Some thoughts toward more reliable solution techniques for the Boltzmann equation

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Abstract

Techniques for determining electron distribution functions in discharges have evolved along various and widely differing paths. Each has its advantages, and all have disadvantages.

Often overlooked is the time-dependent continuum approach. y With the distinct advantage of representing the dynamics of the discharge in a quantitative manner, this is potentially a very reliable approach for obtaining a solution. It draws on well established computational methods developed over many years in the study of reactive flow, and can be applied to the energy-dependent Boltzmann equation.

The process of discretization introduces inevitable errors, some of which are quite subtle and due to the interaction of time-dependent quantities. Often, the choice of what to discretize is as important as the method used for solution. This presentation focuses on the development of representations which lend themselves to numerical solution by time-dependent finite-difference methods, and which mitigate the deleterious effects of some numerical artifacts which would otherwise arise.

Time-dependent approach:

Advantages:

- Convergence according to physical mechanisms
- Physical instability can be discovered
- Monotonic methods are easily applied
- Non-statistical continuum representation can have huge dynamic range

Problems:

- 6-dimensional Boltzmann equation is too difficult
- 2-term spherical harmonic expansion not well-suited (it can blow up!)

Elliptic closure[1]:

$$\vec{f}_2 = \frac{5}{4}(3F(X)-1)(3\hat{X}\hat{X}-\hat{I})f_0 \qquad \vec{X} = \frac{\vec{f}_1}{3\,f_0} \qquad X = \frac{F(X)}{X} - \frac{2}{\ln\left(\frac{F(X)+X}{F(X)-X}\right)}$$

$$\frac{\partial \eta}{\partial t} + \nabla\cdot\vec{G} - \frac{\partial}{\partial u}\left(\vec{E}\cdot\vec{G}\right) = \left(\frac{\delta\eta}{\delta t}\right)_c$$

$$\frac{\partial \vec{G}}{\partial t} + \nabla\cdot\left(\frac{v^2}{2}\hat{X}\hat{X}(3F(X)-1)\eta\right) + \nabla\left(\frac{1}{2}(1-F(X))\eta\right) - \frac{\partial}{\partial u}\left(\frac{v^2}{2}(3F(X)-1)\vec{E}\cdot\hat{X}\hat{X}\eta\right)$$

$$-\frac{v^2}{2}\vec{E}\frac{\partial}{\partial u}\big((1-F(X))\eta\big) + \frac{e}{m}\vec{E}F(X)\eta = \left(\frac{\delta\vec{G}}{\delta t}\right)_c$$

Where:

$$\eta = 4\pi\, v\, f_0 \qquad \vec{G} = \frac{4\pi}{3}v^2\vec{f}_1$$

Problems:

·Discretization causes violation of anisotropy condition: $|X|<1$

·High frequency artifacts cause derived quantities to be non-monotonic [2,3,4]

Bounded Anisotropy Formulation:

- Use dimensionless anisotropy, X, as fundamental quantity

$$\frac{\partial \eta}{\partial t}+\nabla\cdot\left(v\vec{X}\eta\right)-\frac{\partial}{\partial u}\left(v\vec{E}\cdot\vec{X}\eta\right)=\left(\frac{\delta\eta}{\delta t}\right)_c$$

$$\frac{\partial \vec{X}}{\partial t}+\nabla\cdot\left(vG(X)\vec{X}\vec{X}\right)+v\vec{X}\cdot\nabla\vec{X}-\frac{\partial}{\partial u}\left(vG(X)\left(\vec{E}\cdot\vec{X}\right)\vec{X}\right)-v\vec{E}\vec{X}\frac{\partial\vec{X}}{\partial u}=$$

$$-vG(X)\vec{X}\vec{X}\frac{1}{\eta}\nabla\eta-\frac{v}{\eta}\nabla(\eta H(X))+G(X)(\vec{E}\cdot\vec{X})\vec{X}\frac{v}{\eta}\frac{\partial\eta}{\partial u}+\vec{E}\frac{v^2}{\eta}\frac{\partial}{\partial u}(\eta H(X)/v)$$

$$+\frac{v}{2u}J(X)\left(\left(\vec{E}\cdot\vec{X}\right)\vec{X}-X^2\vec{E}\right)+\left(\frac{\delta\vec{X}}{\delta t}\right)_c$$

