# An efficient kinetic modeling in plasmas relevant to inertial confinement fusion by using the AWBS transport equation

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Text of abstract.

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#### I. INTRODUCTION

The first attempts of modern kinetic modeling of plasma can be tracked back to the fifties, when Cohen, Spitzer, and Routly (CSR) [1] in detail demonstrated the fact, that in the ionized gas the effect of Coulomb collisions between electrons and ions predominantly results from frequently occurring events of cumulative small deflections rather than occasional close encounters. This effect was originally described by Jeans in [2] and Chandrasekhar [3] proposed to use the diffusion equation model of the Fokker-Planck type (FP) [4].

As a result, a classical paper by Spitzer and Harm (SH) <sup>49</sup> [5] provides the computed electron distribution function <sup>50</sup> spanning from low to high Z plasmas, and more im-<sup>51</sup> portantly, the current and heat flux formulas, which <sup>52</sup> are widely used in almost every plasma hydrodynamic <sup>53</sup> code nowadays. The distribution function is of the form  $f^0 + \mu f^1$ , where  $f^0$  and  $f^1$  are isotropic and  $\mu$ , is the direction cosine between the particle trajectory and some preferred direction in space. It should be emphasized <sup>54</sup> that the SH solution expresses a small perturbation of <sup>55</sup> equilibrium, i.e. that  $f^0$  is the Maxwell-Boltzmann dis-<sup>56</sup> tribution and  $\mu f^1$  represents a very small deviation.

The actual cornerstone of the modern FP simulations  $_{58}$  was set in place by Rosenbluth [6], when he derived  $_{59}$  a simplified form of the FP equation for a finite expan- $_{60}$  sion of the distribution function, where all the terms are computed according to plasma conditions, including  $f^0$ , which of course needs to tend to the Maxwell-Boltzmann distribution.

In is the purpose of this paper to present an efficient alternative to FP model based on the Albritton-Williams-Bernstein-Swartz collision operator (AWBS) [7]. In Section II we propose a modified form of the AWBS collision operator, where its important properties are further presented in Section III with the emphasis on its comparison to the full FP solution in local diffusive regime. Section IV focuses on the performance of the AWBS transport equation model compared to modern kinetic codes including FP codes Aladin and Impact, and PIC code Calder, where the cases related to real laser generated plasma conditions are studied. Finally, the most impor-

tant outcomes of our research are concluded in Section V

#### II. THE AWBS KINETIC MODEL

The electrons in plasma can be modeled by the deterministic Vlasov model of charged particles

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \tilde{\boldsymbol{E}} \cdot \nabla_{\boldsymbol{v}} f = C_{ee}(f) + C_{ei}(f), \quad (1)$$

where  $f(t, \boldsymbol{x}, \boldsymbol{v})$  represents the density function of electrons at time t, spatial point  $\boldsymbol{x}$ , and velocity  $\boldsymbol{v}$ , and  $\tilde{\boldsymbol{E}} = \frac{q_e}{m_e} \boldsymbol{E}$  is the existing electric field in plasma.

The generally accepted form of the electron-electron collision operator  $C_{ee}$  is the Fokker-Planck form published by Landau [8]

$$C_{FP}(f) = \Gamma \int \nabla_{\boldsymbol{v}} \nabla_{\boldsymbol{v}} (\boldsymbol{v} - \tilde{\boldsymbol{v}}) \cdot (f \nabla_{\tilde{\boldsymbol{v}}} f - f \nabla_{\boldsymbol{v}} f) \, d\tilde{\boldsymbol{v}}, \tag{2}$$

where  $\Gamma = \frac{q_e^4 \ln \Lambda}{4\pi e^2 m_e^2}$  and  $\ln \Lambda$  is the Coulomb logarithm. In principal, the electron-ion collision operator  $C_{ei}$  could be expressed in the form similar to (2), but since ions are considered to be motionless compared to electrons, the scattering operator, i.e. no change in the velocity magnitude, expressed in spherical coordinates is widely accepted

$$C_{ei}(f) = \frac{\nu_{ei}}{2} \left( \frac{\partial}{\partial \mu} \left( (1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), (3)$$

where  $\mu = \cos(\phi)$ ,  $\phi$  and  $\theta$  are the polar and azimuthal angles, and  $\nu_{ei} = \frac{Zn_e\Gamma}{v^3}$  is the electron-ion collision frequency.

Fish introduced an alternative form of  $C_{ee}$  in [9] referred to as high-velocity limit electron collision operator

$$C_H(f) = v\nu_e \frac{\partial}{\partial v} \left( f + \frac{v_{th}^2}{v} \frac{\partial f}{\partial v} \right) + \frac{\nu_e}{2} \left( 1 - \frac{v_{th}^2}{2v^2} \right) \left( \frac{\partial}{\partial \mu} \left( (1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \tag{4}$$

where  $\nu_e = \frac{n_e \Gamma}{v^3}$  is the electron-electron collision frequency and  $v_{th} = \sqrt{\frac{k_B T_e}{m_e}}$  is the electron thermal velocity. The linear form of  $C_H$  arises from an assumption that the fast electrons predominantly interact with

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the thermal (slow) electrons, which simplifies importantly the nonlinear form (2).

The aim of this work is to use a yet simpler form of the electron-electron collision operator, i.e. the AWBS formulation [7], where we propose the following form

$$C_{AWBS}(f) = v \frac{\nu_e}{2} \frac{\partial}{\partial v} (f - f_M) + \frac{\nu_{ei} + \frac{\nu_e}{2}}{2} \left( \frac{\partial}{\partial \mu} \left( (1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \quad (5)^{10}$$

where  $f_M$  is the Maxwell-Boltzmann equilibrium distri-<sub>108</sub> bution.  $C_{AWBS}$  represents the complete  $C_{ee} + C_{ei}$  collision operator in (1).

