Scalable deterministic numerical methods for the Boltzmann equation

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1 Boltzmann Equation summary

The Boltzmann equation is a nonlinear integro-differential equation that describes the evolution of the particle density function $f : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{R}_0^+$. Independent variables for the above density function denotes, time (t), position vector (x), and the velocity (v). For a fixed time t, $f(x, v, t)dxdv$ represent the number of particles for the phase space volume element $dxdv$.

We can write the Boltzmann equation in the absence of external force field can be written as below.

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\epsilon} Q(f, f) \text{ for } x, v \in \mathbb{R}^3 \tag{1}$$

In the presence of external force field (e.g., electromagnetic field) $L(x, t) : \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{R}$, the full Boltzmann equations can be written as,

$$\partial_t f + v \cdot \nabla_x f + L \cdot \nabla_v f = \frac{1}{\epsilon} Q(f, f) \text{ for } x, v \in \mathbb{R}^3 \tag{2}$$

The ϵ is known as the Knudsen number (dimensionless number, $\epsilon > 0$), Q is the collision operator.

Note: Unless stated otherwise, v', v'_* denotes the post-collision velocities and v, v_* denotes the pre-collision velocities of a binary collision.

The collision operator (i.e., capture the physics of the collisions) can be broken up to two main parts,

1. Gain term ($C^+(f, f)$) : For a fixed (t, x) how many particles created with velocity v.
2. Loss term ($C^-(f, f)$) : For a fixed (t, x) how many particles are lost with velocity v.

which are defined as follows.

1.1 Multi-species binary collisions

Let f_e, f_o, denotes the distribution functions for electrons and heavy particles respectively.

2 Electron - Ar collisions

Assuming, that the neutral Ar atoms have $n_0\delta(0)$ distribution in the velocity space, where n_0 denotes the Ar density, and collision kernel B approximation from experimental data, the above collusion operator simplifies to,

$$C(f) = n_0 \int_{S^2} (f(v') - f(v)) \|v\| \, \sigma(\|v\|, \omega) d\omega \tag{3}$$

2.1 Total and differential cross section

For a given total cross section value, the differential cross section, can be computed as follows[1], where $\varepsilon = \frac{1}{2}mv^2$

$$\sigma(\varepsilon, \chi) = \frac{\sigma(\varepsilon)\varepsilon}{4\pi(1 + \varepsilon \sin^2(\chi/2)) \ln(1 + \varepsilon)} \tag{4}$$

2.2 Post-collision velocity

The scattering velocity direction is computed based on using following notations. Assumes vector coordinates w.r.t. basis $\hat{e_i}, \hat{e_j}$ and $\hat{e_k}$.

- v_0, $\hat{v_0}$: pre-collision velocity, unit vector along v_0
- v_1, $\hat{v_1}$: scattered (post-collision) velocity, unit vector along v_1
- χ : scattering angle, i.e., the angle between vectors, $\hat{v_1}$ and $\hat{v_0}$
- ϕ : angle between v_1 projection onto $v_0 \times (v_0 \times e_i)$, $v_0 \times e_i$ plane, and vector $v_0 \times (v_0 \times e_i)$
- θ : angle between $\hat{v_0}$ and $\hat{e_i}$, i.e., $cos\theta = \hat{v_0} \cdot \hat{e_i}$

The angle θ can be computed from v_0, and χ, ϕ are taken to represent the solid angle for the collision event. The scattered velocity can be decomposed along the orthonormal basis vectors, $\hat{E_0} = \hat{v_0}$, $\hat{E_1} = \frac{\hat{v_0} \times e_i}{\sin\theta}$, and $\hat{E_2} = \hat{v_0} \times \hat{E_1}$. Therefore, the scattered direction unit vector can be written,

$$\hat{v_1} = \cos\chi\hat{v_0} + \sin\chi sin\phi(\frac{\hat{v_0} \times \hat{e_i}}{\sin\theta}) + \sin\chi cos\phi(\hat{v_0} \times \frac{\hat{v_0} \times \hat{e_i}}{\sin\theta}) \tag{5}$$

We can see that, $\hat{v_1} \cdot \hat{v_1} = 1$, and $\hat{v_1} \cdot \hat{v_0} = \cos\chi$. When $\theta = 0$, we can pick $\hat{E_0} = \hat{e_i}$, $\hat{E_1} = \hat{e_j}$ and $\hat{E_2} = \hat{e_k}$ as the basis to derive the scattering direction.

In spherical coordinates, for a given incident vector (v_r, θ, ϕ) that is not parallel to $\hat{e_i}$, and scattering angle (χ, γ), we can compute the direction of the scattered particle as

$$\theta' = \left\{ \cos^{-1}\left(\frac{\cos(\theta)\left(\cos(\gamma)\sin(\theta)\sin(\chi)\cos(\phi)+\cos(\chi)\sqrt{1-\sin^2(\theta)\cos^2(\phi)}\right)-\sin(\gamma)\sin(\theta)\sin(\chi)\sin(\phi)}{\sqrt{1-\sin^2(\theta)\cos^2(\phi)}} \right) \right. \tag{6}$$

$$\phi' = \tan^{-1}\left(\frac{\sin(\chi)\left(\cos(\gamma)\sin^2(\theta)\sin(\phi)\cos(\phi)+\sin(\gamma)\cos(\theta)\right)+\sin(\theta)\cos(\chi)\sin(\phi)\sqrt{1-\sin^2(\theta)\cos^2(\phi)}}{\sin(\theta)\cos(\chi)\cos(\phi)\sqrt{1-\sin^2(\theta)\cos^2(\phi)}-\cos(\gamma)\sin(\chi)\left(\sin^2(\theta)\sin^2(\phi)+\cos^2(\theta)\right)} \right) \tag{7}$$

If the incident vector is parallel to the $\hat{e}_i$, we can compute the above,

$$\theta' = \left\{\cos^{-1}(\cos(\gamma)\sin(\chi))\right\} \tag{8}$$

$$\phi' = \tan^{-1}(\sin(\gamma)\tan(\chi)) \tag{9}$$

$$\tag{10}$$

2.3 G0 : $e + Ar \rightarrow e + Ar$ collision operator

$$C_{G0}(f) = n_0 \int_\chi \int_\phi (f(v_1) - f(v_0)) \|v_0\| \sigma_{G0}(\|v_0\|, \omega) \sin\chi d\phi d\chi \tag{11}$$

Let $\varepsilon_0 = 1/2m \|v_0\|_2^2$, $\varepsilon_1 = 1/2m \|v_1\|_2^2$, for inelastic collisions the energy lost, modeled based on [1], (relative energy loss)

$$\Delta\varepsilon = \frac{2m(1 - cos\chi)}{M} \tag{12}$$

where, m, M denotes the mass of the electron and the argon atom. Therefore the magnitude of the scattered velocity, can be written as,

$$\|v_1\| = \|v_0\| \sqrt{1 - \frac{2m(1 - cos\chi)}{M}} \tag{13}$$

where the direction of v_1 is specified by $\hat{v_1}$ in (5).

2.4 G1 : $e + Ar \rightarrow e + Ar^*$ collision operator

$$C_{G1}(f) = n_0 \int_\chi \int_\phi (f(v_1) - f(v_0)) \|v_0\| \sigma_{G1}(\|v_0\|, \omega) \sin\chi d\phi d\chi \tag{14}$$

Let ε_{exc} be the energy threshold to trigger an excitation reaction, then we can write,

$$\frac{1}{2}mv_0^2 - \varepsilon_{exc} = \frac{1}{2}mv_1^2 \tag{15}$$

$$\|v_1\| = \sqrt{\|v_0\|^2 - \frac{2\varepsilon_{exc}}{m}} \tag{16}$$

where the direction of v_1 is specified by $\hat{v_1}$ in (5). Note that, we use excitation threshold of $\varepsilon_{exc} = 11.5eV$.

2.5 G2 : $e + Ar \rightarrow e + Ar^+ + e$ collision operator

- v_1 : velocity of the scattered electron
- v_2 : velocity of the ejected electron from Ar.

$$C_{G2}(f) = n_0 \int_\chi \int_\phi (f(v_1) + f(v_2) - f(v_0)) \left\| v_0 \right\| \sigma_{G2}(\left\| v_0 \right\|, \omega) \sin \chi d\phi d\chi \quad (17)$$

Let ε_{ion} be the energy threshold for the ionization reaction, then as in [1] we split the $\varepsilon_0 - \varepsilon_{ion}$ equally among scattered and the ejected electron. i.e., $\varepsilon_1 = 0.5(\varepsilon_0 - \varepsilon_{ion})$, $\varepsilon_2 = 0.5(\varepsilon_0 - \varepsilon_{ion})$. Therefore, we can derive the velocity magnitudes of the scattered and ejected electrons as follows.

$$\left\| v_1 \right\| = \sqrt{\frac{1}{2} \left\| v_0 \right\|^2 - \frac{\varepsilon_{ion}}{m}} \quad (18)$$

$$\left\| v_2 \right\| = \sqrt{\frac{1}{2} \left\| v_0 \right\|^2 - \frac{\varepsilon_{ion}}{m}} \quad (19)$$

The direction of v_1 is given by $\hat{v_1}$ as in (5) and the direction of the v_2 derived based on the momentum conservation, assuming the momentum change in the Ar atom is negligible.

$$mv_0 + Mv = Mv + mv_1 + mv_2 \quad (20)$$

$$\hat{v_2} = \frac{v_0 - v_1}{\left\| v_0 - v_1 \right\|} \quad (21)$$

3 Maxwell-Boltzmann distribution (Maxwellian)

A particularly important velocity distribution function is the Maxwell-Boltzmann distribution, or Maxwellian. It describes the spread of velocities for a gas which is in thermal equilibrium. Maxwellian in d dimensional velocity space can be written as,

$$M(v) = A \exp(-\frac{mv^2}{2k_B T}) \quad (22)$$

using the number density equation, we can derive the coefficient A as follows,

$$M(v) = \frac{n}{(\sqrt{\pi} v_{th})^d} \exp\left(-(\frac{v}{v_{th}})^2\right) \quad (23)$$

where, v_{th} defined as,

$$v_{th} = \sqrt{\frac{2kT}{m}} \quad (24)$$

4 Collision Operator

The term $v \cdot \nabla_x f$ makes the distribution $f(v)$ at fixed (t, x) coupled with $f(v)$ defined in neighboring x. In operator splitting methods, Boltzmann equation is split in to "transport" and "collision" part. First we are going to focus on the collision part, given by,

$$\partial_t f = \frac{1}{\epsilon} C(f, f) \tag{25}$$

5 Collision operator for electron-neutral elastic collisions

Note: The below derivation only valid for 2-body elastic collisions. For inelastic collisions require jacobian term in the strong form. Without the proper jacobian term, we the derived weak form does not obey the mass conservation. Let $f_e(v, t)$ be the electron density and $f_o(v, t) = \delta(v)$ for all (t, x). Then the evolution of the f_e can be written as,

$$\partial_t f_e(v, t) = C(f_e, f_0) \tag{26}$$

Let $(v', v'_*) \to (v, v_*)$ be the pre and post collision velocities. The assumption $f_o(v, t) = \delta(v)$, implies neutral particles are mostly centered at velocity 0. We can write the pre collision velocities as, $v' = v'(v, \omega)$.

With these assumptions, the generic collision operator, for fixed time t can be simplified for follows.

$$C(f_e, f_0) = \int_{\mathbb{R}^3} \int_{S^2} B(|v - v_*|, \omega)(f_e(v') f_0(v'_*) - f_e(v) f_0(v_*)) d\omega dv_* \tag{27}$$

Change of the integral order (assumes that the integral is finite) with properties of the Dirac's delta function, we can write,

$$C(f_e, f_0) = \int_{S^2} B(|v|, \omega)(f_e(v') - f_e(v)) d\omega \tag{28}$$

Then we can write the final evolution equation as,

$$\partial_t f_e(v, t) = \int_{S^2} B(|v|, \omega)(f_e(v', t) - f_e(v, t)) d\omega \tag{29}$$

Since we know the above evolution will reach the Maxwellian at $t \to \infty$, we approximate $f_e(v, t)$ as follows, where $M(v)$ denotes the Maxwellian,

$$f_e(v, t) = M(v)[1 + h(v, t)] \tag{30}$$

The idea is that when $t \to \infty$ the time dependent, $h(v, t) \to 0$. Assuming that $\phi(v)$ is our test function with required properties. We can write the variational form for the above as,

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^3} f_e(v, t) \phi(v) dv = \int_{\mathbb{R}^3} \int_{S^2} B(|v|, \omega)(f_e(v', t) - f_e(v, t)) \phi(v) d\omega dv \tag{31}$$

Let $P_i(v)$ be orthonormal polynomial basis with the weighted inner product in the velocity space, where $w(v)$ denotes tha weight function.

$$\int_V w(v)P_i(v)P_j(v)dv = k_i\delta_{ij} \tag{32}$$

Assuming finite dimensional expansion for fixed time t, on $f(v,t)$, we can write,

$$f(v,t) \approxeq \bar{f}(v,t) = M(v)\sum_{j=0}^{N_v} f_j(t)P_j(v) \tag{33}$$

For the above, By substituting, basis expansion for $f(v,t)$ we can write,

$$\partial_t \int_{\mathbb{R}^3} M(v)\sum_{j=0}^{N_v} f_j(t)P_j(v)\phi(v)dv = \tag{34}$$

$$\int_{\mathbb{R}^3}\int_{S^2} M(v')\sum_{j=0}^{N_v} f_j(t)P_j(v')B(|v|,\omega)\phi(v)d\omega dv$$

$$-\int_{\mathbb{R}^3}\int_{S^2} M(v)\sum_{j=0}^{N_v} f_j(t)P_j(v)B(|v|,\omega)\phi(v)d\omega dv \tag{35}$$

By choosing $\phi(v) = P_i(v)$, we can further simplify,

$$\mathrm{diag}(k_i')\partial_t f_i = \sum_{j=0}^{N_v} L_{ij}f_j(t) \tag{36}$$

where,

$$L_{ij} = \int_{\mathbb{R}^3}\int_{S^2}(M(v')P_i(v)P_j(v') - M(v)P_i(v)P_j(v))B(|v|,\omega)d\omega dv \tag{37}$$

$$k_i' = \int_{\mathbb{R}^3} M(v)P_i(v)^2 dv \tag{38}$$

5.1 Issue of mass conservation when used in inelastic collisions

For any smooth distribution, $f(v) = M(v_\alpha)\sum_{klm} f_{klm}\phi_{klm}(v_\alpha)$, and we can write,

$$\int_{\mathbb{R}^3} f dv = const. \tag{39}$$

$$\frac{d}{dt}\int_{\mathbb{R}^3} f dv = 0 \tag{40}$$

$$\int_{\mathbb{R}^3} \partial_t f dv = \int_{\mathbb{R}^3} c(f)dv = 0 \tag{41}$$

$$\tag{42}$$

We can further write,

$$\int_{\mathbb{R}^3} c(f)dv = \sum_{klm} f_{klm} \int_{\mathbb{R}^3} \int_{S^2} \big(M(v'/\alpha)\phi_{klm}(v'/\alpha) - M(v/\alpha)\phi_{klm}(v/\alpha)\big) \tag{43}$$

$$\times \left\|v\right\| \sigma(\left\|v\right\|, \omega) d\omega dv, \ \forall f(v,t) \tag{44}$$

$$\implies \int_{\mathbb{R}^3} \int_{S^2} \big(M(v'/\alpha)\phi_{klm}(v'/\alpha) - M(v/\alpha)\phi_{klm}(v/\alpha)\big) \left\|v\right\| \tag{45}$$

$$\times\sigma(\left\|v\right\|, \omega) d\omega dv = 0 \forall klm \tag{46}$$

But the above is not satisfied, take const polynomial $\phi_{000}(x) = 1/2\sqrt{\pi}$ with $v' \neq v$.

