Solving the Boltzmann equation for electron kinetics using Petrov-Galerkin approach

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- **Importance:** Distribution function of electrons defines transport and reaction properties
  $\rightarrow$ Need to couple plasma model with electron kinetics (Y3)
- Evolution of $f = f(\boldsymbol{x}, \boldsymbol{v}, t)$ obeys the **Boltzmann equation**

$$\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f - \boldsymbol{E} \cdot \nabla_{\boldsymbol{v}} f = \sum_a C_a(f)$$

where, for example, in case of $a =$ elastic collisions

$$C_a(f) = n_0 \int_{S^2} v \underbrace{\sigma_a(v, \omega)}_{\text{scat. cross sec.}} \left(f(v') - f(v)\right) \, \mathrm{d}\omega$$

- **Main challenge**: 6+1 dimensions
- **Idea**: FEM in $\boldsymbol{x}$, spectral in $\boldsymbol{v}$
- **Currently (Y1)**: spatially homogeneous case $f = f(\boldsymbol{v}, t)$

$$\partial_t f = \sum_a C_a(f)$$

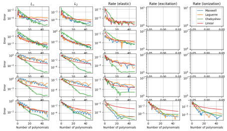
to investigate efficient velocity-space discretizations

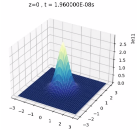
- **Approach:** Petrov-Galerkin
  - Nearly isotropic and symmetric f $\rightarrow$ employ spherical harmonics

$$f(\boldsymbol{v}) = \sum_{k,l,m} h_{k,l,m}(t) \Phi_k(v) \underbrace{Y_{lm}(v_\theta, v_\phi)}_{\text{sph. harm.}} \quad \rightarrow \quad \text{ODEs for } h_{k,l,m}(t)$$

Results:

- Investigating choice of $\Phi_k(v)$:
  - Tested Laguerre, Maxwell, Chebyshev, Linear polys using Bolsig+ data
- Solver implementation:
  - Python
  - Tenzorized 5D integrations: 0.0093s vs 5.2256s loop-based
  - Arbitrary choice of $\Phi_k(v)$
  - Reactions implemented: Elastic, Excitation, Ionization
  - Testing and verification are underway





Boltzmann equation

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$$\partial_t f = \sum C_a(f)$$

Petrov-Galerkin approach

- Weak formulation: $\partial_t f = \sum_a C_a(f) \quad \rightarrow \quad \partial_t \int_{R^3} f\phi(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} = \sum_a \int_{R^3} C_a(f)\phi(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}$

- Solution as a perturbed Maxwellian:

$$f(\boldsymbol{v}) = M(v)h(\boldsymbol{v},t), \qquad M(v) = n_e \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}}$$

- Expansion in basis functions:

$$h(\boldsymbol{v},t) = \sum_{k,l,m} h_{k,l,m}(t)\Phi_k(v)\underbrace{Y_{lm}(v_\theta,v_\phi)}_{\text{sph. harm.}}, \qquad \phi(\boldsymbol{v}) = \Phi_p(v)\underbrace{Y_{qs}(v_\theta,v_\phi)}_{\text{sph. harm.}}$$

- Resulting system of ODEs:

$$\sum_{k,l,m} M^{k,l,m}_{p,q,s}\partial_t h_{k,l,m}(t) = \sum_{k,l,m} L^{k,l,m}_{p,q,s} h_{k,l,m}(t)$$

Investigation of different bases

- Choice of basis functions in radial direction

$$\text{Assoc. Laguerre poly:} \quad \Phi_n(v) = L_n(v^2), \qquad \int_0^{+\infty} v^2 e^{-v^2} L_n(v^2) L_{n'}(v^2)\,\mathrm{d}v \sim \delta_{nn'}$$

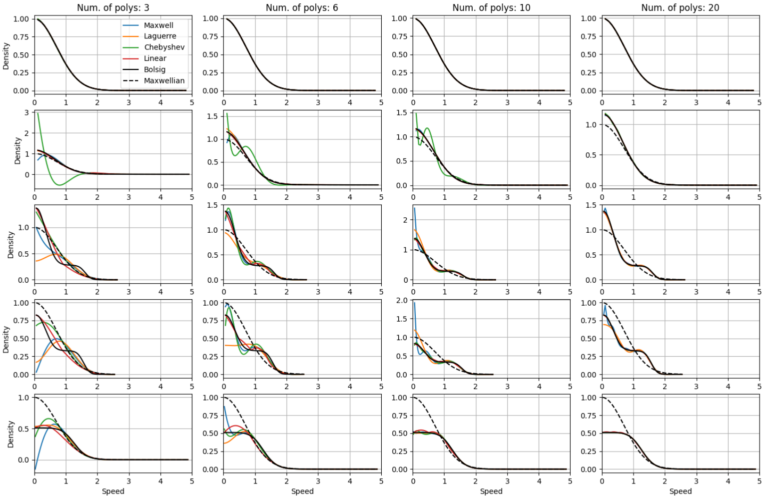
$$\text{Maxwell (speed) poly:} \quad \Phi_n(v) = P_n(v), \qquad \int_0^{+\infty} v^2 e^{-v^2} P_n(v) P_{n'}(v)\,\mathrm{d}v \sim \delta_{nn'}$$