Where:

$$G(X)=\frac{1}{2X^2}\left(3F(X)-1\right)-1$$

$$H(X)=\frac{1}{2}\left(1-F(X)\right)$$

$$J(X)=\frac{1}{2X^2}\left(3F(X)-1\right)$$

Note:

$$\left(\frac{\delta\vec{X}}{\delta t}\right)_c=\frac{1}{\eta}\sum_i(\nu_T(v')-\nu_M(v'))\eta(v')\vec{X}(v')-\nu_T(v')\eta(v')\vec{X}(v)$$

Depends *only on in-scattering*, and:

$$X=|\vec{X}|\rightarrow 1 \qquad \frac{\partial X}{\partial t}\rightarrow\left(\frac{\delta X}{\delta t}\right)_c$$

Problem:

- Roundoff/truncation error lead to violations of |X|<1

Unbounded Anisotropy Formulation:

$$\vec{Y} = \frac{\vec{X}}{\sqrt{1-X^2}} \qquad\qquad \vec{X} = \frac{\vec{Y}}{\sqrt{1+Y^2}}$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot \left(v \vec{X} \eta \right) - \frac{\partial}{\partial u}\left(v \vec{E} \cdot \vec{X} \eta \right) = \left(\frac{\delta \eta}{\delta t} \right)_c$$

$$\begin{aligned}
\frac{\partial \vec{Y}}{\partial t} + \nabla \cdot \left(v\, G(X) \vec{X}\, \vec{Y} \right) + v \vec{X} \cdot \nabla \vec{Y} - \frac{\partial}{\partial u}\left(vG(X) \left(\vec{E} \cdot \vec{X} \right) \vec{Y} \right) - v \vec{E}\, \vec{X} \frac{\partial \vec{Y}}{\partial u} \quad &= \\
Y^2 \vec{Y} \frac{\partial}{\partial u}\left(vG(X)(\vec{E} \cdot \vec{X}) \right) - v\, G(X)(1+Y^2)\, \vec{Y}\, \vec{X} \cdot \frac{1}{\eta} \nabla \eta & \\
- v \sqrt{1+Y^2} \left(1 + \vec{Y}\, \vec{Y} \cdot \right) \frac{1}{\eta} \nabla \left(\eta H(X) \right) & \\
- vY^2 \vec{Y} \nabla \cdot \left(G(X) \vec{X} \right) + (1+Y^2) G(X) \left(\vec{E} \cdot \vec{X} \right) \vec{Y} \frac{v}{\eta} \frac{\partial \eta}{\partial u} & \\
+ \frac{v^2}{\eta} \frac{\partial (\eta H(X)/v)}{\partial u} \sqrt{1+Y^2} \left(\vec{E} + \vec{Y} \left(\vec{Y} \cdot \vec{E} \right) \right) & \\
+ \frac{v}{2u} J(X) \left(\left(\vec{E} \cdot \vec{X} \right) \vec{Y} - XY \vec{E} \right) + \left(\frac{\delta \vec{Y}}{\delta t} \right)_c &
\end{aligned}$$

Where:

$$\left(\frac{\delta \vec{Y}}{\delta t} \right)_c = \sqrt{1+Y^2} \left(1 + \vec{Y}\, \vec{Y} \cdot \right) \left(\frac{\delta \vec{X}}{\delta t} \right)_c$$

Advantages:

- Provides monotonicity of derived quantities
- $|X|<1$ strictly enforced, without artificial limiting
- Very reliable solutions over a wide range of conditions