5.2 Hermite Polynomials

Let $H_k(x)$ be the sequence of Hermite polynomials, defined on $(\infty, infty)$ and are orthogonal with respect to the weight function $w(x) = \exp(-x^2/2)$. More precisely we can write,

$$\int_{-\infty}^{\infty} w(x) H_i(x) H_j(x) dx = \sqrt{2\pi} n! \delta_{ij} \tag{47}$$

where the polynomials can be generated using,

$$H_k(x) = (-1)^k \exp(x^2/2) \frac{d^k}{dx^k} \exp(-x^2/2) \tag{48}$$

. The corresponding Gauss-Hermite quadrature can be defined as,

$$\int_{-\infty}^{\infty} w(x) f(x) \approx \sum_{q=1}^{n} w_i f(x_i) \tag{49}$$

where, x_i are the roots of $H_n(x)$, and w_i are the corresponding weights for the Gaussian quadrature.

6 Maxwellian polynomials with spherical coordinates

For the electron-Boltzmann equation, the generalized weak form of the collision operator can be written as follows (note: velocity should be normalized by the thermal velocity).

$$L_{ij} = n_0 \int_{\mathbb{R}^3} \int_{S^2} (M(v') P_i(v) P_j(v') - M(v) P_i(v) P_j(v)) B(|v|, \omega) d\omega dv \tag{50}$$

$$M_{ij} = \int_{\mathbb{R}^3} M(v) P_i(v) P_j(v) dv \tag{51}$$

In spherical coordinates, the above becomes,

$$L^{p,q,s}_{k,l,m} = n_0 \int_0^{+\infty} v^2 P^p\left(\frac{v}{v_{\text{th}}}\right) \int_{S^2}\int_{S^2} B(v,\omega) Y^{qs}(v_\theta, v_\phi) \times$$
$$\times \left(M(v')P_k\left(\frac{v'}{v_{\text{th}}}\right) Y_{lm}\big(v'_\theta, v'_\phi\big) - M(v)P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\phi)\right)\, d\omega\, dv_\omega\, dv$$

$$M^{p,q,s}_{k,l,m} = \int_0^{+\infty} v^2 M(v) P^p\left(\frac{v}{v_{\text{th}}}\right) P_k\left(\frac{v}{v_{\text{th}}}\right) \delta^{qs}_{lm}\, dv$$

6.1 Tensorized computation of $L^{p,q,s}_{k,l,m}$

$$L^{p,q,s}_{k,l,m} = L^{+}{}^{p,q,s}_{k,l,m} - L^{-}{}^{p,q,s}_{k,l,m}$$

where,

$$L^{+}{}^{p,q,s}_{k,l,m} = n_0 \int_{v_r} \int_{S^2(v_\theta,v_\phi)} \int_{S^2(\chi,\gamma)} v^2 M(v') P^p\left(\frac{v}{v_{\text{th}}}\right) Y^{qs}(v_\theta, v_\phi) \times$$
$$P_k\left(\frac{v'}{v_{\text{th}}}\right) Y_{lm}\big(v'_\theta, v'_\phi\big) |v| \sigma(|v|, \chi) d\omega dv_\omega dv$$
$$L^{-}{}^{p,q,s}_{k,l,m} = n_0 \int_{v_r} \int_{S^2(v_\theta,v_\phi)} \int_{S^2(\chi,\gamma)} v^2 M(v) P^p\left(\frac{v}{v_{\text{th}}}\right) Y^{qs}(v_\theta, v_\phi) \times$$
$$P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\phi) |v| \sigma(|v|, \chi) d\omega dv_\omega dv$$

The list of tensors that can be precomputed

- V_r - quadrature points on the radial direction (incident velocities)
- W_r - quadrature weights on the radial direction
- V_θ - quadrature points on the polar direction
- W_θ - quadrature weights for theta
- V_ϕ - quadrature points on the azimuthal direction
- S_χ - quadrature points on the scattering angle
- S_γ - quadrature points on the azimuthal angle (for scattering direction)
- W_χ - quadrature weights
- $\sigma_{r\chi}$ - differential cross section tensor (rank 2)

- $Y_{lm}^{\theta\phi}$ - lm-mode spherical harmonic function evaluated at (V_θ, V_ϕ). The sparse version (i.e., for given l mode not selecting all the m modes) , but generally can be considered as rank 4 tensor.
- M_r - Maxwellian times v_r evaluated at V_r
- P_{kr} - k^{th} Maxwell polynomial evaluated at the V_r r^{th} location.

Notation : Same index up-down denotes contraction, $\otimes$ for kronecker product, same level index, same index (i.e., up-up, down down) denotes the element-wise multiplication. The total cross section σ_r, can be written as,

$$\sigma_r = \frac{\pi}{|S\chi|}\sigma_{r,\chi}W^{\chi} \tag{52}$$

The weighted spherical harmonic tensor,

$$\tilde{Y}_{\theta\phi}^{qsr} = \left(Y_{\theta\phi}^{qs}W_\theta \frac{\pi}{|V\chi|}\right) \tag{53}$$

Then we can write,

$$L^{-}{}^{p,q,s}_{k,l,m} = ((P_r^p W_r \sigma_r)(P_k^r M^r)) \otimes Y_{lm}^{\theta\phi}\tilde{Y}_{\theta\phi}^{qs} \tag{54}$$

$$L^{-}{}^{p,q,s}_{k,l,m} = ((P_r^p W_r \sigma_r)(P_k^r M^r)) \otimes \delta^{qs}\delta_{lm} \tag{55}$$

More additional tensors that we need to compute the L^+ component.

- $S_{r'\theta'\phi'}^{r\theta\phi\chi\gamma}$: Scattering velocity tensor, for each $v = (r, \theta, \phi)$ and scattering solid angle (χ, γ) computes (r', θ', ϕ') scattered or newly created particle velocity (i.e., in G2 ejected electron). This is a rank 8 tensor where it might be too expensive to compute. For cases $G0$, $G1$ we can compute $S_{r'\theta'\phi'}^{r\theta\phi\chi\gamma} = S^r{}_{r'} \otimes S_{\theta'\phi'}^{\theta\phi\chi\gamma}$ since radial component only depends on energy, while for reactions like $G2$ it's depends on both energy and direction (i.e., for momentum conservation).
- $P_k^{r\theta\phi\chi\gamma}$ - radial polynomial evaluated at differed velocity for given incident particle $(r, \theta, \phi, \chi, \gamma)$
- $M^{r\theta\phi\chi\gamma}$ - Maxwellian times v_r evaluated for the differed particle for a given incident particle $(r, \theta, \phi, \chi, \gamma)$
- $Y_{lm}^{r\theta\phi\chi\gamma}$ - lm spherical harmonic mode evaluated differed particle direction for a given incident particle $(r, \theta, \phi, \chi, \gamma)$
- $\sigma^{r\theta\phi\chi\gamma}$ - differential cross section broadcasted on scattering cross section angles.
- $B_{pqs}^{r\theta\phi}$ - pqs basis evaluated at the incident grid.

For the general case, of the differed particle, (i.e., differed particle all velocity components are functions of $r, \theta, \phi, \chi, \gamma$) we can write the following. Note, A is obtained for contraction on the γ azimuthal of angle of the scattered particle, B is obtained with contraction on the polar angle of the scattering direction, C is obtained contraction on (θ, ϕ) for the velocity space angular directions, and finally L^+ obtained using radical direction contraction.

$$A^{r\theta\phi}_{klm} = (P^{r\theta\phi\chi\gamma}_k M^{r\theta\phi\chi\gamma} Y^{r\theta\phi\chi\gamma}_{lm}) W\gamma W_\chi \tag{56}$$

$$L^{+\,p,q,s}_{\;k,l,m} = B^{r\theta\phi}_{pqs} A^{r\theta\phi}_{klm} W_\phi W_\theta W_r \tag{57}$$

6.2 Distribution moments in basis expansion

Let $f(v) = M(v_\alpha) \sum_{klm} f_{klm} \phi_{klm}(v_\alpha)$, where $v_\alpha = v/\alpha$. Then we can write the zeroth moment (number of species particles) of the distribution,

$$n_e = \int_{R^3} f(v) dv \tag{58}$$

$$\tag{59}$$

which can be written as,

$$n_e = q^{klm} f_{klm} \tag{60}$$

where,

$$q_{klm} = \int_{\mathbb{R}^3} M(v_\alpha) \phi_{klm}(v_\alpha) dv = 0 \text{ if } klm \neq 000 \tag{61}$$

$$q_{000} = \int_{\mathbb{R}^3} M(v_\alpha) \phi_{klm}(v_\alpha) dv = \frac{n}{4\pi} \tag{62}$$

6.3 Varying thermal velocity

Let α, β be two thermal velocities, and their corresponding normalized velocity be $v_\alpha = v/\alpha, v_\beta = v/\beta$. Let $f(v) = M(v_\alpha) h(v_\alpha)$. Let $h^{(\alpha)}$ be the basis coefficients w.r.t. the chosen basis. Let us try to expand $f(v)$ using maxwellian at different temperature say at β, let $h^{(\beta)}$ be the coefficients for the expansion.

$$M^{(\beta)} h^{(\beta)} = W^{(\alpha)} h^{(\alpha)} \tag{63}$$

where,

$$M^{(\beta)}_{ij} = \int_v \int_{S^2} M(v_\beta) \phi_i(v_\beta) \phi_j(v_\beta) d\omega dv = \frac{n}{4\pi} \delta_{ij} \tag{64}$$

$$W^{(\alpha)}_{ij} = \int_v \int_{S^2} M(v_\alpha) \phi_i(v_\beta) \phi_j(v_\alpha) d\omega dv \tag{65}$$

For $W_i j^{(\alpha)}$, let i=0, then we can write (Note : $\phi_0(v_\beta) = 1$)

$$W_{0j}^{(\alpha)} = \int_v \int_{S^2} M(v_\alpha)\phi_0(v_\beta)\phi_j(v_\alpha) d\omega dv$$
$$W_{0j}^{(\alpha)} = \int_v \int_{S^2} M(v_\alpha)\phi_j(v_\alpha) d\omega dv = \frac{n}{4\pi}\delta_{0j}$$

Therefore, we can write $h_0^{(\beta)} = h_0^{(\alpha)}$. There zeroth coefficient always match hence we should preserve zeroth moment of the distribution under basis change.