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The complete form of collision operator (5) was previously introduced in [10, 11], nevertheless, we intentionally use a half of the electron-electron collisional frequency modification  $\frac{\nu_e}{2}$ , because this formulation provides very promising results compared to the full FP operator as emphasized in Section III.

The Maxwell-Boltzmann averaged e-e scattering in (4) $_{112}^{111}$  can be approximated as  $\nu_e \int \left(1 - \frac{v_{th}^2}{2v^2}\right) f_M 4\pi v^2 \, \mathrm{d}v = \frac{\nu_e}{2}$ . 113

# III. BGK, AWBS, AND FOKKER-PLANCK MODELS IN LOCAL DIFFUSIVE REGIME

In a broad analysis of the electron transport, any qual-120 itative information about its properties are highly wel-121 come. Even better, if one can extract some qualitative information, which provides comparative and reliable re-123 sults in a clear way, the confidence of using a transport model, e.g. (5), can lead to efficient yet relatively cheap computation cost predictions of real physics.

In this paper, we can try to find an approximate solution to the so-called local diffusive regime of electro transport, where the diffusive regime, in general, refers to a low anisotropy in angle given by  $\mu$ , and local means that the mean free path of electrons  $\lambda_{ei}$  is rather restricted compared to the plasma spatial scale. In the words of mathematics this corresponds to the first order expansion in  $\lambda_{ei}$  and  $\mu$  of the distribution function as

$$\tilde{f}(z,v,\mu) = f^0(z,v) + f^1(z,v)\lambda_{ei}\mu, \tag{6}$$

where z is the spatial coordinate along the axis z, v the magnitude of transport velocity, and  $\lambda_{ei} = \frac{v}{\nu_{ei}} = \frac{v^4}{Zn_e\Gamma}$ . In other words, one can say that by evaluating numerically  $\tilde{f}$  in (6), we accept some error of the order125  $O(\lambda_{ei}^2) + O(\mu^2)$ . The expansion in a small parameter  $\lambda_{ei}$  is also coherent with a time-steady approximation due to the relation between the mean free path and collision frequency, where the higher the collision frequency the more steady the solution.

In order to start, we express the time-steady left hand<sub>127</sub> side of (1) in 1D and insert the approximation (6), which<sub>128</sub>

leads to

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$$\mu \left( \frac{\partial \tilde{f}}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial \tilde{f}}{\partial v} \right) + \frac{\tilde{E}_z (1 - \mu^2)}{v^2} \frac{\partial \tilde{f}}{\partial \mu} = \mu \left( \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f^0}{\partial v} \right) + \frac{\tilde{E}_z \lambda_{ei}}{v^2} f^1 + O(\mu^2), \quad (7)$$

and is truncated for low anisotropy, i.e. with error  $O(\mu^2)$ .

## A. The BGK local diffusive electron transport

Even though the BGK plasma collisional operator [12]

$$\frac{1}{v}C_{BGK}(\tilde{f}) = \frac{\tilde{f} - f_M}{\lambda_e} + \frac{1}{2\lambda_{ei}} \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \tilde{f}}{\partial \mu}, \quad (8)$$

where  $\lambda_e = Z\lambda_{ei}$ , is not actually used in our nonlocal transport simulations, we consider it useful to include this simplest form of the Boltzmann transport collision operator, because of two reasons: a) it can be treated analytically in the local diffusive regime; and b) it represents the so-called phenomenological collision operator by explicitly using the Maxwell-Boltzmann equilibrium distribution  $f_M$ , which proves to be very useful in coupling of the nonlocal electron transport to hydrodynamics.

If one applies the action of the right hand side, i.e. of (8), on the approximation (6) and sets the result to be equal to the left hand side (7), the corresponding terms in  $\mu$  are governed by the following equations

$$f^{0} = f_{M} + \frac{\tilde{E}_{z}}{v^{2}} f^{1} Z \lambda_{ei}^{2}, \tag{9}$$

$$f^{1} = -\frac{Z}{Z+1} \left( \frac{\partial f^{0}}{\partial z} + \frac{\tilde{E}_{z}}{v} \frac{\partial f^{0}}{\partial v} \right), \tag{10}$$

i.e.  $f^0 = f_M + O(\lambda_{ei}^2)$  and  $f^1 = -\frac{Z}{Z+1} \left( \frac{\partial f_M}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f_M}{\partial v} \right)$ . Now the electric current expressing the contribution of every electron naturally tends to zero, i.e. the *quasineutrality* constraint, which lead to an analytic formula of the self-consistent electric field

$$\mathbf{j} \equiv q_e \int \mathbf{v}\tilde{f} \,d\mathbf{v} = \mathbf{0} \to \tilde{\mathbf{E}} = v_{th}^2 \left( \frac{\nabla \rho}{\rho} + \frac{5}{2} \frac{\nabla T}{T} \right).$$
(11)

Consequently, based on (9), (10), and (11), the analytic formula (6) of the electron distribution function reads

$$\tilde{f} = f_M - \frac{Z}{Z+1} \left( \frac{v^2}{2v_{th}^2} - 4 \right) \frac{1}{T} \frac{\partial T}{\partial z} f_M \lambda_{ei} \mu, \qquad (12)$$

which is nothing else than the famous Lorentz electronion collision gas model [13] scaled by a constant depending on Z, naturally arising from the BGK model (8).

