An efficient kinetic modeling in plasmas by using the AWBS transport equation

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Abstract

The AWBS Boltzmann transport equation for electrons equipped with a simplified e-e collision operator [**?**] provides an efficient, yet physically relevant, kinetic extension compared the classical Spitzer-Harm heat flux (SH) based on local approximation and flux-limiting. This classical approach is widely used in plasma kinetics models coupled to hydrodynamics. Even though SH reflects the electron-electron collision effect, the essential physical properties of the electron transport cannot be modeled with an explicitly local model. A simple form of the AWBS model opens a way to couple kinetics to hydrodynamic codes while describing the important physics correctly. Since the electron-electron collision effect becomes especially important in the case of low ion potential, we focus on presenting results related to low Z plasmas.

Keywords: kinetics; hydrodynamics; nonlocal electron transport; laser-heated plasmas.

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1. Introduction

2. The AWBS nonlocal transport model

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \tilde{\boldsymbol{E}} \cdot \nabla_{\boldsymbol{v}} f = v \frac{\nu_e}{2} \frac{\partial}{\partial v} \left(f - f_M \right) + \frac{\nu_{ei} + \frac{\nu_e}{2}}{2} \frac{\partial^2 f}{\partial \boldsymbol{n}^2}, \tag{1}$$

[1]

3. BGK, AWBS, and Fokker-Planck models in diffusive regime

We can try to find an approximate solution while using the first term of expansion in λ_e and muas

$$\tilde{f}(z, v, \mu) = f^0(z, v) + f^1(z, v) \lambda_{ei} \mu. \tag{2}$$

3.1. The BGK diffusive electron transport

$$\boldsymbol{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} \frac{\partial f}{\partial v} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_\phi - v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_\theta + v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_\phi}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \\ \frac{(f_M - f)}{\lambda^e} + \frac{1}{2\lambda^{ei}} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \tag{3}$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path. We also approximate $\lambda_e = \bar{Z} \lambda_{ei}$.

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\boldsymbol{B}} = \tilde{B}_z \boldsymbol{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z} \boldsymbol{e}_z$ and appropriately $\tilde{\boldsymbol{E}} = \tilde{E}_z \boldsymbol{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} = \tilde{E}_z \cos(\phi) = \mu$ and $\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_\phi = -\tilde{E}_z \sin(\phi)$. As a result, the analyzed BGK equation reads

$$\mu \frac{\partial}{\partial z} \left(f^0 + f^1 \lambda_{ei} \mu \right) + \frac{1}{v} \left[\tilde{E}_z \mu \frac{\partial}{\partial v} \left(f^0 + f^1 \lambda_{ei} \mu \right) - \frac{\tilde{E}_z \sin(\phi)}{v} \frac{\partial}{\partial \phi} \left(f^0 + f^1 \lambda_{ei} \mu \right) \right] = \\ \frac{(f_M - (f^0 + f^1 \lambda_{ei} \mu))}{\lambda_e} + \frac{1}{2\lambda_{ei}} \frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial}{\partial \mu} \left(f^0 + f^1 \lambda_{ei} \mu \right) \right), \tag{4}$$

$$\mu\frac{\partial f^0}{\partial z} + \mu^2\frac{\partial}{\partial z}\left(f^1\lambda_{ei}\right) + \frac{\tilde{E}_z}{v}\left[\mu\frac{\partial f^0}{\partial v} + \mu^2\frac{\partial}{\partial v}\left(f^1\lambda_{ei}\right) + \frac{1-\mu^2}{v}f^1\lambda_{ei}\right] = \frac{f_M - f^0}{\bar{Z}\lambda_{ei}} - \mu\frac{1}{\bar{Z}}f^1 - \mu f^1, \quad (5)$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, ...$ equations

$$\begin{aligned} \frac{f_M - f^0}{\bar{Z}\lambda_{ei}} &= \frac{\tilde{E}_z}{v^2}f^1\lambda_{ei}, \\ \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v} &= -\frac{1}{\bar{Z}}f^1 - f^1, \\ \frac{\partial}{\partial z}\left(f^1\lambda_{ei}\right) + \frac{\tilde{E}_z}{v}\left[\frac{\partial}{\partial v}\left(f^1\lambda_{ei}\right) - \frac{1}{v}f^1\lambda_{ei}\right] &= 0, \end{aligned}$$

which lead to the definitions

$$\begin{aligned} f^0 &= f_M + \frac{1}{v}f^1\bar{Z}\lambda_{ei}^2, && (6) \\ f^1 &= -\frac{\bar{Z}}{\bar{Z}+1}\left[\frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v}\right] \\ &= -\frac{\bar{Z}}{\bar{Z}+1}\left[\frac{1}{\rho}\frac{\partial \rho}{\partial z} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial z} - \frac{\tilde{E}_z}{v_{th}^2}\right]f_M && (7) \end{aligned}$$