6.4 Bounds on the tails for the basis change

The thermal velocity basis change operator is given by, (65), using orthogonality in the angular directions we can only operate in the radial direction. Therefore, the above simplifies to following (note that we can consider scaling of the 1d Maxwellian)

$$W_{ij} = \int_{\mathbb{R}} M(v_\alpha)P_i(v_\beta)P_j(v_\alpha) dv \tag{66}$$

Let $\epsilon > 0$, $\alpha = \beta + \epsilon$. Then we can write the simplified W_{ij} as,

$$W_{ij} = \frac{n}{\sqrt{\pi}^3} \int_{\mathbb{R}} \exp(-v_\alpha^2) P_i(v_\alpha(1 + \frac{\epsilon}{\beta})) P_j(v_\alpha) \frac{dv}{\alpha} \tag{67}$$

$$\tag{68}$$

7 Advection term

7.1 Eulerian approach

Advection (acceleration) term

$$\partial_t f + \mathbf{E}\cdot\nabla_{\mathbf{v}} f = C[f]$$

In spherical coordinates

$$\nabla_{\mathbf{v}} = \hat{\mathbf{v}}_r \frac{\partial}{\partial v} + \hat{\mathbf{v}}_\theta \frac{1}{v}\frac{\partial}{\partial v_\theta} + \hat{\mathbf{v}}_\varphi \frac{1}{v\sin(v_\theta)}\frac{\partial}{\partial v_\varphi}$$

$$\mathbf{E} = E\hat{\mathbf{z}} = E\left(\cos(v_\theta)\hat{\mathbf{v}}_r - \sin(v_\theta)\hat{\mathbf{v}}_\theta\right)$$

$$\mathbf{E}\cdot\nabla_{\mathbf{v}} f = E\left(\cos(v_\theta)\frac{\partial f}{\partial v} - \sin(v_\theta)\frac{1}{v}\frac{\partial f}{\partial v_\theta}\right)$$

Expansion in terms of Maxwell polynomials and spherical harmonics

$$f = \sum_{klm} a_{klm}\Phi_{kl}\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\varphi)$$

Spherical harmonics

$$Y_{lm}(v_\theta, v_\varphi) = U_{lm} P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi)$$

$$U_{lm} = \begin{cases} (-1)^m\sqrt{2}\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|!}}, & m \neq 0 \\ \sqrt{\frac{2l+1}{4\pi}}, & m = 0 \end{cases}$$

$$\alpha_m(v_\varphi) = \begin{cases} \sin(|m|\phi), & m < 0 \\ 1, & m = 0 \\ \cos(m\phi), & m > 0 \end{cases}$$

Useful relationships

$$\begin{aligned} xP_l^m(x) &= \frac{l+m}{2l+1}P_{l-1}^m(x) + \frac{l-m+1}{2l+1}P_{l+1}^m(x) \\ &= \alpha_M(l,m)P_{l-1}^m(x) + \beta_M(l,m)P_{l+1}^m(x) \\ (1-x^2)\frac{d}{dx}P_l^m(x) &= \frac{(l+1)(l+m)}{2l+1}P_{l-1}^m(x) - \frac{l(l-m+1)}{2l+1}P_{l+1}^m(x) \\ &= \alpha_D(l,m)P_{l-1}^m(x) + \beta_D(l,m)P_{l+1}^m(x) \end{aligned}$$

Now we can show

$$
\begin{aligned}
\cos(v_\theta)Y_{lm}(v_\theta, v_\varphi) &= \cos(v_\theta)U_{lm}P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi) \\
&= \cos(v_\theta)U_{lm}P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi) \\
&= U_{lm}\left(\alpha_M(l,|m|)P_{l-1}^{|m|}(\cos(v_\theta)) + \beta_M(l,|m|)P_{l-1}^{|m|}(\cos(v_\theta))\right)\alpha_m(v_\varphi) \\
&= \alpha_M(l,|m|)\frac{U_{lm}}{U_{(l-1)m}}Y_{(l-1)m}(v_\theta, v_\varphi) + \beta_M(l,|m|)\frac{U_{lm}}{U_{(l+1)m}}Y_{(l+1)m}(v_\theta, v_\varphi) \\
&= A_M(l,m)Y_{(l-1)m}(v_\theta, v_\varphi) + B_M(l,m)Y_{(l+1)m}(v_\theta, v_\varphi)
\end{aligned}
$$

$$
\begin{aligned}
-\sin(v_\theta)\frac{d}{dv_\theta}Y_{lm}(v_\theta, v_\varphi) &= -\sin(v_\theta)U_{lm}\frac{d}{dv_\theta}P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi) \\
&= (\sin(v_\theta))^2\, U_{lm}\frac{d}{d\cos(v_\theta)}P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi) \\
&= \left(1-(\cos(v_\theta))^2\right)U_{lm}\frac{d}{d\cos(v_\theta)}P_l^{|m|}(\cos(v_\theta))\alpha_m(v_\varphi) \\
&= U_{lm}\left(\alpha_D(l,|m|)P_{l-1}^{|m|}(\cos(v_\theta)) + \beta_D(l,|m|)P_{l-1}^{|m|}(\cos(v_\theta))\right)\alpha_m(v_\varphi) \\
&= \alpha_D(l,|m|)\frac{U_{lm}}{U_{(l-1)m}}Y_{(l-1)m}(v_\theta, v_\varphi) + \beta_D(l,|m|)\frac{U_{lm}}{U_{(l+1)m}}Y_{(l+1)m}(v_\theta, v_\varphi) \\
&= A_D(l,m)Y_{(l-1)m}(v_\theta, v_\varphi) + B_D(l,m)Y_{(l+1)m}(v_\theta, v_\varphi)
\end{aligned}
$$

Substituting into advection term

$$
\begin{aligned}
\mathbf{E}\cdot\nabla_{\mathbf{v}}f &= E\left(\cos(v_\theta)\frac{\partial f}{\partial v} - \sin(v_\theta)\frac{1}{v}\frac{\partial f}{\partial v_\theta}\right) \\
&= E\sum_{klm}a_{klm}\left(\frac{d}{dv}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right)\left(A_M(l,m)Y_{(l-1)m}(v_\theta, v_\varphi) + B_M(l,m)Y_{(l+1)m}(v_\theta, v_\varphi)\right)\right. \\
&\left.+\frac{1}{v}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right)\left(A_D(l,m)Y_{(l-1)m}(v_\theta, v_\varphi) + B_D(l,m)Y_{(l+1)m}(v_\theta, v_\varphi)\right)\right) \\
&= E\sum_{klm}a_{klm}\left(\left(A_M(l,m)\frac{d}{dv}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right) + A_D(l,m)\frac{1}{v}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right)\right)Y_{(l-1)m}(v_\theta, v_\varphi)\right. \\
&\left.+\left(B_M(l,m)\frac{d}{dv}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right) + B_D(l,m)\frac{1}{v}\Phi_{kl}\left(\frac{v}{v_{\mathrm{th}}}\right)\right)Y_{(l+1)m}(v_\theta, v_\varphi)\right)
\end{aligned}
$$

Projecting onto test functions

$$
\begin{aligned}
&\int \mathbf{E}\cdot\nabla_{\mathbf{v}} f \Psi_{pq}\left(\tfrac{v}{v_{\rm th}}\right) Y_{qs}(\theta,\phi) v^2\, dv\, dv_\omega \\
&= E\int\sum_k \left(a_{k(q+1)s}\left(A_M(q+1,s)\frac{d}{dv}\Phi_{k(q+1)}\left(\frac{v}{v_{\rm th}}\right) + A_D(q+1,s)\frac{1}{v}\Phi_{k(q+1)}\left(\frac{v}{v_{\rm th}}\right)\right)\right. \\
&\left. + a_{k(q-1)s}\left(B_M(q-1,s)\frac{d}{dv}\Phi_{k(q-1)}\left(\frac{v}{v_{\rm th}}\right) + B_D(q-1,s)\frac{1}{v}\Phi_{k(q-1)}\left(\frac{v}{v_{\rm th}}\right)\right)\right)\Psi_{pq}\left(\tfrac{v}{v_{\rm th}}\right) v^2\, dv
\end{aligned}
$$

Non-dimensionalizing integrands

$$
\begin{aligned}
&= E v_{\rm th}^2 \int\sum_k \left(a_{k(q+1)s}\left(A_M(q+1,s)\frac{d}{dx}\Phi_{k(q+1)}(x) + A_D(q+1,s)\frac{1}{x}\Phi_{k(q+1)}(x)\right)\right. \\
&\left. + a_{k(q-1)s}\left(B_M(q-1,s)\frac{d}{dx}\Phi_{k(q-1)}(x) + B_D(q-1,s)\frac{1}{x}\Phi_{k(q-1)}(x)\right)\right)\Psi_{pq}(x) x^2\, dx
\end{aligned}
$$

Differentiating by parts

$$
\begin{aligned}
= E v_{\rm th}^2 \int\sum_k \Bigg(a_{k(q+1)s}\Bigg(& \left(A_M(q+1,s) - \frac{1}{2}A_D(q+1,s)\right)\Psi_{pq}(x)\frac{d}{dx}\Phi_{k(q+1)}(x) \\
& - \frac{1}{2}A_D(q+1,s)\Phi_{k(q+1)}(x)\frac{d}{dx}\Psi_{pq}(x)\Bigg) \\
+ a_{k(q-1)s}\Bigg(& \left(B_M(q-1,s) - \frac{1}{2}B_D(q-1,s)\right)\Psi_{pq}(x)\frac{d}{dx}\Phi_{k(q-1)}(x) \\
& - \frac{1}{2}B_D(q-1,s)\Phi_{k(q-1)}(x)\frac{d}{dx}\Psi_{pq}(x)\Bigg)\Bigg) x^2\, dx
\end{aligned}
$$

Writing in a more compact form

$$
\begin{aligned}
&= E v_{\rm th}^2 \sum_k a_{k,q+1,s}\left(\left(A_M(q+1,s) - \frac{1}{2}A_D(q+1,s)\right) C_{p,k}^{q,\Psi d\Phi +} - \frac{1}{2}A_D(q+1,s) C_{p,k}^{q,\Phi d\Psi +}\right) \\
&+ E v_{\rm th}^2 \sum_k a_{k,q-1,s}\left(\left(B_M(q-1,s) - \frac{1}{2}B_D(q-1,s)\right) C_{p,k}^{q,\Psi d\Phi -} - \frac{1}{2}B_D(q-1,s) C_{p,k}^{q,\Phi d\Psi -}\right)
\end{aligned}
$$

where

$$
\begin{aligned}
C^{q,\Psi d\Phi+}_{p,k} &= \int \Psi_{p,q}(x)\frac{d}{dx}\Phi_{k,q+1}(x)x^2\,dx \\
C^{q,\Psi d\Phi-}_{p,k} &= \int \Psi_{p,q}(x)\frac{d}{dx}\Phi_{k,q-1}(x)x^2\,dx \\
C^{q,\Phi d\Psi+}_{p,k} &= \int \Phi_{k,q+1}(x)\frac{d}{dx}\Psi_{p,q}(x)x^2\,dx \\
C^{q,\Phi d\Psi-}_{p,k} &= \int \Phi_{k,q-1}(x)\frac{d}{dx}\Psi_{p,q}(x)x^2\,dx
\end{aligned}
$$

Potentially these can be found analytically and tried to do that for Laguerre polynomials but the results are quite messy. So, it seems to be more convenient just to compute those numerically.

7.1.1 Case of Maxwell polynomials

$$
\begin{aligned}
\Phi_{kl}(x) &= e^{-x^2}x^l P^{(2l+2)}_k(x) \\
\Psi_{pq}(x) &= x^q P^{(2q+2)}_p(x)
\end{aligned}
$$

$$
\int\limits_0^\infty \Phi_{kq}(x)\Psi_{pq}(x)x^2\,dx = \int\limits_0^\infty e^{-x^2}x^{2q+2}P^{(2q+2)}_k(x)P^{(2q+2)}_p(x)\,dx = \delta_{k,p}
$$

$$
\begin{aligned}
\Psi_{p,q}(x)\frac{d}{dx}\Phi_{k,q+1}(x) &= e^{-x^2}x^{2q}P^{(2q+2)}_p(x)\left(\left((q+1)-2x^2\right)P^{(2q+4)}_k + x\sum_{j=0}^{k-1}D^{(2q+4)}_{j,k}P^{(2q+4)}_j\right) \\
\Psi_{p,q}(x)\frac{d}{dx}\Phi_{k,q-1}(x) &= e^{-x^2}x^{2q-2}P^{(2q+2)}_p(x)\left(\left((q-1)-2x^2\right)P^{(2q)}_k + x\sum_{j=0}^{k-1}D^{(2q)}_{j,k}P^{(2q)}_j\right) \\
\Phi_{k,q+1}(x)\frac{d}{dx}\Psi_{p,q}(x) &= e^{-x^2}x^{2q}P^{(2q+4)}_k(x)\left(qP^{(2q+2)}_p + x\sum_{j=0}^{p-1}D^{(2q+2)}_{j,p}P^{(2q+2)}_j\right) \\
\Phi_{k,q-1}(x)\frac{d}{dx}\Psi_{p,q}(x) &= e^{-x^2}x^{2q-2}P^{(2q)}_k(x)\left(qP^{(2q+2)}_p + x\sum_{j=0}^{p-1}D^{(2q+2)}_{j,p}P^{(2q+2)}_j\right)
\end{aligned}
$$

where differentiation matrices

$$
\frac{d}{dx}P^{(l)}_k(x) = \sum_{j=0}^{k-1}D^{(l)}_{j,k}P^{(l)}_j(x)
$$

are assembled as

$$
\begin{aligned}
D^{(l)}_{k-1,k} &= \frac{k}{\beta^{(l)}_k} \\
D^{(l)}_{k-2,k} &= \frac{\sum_{j=0}^{k-1} \alpha^{(l)}_j - k\alpha^{(l)}_{k-1}}{\sqrt{\beta^{(l)}_k \beta^{(l)}_{k-1}}} \\
D^{(l)}_{k-3,k} &= \frac{2\sqrt{\beta^{(l)}_{k-1}\beta^{(l)}_k} - \sqrt{\beta^{(l)}_{k-1}} D^{(l)}_{k-1,k} - \alpha^{(l)}_{k-2} D^{(l)}_{k-2,k}}{\sqrt{\beta^{(l)}_{k-2}}} \\
D^{(l)}_{j,k} &= -\frac{\sqrt{\beta^{(l)}_{j+2}} D^{(l)}_{j+2,k} + \alpha^{(l)}_{j+1} D^{(l)}_{j+1,k}}{\sqrt{\beta^{(l)}_{j+1}}}, \quad 0 \le j \le k-4
\end{aligned}
$$

7.1.2 Case of Laguerre polynomials

$$
\begin{aligned}
\Phi_{kl}(x) &= e^{-x^2} x^l L^{(l+1/2)}_k\big(x^2\big) \\
\Psi_{pq}(x) &= x^q L^{(q+1/2)}_p\big(x^2\big)
\end{aligned}
$$

$$
\frac{d}{dx} L^{(l)}_k\big(x^2\big) = 2x \frac{d}{dx^2} L^{(l)}_k\big(x^2\big) = -2x L^{(l+1)}_{k-1}\big(x^2\big)
$$

$$
\begin{aligned}
\Psi_{p,q}(x) \frac{d}{dx} \Phi_{k,q+1}(x) &= e^{-x^2} x^{2q} L^{(q+1/2)}_p \Big(\big((q+1) - 2x^2\big) L^{(q+3/2)}_k - 2x^2 L^{(q+5/2)}_{k-1} \Big) \\
\Psi_{p,q}(x) \frac{d}{dx} \Phi_{k,q-1}(x) &= e^{-x^2} x^{2q-2} L^{(q+1/2)}_p \Big(\big((q-1) - 2x^2\big) L^{(q-1/2)}_k - 2x^2 L^{(q+1/2)}_{k-1} \Big) \\
\Phi_{k,q+1}(x) \frac{d}{dx} \Psi_{p,q}(x) &= e^{-x^2} x^{2q} L^{(q+3/2)}_k \Big(q L^{(q+1/2)}_p - 2x^2 L^{(q+3/2)}_{p-1} \Big) \\
\Phi_{k,q-1}(x) \frac{d}{dx} \Psi_{p,q}(x) &= e^{-x^2} x^{2q-2} L^{(q-1/2)}_k \Big(q L^{(q+1/2)}_p - 2x^2 L^{(q+3/2)}_{p-1} \Big)
\end{aligned}
$$