### B. The AWBS local diffusive electron transport

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The main object of this work presented in Sec II simplifies in 1D to a relatively simple form of the Boltzmann transport collision operator (compared to (2))

$$\frac{1}{v}C_{AWBS}(f) = \frac{v}{2\lambda_e} \frac{\partial}{\partial v} (f - f_M) 
+ \frac{1}{2} \left( \frac{1}{\lambda_{ei}} + \frac{1}{2\lambda_e} \right) \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial f}{\partial \mu}.$$
(13)

Similarly to the BGK model, AWBS 13 is also referred to as a phenomenological model, since it explicitly uses the Maxwell-Boltzmann equilibrium distribution  $f_M$ , and also, makes it a very attractive model of the non-local electron transport to be coupled to hydrodynamics via the plasma electron temperature and density.

A qualitative information about the AWBS model is obtained while repeating the action on (6) by the left hand side (7) and by the right hand side (13) and setting the equality. The corresponding terms in  $\mu$  are then governed by the following equations

$$\frac{\partial}{\partial v} \left( f^0 - f_M \right) = \frac{\dot{E}_z}{v^3} f^1 2Z \lambda_{ei}^2, \qquad (14)$$

$$v = \partial \left( f^1 \lambda_{ei} \right) = 2Z + 1 \quad \partial f^0 = \tilde{E}_z \partial f^0 \quad (15)$$

$$\frac{v}{2Z\lambda_{ei}}\frac{\partial (f^1\lambda_{ei})}{\partial v} - \frac{2Z+1}{2Z}f^1 = \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v}, (15)$$

i.e.  $f^0 = f_M + O(\lambda_{ei}^2)$ , however, the  $f^1$  does not have a straightforward analytic formula. In reality,  $f^1$  arises from the ordinary differential equation (by inserting  $f_M$  into (15))

$$\frac{\partial f^{1}}{\partial v} + \frac{1}{v}(3 - 2Z)f^{1} =$$

$$\frac{2Z}{v} \left( \frac{1}{\rho} \frac{\partial \rho}{\partial z} + \left( \frac{v^{2}}{2v_{th}^{2}} - \frac{3}{2} \right) \frac{1}{T} \frac{\partial T}{\partial z} - \frac{\tilde{E}_{z}}{v_{th}^{2}} \right) f_{M}. \quad (16)$$

We will stick with a numerical solution of (16), where the details about the resulting distribution function can be found in Section III D.

# C. The Fokker-Planck local diffusive electron transport

The Fokker-Plank (2) collision operator can be also written as [14]

$$\frac{1}{v}C_{FP}(f) = \frac{\Gamma}{v} \left( 4\pi f^2 + \frac{\nabla_{\boldsymbol{v}}\nabla_{\boldsymbol{v}}f : \nabla_{\boldsymbol{v}}\nabla_{\boldsymbol{v}}g}{2} \right), \quad (17)$$

where  $g(\boldsymbol{v}) = \int |\boldsymbol{v} - \tilde{\boldsymbol{v}}| f(\tilde{\boldsymbol{v}}) \, \mathrm{d}\tilde{\boldsymbol{v}}$  is the Rosenbluth potential [6]. Since we are interested in the approximate solution in the local diffusive regime, it is convenient to use a low anisotropy approximation  $\tilde{g} = g^0(f^0) + g^1(f^1) \lambda_{ei} \mu$ , which arises based on Eq. 45 of [6].

For a better clarity we present the action of (17) in 1D

$$C_{FP}(\tilde{f}) = \Gamma \left( 4\pi f^{02} + \frac{1}{2} \frac{\partial^2 f^0}{\partial v^2} \frac{\partial^2 g^0}{\partial v^2} + \frac{1}{v^2} \frac{\partial f^0}{\partial v} \frac{\partial g^0}{\partial v} \right)$$

$$+ \frac{\mu}{Zn_e} \left[ 8\pi f^0 f^1 v^4 - v \left( \frac{\partial f^0}{\partial v} g^1 + \frac{\partial g^0}{\partial v} f^1 \right) \right]$$

$$+ \frac{1}{v^2} \left( \frac{\partial f^0}{\partial v} \frac{\partial (g^1 v^4)}{\partial v} + \frac{\partial g^0}{\partial v} \frac{\partial (f^1 v^4)}{\partial v} \right)$$

$$+ \frac{1}{2} \left( \frac{\partial^2 f^0}{\partial v^2} \frac{\partial^2 (g^1 v^4)}{\partial v^2} + \frac{\partial^2 g^0}{\partial v^2} \frac{\partial^2 (f^1 v^4)}{\partial v^2} \right) \right] + O(\lambda_{ei}^2, \mu^2), \tag{18}$$

truncated by the quadratic terms in the angular anisotropy and the transport localization.

If once more repeated the action on (6) by the left hand side (7) and by the right hand side (17) and setting the equality, the equation governing  $f^0$  corresponding to  $\mu^0$  takes the form

$$4\pi f^{0^2} + \frac{1}{2} \frac{\partial^2 f^0}{\partial v^2} \frac{\partial^2 g^0}{\partial v^2} + \frac{1}{v^2} \frac{\partial f^0}{\partial v} \frac{\partial g^0}{\partial v} = \frac{\tilde{E}_z}{v^5} f^1 Z n_e \lambda_{ei}^2 - \frac{2}{v^2} \left( \frac{\partial f^1 \lambda_{ei}}{\partial v} - \frac{f^1 \lambda_{ei}}{v} \right) \left( \frac{\partial g^1 \lambda_{ei}}{\partial v} - \frac{g^1 \lambda_{ei}}{v} \right), \quad (19)$$

where the fundamental property of the Fokker-Planck collision operator tending to the Maxwell-Boltzmann distribution  $f_M$  [15], leads to  $f^0 = f_M + O(\lambda_{ei}^2)$ , where we write an explicit form of the quadratic term  $O(\lambda_{ei}^2)$  obtained from the truncation (18). The equality corresponding to  $\mu$  takes the form