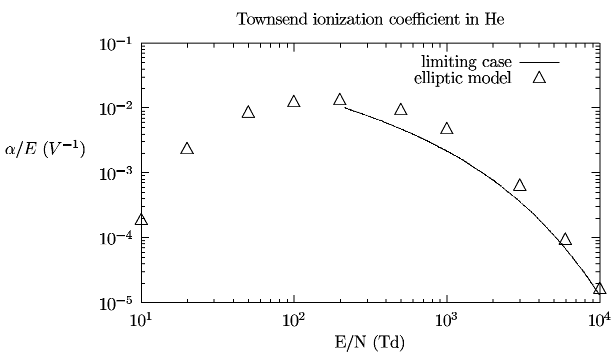
0-d Example: Townsend discharge in He; forward scattering [5]

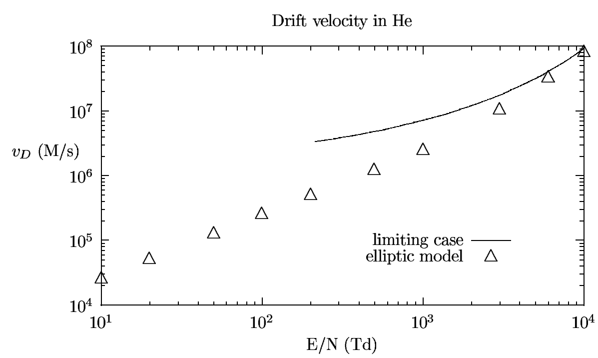
$$\frac{\partial \eta}{\partial t} - \frac{\partial}{\partial u}(v E X \eta) = -\alpha v X \eta + \left(\frac{\delta \eta}{\delta t}\right)_c$$

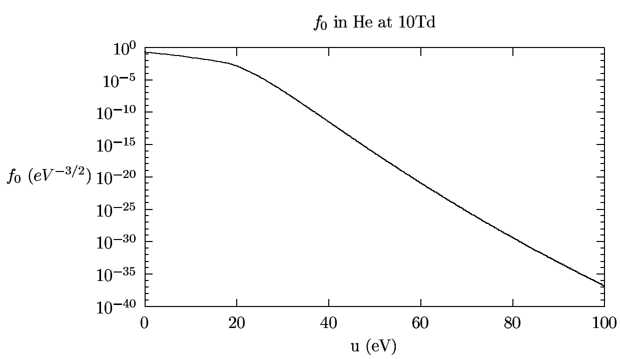
$$\frac{\partial Y}{\partial t} - v E X K(X) \frac{\partial Y}{\partial u} = -\alpha v (1+Y^2)^{\frac{3}{2}} (F(X) - X^2)$$

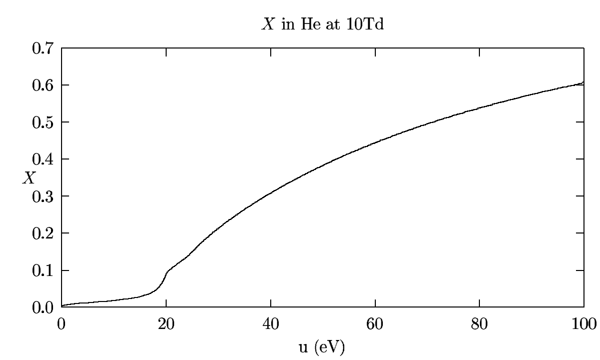
$$+ (1+Y^2)^{\frac{3}{2}} v E \left(G(X) \frac{X^2}{u} + (F(X) - X^2) \frac{v}{\eta} \frac{\partial \eta / v}{\partial u} \right) - (1+Y^2) \left(\frac{\delta X}{\delta t}\right)_c$$