7.2 Lagrangian approach with operator splitting

$$\partial_t f + \mathbf{E}\cdot\nabla_{\mathbf{v}} f = C[f]$$

Given advection time step Δt, a second order operator splitting:

$$\begin{cases} \partial_t f^{(0)} + \mathbf{E}\cdot\nabla_{\mathbf{v}} f^{(0)} = 0, \quad t_n < t \le t_n + \frac{1}{2}\Delta t \\ f^{(0)}(t_n) = f(t_n) \end{cases}$$
$$\begin{cases} \partial_t f^{(1)} = C[f^{(1)}], \quad t_n < t \le t_n + \Delta t \\ f^{(1)}(t_n) = f^{(0)}\left(t_n + \frac{1}{2}\Delta t\right) \end{cases}$$
$$\begin{cases} \partial_t f^{(2)} + \mathbf{E}\cdot\nabla_{\mathbf{v}} f^{(2)} = 0, \quad t_n + \frac{1}{2}\Delta t < t \le t_n + \Delta t \\ f^{(2)}(t_n) = f^{(1)}(t_n + \Delta t) \end{cases}$$
$$f(t_n + \Delta t) = f^{(2)}(t_n + \Delta t)$$

$$f = \sum a_{klm}(t)\psi_{klm}(\mathbf{v}) = \sum a_{klm}(t)\tilde{\psi}_{klm}(\mathbf{v} - \mathbf{v}_0)$$

$$\tilde{\psi}_{klm}(\mathbf{v}) = \exp\left(-\left(\frac{\mathbf{v}}{v_{\text{th}}}\right)^2\right) P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\varphi)$$
$$\tilde{\phi}_{klm}(\mathbf{v}) = P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\varphi)$$

Collisional term in "physical" system of coordinates:

$$\sum \partial_t a_{klm}(t) \int\limits_{R^3} \psi_{klm}(\mathbf{v})\phi_{pqs}(\mathbf{v}) d\mathbf{v}$$
$$= \sum a_{klm}(t) \int\limits_{R^3}\int\limits_{S^2} \psi_{klm}(\mathbf{v}) B(\mathbf{v},\omega)\left(\phi_{pqs}\big(\mathbf{v}^{\text{post}}(\mathbf{v},\omega)\big) - \phi_{pqs}(\mathbf{v})\right) d\mathbf{v}$$

Substituting shifted basis and test functions

$$\sum \partial_t a_{klm}(t) \int\limits_{R^3} \tilde{\psi}_{klm}(\mathbf{v} - \mathbf{v}_0)\tilde{\phi}_{pqs}(\mathbf{v} - \mathbf{v}_0) d\mathbf{v} d\omega$$
$$= \sum a_{klm}(t) \int\limits_{R^3}\int\limits_{S^2} \tilde{\psi}_{klm}(\mathbf{v} - \mathbf{v}_0) B(\mathbf{v},\omega)\left(\tilde{\phi}_{pqs}\big(\mathbf{v}^{\text{post}}(\mathbf{v},\omega) - \mathbf{v}_0\big) - \tilde{\phi}_{pqs}(\mathbf{v} - \mathbf{v}_0)\right) d\mathbf{v} d\omega$$

Shifting integration variable $\mathbf{v} = \mathbf{v}_0 + \mathbf{u}$

$$\begin{aligned}
&\sum \partial_t a_{klm}(t) \int\limits_{R^3} \tilde{\psi}_{klm}(\mathbf{u}) \tilde{\phi}_{pqs}(\mathbf{u}) d\mathbf{v} d\omega \\
= &\sum a_{klm}(t) \int\limits_{R^3} \int\limits_{S^2} \tilde{\psi}_{klm}(\mathbf{u}) B(\mathbf{u} + \mathbf{v}_0, \omega) \left(\tilde{\phi}_{pqs}\big(\mathbf{v}^{\text{post}}(\mathbf{u} + \mathbf{v}_0, \omega) - \mathbf{v}_0\big) - \tilde{\phi}_{pqs}(\mathbf{u}) \right) d\mathbf{u} d\omega
\end{aligned} \tag{69}$$

Overall algorithm: given $\mathbf{v}_0$, a_{klm} at t_n:

1. $\mathbf{v}_0 \leftarrow \mathbf{v}_0 - \int\limits_{t_n}^{t_n + \frac{1}{2}\Delta t} \mathbf{E}(\tau) d\tau$
2. Solve (69) from t_0 to $t_0 + \Delta t$
3. $\mathbf{v}_0 \leftarrow \mathbf{v}_0 - \int\limits_{t_n + \frac{1}{2}\Delta t}^{t_n + \Delta t} \mathbf{E}(\tau) d\tau$

$$\begin{aligned}
\psi_{pqs}(\mathbf{v}) &= \tilde{\psi}_{pqs}(\mathbf{v} - \mathbf{v}_0) \\
\phi_{pqs}(\mathbf{v}) &= \tilde{\phi}_{pqs}(\mathbf{v} - \mathbf{v}_0)
\end{aligned}$$

8 Numerical evaluation

This section presents, a numerical evaluation of the spatially homogeneous Boltzmann equation without external force field. Recall, under the above assumptions we can write the collision source term as (70),

$$\partial_t f_e(v,t) = \sum_k n_k C_k(f_e) \tag{70}$$

where the C_k denotes the collision operator for the k^{th} collision. We consider the following experiments in the study.

- G0: $e + Ar \rightarrow e + Ar$
- G1: $e + Ar \rightarrow e + Ar^{*}$
- G2: $e + Ar \rightarrow e + Ar^{+} + e$

The post collision velocities for the above collisions are summerized in §2.

8.1 Handling changing temperature

Due to the kinetic energy loss in $e-Ar$ collisions, the thermal velocity decreases with the time. Since we use quadrature points on the normalized velocity (i.e., $\frac{v}{v_t h}$) we need transform the solution from one temperature to another. If the temperature drop is significant and if we don't have enough basis functions in the radial direction, the projection between temperature cause an aliasing effect and gives larger tails.

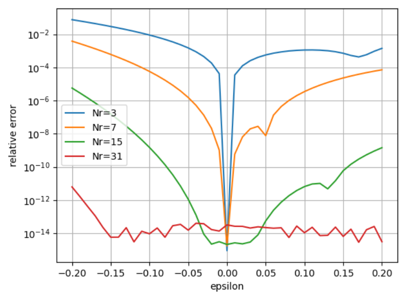
Let T_α be the current temperature and we want to transform the solution to $T_\beta = T_\alpha(1+\epsilon)$ where $\epsilon \in [-a, a]$ for $a > 0$.

$$W_{ij} = \int_{\mathbb{R}} M(v_\alpha) P_i(v_\beta) P_j(v_\alpha) dv \tag{71}$$

Let $\epsilon > 0$, $\alpha = \beta + \epsilon$. Then we can write the simplified W_{ij} as,

$$W_{ij} = \frac{n}{\sqrt{\pi}^3} \int_{\mathbb{R}} \exp(-v_\alpha^2) P_i(v_\alpha(1+\frac{\epsilon}{\beta})) P_j(v_\alpha) \frac{dv}{\alpha} \tag{72}$$

$$\tag{73}$$



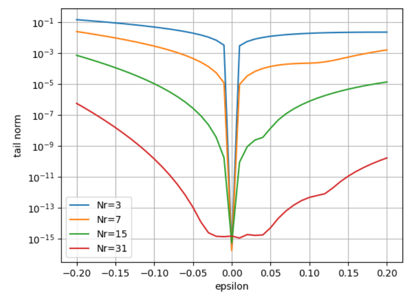


Figure 1: The left most figure shows the $f(v)$ expansion evaluated at uniform grid in the radial direction followed by normed difference computation for increasing N_r polynomials. For a given Maxwellian distribution (i.e., $h^\alpha = 1$) we compute the projection of the solution to $T_\beta = T_\alpha(1+\epsilon)$ with computed $W_{\beta\alpha}$, where $h^\beta = W_{\beta\alpha}h^\alpha$. The right most figure shows the tail of the computed h^β with increasing polynomials in the radial direction.

9 Numerical results with picewise linear synthetic cross section data

Experimental setup summary.

- Collision operator assembled using composite Simpson rule with 1601 points in the radial direction.

References

[1] Vahid Vahedi and Maheswaran Surendra. A monte carlo collision model for the particle-in-cell method: applications to argon and oxygen discharges. *Computer Physics Communications*, 87(1-2):179–198, 1995.

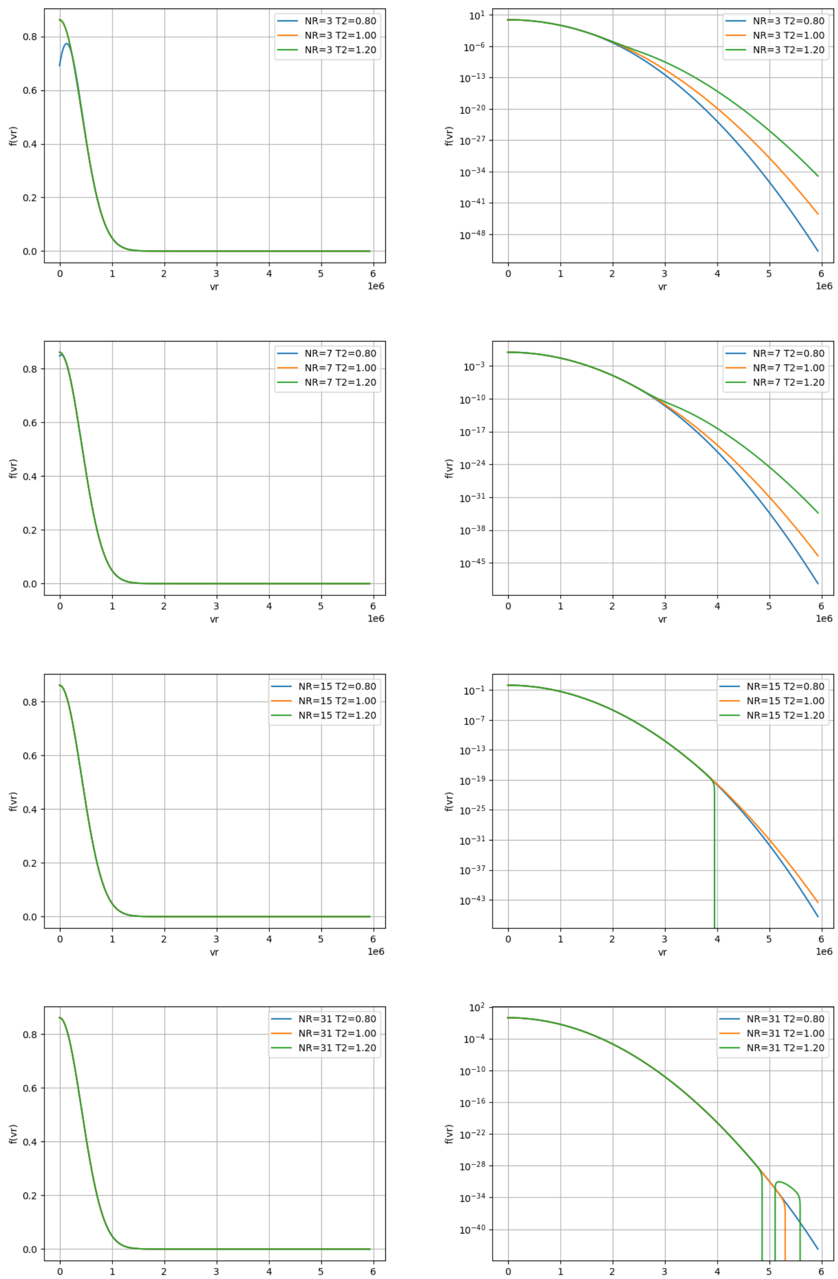


Figure 2: For each row the the right most figure shows the log scale to emphasis the variation in the tails of the distribution function. Each row corresponds to a temperature change indicated byt the ϵ parameter, and projected coefficient evaluated at a uniformly space grid of 10^5 points in the range of $(0, 6V_th)$.

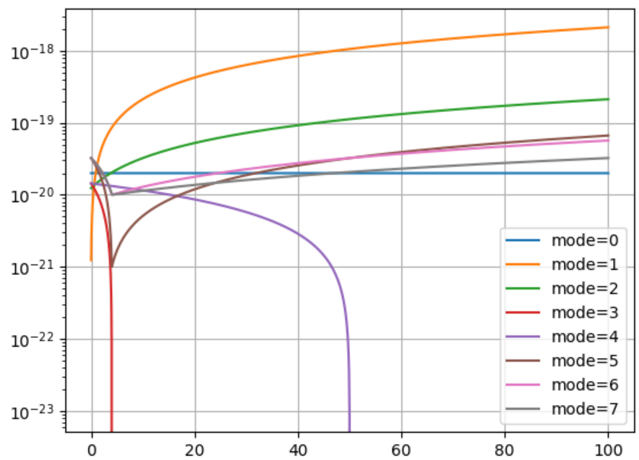


Figure 3: Total cross-section plots with different synthetic functions. For modes 3,4,5,6 the kink is at an exact quadrature point while mode 7 kink location is not co-located with a quadrature point. For all the experiment differential cross-section computed with uniform distribution.

