}]g_{\text{tr}}^\lambda & \text{if } g_{\text{tr}} = v,\\ \frac{\pi c}{2k^2}\ \frac{e^{-k(g_{\text{tr}}-v)^2}}{g_{\text{tr}}-v}\ \frac{g_{\text{tr}}^{1+\lambda}}{v} & \text{if } g_{\text{tr}} > v.\end{cases}$$

In particular,

- *For $g_{\text{tr}} > v$, $\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) \to 0$ exponentially as $g_{\text{tr}} \to \infty$*
- *For $\lambda = 0$ and $g_{\text{tr}} \gtrsim v \gg 0$,*

$$\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) \approx \frac{\pi c}{2k^2}\frac{e^{-k(g_{\text{tr}}-v)^2}}{g_{\text{tr}} - v}.$$

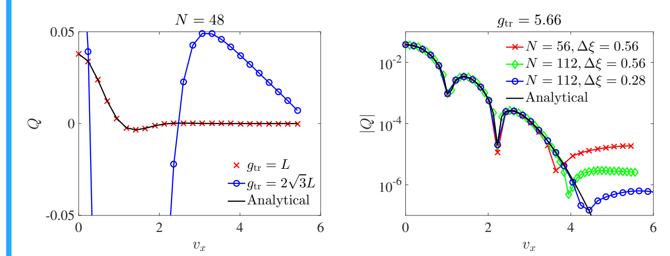
Strategy for choosing g_{tr}

To ensure $Q^{\text{tr}} \approx Q$ at $\mathbf{v}$, choose g_{tr} slightly larger than v.

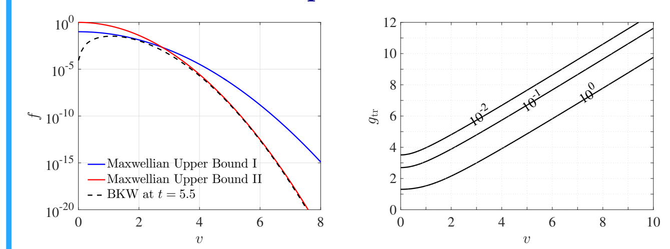
Numerical Method

- **Method I for g_{tr}:** Choose c: $f_0(\boldsymbol{v}) \le c\, e^{-(3/2E_0)v^2}$, so width agrees with that of limiting Maxwellian.
- **Method II for g_{tr}:** Tightest Maxwell$^{\text{n}}$ bound for f_0.
- Ensure f^{tr} is accurate on $[0, v_*]$ by choosing g_{tr} so that $\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) < 10^{-1}$ for all $v \le v_*$.
- Discretize $\mathbb{R}^3$ using N^3 points on $[-L, L]^3$.
- Compute integral for Q^{tr} via spectrally accurate trapezoid rule with N sufficiently large, as in [1].
- Solve ODE system using multistep 4th-order Adams-Bashforth method.
- Enforce conservation of moments using a Lagrangian projection of [1].