$$\frac{1}{Zn_e} \left[ \frac{1}{2} \left( \frac{\partial^2 f_M}{\partial v^2} \frac{\partial^2 (g^1 v^4)}{\partial v^2} + \frac{\partial^2 g_M}{\partial v^2} \frac{\partial^2 (f^1 v^4)}{\partial v^2} \right) \right. \\
+ \frac{1}{v^2} \left( \frac{\partial f_M}{\partial v} \frac{\partial (g^1 v^4)}{\partial v} + \frac{\partial g_M}{\partial v} \frac{\partial (f^1 v^4)}{\partial v} \right) \\
- v \left( \frac{\partial f_M}{\partial v} g^1 + \frac{\partial g_M}{\partial v} f^1 \right) + 8\pi f_M f^1 v^4 \right] - v f^1 \\
= v \frac{\partial f_M}{\partial z} + \tilde{E}_z \frac{\partial f_M}{\partial v}, \quad (20)$$

which is the equation governing the unknown  $f^1$ .

In principle, the solution to the equation (20) is very ambitious, as demonstrated in [1, 3, 6], fortunately, one can use the explicit evaluation of the electron distribution function published in [5], which takes the following form

$$f^{1}(z,v) = \frac{1}{\lambda_{ei}} \frac{m_e^2}{4\pi q_e^4 \ln \Lambda} \frac{v_{2th}^4}{Z}$$

$$\left(2d_T(v/v_{2th}) + \frac{3}{2} \frac{\gamma_T}{\gamma_E} d_E(v/v_{2th})\right) \frac{f_M}{n_e} \frac{1}{T} \frac{\partial T_e}{\partial z}, \quad (21)$$

where  $d_T(x) = ZD_T(x)/B$ ,  $d_E(x) = ZD_E(x)/A$ ,  $\gamma_T$ , and  $\gamma_E$  are represented by numerical values in TABLE I, TABLE II, and TABLE III in [5], and  $v_{2th} = \sqrt{\frac{k_B T_e}{2m_e}}$ .

	Z=1	Z=2	Z=4	Z = 16	Z = 116
$ar{\Delta}oldsymbol{q}_{AWBS}$	0.057	0.004	0.038	0.049	0.004

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TABLE I. Relative error  $\bar{\Delta}q_{AWBS} = |q_{AWBS} - q_{SH}|/q_{SH_{196}}$  of the AWBS kinetic model equation (5) showing the discrepancy (maximum around 5%) with respect to the original solution of the heat flux given by numerical solution in Spitzer and Harm [5].

# D. Summary of the BGK, AWBS, and Fokker-Planck local diffusive transport

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Ever since the SH paper [5], the effect of microscopic electron transport on the current  $\int q_e \boldsymbol{v} \tilde{f} \, d\boldsymbol{v}$  and the heat flux  $\int \frac{m_e |\boldsymbol{v}|^2}{2} \boldsymbol{v} \tilde{f} \, d\boldsymbol{v}$  in plasmas under local diffusive conditions has been understood. By overcoming some delicate aspects of the numerical solution to (20) presented in the CSR paper [1], the effect of electron-electron collisions was properly quantified and the correct dependence on Z of the heat flux  $\boldsymbol{q}$  was approximated as

$$q = \frac{Z + 0.24}{Z + 4.2} q_L, \tag{22}$$

where  $q_L = \kappa T_e^{\frac{5}{2}} \nabla T_e$  is the heat flux given by Lorentz [13]. In order to follow the SH Z-dependence of heat flux,<sub>199</sub> the BGK operator needs to be scaled as

$$\frac{Z+4.2}{Z+0.24}\frac{Z}{Z+1}\left[\nu_e\left(\tilde{f}-f_M\right)+\frac{\nu_{ei}}{2}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial\tilde{f}}{\partial\mu}\right],$$

which leads to a scaled Lorentz\* distribution function

$$\tilde{f} = f_M - \frac{Z + 0.24}{Z + 4.2} \left( \frac{v^2}{2v_{th}^2} - 4 \right) \frac{1}{T} \frac{\partial T}{\partial z} f_M \lambda_{ei} \mu, \quad (23)_{207}^{206}$$

which obeys the Z-dependence (22).

On the contrary, the modified form of the AWBS col-210 lision operator (5) provides a very precise heat flux Z-211 dependence without introducing any scaling. Indeed,212 TABLE I shows the relative error (maximum around 5%)213 of the heat flux modeled by (5) vs. SH results represented by (22). It should be noted that the error is calculated with respect to original values presented in TABLE III in [5].

Nevertheless, the electron-electron collisions effect rep-216 resented by (22) provides only an integrated information 217 about the heat flux magnitude. If one takes a closure look at the distribution function itself, the conformity of the modified AWBS collision operator is even more emphasize as can be seen in FIG. 1 showing the flux moment in spherical coordinates of velocity

$$q_1 = \frac{m_e v^2}{2} v f_1 v^2,$$

where  $f_1$  is the anisotropic part of the distribution function, i.e.  $f_1 = f^1 \lambda_{ei}$  ( $\mu = 1$ ) in the local diffusive transport.

In the case of the high Z Livermorium plasma (Z=116), AWBS exactly aligns with the Lorentz gas limit. In the opposite case of the low Z Hydrogen plasma (Z=1), the AWBS distribution function approaches significantly the numerical SH solution. Overall BGK behavior is consistent with the scaled Lorentz\* distribution function (23) for any Z.