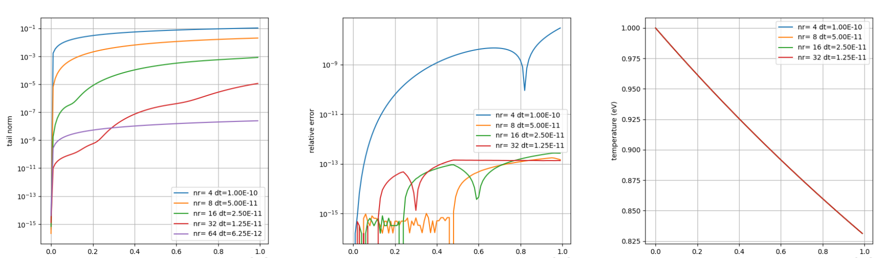


Figure 4: Mode 0

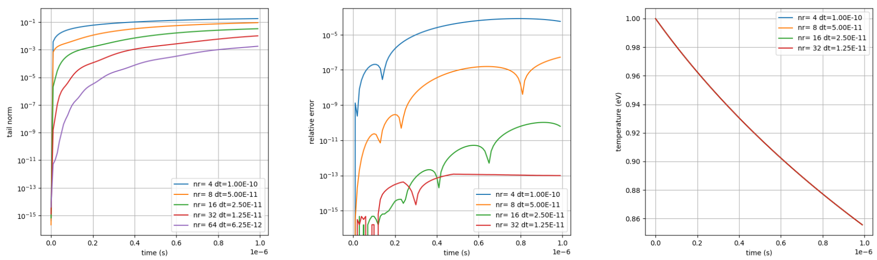


Figure 5: Mode 1

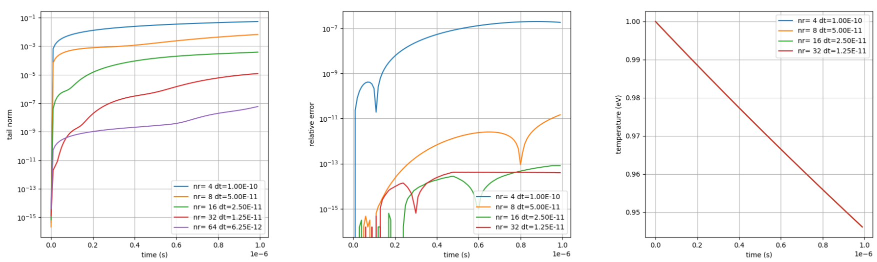


Figure 6: Mode 2

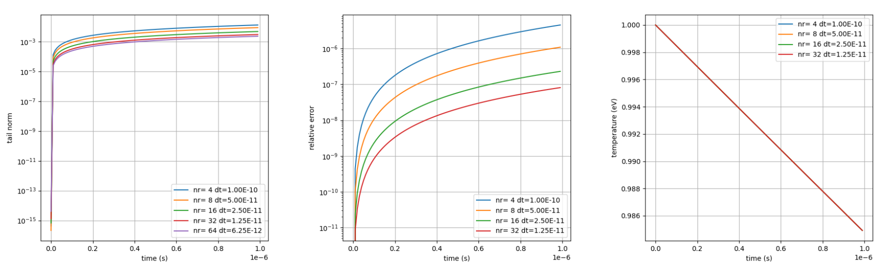


Figure 7: Mode 3

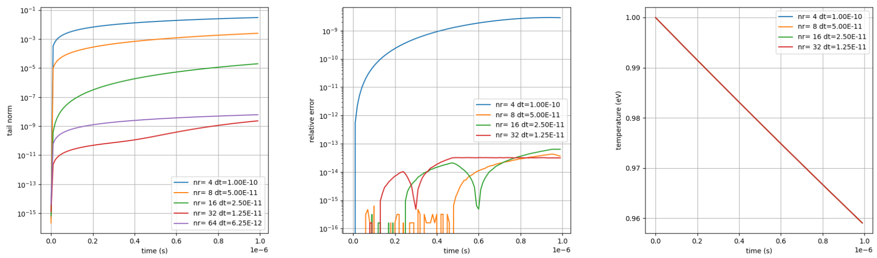


Figure 8: Mode 4

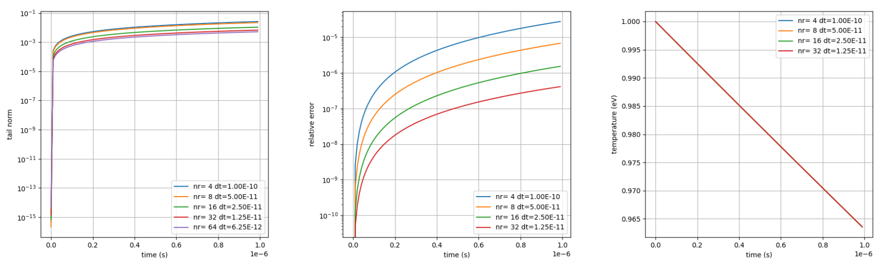


Figure 9: Mode 5

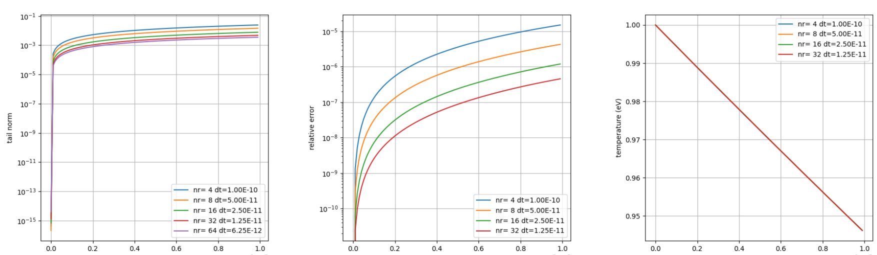


Figure 10: Mode 6

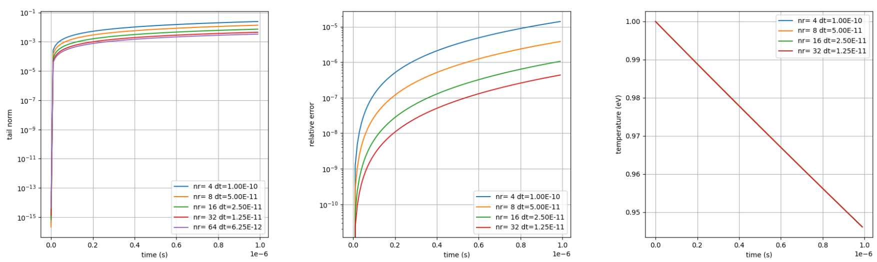


Figure 11: Mode 7

A Derivation of Collision operators

A.1 Binary reactions

We start with reactions of the type

$$\mathrm{Ar} + e \longrightarrow \tilde{\mathrm{Ar}} + e$$

where $\tilde{\mathrm{Ar}} = \mathrm{Ar}$ in the case of elastic collisions and $\tilde{\mathrm{Ar}} = \mathrm{Ar}^*$ in the case of excitation events. Let us denote the expressions that map given pre-collisional velocities $\mathbf{v}_e$, $\mathbf{v}_0$ to post-collisional velocities as

$$\begin{aligned}
\mathbf{v}_e^{\text{post}} &= \mathbf{v}_e^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega) \\
\mathbf{v}_0^{\text{post}} &= \mathbf{v}_0^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)
\end{aligned}$$

where $\omega \in S^2$ is the vector defining along which directions velocities change in the reaction. Specifically, from the conservation of momentum and energy it can be derived that

$$\begin{aligned}
\mathbf{v}_e^{\text{post}} &= \mathbf{v}_e + \frac{\alpha}{m_e}\omega, \\
\mathbf{v}_0^{\text{post}} &= \mathbf{v}_0 - \frac{\alpha}{m_0}\omega,
\end{aligned}$$

where

$$\alpha = \frac{u + \sqrt{u^2 - 4\Delta E \mu}}{2\mu}, \quad u = \omega \cdot (\mathbf{v}_0 - \mathbf{v}_e), \quad \mu = \frac{m_e + m_0}{2 m_e m_0}$$

and ΔE denotes the energy loss during the reaction ($\Delta E = 0$ for elastic collisions). Note that if $\Delta E = 0$, then

$$\begin{aligned}
\mathbf{v}_e^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega) &= \mathbf{v}_e, \\
\mathbf{v}_0^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega) &= \mathbf{v}_0,
\end{aligned}$$

for $\omega \cdot (\mathbf{v}_0 - \mathbf{v}_e) < 0$, that is, no collision happens.

The inverse map (assuming it exists and well-defined) is denoted as

$$\mathbf{v}_e^{\mathrm{pre}} = \mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega)$$
$$\mathbf{v}_0^{\mathrm{pre}} = \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega)$$

where $\mathbf{v}_e$, $\mathbf{v}_0$ now represent the post-collision velocities. Thus we have

$$\mathbf{v}_e = \mathbf{v}_e^{\mathrm{pre}}\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \omega\big)$$
$$\mathbf{v}_0 = \mathbf{v}_0^{\mathrm{pre}}\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \omega\big)$$

Let us denote the collision kernel of reaction as $B(\mathbf{v}_e, \mathbf{v}_0, \omega)$ which is a function of pre-collision velocities $\mathbf{v}_e$, $\mathbf{v}_0$ and the direction of velocity change ω. The number of electrons with velocity $\mathbf{v}_e$ that will participate in the reaction and, thus, lost is given by

$$C^- = \int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0)\, d\mathbf{v}_0\, d\omega$$

The number of electrons with the same velocity created in the reaction is given by

$$C^+ = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}'_e, \mathbf{v}'_0, \omega) f_e(\mathbf{v}'_e) f_0(\mathbf{v}'_0) \delta\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}'_e, \mathbf{v}'_0, \omega) - \mathbf{v}_e\big)\, d\mathbf{v}'_0\, d\mathbf{v}'_e\, d\omega$$

where we integrate over all possible pre-collision velocities $\mathbf{v}'_e$, $\mathbf{v}'_0$ but pick out only those that result in post-collision electron velocity $\mathbf{v}_e$ (thanks to the delta function). Note that in the expression for C^- symbols $\mathbf{v}_e$, $\mathbf{v}_0$ have the meaning of pre-collision velocity, while in the expression for C^+ those are denoted by $\mathbf{v}'_e$, $\mathbf{v}'_0$.

Remark. One could define C^- in an analogous to C^+ way. That is, consider reactions for all possible pre-collision velocities $\mathbf{v}'_e$, $\mathbf{v}'_0$ but select only those that lead to loss of electrons with velocity $\mathbf{v}_e$

$$C^- = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}'_e, \mathbf{v}'_0, \omega) f_e(\mathbf{v}'_e) f_0(\mathbf{v}'_0) \delta(\mathbf{v}'_e - \mathbf{v}_e)\, d\mathbf{v}'_0\, d\mathbf{v}'_e\, d\omega.$$

We understand C^- and C^+ as operators acting on functions of variable $\mathbf{v}_e$. Their weak forms are given by

$$\int\limits_{R^3} C^- \phi(\mathbf{v}_e)\, d\mathbf{v}_e = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0) \phi(\mathbf{v}_e)\, d\mathbf{v}_e\, d\mathbf{v}_0\, d\omega$$

$$\begin{aligned}\int\limits_{R^3} C^+ \phi(\mathbf{v}_e)\, d\mathbf{v}_e &= \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}'_e, \mathbf{v}'_0, \omega) f_e(\mathbf{v}'_e) f_0(\mathbf{v}'_0) \phi\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}'_e, \mathbf{v}'_0, \omega)\big)\, d\mathbf{v}'_0\, d\mathbf{v}'_e\, d\omega \\ &= \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0) \phi\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\big)\, d\mathbf{v}_0\, d\mathbf{v}_e\, d\omega\end{aligned}$$

where we integrated out the delta function and renamed dummy variables. Thus the weak form of the total collision operator $C = C^+ - C^-$ can be written as

$$\int\limits_{R^3} C\phi(\mathbf{v}_e)\,d\mathbf{v}_e = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0)\left(\phi\big(\mathbf{v}_e^{\mathrm{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\big) - \phi(\mathbf{v}_e)\right)\,d\mathbf{v}_0\,d\mathbf{v}_e\,d\omega$$

While for our purposes this formulation is all we need, for completeness sake we derive a strong form of the collision operator. To do so, we perform a change of variables in the weak form of gain operator C^+ according to:

$$\begin{aligned}\mathbf{v}_e' &= \mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega)\\ \mathbf{v}_0' &= \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega)\end{aligned}$$

As result we get

$$\begin{aligned}\int\limits_{R^3} C^+\phi(\mathbf{v}_e)\,d\mathbf{v}_e = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} & B(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega), \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega), \omega)\times\\ & \times f_e(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega)) f_0(\mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e'', \mathbf{v}_0'', \omega))\phi(\mathbf{v}_e'')|J(\mathbf{v}_e'', \mathbf{v}_0'', \omega)|\,d\mathbf{v}_0''\,d\mathbf{v}_e''\,d\omega\end{aligned}$$

or, after renaming dummy variables,

$$\begin{aligned}\int\limits_{R^3} C^+\phi(\mathbf{v}_e)\,d\mathbf{v}_e = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} & B(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \omega)\times\\ & \times f_e(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega)) f_0(\mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega))\phi(\mathbf{v}_e)|J(\mathbf{v}_e, \mathbf{v}_0, \omega)|\,d\mathbf{v}_0\,d\mathbf{v}_e\,d\omega\end{aligned}$$

where $J(\mathbf{v}_e, \mathbf{v}_0, \omega) = \frac{\partial\left(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\right)}{\partial(\mathbf{v}_e, \mathbf{v}_0)}$ is the Jacobian of the transformation of variables. Note that in this last expression $\mathbf{v}_e$, $\mathbf{v}_0$ can be interpreted as post-collision velocities. Combining it with the weak form of the loss operator (where $\mathbf{v}_e$, $\mathbf{v}_0$ actually stand for pre-collision velocities) we obtain

$$\begin{aligned}\int\limits_{R^3} C\phi(\mathbf{v}_e)\,d\mathbf{v}_e = \int\limits_{R^3}\int\limits_{R^3}\int\limits_{S^2} & \phi(\mathbf{v}_e)\,d\mathbf{v}_0\,d\mathbf{v}_e\,d\omega\times\\ & \times\big(B^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega) f_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega)|J(\mathbf{v}_e, \mathbf{v}_0, \omega)|\\ & \qquad - B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0)\big)\end{aligned}$$

where notation $x^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega) = x(\mathbf{v}_e^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\mathrm{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \omega)$ is used. Thus, a strong form of the total collision operator for general binary reactions can be written as

$$C = \int\limits_{R^3}\int\limits_{S^2} \left(f_e^{\mathrm{pre}} f_0^{\mathrm{pre}} B^{\mathrm{pre}}|J| - f_e f_0 B\right)\,d\mathbf{v}_0\,d\omega$$