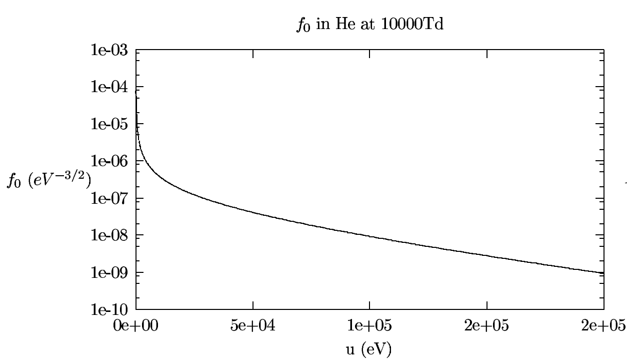
$$K(X) = \frac{1}{X} \frac{dF(X)}{dX} - 1$$

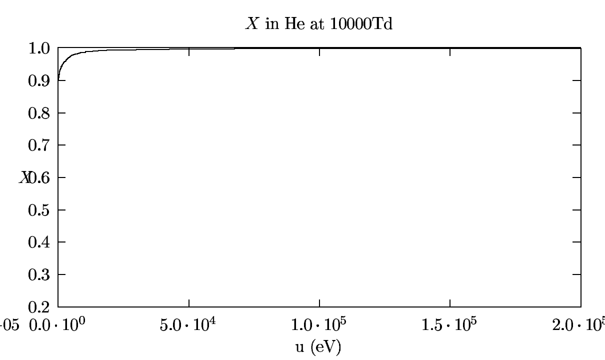




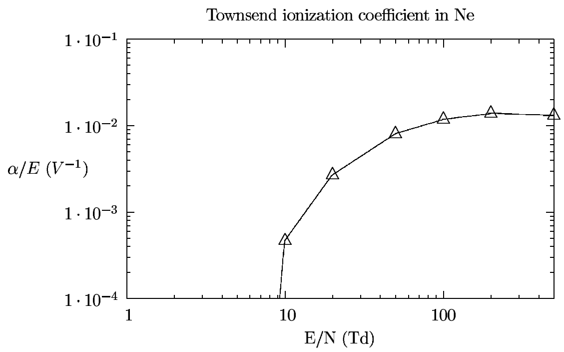


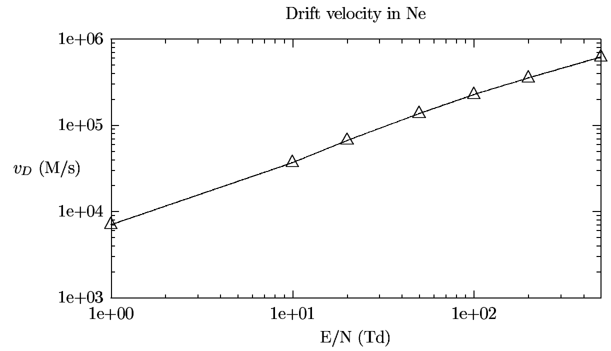


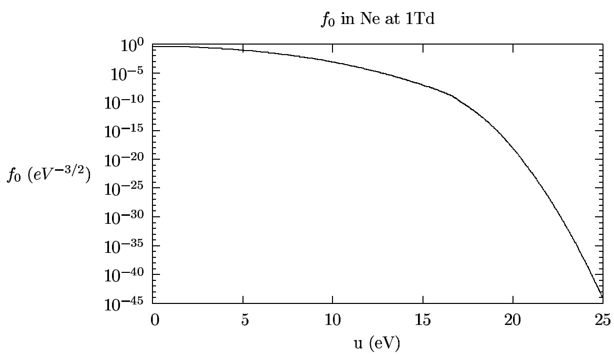


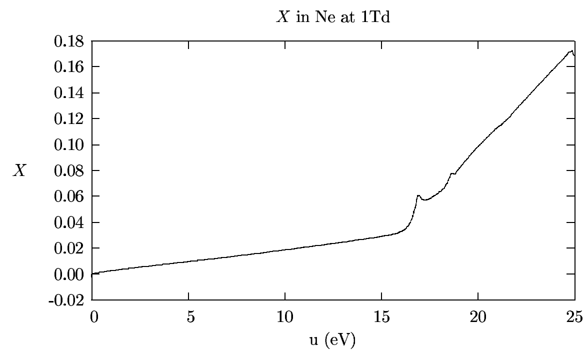


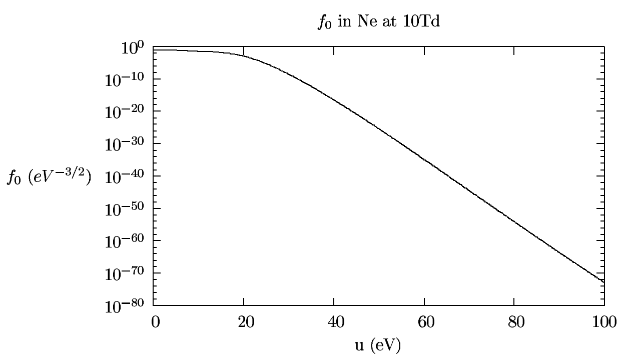
0-d Example: Townsend discharge in Ne; energy sharing, no forward scattering

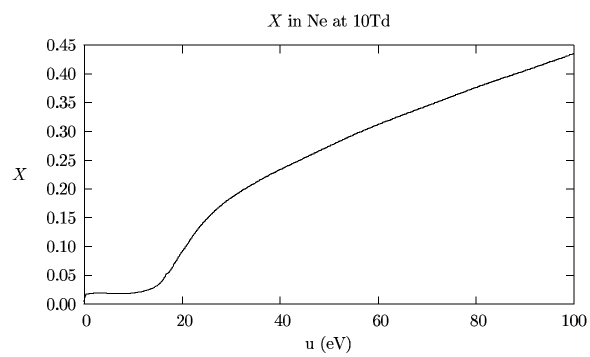


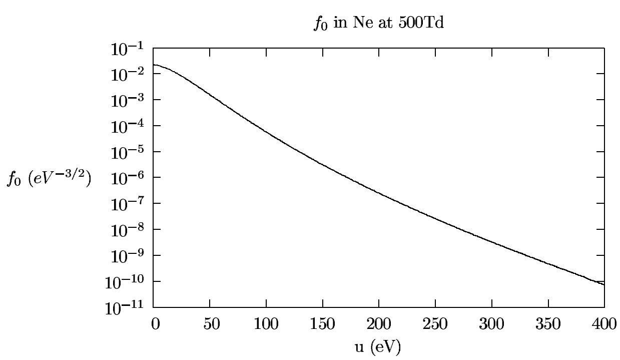


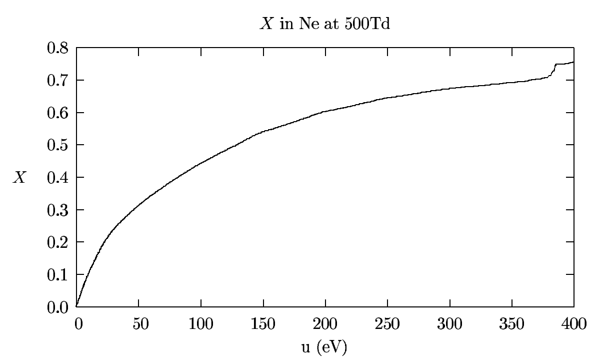












Summary:

- Unbounded anisotropy, "Y", formulation is presented
- Time-dependent solutions are possible
- Low phase-error monotonic methods can be used
- A very wide range of conditions is tolerated
- Ill effects of terracing, and energy migration to higher spatial frequencies, are mitigated
- Non-physical representations of anisotropy are avoided

References:

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