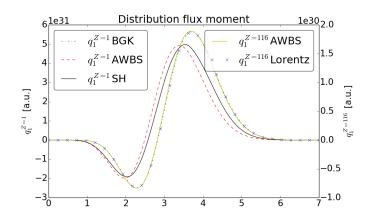


FIG. 1. The flux velocity moment of the anisotropic part of the electron distribution function in low Z=1 and high Z=116 plasmas in diffusive regime.

If one observes the  $f^1$  equations of each of the model, i.e. (10), (16), and (20), it turns out to be clear that the terms containing derivatives with respect to v address important physical mechanisms of electron-electron collisions in plasma. In other words, even a simple linear first derivative term in the modified AWBS collision operator (5) (red dashed line) provides a significant model improvement with respect to the SH (Fokker-Planck) solution (solid black line) and compared to the simplest BGK model (dashed-dot blue line) in FIG. 1.

At last, we provide a qualitative information with respect to the dominant velocity of electrons contributing to the heat flux. In the high Z case all the models give  $3.7 \times v_{th}$ , while SH solution gives  $3.5 \times v_{th}$  and AWBS  $3.4 \times v_{th}$  in the case of low Z plasmas, thus showing the right tendency of the maximum velocity shift modeled by the modified AWBS collision operator (5).

# IV. BENCHMARKING THE AWBS NONLOCAL TRANSPORT MODEL

After having shown several encouraging properties of the AWBS transport equation defined by (5) under local diffusive conditions in Sec. III, this section provides a broader analysis of the electron transport and focuses on analysis its behavior under variety of conditions in plasmas. In principle, this is characterized by allowing that electron mean free path can be arbitrarily long,<sup>244</sup> which leads to so-called nonlocal electron transport ex-<sup>245</sup> tensively investigated in numerous publications [10, 16–<sup>246</sup> 21], where the Fokker-Planck modeling of electrons in plasma represents the essential tool. Being so, we introduce our implementation of the AWBS transport equation called AP1, where its results are further benchmarked against simulation results provided by Aladin, Impact FP codes, and Calder a collisional Particle-In-<sup>247</sup> Cell code. Their description follows in the next section. <sup>248</sup>

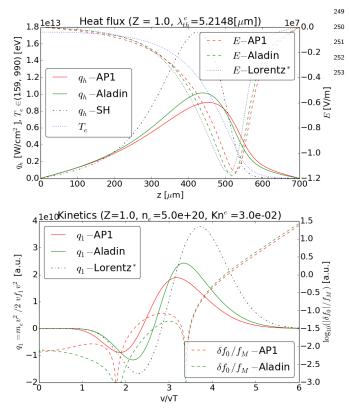


FIG. 2. Snapshot 20 ps. Left: correct steady solution of heat flux. Right: Aladins results are correct. Velocity limit  $4.4 \ v_{th}$ ..

# A. AP1 implementation

AP1 represents the abbreviation AWBS-P1, i.e. the use of collision operator (5) and the P1 angular discretization, i.e. the lowest order anisotropy approximation. AP1 in general belongs to the so-called angular<sup>254</sup> moments method and the electron distribution function takes the form

$$\tilde{f} = \frac{f_0}{4\pi} + \frac{3}{4\pi} \boldsymbol{n} \cdot \boldsymbol{f_1},$$

which consists of the isotropic part  $f_0 = \int_{4\pi} \tilde{f} d\mathbf{n}$  and the directional part  $\mathbf{f_1} = \int_{4\pi} \mathbf{n} \tilde{f} d\mathbf{n}$ , where  $\mathbf{n}$  is the transport direction (the solid angle).

The first two angular moments applied to the steady form of (1) with collision operator (5) lead to the AP1 model equations

$$v\frac{\nu_e}{2}\frac{\partial}{\partial v}\left(f_0 - 4\pi f_M\right) = v\nabla \cdot \boldsymbol{f_1} + \tilde{\boldsymbol{E}} \cdot \frac{\partial \boldsymbol{f_1}}{\partial v} + \frac{2}{v}\tilde{\boldsymbol{E}} \cdot \boldsymbol{f_1}(24)$$

$$v\frac{\nu_e}{2}\frac{\partial \mathbf{f_1}}{\partial v} - \nu_{scat}\mathbf{f_1} = \frac{v}{3}\nabla f_0 + \frac{\tilde{\mathbf{E}}}{3}\frac{\partial f_0}{\partial v},\tag{25}$$

where  $\nu_{scat} = \nu_{ei} + \frac{\nu_e}{2}$ . The strategy of solving (24) and (25) resides in integrating  $\frac{\partial f_0}{\partial v}$  and  $\frac{\partial f_1}{\partial v}$  in velocity magnitude while starting the integration from infinite velocity to zero velocity, which corresponds to decelerating electrons. It should be noted, that in practice we start the integration from  $v = 7v_{th}$ , which represents a sufficiently high velocity.

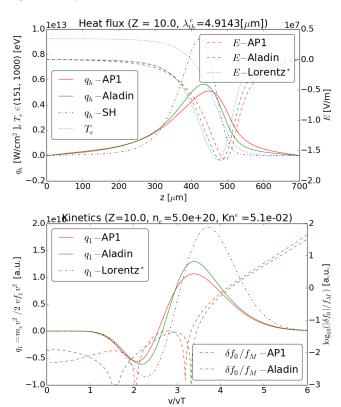


FIG. 3. Snapshot 12 ps. Left: correct steady solution of heat flux. Right: correct comparison to kinetic profiles at point 442  $\mu$ m by Aladin. Velocity limit 3.4  $v_{th}$ .