In case of elastic collisions it can be shown that $|J| = 1$ and

$$\begin{aligned} B^{\text{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega) &= B(\mathbf{v}_e^{\text{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \mathbf{v}_0^{\text{pre}}(\mathbf{v}_e, \mathbf{v}_0, \omega), \omega) \\ &= B(|\mathbf{v}_e^{\text{pre}} - \mathbf{v}_0^{\text{pre}}|, |\,(\mathbf{v}_e^{\text{pre}} - \mathbf{v}_0^{\text{pre}}) \cdot \omega|) \\ &= B(|\mathbf{v}_e - \mathbf{v}_0|, |\,(\mathbf{v}_e - \mathbf{v}_0) \cdot \omega|) \\ &= B(\mathbf{v}_e, \mathbf{v}_0, \omega) \end{aligned}$$

and the collision operator becomes the familiar

$$C = \int\limits_{R^3} \int\limits_{S^2} (f_e^{\text{pre}} f_0^{\text{pre}} - f_e f_0)\, B\, d\mathbf{v}_0\, d\omega$$

In the derivation above we assumed that the collision kernel $B = B(\mathbf{v}_e, \mathbf{v}_0, \omega)$ is known. However, for electron-heavy particle collisions information is available in terms of collisional cross sections $\sigma = \sigma(|\mathbf{v}_e|, \chi, \theta)$, where $\mathbf{v}_e$ is the velocity of the incident electron in the frame of reference of the heavy particle, and χ, θ are angles of scattering. It is usually assumed that collisions occur axisymmetrically, that is $\sigma = \sigma(|\mathbf{v}_e|, \chi)$

$$C^- = \int\limits_{R^3} \int\limits_{R^3} \int\limits_0^{\pi} \int\limits_0^{2\pi} |\mathbf{v}_e' - \mathbf{v}_0'| \sigma(|\mathbf{v}_e' - \mathbf{v}_0'|, \chi) f_e(\mathbf{v}_e') f_0(\mathbf{v}_0') \delta(\mathbf{v}_e' - \mathbf{v}_e)\, d\mathbf{v}_0'\, d\mathbf{v}_e' \sin(\chi)\, d\chi\, d\theta.$$

$$C^+ = \int\limits_{R^3} \int\limits_{R^3} \int\limits_0^{\pi} \int\limits_0^{2\pi} |\mathbf{v}_e' - \mathbf{v}_0'| \sigma(|\mathbf{v}_e' - \mathbf{v}_0'|, \chi) f_e(\mathbf{v}_e') f_0(\mathbf{v}_0') \delta\big(\mathbf{v}_e^{\text{post}}(\mathbf{v}_e', \mathbf{v}_0', \chi, \theta) - \mathbf{v}_e\big)\, d\mathbf{v}_0'\, d\mathbf{v}_e' \sin(\chi)\, d\chi\, d\theta.$$

A.2 Ionization

Let's consider the following ionization reaction.

$$e + Ar \to e + Ar^{+} + e \tag{74}$$

For a given pre-collision velocities $\mathbf{v_e}, \mathbf{v_0}$, let $\mathbf{v}_e^{post}(\mathbf{v_e}, \mathbf{v_0}, \omega), \mathbf{v}_0^{post}(\mathbf{v_e}, \mathbf{v_0}, \omega)$, $\mathbf{u}_e^{post}(\mathbf{v_e}, \mathbf{v_0}, \omega)$ be the post velocity maps of the scattered, ionized Ar and ejected electron.

Following the same derivation we can write the collision operator for ionization,

$$\int_{R^3} C\phi(\mathbf{v}_e)\, d\mathbf{v}_e = \int_{R^3}\int_{R^3}\int_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0) \times \tag{75}$$

$$\Big(\phi\big(\mathbf{v}_e^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\big) + \phi\big(\mathbf{u}_e^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\big) - \phi(\mathbf{v}_e)\Big)\, d\mathbf{v}_0\, d\mathbf{v}_e\, d\omega \tag{76}$$

A.3 Recombination

Let's consider the following recombination reaction.

$$e + Ar^{+} + e \to e + Ar \tag{77}$$

Let $\mathbf{v}_e$, $\mathbf{v}_0$, and $\mathbf{u}_e$ be the velocities of the 3-body collision and the post collision velocities are given by $\mathbf{v}_e^{post}(\mathbf{v}_e, \mathbf{v}_0, \omega)$ and $\mathbf{v}_0^{post}(\mathbf{v}_e, \mathbf{v}_0, \omega)$.

$$\int_{R^3} C\phi(\mathbf{v}_e)\, d\mathbf{v}_e = \int_{R^3}\int_{R^3}\int_{R^3}\int_{S^2} B(\mathbf{v}_e, \mathbf{v}_0, \omega) f_e(\mathbf{u}_e) f_e(\mathbf{v}_e) f_0(\mathbf{v}_0) \times \tag{78}$$

$$\Big(\phi\big(\mathbf{v}_e^{\text{post}}(\mathbf{v}_e, \mathbf{v}_0, \omega)\big) - \phi(\mathbf{v}_e)\Big)\, d\mathbf{v}_0\, d\mathbf{u}_e\, d\mathbf{v}_e\, d\omega \tag{79}$$

B Analysis of projection operator

Consider a distribution function given as an expansion in terms of Maxwell polynomials based on thermal velocity v_0

$$f_0(v) = \frac{1}{\left(\sqrt{\pi}v_0\right)^3} e^{-\left(\frac{v}{v_0}\right)^2} \sum_{j=0}^{N} a_j P_j\left(\frac{v}{v_0}\right)$$

We are interested in obtaining the same distribution function in a different basis corresponding to thermal velocity v_1

$$f_1(v) = \frac{1}{\left(\sqrt{\pi}v_1\right)^3} e^{-\left(\frac{v}{v_1}\right)^2} \sum_{j=0}^{N} b_j P_j\left(\frac{v}{v_1}\right)$$

A natural way of obtaining coefficients b_i from known coefficients a_i is to ensure that the action of both distribution functions onto a chosen set of test functions coincides

$$\int_R v^2 f_0(v)\phi(v)\,dv = \int_R v^2 f_1(v)\phi(v)\,dv$$

Choosing polynomial functions up to order N (more precisely, Maxwell polynomials $P_i\left(\frac{v}{v_1}\right)$ for sake of convenience) as the set of test functions one gets (using orthogonality)

$$b_i \int_R \left(\frac{v}{v_1}\right)^2 e^{-\left(\frac{v}{v_1}\right)^2} P_i^2\left(\frac{v}{v_1}\right) d\left(\frac{v}{v_1}\right) = \sum_{j=0}^{N} a_j \int_R \left(\frac{v}{v_0}\right)^2 e^{-\left(\frac{v}{v_0}\right)^2} P_j\left(\frac{v}{v_0}\right) P_i\left(\frac{v}{v_1}\right) d\left(\frac{v}{v_0}\right)$$

Note that automatically $b_0 = a_0$, which can be interpreted as mass conservation during projection. Let us denote $\mathbf{a} = (a_0, \ldots, a_N)^T$ and $\mathbf{b} = (b_0, \ldots, b_N)^T$, then the transformation from one expansion to another one can be written as

$$\mathbf{b} = \Pi\mathbf{a}$$

where elements of matrix Π are given by

$$\Pi_{i,j} = \int_R \left(\frac{v}{v_0}\right)^2 e^{-\left(\frac{v}{v_0}\right)^2} P_j\left(\frac{v}{v_0}\right) P_i\left(\frac{v}{v_1}\right) d\left(\frac{v}{v_0}\right) \Big/ \int_R \left(\frac{v}{v_1}\right)^2 e^{-\left(\frac{v}{v_1}\right)^2} P_i^2\left(\frac{v}{v_1}\right) d\left(\frac{v}{v_1}\right)$$

Assume that the relation between thermal velocities v_0 and v_1 are given by relative change ε as

$$v_1 = v_0\,(1+\varepsilon)$$

Then the expression for $\Pi_{i,j}$ can be written as

$$\Pi_{i,j} = \Pi_{i,j}(\varepsilon) = \int_R x^2 e^{-x^2} P_i\left(\frac{x}{1+\varepsilon}\right) P_j(x)\,dx \Big/ \int_R x^2 e^{-x^2} P_i^2(x)\,dx$$

B.1 Preliminary experimental observations

Figure B.1 (a) shows the eiganvalues of the projection operator for a few different values of ε. As one can see, if $\varepsilon > 0$ (projection to a higher temperature) then all eigenvalues seem to be less than one. On the other hand, if $\varepsilon < 0$ (projection to a lower temperature) then all eigenvalues appear to be greater than one, which might indicate of a very unstable behavior. Indeed, all information, including errors, gets amplified during projection.

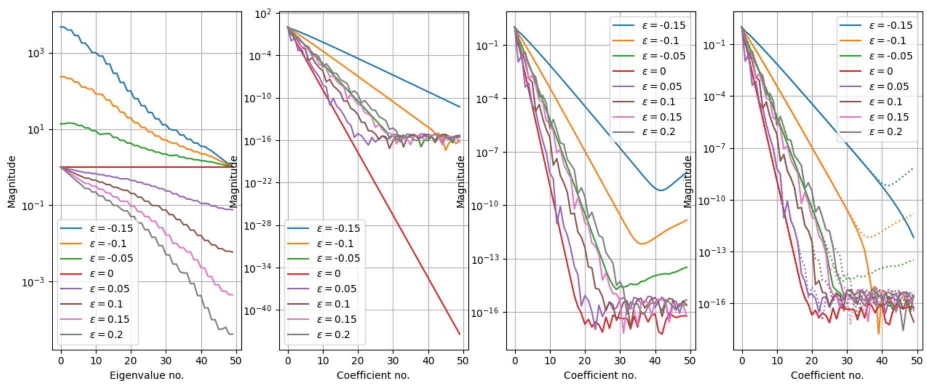


Figure 12: (a) Eigenvalues of projection operator for different ε; (b) Projection of clean data; (c) Projection of polluted data; (d) Projection of polluted data with small steps and thresholding

To inspect the behavior of the projection operator more closely, let us consider projection of a series which coefficients are given by $a_i = \exp(-100i)$. The results of projection with different ε are given in Figure B.1 (b) and, at the first glance, do not indicate of any instabilities. However, this is likely due to coefficients a_i decaying very fast. Indeed, if we add a random noise to coefficients a_i then the projection results seem to stay stable only if $\varepsilon > 0$ while for $\varepsilon < 0$ high-order coefficients growing uncontrollably (see Figure B.1 (c)).

A possible fix could be to use multiple small projection steps with zeroing all coefficients below a chosen threshold after each sub-step. The example of such a strategy is given in Figure B.1 (d) where a target relative change $\varepsilon_0 = 0.001$ was used (that is, the number of sub-steps and their size are chosen as $m = \text{ceil}\left(\frac{\log(1+\varepsilon)}{\log(1+\varepsilon_0)}\right)$ and $\tilde{\varepsilon} = \sqrt[n]{1+\varepsilon} - 1$). This strategy produces almost identical results as in the case of one full step and does not result in an uncontrollable growth of high-order coefficients for $\varepsilon < 0$. However, it is unclear whether there are any growing instabilities in the low-order part of the spectrum which are not seen due to large values of the coefficients there.