$$\text{Chebyshev poly:} \quad \Phi_n(v) = C_n(v), \qquad \int_{-1}^{1} (1 - v^2)^{-\frac{1}{2}} C_n(v) C_{n'}(v)\,\mathrm{d}v \sim \delta_{nn'}$$

$$\text{Linear interp:} \quad \Phi_n(v) = N_n(v), \qquad N_n(v) = 1 - \frac{|x - x_n|}{\Delta x}, \quad x_{n-1} < x < x_{n+1}$$

Investigation of different bases

- Bolsig+ data for Ar
- Included reactions:
  - Elastic:
    $e + \text{Ar} \rightarrow e + \text{Ar}$
  - Excitation:
    $e + \text{Ar} \rightarrow e + \text{Ar}^*$
  - Ionization:
    $e + \text{Ar} \rightarrow e + \text{Ar}^+ + e$
- Electric field E/N:
  - 1×10^{-26} V $\cdot$ m^2
  - 1×10^{-24} V $\cdot$ m^2
  - 7×10^{-24} V $\cdot$ m^2
  - 1×10^{-23} V $\cdot$ m^2
  - 6×10^{-19} V $\cdot$ m^2



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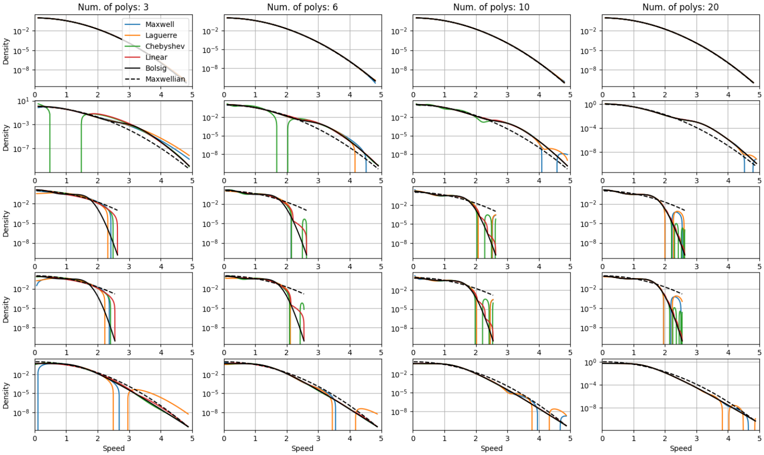
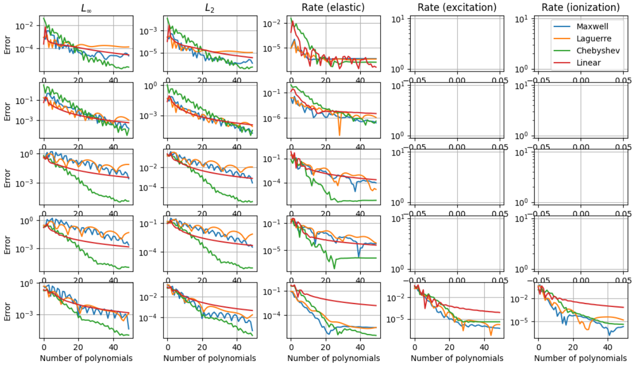


Investigation of different bases

- Error measures
  - EDF f itself: L_∞, L_2
  - Reaction rate
    $k_a = \gamma \int \varepsilon \sigma_a f \, \mathrm{d}\varepsilon$
    where
    $a =$ elastic, excitation, collision
- Takeaways:
  - No obvious choice
  - Needs further investigation



Solver implementation

- Python
- 5-dimensional integrations:
  - Tenzorized implementation
  - 0.0093s vs 5.2256s loop-based
- Flexible choice of basis functions in radial directions
- Reactions implemented
  - Elastic: $e + \mathrm{Ar} \rightarrow e + \mathrm{Ar}$
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- Currently: testing and verification