#### 1. Nonlocal electric field treatment

Similarly to (11), one can obtain the model equation of the electric field  $\tilde{E}$  by evaluating the zero current condition (a velocity integration of (25))

$$\int_{v} \left( \frac{\frac{\nu_{e}}{2} v^{2}}{\nu_{scat}} \frac{\partial \mathbf{f_{1}}}{\partial v} - \frac{v^{2}}{3\nu_{scat}} \nabla f_{0} - \frac{v}{3\nu_{scat}} \frac{\partial f_{0}}{\partial v} \tilde{\mathbf{E}} \right) v^{2} dv = 0,$$
(26)

$\overline{\mathrm{Kn}^e}$	$10^{-4}$	$10^{-3}$	$10^{-2}$	10 <sup>-1</sup>	1
$v_{lim}/v_{th}$	70.8	22.4	7.3	3.1	1.8

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TABLE II.  $\sqrt{3}v^{\frac{\nu_e}{2}} > |\tilde{\boldsymbol{E}}|$ .

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from which it is easy to express  $\tilde{\boldsymbol{E}}$  once  $f_0$  and  $\boldsymbol{f_1}$  are  $_{292}$  known, or in other words, the integral-differential model  $_{293}$  equations need to be solved simultaneously, which is achieved by k-iteration of  $f_0^k(\tilde{\boldsymbol{E}}^k), f_1^k(\tilde{\boldsymbol{E}}^k)$ , i.e. (24), (25), and  $\tilde{\boldsymbol{E}}^{k+1}(f_0^k, f_1^k)$ , i.e. (26), until the current evaluation (26) converges to zero. In principle, our concept of k-iteration resembles to the embedded nonlinear iteration of the implicit E field introduced in [22]. The first iteration starts with  $\tilde{\boldsymbol{E}} = \boldsymbol{0}$  in (24) and (25) and usually less than 10 iterations is sufficient to obey the quasineutrality constraint.

Interestingly, we have encountered a very specific prop-295 erty of the AP1 model with respect to the electric field296 magnitude. The easiest way how to demonstrate this is297 to write the model equations (24) and (25) in 1D and298 eliminate one of the partial derivatives with respect to v.299 In the case of elimination of  $\frac{\partial f_0}{\partial v}$  one obtains the following300 equation

$$\left(v\frac{\nu_e}{2} - \frac{2\tilde{E}_z^2}{3v\nu_e}\right)\frac{\partial f_{1_z}}{\partial v} = \frac{2\tilde{E}_z}{3\nu_e}\frac{\partial f_{1_z}}{\partial z} + \frac{4\pi\tilde{E}_z}{3}\frac{\partial f_M}{\partial v} + \frac{v}{3}\frac{\partial f_0}{\partial z} + \left(\frac{4\tilde{E}_z^2}{3v^2\nu_e} + \left(\nu_{ei} + \frac{\nu_e}{2}\right)\right)f_{1_z}.$$
(27)

It is convenient to write the left hand side of  $(27)^{304}$  as  $\frac{2}{3v\nu_e}\left(\left(\sqrt{3}v\frac{\nu_e}{2}\right)^2 - \tilde{E}_z^2\right)$  from where it is clear that  $^{305}_{306}$  the bracket is negative if  $\sqrt{3}v\frac{\nu_e}{2} = \sqrt{3}\frac{n_e\Gamma}{2v^2} < |\tilde{E}|$ , i.e.<sub>307</sub> there is a velocity limit for a given magnitude  $|\tilde{E}|$ , when<sub>308</sub> the collisions are no more fully dominant and the electric field introduces a comparable effect to friction in the electron transport.

Since the last term on the right hand side of (27) is dominant, the solution behaves as<sub>310</sub>  $f_1 \sim \exp\left(-\left(\frac{4\tilde{E}_z^2}{3v^2\nu_e} + \left(\nu_{ei} + \frac{\nu_e}{2}\right)\right) / \left(v\frac{\nu_e}{2} - \frac{2\tilde{E}_z^2}{3v\nu_e}\right) v\right),_{311}$  which becomes ill-posed for velocities above the limit.

In order to provide a stable model, we introduce a reduced electric field  $\,^{\rm 31}$ 

$$|\tilde{\boldsymbol{E}}_{red}| = \sqrt{3}v\frac{\nu_e}{2},\tag{28}$$

ensuring that the bracket on the left hand side of (27) remains positive. Further more we define two quantities <sup>314</sup>

$$\omega_{red} = rac{| ilde{m{E}}_{red}|}{| ilde{m{E}}|}, \quad 
u_{scat}^E = rac{| ilde{m{E}}| - | ilde{m{E}}_{red}|}{v}.$$

introducing the reduction factor of the electric field  $\omega_{red}$  and the compensation of the electric field effect in terms of scattering  $\nu_{scat}^E$ . Consequently, the AP1 model (24), (25), and (26) can be formulated as well posed with the help of  $\omega_{red}$  and  $\nu_{scat}^E$ . However, before doing so, we introduce a slightly different approximation to the electron distribution function as

$$\tilde{f} = \frac{4\pi f_M + \delta f_0}{4\pi} + \frac{3}{4\pi} \boldsymbol{n} \cdot \boldsymbol{f_1}.$$
 (29)

where  $\delta f_0$  represents the departure of isotropic part from the Maxwell-Boltzmann equilibrium distribution  $f_M$ . Then, the stable AP1 model reads

$$v\frac{\nu_{e}}{2}\frac{\partial\delta f_{0}}{\partial v} = v\nabla\cdot\boldsymbol{f_{1}} + \tilde{\boldsymbol{E}}\cdot\left(\omega_{red}\frac{\partial\boldsymbol{f_{1}}}{\partial v} + \frac{2}{v}\boldsymbol{f_{1}}\right), \quad (30)$$