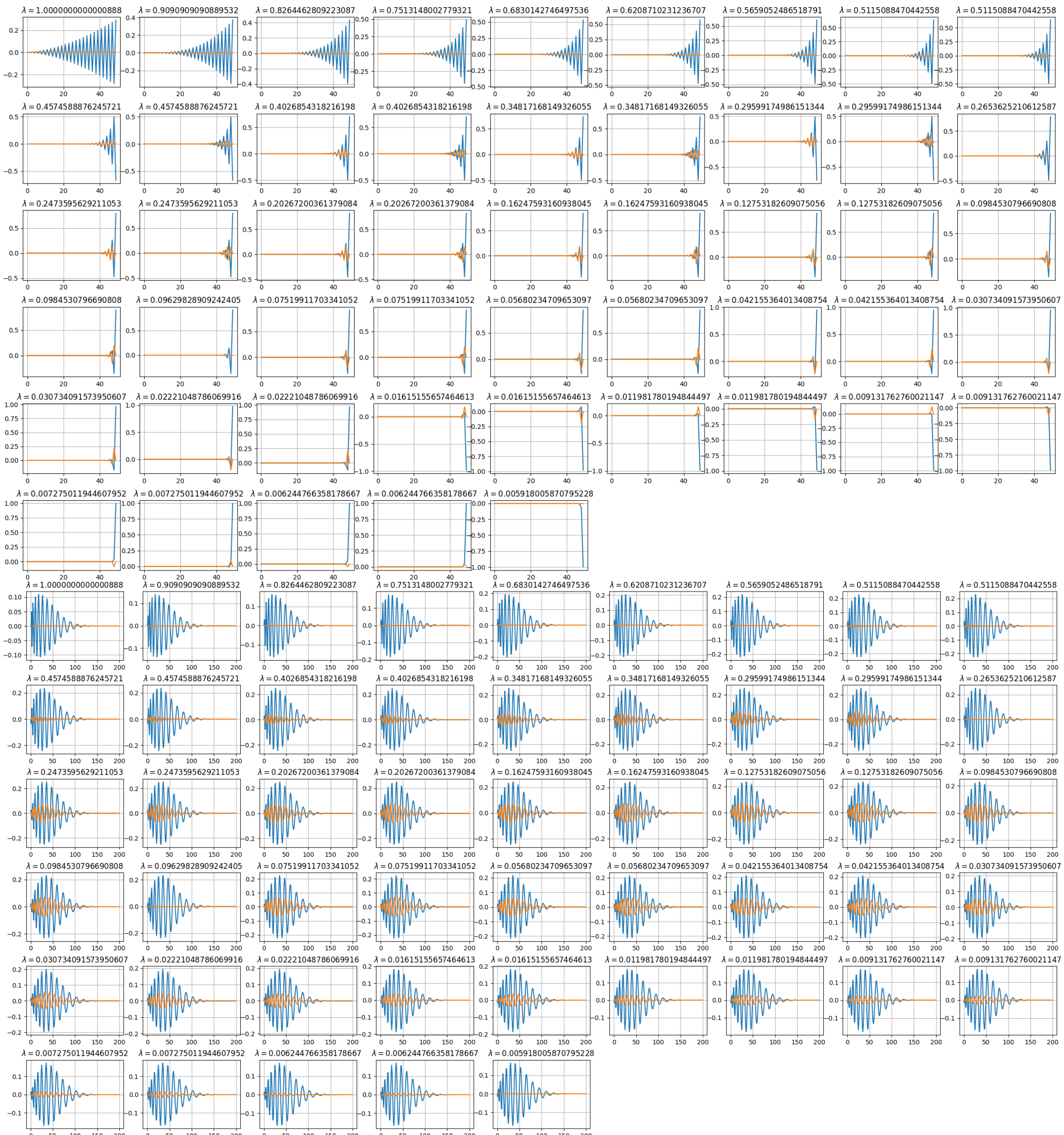


Figure 13: Eigenvectors (top) and their visualization (bottom) for $\varepsilon = 0.1$

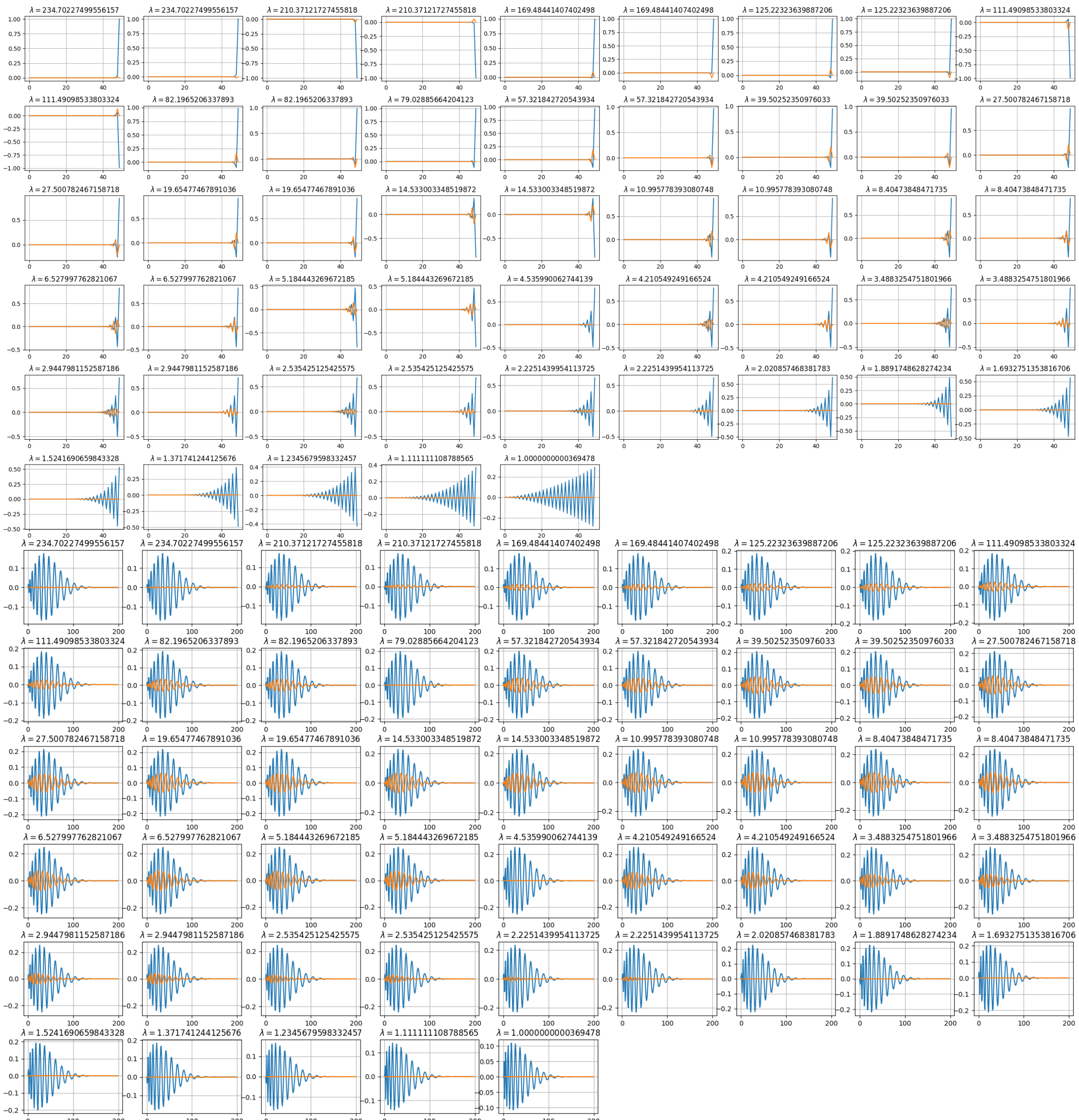


Figure 14: Eigenvectors (top) and their visualization (bottom) for $\varepsilon = -0.1$

C Advection term (initial poor attempt)

Advection (acceleration) term

$$\partial_t f + \mathbf{E} \cdot \nabla_{\mathbf{v}} f = 0$$

In spherical coordinates

$$\nabla_{\mathbf{v}} = \hat{\mathbf{v}}_r \frac{\partial}{\partial v} + \hat{\mathbf{v}}_\theta \frac{1}{v} \frac{\partial}{\partial v_\theta} + \hat{\mathbf{v}}_\varphi \frac{1}{v \sin(v_\theta)} \frac{\partial}{\partial v_\varphi}$$

$$\mathbf{E} = E\hat{\mathbf{z}} = E \left(\cos(v_\theta) \hat{\mathbf{v}}_r - \sin(v_\theta) \hat{\mathbf{v}}_\theta \right)$$

$$\mathbf{E} \cdot \nabla_{\mathbf{v}} f = E \left(\cos(v_\theta) \frac{\partial f}{\partial v} - \sin(v_\theta) \frac{1}{v} \frac{\partial f}{\partial v_\theta} \right)$$

Expansion in terms of Maxwell polynomials and spherical harmonics

$$f = A \exp\left(- \left(\frac{v}{v_{\text{th}}} \right)^2 \right) \sum_{klm} a_{klm} P_k\left(\tfrac{v}{v_{\text{th}}} \right) Y_{lm}(v_\theta, v_\varphi)$$

Differentiation and lifting matrices

$$P'_k(x) = \sum_{j=0}^{N_r} d_{jk} P_j(x) \quad \to \quad \sum_{k=0}^{N_r} a_k P'_k(x) = \sum_{k=0}^{N_r} \sum_{j=0}^{N_r} d_{jk} a_k P_j(x) = \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} d_{jk} a_k \right) P_j(x)$$

$$x P_k(x) = \sum_{j=0}^{N_r} l_{jk} P_k(x) \quad \to \quad \sum_{k=0}^{N_r} a_k x P_k(x) = \sum_{k=0}^{N_r} \sum_{j=0}^{N_r} l_{jk} a_k P_j(x) = \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} l_{jk} a_k \right) P_j(x)$$

where d_{jk} and l_{jk} are calculated from recursive coefficients generating polynomials

$$\begin{aligned}
\left(e^{-x^2} P_k(x) \right)' = -2x e^{-x^2} P_k(x) + e^{-x^2} P'_k(x) &= e^{-x^2} \sum_{j=0}^{N_r} \left(d_{jk} - 2 l_{jk} \right) P_j(x) \\
&= e^{-x^2} \sum_{j=0}^{N_r} g_{jk} P_j(x)
\end{aligned}$$

$$\frac{\partial f}{\partial v} = \frac{1}{v_{\text{th}}} A \exp\left(- \left(\frac{v}{v_{\text{th}}} \right)^2 \right) \sum_{lm} \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} g_{jk} a_{klm} \right) P_j \left(\frac{v}{v_{\text{th}}} \right) Y_{lm}(v_\theta, v_\varphi)$$

$$\frac{1}{v}\frac{\partial f}{\partial v_\theta} = \frac{1}{v} A \exp\left(-\left(\frac{v}{v_{\text{th}}}\right)^2\right) \sum_{klm} a_{klm} P_k\left(\frac{v}{v_{\text{th}}}\right) \frac{\partial}{\partial v_\theta} Y_{lm}(v_\theta, v_\varphi)$$

$$\begin{aligned}
&\int \cos(v_\theta) \frac{\partial f}{\partial v} P_p\left(\frac{v}{v_{\text{th}}}\right) Y_{qs}(v_\theta, v_\varphi) v^2 \, dv \, dv_\omega \\
&= \frac{1}{v_{\text{th}}} A \sum_{lm} \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} g_{jk} a_{klm}\right) \left(\int \exp\left(-\left(\frac{v}{v_{\text{th}}}\right)^2\right) P_j\left(\frac{v}{v_{\text{th}}}\right) P_p\left(\frac{v}{v_{\text{th}}}\right) v^2 \, dv\right) \\
&\qquad \times \left(\int \cos(v_\theta) Y_{lm}(v_\theta, v_\varphi) Y_{qs}(v_\theta, v_\varphi) \, dv_\omega\right) \\
&= v_{\text{th}}^2 A \sum_{lm} \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} g_{jk} a_{klm}\right) M_p \delta_{j,p} \Psi_{lmqs} = v_{\text{th}}^2 A \sum_{lm} \left(\sum_{k=0}^{N_r} g_{pk} a_{klm}\right) M_p \Psi_{lmqs}
\end{aligned}$$

$$\begin{aligned}
&\int \sin(v_\theta) \frac{1}{v} \frac{\partial f}{\partial v_\theta} P_p\left(\frac{v}{v_{\text{th}}}\right) Y_{qs}(v_\theta, v_\varphi) v^2 \, dv \, dv_\omega = \\
&A \sum_{lm} \sum_{j=0}^{N_r} \left(\sum_{k=0}^{N_r} g_{jk} a_{klm}\right) \left(\int \exp\left(-\left(\frac{v}{v_{\text{th}}}\right)^2\right) P_j\left(\frac{v}{v_{\text{th}}}\right) P_p\left(\frac{v}{v_{\text{th}}}\right) v \, dv\right) \\
&\qquad \times \left(\int \sin(v_\theta) Y_{qs}(v_\theta, v_\varphi) \frac{\partial}{\partial v_\theta} Y_{lm}(v_\theta, v_\varphi) \, dv_\omega\right)
\end{aligned}$$

$$\begin{aligned}
&\int \exp\left(-\left(\frac{v}{v_{\text{th}}}\right)^2\right) P_j\left(\frac{v}{v_{\text{th}}}\right) P_p\left(\frac{v}{v_{\text{th}}}\right) v \, dv = v_{\text{th}}^2 \int e^{-x^2} P_j(x) P_p(x) x \, dx \\
&= -\frac{v_{\text{th}}^2}{2} \int x^2 \left(e^{-x^2} P_j(x) P_p(x)\right)' \, dx \\
&= -\frac{v_{\text{th}}^2}{2} \int x^2 e^{-x^2} \left(-2x P_j(x) P_p(x) + P_j'(x) P_p(x) + P_j(x) P_p'(x)\right) \, dx \\
&= \frac{v_{\text{th}}^2}{2} \int x^2 e^{-x^2} \left(\sum_k 2 l_{kj} P_k(x) P_p(x) - \sum_k d_{kj} P_k(x) P_p(x) - \sum_k d_{kp} P_j(x) P_k(x)\right) \, dx \\
&= \frac{v_{\text{th}}^2}{2} \left(\sum_k 2 l_{kj} \int x^2 e^{-x^2} P_k(x) P_p(x) \, dx - \sum_k d_{kj} \int x^2 e^{-x^2} P_k(x) P_p(x) \, dx - \sum_k d_{kp} \int x^2 e^{-x^2} P_j(x) P_k(x) \, dx\right) \\
&= -\frac{v_{\text{th}}^2}{2} \left(\sum_k g_{kj} M_p \delta_{k,p} + \sum_k d_{kp} M_j \delta_{k,j}\right) = -\frac{v_{\text{th}}^2}{2} \left(g_{pj} M_p + d_{jp} M_j\right)
\end{aligned}$$

$$\int \sin(v_\theta)\frac{1}{v}\frac{\partial f}{\partial v_\theta}P_p\left(\tfrac{v}{v_{\text{th}}}\right)Y_{qs}(v_\theta,v_\varphi)v^2\,dv\,dv_\omega = \\ -\frac{v_{\text{th}}^2}{2}A\sum_{lm}\sum_{j=0}^{N_r}\left(\sum_{k=0}^{N_r}g_{jk}a_{klm}\right)(g_{pj}M_p+d_{jp}M_j)\,\Phi_{lmqs}$$

$$\int \mathbf{E}\cdot\nabla_{\mathbf{v}}fP_p\left(\tfrac{v}{v_{\text{th}}}\right)Y_{qs}(\theta,\phi)v^2\,dv\,dv_\omega \\ = Ev_{\text{th}}^2A\sum_{lm}\left(\sum_{k=0}^{N_r}g_{pk}a_{klm}\right)M_p\Psi_{lmqs}+\frac{v_{\text{th}}^2}{2}A\sum_{lm}\sum_{j=0}^{N_r}\left(\sum_{k=0}^{N_r}g_{jk}a_{klm}\right)(g_{pj}M_p+d_{jp}M_j)\,\Phi_{lmqs} \\ = E\sum_{klm}\epsilon_{pqsklm}a_{klm}$$

$$\epsilon_{pqsklm} = v_{\text{th}}^2A\left(g_{pk}M_p\Psi_{lmqs}+\frac{1}{2}\sum_{j=0}^{N_r}g_{jk}\,(g_{pj}M_p+d_{jp}M_j)\,\Phi_{lmqs}\right)$$

Let the polynomials on the radial direction is defined as,

$$P_{kl} = b_k(x)x^l \tag{80}$$

where b_k be the k^{th} bspline polynomial.