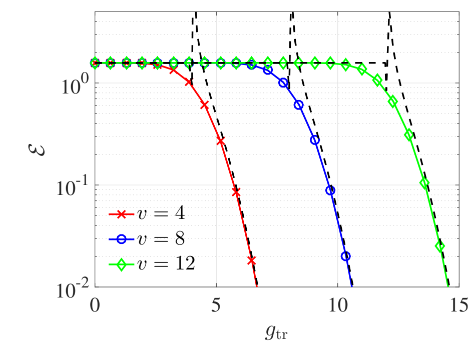
Results for BKW pdf



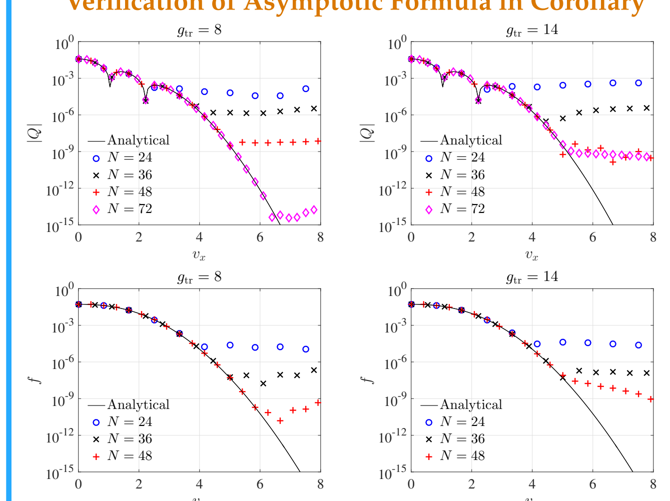
Smaller $\Delta\xi$ better captures the oscillations of $\widehat{G}^{\text{tr}}$



Maxwellian upper bounds and contour plot of $\mathcal{E}_{\text{rel}}$



Verification of Asymptotic Formula in Corollary



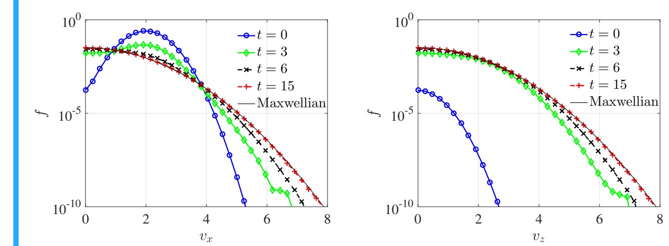
Validation of Method for Choosing g_{tr}

Results for Mixs of Maxwellians

$$f_{\text{mix}}(\boldsymbol{v}) = (1-\omega)f(\boldsymbol{v} - \boldsymbol{v}_1, T_1) + \omega f(\boldsymbol{v} - \boldsymbol{v}_2, T_2),$$

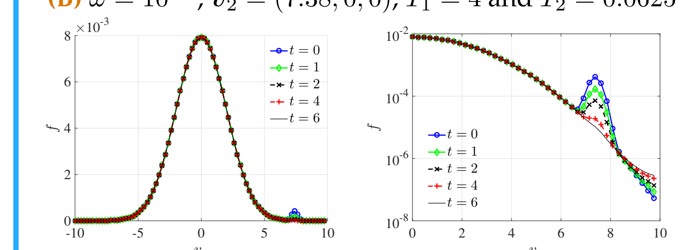
$$\text{where } f(\boldsymbol{v}, T) = (2\pi T)^{-3/2}\exp(-v^2/2T).$$

(A) $\omega = 0.5$, $\boldsymbol{v}_1 = (2, 0, 0)$, $\boldsymbol{v}_2 = -\boldsymbol{v}_1$, and $T_1 = T_2 = 0.25$.



Chose $g_{\text{tr}} = 10$ to ensure $\mathcal{E}_{\text{rel}}(g_{\text{tr}}, v) < 10^{-1}$ for $v \le 6$.

(B) $\omega = 10^{-4}$, $\boldsymbol{v}_2 = (7.38, 0, 0)$, $T_1 = 4$ and $T_2 = 0.0625$



Bound based on dominant Maxwellian gives $g_{\text{tr}} = 10$.

Conclusions

1. 1st explicit study of accuracy of deterministic computation of low-probability tails for Boltzmann eq.
2. g_{tr} plays important role in computational accuracy.
3. $\exists$ trade off between errors in truncation of Q and numerical computation of Q^{tr}.
4. Error estimate applies to related methods.

References

[1] I. M. Gamba and S. H. Tharkabhushanam. Spectral-Lagrangian methods for collisional models of non-equilibrium statistical states. *Journal of Computational Physics*, 228:2012–2036, 2009.

[2] J. Zweck, Y. Chen, M.J. Goeckner, and Y. Shen. Spectral computation of low probability tails for the homogeneous Boltzmann equation. *Applied Numerical Mathematics*, 162(4):301–317, 2021.