$$v\frac{\nu_{e}}{2}\frac{\partial\boldsymbol{f_{1}}}{\partial v} = \tilde{\nu}_{scat}\boldsymbol{f_{1}} + \frac{v}{3}\nabla\left(4\pi f_{M} + \delta f_{0}\right)$$

$$+\frac{\tilde{\boldsymbol{E}}}{3}\left(4\pi\frac{\partial f_{M}}{\partial v} + \omega_{red}\frac{\partial\delta f_{0}}{\partial v}\right), \quad (31)$$

where  $\tilde{\nu}_{scat} = \nu_{ei} + \nu_{scat}^E + \frac{\nu_e}{2}$ . The reason for keeping  $f_M$  in the distribution function approximation (29) can be seen in the last term on the right hand side of (31), which provides the effect of electric field on directional quantities as current or heat flux. In principle, the explicit use of  $f_M$  ensures the proper effect of  $\tilde{E}$  if  $\delta f_0 \ll f_M$ , i.e. no matter what the reduction  $\omega_{red}$  is. Apart from its stability, it also exhibits much better convergence of the electric field, which is now given by the zero current condition of (31) as

$$\tilde{\mathbf{E}} = \frac{\int_{v} \left( \frac{\nu_{e}}{2\tilde{\nu}_{scat}} v^{2} \frac{\partial \mathbf{f}_{1}}{\partial v} - \frac{v^{2}}{3\tilde{\nu}_{scat}} \nabla \left( 4\pi f_{M} + \delta f_{0} \right) \right) v^{2} dv}{\int_{v} \frac{v}{3\tilde{\nu}_{scat}} \left( 4\pi \frac{\partial f_{M}}{\partial v} + \omega_{red} \frac{\partial \delta f_{0}}{\partial v} \right) v^{2} dv}.$$
(32)

For practical reasons we present in TABLE II some explicit values of velocity limit corresponding to varying transport conditions expressed in terms of Knudsen number  $\mathrm{Kn}^e = \frac{\lambda_e |\nabla T_e|}{|\nabla T_e|}$ , where  $\frac{T_e}{|\nabla T_e|}$  stands for the length scale of plasma.

# B. Aladin, Impact, and Calder kinetic codes

- Brief description of the Aladin code FIG. 2, FIG. 3.
- Brief description of the Impact code FIG. 4.
- Brief description of the Calder code FIG. 5.

### C. Large temperature variations tests

### 1. Heat-bath problem

The first test case is a simple non-linear heat-bath problem, in which the initial temperature is tanh(z).

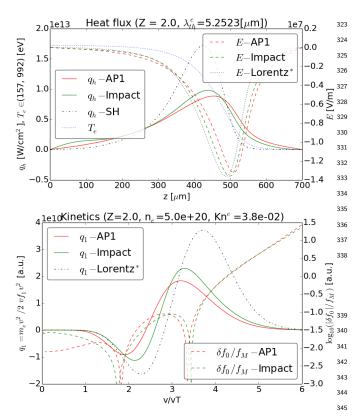


FIG. 4. Snapshot 12 ps. Left: correct steady solution of heat flux. Right: correct comparison to kinetic profiles at point 437  $\mu$ m by Impact. Velocity limit 4.0  $v_{th}$ .

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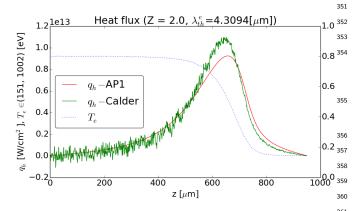


FIG. 5. Snapshot 11 ps. Left: correct steady solution of  $^{362}$  heat flux. Right: Kinetic profiles at point of maximum flux $^{363}$  by AP1. Kinetics profiles by CALDER should be added. Ve- $^{364}$  locity limit 3.8  $v_{th}$ .

The total computational box size is 700  $\mu$ m in the case<sub>369</sub> of Aladin and Impact and 1000  $\mu$ m in the case of Calder.<sub>370</sub> The Knudsen number has been varied to address a broad<sub>371</sub> range of nonlocality of the electron transport correspond-<sub>372</sub> ing to the laser-heated plasma conditions, i.e. Kn<sup>e</sup>  $\in$ <sub>373</sub> (0.0001, 1). The variation of Kn<sup>e</sup> arises from the vari-<sub>374</sub>

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ation of the electron density  $n_e \in (10^{19}, 10^{23}) \text{ cm}^{-3}$  or the slope of the temperature profile  $s \in (25, 2500) \mu \text{m}$ . The coulomb logarithm was held fixed throughout,  $\ln \Lambda = 7.09$ .

We now investigate the accuracy of the AP1, Aladin, Impact and Calder codes in calculating the heat flow in the case where we have a large relative temperature variation. We consider the case of an initial temperature profile consisting of a ramp connecting two large hot and cold regions (baths). This has the advantages of allowing simple reflective boundary conditions and not requiring any external heating/cooling mechanisms that would also need to be carefully calibrated between codes.

The hot and cold baths had temperatures of T 0 and  $0.15\mathrm{T}$  0; these were connected by a cubic ramp given by

## tanh(z)

For these simulations the electron density, Coulomb logarithm and ionisation were all kept constant and uniform.

Aladin and Impact simulations showed an evolution of the heat flow from the local (due to initialising as a Maxwellian) to the nonlocal, with a reduced peak, over an initial transient phase (over which the temperature ramp flattened some- what). The transient phase was considered over when the ratio of the VFP heat flow to the expected local heat flow stopped decreasing. After the transient phase this ratio begins to slowly increase as the thermal conduction flattens the temperature ramp and the ratio of the scalelength to mfp increases (i.e. the thermal transport slowly becomes more local). We then took the temperature profile from Aladin/Impact/Calder and used our AP1 implementation to calculate the heat flow they would predict given this profile.