For expansion using bspline polynomials in the radial direction we can write,

$$f(\mathbf{v}) = \sum_{klm}a_{klm}P_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)Y_{lm}(v_\theta,v_\varphi) \tag{81}$$

$$\partial_v f = \frac{1}{v_{\text{th}}}\sum_{klm}a_{klm}P'_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)Y_{lm}(v_\theta,v_\varphi) \tag{82}$$

$$\frac{1}{v}\partial_{v_\theta} f = \sum_{klm}a_{klm}P_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)\partial_{v_\theta}Y_{lm}(v_\theta,v_\varphi) \tag{83}$$

$$\int\int \cos(v_\theta)\frac{\partial f}{\partial v}P_{pq}\left(\frac{v}{v_{\text{th}}}\right)Y_{qs}(v_\theta,v_\varphi)v^2\,dv\,dv_\omega = \\ \sum_{klm}a_{klm}\int\int\frac{v^2}{v_{\text{th}}}P'_{kl}\left(\frac{v}{v_{\text{th}}}\right)P_{pq}\left(\frac{v}{v_{\text{th}}}\right)\cos(v_\theta)Y_{lm}(v_\theta,v_\varphi)Y_{qs}(v_\theta,v_\varphi)\,dv\,dv_\omega = \\ \sum_{klm}a_{klm}\int\frac{v^2}{v_{\text{th}}}P'_{kl}\left(\frac{v}{v_{\text{th}}}\right)P_{pq}\left(\frac{v}{v_{\text{th}}}\right)dv\Psi_{lmqs} \tag{84}$$

$$
\begin{aligned}
&\int\int \sin(v_\theta)\frac{1}{v}\frac{\partial f}{\partial v_\theta}P_{pq}\left(\tfrac{v}{v_{\text{th}}}\right)Y_{qs}(v_\theta,v_\varphi)v^2\,dv\,dv_\omega = \\
&\sin(v_\theta)\left(\sum_{klm}a_{klm}P_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)\partial_{v_\theta}Y_{lm}(v_\theta,v_\varphi)\right)P_{pq}\left(\tfrac{v}{v_{\text{th}}}\right)Y_{qs}(v_\theta,v_\varphi)v\,dv\,dv_\omega = \\
&\sum_{klm}a_{klm}\int vP_{pq}\left(\tfrac{v}{v_{\text{th}}}\right)P_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)dv\int \sin(v_\theta)\partial_{v_\theta}Y_{lm}(v_\theta,v_\varphi)Y_{qs}(v_\theta,v_\varphi)\,dv_\omega = \\
&\qquad\qquad\sum_{klm}a_{klm}\int vP_{pq}\left(\tfrac{v}{v_{\text{th}}}\right)P_{kl}\left(\tfrac{v}{v_{\text{th}}}\right)dv\phi_{lmqs}
\end{aligned}
$$

C.1 Case of Laguerre polynomials (fancy attempt)

An attempt to compute advection operator analytically in the case of Laguerre polynomials. There are some mistakes early on that propagates throughout the derivations. However, it still gives an overall idea how to proceed. Maybe will revisit later.

$$
\begin{aligned}
L_0^{(l)}(x) &= 1 \\
L_1^{(l)}(x) &= 1 + l - x \\
L_{k+1}^{(l)}(x) &= \frac{(2k+1+l-x)L_k^{(l)}(x) - (k+l)L_{k-1}^{(l)}(x)}{k+1}
\end{aligned}
$$

$$
\int_0^\infty e^{-x}x^l L_k^{(l)}(x)L_p^{(l)}(x)\,dx = \frac{\Gamma(p+l+1)}{n!}\delta_{k,p}
$$

$$
\tilde{L}_k^{(l)} = L_k^{(l+1/2)}
$$

$$
\begin{aligned}
\Phi_{kl}(x) &= e^{-x^2}x^l\tilde{L}_k^{(l)}\left(x^2\right) \\
\Psi_{pq}(x) &= x^q\tilde{L}_p^{(q)}\left(x^2\right)
\end{aligned}
$$

$$
\begin{aligned}
\int_0^\infty \Phi_{kq}(x)\Psi_{pq}(x)x^2\,dx &= \int_0^\infty e^{-x^2}x^{2q+2}\tilde{L}_k^{(q)}\left(x^2\right)\tilde{L}_p^{(q)}\left(x^2\right)dx \\
&= \frac{1}{2}\int_0^\infty e^{-y}y^{q+1/2}\tilde{L}_k^{(q)}(y)\tilde{L}_p^{(q)}(y)\,dx \\
&= N_{p,q}\delta_{k,p}
\end{aligned}
$$

Useful formulae

$$
\begin{aligned}
\tilde{L}_k^{(l+1)}(x^2) &= \sum_{j=0}^{k} \tilde{L}_j^{(l)}(x^2) \\
\tilde{L}_k^{(l)}(x^2) &= \tilde{L}_k^{(l+1)}(x^2) - \tilde{L}_{k-1}^{(l+1)}(x^2) \\
x^2 \tilde{L}_k^{(l+1)}(x^2) &= (k+l+3/2)\tilde{L}_k^{(l)}(x^2) - (k+1)\tilde{L}_{k+1}^{(l)}(x^2) \\
\frac{d}{dx^2}\tilde{L}_k^{(l)}(x^2) &= -\tilde{L}_{k-1}^{(l+1)}(x^2) \\
\frac{d}{dx}\tilde{L}_k^{(l)}(x^2) &= 2x\frac{d}{dx^2}\tilde{L}_k^{(l)}(x^2) = -2x\tilde{L}_{k-1}^{(l+1)}(x^2)
\end{aligned}
$$

$$
\begin{aligned}
&\Psi_p^{(q)}(x)\frac{d}{dx}\Phi_k^{(q+1)}(x) = x^q\tilde{L}_p^{(q)}\frac{d}{dx}e^{-x^2}x^{q+1}\tilde{L}_k^{(q+1)} \\
&= x^q\tilde{L}_p^{(q)}\left(-2e^{-x^2}x^{q+2}\tilde{L}_k^{(q+1)}(x^2) + (q+1)e^{-x^2}x^q\tilde{L}_k^{(q+1)}(x^2) - 2e^{-x^2}x^{q+2}\tilde{L}_{k-1}^{(q+2)}(x^2)\right) \\
&\qquad = -2x^q\tilde{L}_p^{(q)}e^{-x^2}x^q\left((k+q+3/2)\tilde{L}_k^{(q)} - (k+1)\tilde{L}_{k+1}^{(q)}\right) \\
&+ (q+1)x^q\tilde{L}_p^{(q)}e^{-x^2}x^q\sum_{j=0}^{k}\tilde{L}_j^{(q)} - 2x^{q+1}\left(\tilde{L}_p^{(q+1)} - \tilde{L}_{p-1}^{(q+1)}\right)e^{-x^2}x^{q+1}\sum_{j=0}^{k-1}\tilde{L}_j^{(q+1)} \\
&= -2\Psi_p^{(q)}\left((k+q+3/2)\Phi_k^{(q)} - (k+1)\Phi_{k+1}^{(q)}\right) + (q+1)\Psi_p^{(q)}\sum_{j=0}^{k}\Phi_j^{(q)} - 2\left(\Psi_p^{(q+1)} - \Psi_{p-1}^{(q+1)}\right)\sum_{j=0}^{k-1}\Phi_j^{(q+1)}
\end{aligned}
$$

$$
\begin{aligned}
\int_0^\infty \Psi_p^{(q)}(x)\frac{d}{dx}\Phi_k^{(q+1)}(x) &= -2N_p^{(q)}\left((k+q+3/2)\delta_{p,k} - (k+1)\delta_{p,k+1}\right) + (q+1)N_p^{(q)}\sum_{j=0}^{k}\delta_{p,j} \\
&\quad - 2\left(N_p^{(q+1)}\sum_{j=0}^{k-1}\delta_{p,j} - N_{p-1}^{(q+1)}\sum_{j=0}^{k-1}\delta_{p-1,j}\right)
\end{aligned}
$$

Warning: what's below is not correct (forgot 1/2 in Laguerre index)

$$
\begin{aligned}
\Phi_{k,q+1}(x)\frac{d}{dx}\Psi_{p,q}(x) &= e^{-x^2}x^{q+1}L_k^{(q+1)}(x^2)\left(qx^{q-1}L_p^{(q)}(x^2) + x^q\frac{d}{dx}L_p^{(q)}(x^2)\right) \\
&= e^{-x^2}x^q\sum_{j=0}^{k}L_j^{(q)}(x^2)qx^qL_p^{(q)}(x^2) - \Phi_{k,q+1}(x)2x^{q+1}L_{p-1}^{(q+1)}(x^2) \\
&= q\sum_{j=0}^{k}\Phi_{j,q}(x)\Psi_{p,q}(x) - 2\Phi_{k,q+1}(x)\Psi_{p-1,q+1}(x)
\end{aligned}
$$

$$\int_0^\infty \Phi_{k,q+1}(x)\frac{d}{dx}\Psi_{p,q}(x)x^2\,dx = q\sum_{j=0}^{k} N_{p,q}\delta_{p,j} - 2N_{p,q+1}\delta_{p-1,k}$$
$$= q\sum_{j=0}^{k} N_{p,q}\delta_{p,j} - 2N_{p,q+1}\delta_{p,k+1}$$

$$\begin{aligned}
\Phi_{k,q-1}(x)\frac{d}{dx}\Psi_{pq}(x) &= e^{-x^2}x^{q-1}L_k^{(q-1)}\left(x^2\right)\frac{d}{dx}x^q L_p^{(q)}\left(x^2\right) \\
&= e^{-x^2}x^{q-1}L_k^{(q-1)}\left(x^2\right)\left(qx^{q-1}L_p^{(q)}\left(x^2\right) + x^q\frac{d}{dx}L_p^{(q)}\left(x^2\right)\right) \\
&= q\Phi_{k,q-1}(x)\sum_{j=0}^{p}\Psi_{j,q-1}(x) - 2e^{-x^2}x^{q-1}L_k^{(q-1)}\left(x^2\right)x^{q+1}L_{p-1}^{(q+1)}\left(x^2\right) \\
&= q\Phi_{k,q-1}(x)\sum_{j=0}^{p}\Psi_{j,q-1}(x) - 2e^{-x^2}x^q\left(L_k^{(q)}\left(x^2\right) - L_{k-1}^{(q)}\left(x^2\right)\right)x^q\sum_{j=0}^{p-1}L_j^{(q)}\left(x^2\right) \\
&= q\sum_{j=0}^{p}\Phi_{k,q-1}(x)\Psi_{j,q-1}(x) - 2\sum_{j=0}^{p-1}\left(\Phi_{k,q}\left(x^2\right) - \Phi_{k-1,q}\left(x^2\right)\right)\Psi_{j,q}\left(x^2\right)
\end{aligned}$$

$$\int_0^\infty \Phi_{k,q-1}(x)\frac{d}{dx}\Psi_{pq}(x)x^2\,dx = q\sum_{j=0}^{p} N_{k,q-1}\delta_{k,j} - 2\sum_{j=0}^{p-1}\left(N_{k,q}\delta_{k,j} - N_{k-1,q}\delta_{k-1,j}\right)$$

$$\begin{aligned}
&\Psi_{pq}(x)\frac{d}{dx}\Phi_{k,q-1}(x) = x^q L_p^{(q)}\left(x^2\right)\frac{d}{dx}e^{-x^2}x^{q-1}L_k^{(q-1)}\left(x^2\right) \\
&= x^q L_p^{(q)}\left(x^2\right)\left(-2e^{-x^2}x^q L_k^{(q-1)}\left(x^2\right) + (q-1)e^{-x^2}x^{q-2}L_k^{(q-1)}\left(x^2\right) + e^{-x^2}x^{q+1}\frac{d}{dx}L_k^{(q+1)}\left(x^2\right)\right) \\
&= -x^q L_p^{(q)}e^{-x^2}x^q\left(L_k^{(q)} - L_{k-1}^{(q)}\right) + (q-1)x^{q-1}\sum_{j=0}^{p}L_j^{(q-1)}e^{-x^2}x^{q-1}L_k^{(q-1)} - 2x^q L_p^{(q)}e^{-x^2}x^q L_{k-1}^{(q)} \\
&\qquad = -\Psi_p^{(q)}\Phi_k^{(q)} + \Psi_p^{(q)}\Phi_{k-1}^{(q)} + (q-1)\sum_{j=0}^{p}\Psi_j^{(q-1)}\Phi_k^{(q-1)} - 2\Psi_p^{(q)}\Phi_{k-1}^{(q)}
\end{aligned}$$

$$\int_0^\infty \Psi_{pq}(x)\frac{d}{dx}\Phi_{k,q-1}(x)x^2\,dx = -N_p^{(q)}\delta_{p,k} - N_p^{(q)}\delta_{p,k-1} + (q-1)\sum_{j=0}^{p}N_j^{(q-1)}\delta_{j,k}$$