### 2. Hohlraum problem

While comparisons between the AP1 model and VFP codes have previously been performed 8,45 , none have included spatially-inhomogeneous ionisation. As inertial fusion experiments involve steep ionisation and density gradients (for example, at the interface between the helium gas-fill and the ablated gold plasma), it is critical that the AP1 model be tested in such an environment. For evaluating this, the IMPACT [22] VFP code was used due to its ability to simulate inhomogeneous ionisation profiles.

We performed a HYDRA simulation in 1D spherical geometry of a laser-heated gadolinium hohlraum containing a typical helium gas-fill. A leak source was implemented with an area equal to the laser entrance hole to reproduce the energy balance. Electron temperature  $T_e$ , electron density  $n_e$  and ionisation Z profiles (shown in FIG. 7) at 20 nanoseconds were extracted and used as the initial conditions (along with the assumption that the electron distribution function is initially Maxwellian

everywhere) for the IMPACT simulation (which was performed instead in planar geometry). At this point very steep gradients in all three variables were set up with a change from  $T_e=2.5$  keV,  $n_e=5\times10^{20}$  cm<sup>3</sup>, Z = 2 to  $T_e=0.3$  keV,  $n_e=5\times10^{21}$  cm<sup>3</sup>, Z = 39 across approximately 100  $\mu$ m at the helium-gadolinium interface. Spline interpolation was used to increase the spatial resolution near the steep interface for the IMPACT simulations, helping both numerical stability and runtime due to needing a reduced number of nonlinear iterations. For simplicity, the Coulomb logarithm was treated as a constant  $\ln \Lambda_{ei} = \ln \Lambda_{ee} = 2.1484$ . Note that in reality the plasma is only strongly coupled in the colder region of the gadolinium bubble beyond  $\sim 1.7$  mm and  $\ln \Lambda_{ei} \approx 8$ up to  $\sim 1.6$  mm in the hotter corona. Reflective boundary conditions were used here as in the previous section and IMPACT used a timestep of 1.334 fs. The  $n_e$  and Z profiles did not evolve in the IMPACT simulation due to the treatment of the electric field discussed in section II that ensures quasineutrality and the neglection of ion motion and ionisation models.

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As with the VFP simulations in the previous section, there is an initial transient phase where the IMPACT heat flux gradually reduces from the Braginskii prediction as the distribution function rapidly moves away from Maxwellian. Once again this transient phase is considered to be over when the ratio of the peak heat flow to the Braginskii prediction stops reducing. This ratio is not observed to change by more than 5% after the first 5 ps of our 15.7 ps simulation. Therefore, we conclude that it safe to assume the transient phase is over after 5 ps, at which point the temperature front has advanced by approximately 8  $\mu$ m leading to a maximum temperature change of 41% as shown in FIG. 7. In comparing the IM-PACT, AP1, and SNB heat flow profiles we encountered an important subtlety concerning the implementation of the model. A recent SNB model with separate electron ion and electron-electron collision frequencies provides a very good prediction of the preheat into the hohlraum, the peak heat flow to within 16% and an improved estimate of the thermal conduction in the gas-fill region, the latter is still too large by a factor of  $\sim 2$ . This discrepancy could potentially lead to an overestimate of hohlraum temperatures and thus cause issues similar to those aris-428 ing with using an overly restrictive flux limiter.

• Multiple runs analyzing the performance of AP1 $_{431}$  with respect to Aladin/Impact/Calder along wide range of  $\rm Kn^e$  shown in FIG. 6.

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- Realistic hydro simulation setting provided by HY-434
   DRA, a comparison between AP1, Impact, and 435
   SNB shown in FIG. 7.
- Comment on and summarize the velocity limits for 438 all figs.

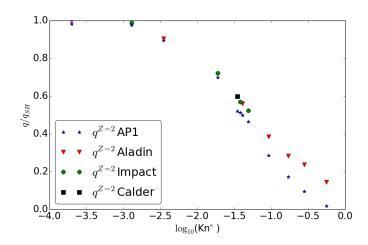


FIG. 6. Simulation results for the case Z=2 computed by AP1/Aladin/Impact/Calder. Every point corresponds to the maximum heat flux in a "tanh" temperature simulation, which can be characterized by Kn. The range of  $\log_{10}(\mathrm{Kn}) \in (0,-4)$  can be expressed as equivalent to the electron density approximate range  $n_e \in (1e19,3.5e22)$  of the 50  $\mu$ m slope tanh case. In the case of Kn = 0.56,  $q_{Aladin}/q_{AP1} \approx 7.9$ .

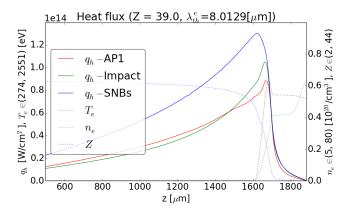


FIG. 7.

# V. CONCLUSIONS

- The most important point is that we introduce a collision operator, which is coherent with the full FP, i.e. no extra dependence on Z.
- Touch pros/contras of linearized FP in Aladin and Impact vs AWBS
- Raise discussion about what is the weakest point of AP1 for high Kns: the velocity limit or phenomenological Maxwellization?
- Summarize useful outcomes related to plasma physics as the tendency of the velocity maximum in  $q_1$  with respect to Z and  $\operatorname{Kn}^e$ .

• Emphasize the good results of Aladin (compared 443 to Impact) and also outstanding results of Calder while being PIC.

#### ACKNOWLEDGMENTS

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