In order to ensure the plasma to be quasi-neutral, the zero-current condition

$$\boldsymbol{j} = \int_0^\infty \int_{4\pi} q_e v \boldsymbol{n} f \,\mathrm{d}\boldsymbol{n}\; v^2 \,\mathrm{d}v = \boldsymbol{0}, \quad (8)$$

can be achieved by providing a consistent electric field in (15), i.e.

$$\tilde{\boldsymbol{E}} = \frac{v_{th}^2 \int_{4\pi} \boldsymbol{n}\otimes\boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha}\left(\frac{\nabla\rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{\nabla T}{T}\right) v^2 \,\mathrm{d}v \,\mathrm{d}\boldsymbol{n}}{\int_{4\pi} \boldsymbol{n}\otimes\boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} v^2 \,\mathrm{d}v \,\mathrm{d}\boldsymbol{n}}, \quad (9)$$

which may be further simplified as

$$\tilde{\boldsymbol{E}} = \frac{\int_0^\infty f_M \frac{1}{2}\frac{\nabla T}{T} v^9 \,\mathrm{d}v}{\int_0^\infty f_M v^7 \,\mathrm{d}v} + v_{th}^2\left(\frac{\nabla\rho}{\rho} - \frac{3}{2}\frac{\nabla T}{T}\right) = v_{th}^2\left(\frac{\nabla\rho}{\rho} + \frac{5}{2}\frac{\nabla T}{T}\right), \quad (10)$$

where it is worth mentioning, that the part $f_M + \frac{v\lambda}{\alpha}\frac{\partial f_1}{\partial v}$ of the distribution does not contribute to the current since it is isotropic. One can write the quasi-neutral distribution function explicitly distinguishing between original part (blue color) and E field correction (red color) as

$$f \approx f_M \left(1 - \frac{\lambda}{\alpha}\boldsymbol{n} \cdot \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2}\right)\frac{\nabla T}{T}\right) + \frac{v\lambda}{\alpha}\frac{\partial f_1}{\partial v}. \tag{11}$$

which leads to the resulting heat flux

$$\boldsymbol{q}_H = \int_{4\pi}\int_0^\infty \frac{m_e v^2}{2} v\boldsymbol{n} f v^2 \,\mathrm{d}v\,\mathrm{d}\boldsymbol{n} = \frac{4\pi}{3}\frac{m_e}{2}\frac{1}{\alpha\sigma\rho}\int_0^\infty \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2}\right) v^9 f_M \,\mathrm{d}v \frac{\nabla T}{T}.$$

Based on the Gauss integral formula

$$\int v^{2s+1}\exp\left(-\frac{v^2}{2v_{th}^2}\right)\,\mathrm{d}v = \frac{s!\ (2v_{th}^2)^{s+1}}{2}$$

and Maxwell-Boltzmann distribution (**??**) the heat flux can be written as

$$\boldsymbol{q}_H = \frac{4\pi}{3}\frac{m_e}{2}\frac{1}{\alpha\sigma\rho}\frac{\rho}{v_{th}^3\,(2\pi)^{3/2}}\frac{4!\ 2^4 v_{th}^{10}}{T}\left(5 - \frac{3}{2} - \frac{5}{2}\right)\nabla T = \frac{m_e}{\alpha\sigma}\frac{128}{\sqrt{2\pi}}\left(\frac{k_B}{m_e}\right)^{\frac{7}{2}} T^{\frac{5}{2}}\nabla T. \tag{12}$$

In conclusion, equation (12) provides nothing else than the well known Lorentz approximation heat flux and its nonlinearity 2.5 in temperature. What is worth mentioning is the effect of E field (quasi-neutrality), which reduces the flux of about 71.4% (also assuming constant density).

Finally, one can find the approximate solution

$$\tilde{f} = f_M - \lambda_{ei}\frac{\bar{Z}}{\bar{Z}+1}\left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \alpha\right)\frac{\boldsymbol{n}\cdot\nabla T}{T} f_M. \tag{13}$$

3.2. The AWBS diffusive electron transport

The AWBS electron transport equation in 6D reads

$$\boldsymbol{n}\cdot\nabla f + \frac{1}{v}\left[\tilde{\boldsymbol{E}}\cdot\boldsymbol{n}\frac{\partial f}{\partial v} + \frac{\tilde{\boldsymbol{E}}\cdot\boldsymbol{e}_\phi - v\tilde{\boldsymbol{B}}\cdot\boldsymbol{e}_\theta}{v}\frac{\partial f}{\partial \phi} + \frac{\tilde{\boldsymbol{E}}\cdot\boldsymbol{e}_\theta + v\tilde{\boldsymbol{B}}\cdot\boldsymbol{e}_\phi}{v\sin(\phi)}\frac{\partial f}{\partial \theta}\right] =$$

$$\frac{v}{\lambda^e}\frac{\partial}{\partial v}(f - f_M) + \left(\frac{1}{\lambda_{ei}} + \frac{1}{\lambda_e}\right)\frac{1}{2}\left(\frac{\partial}{\partial \mu}\left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right), \tag{14}$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path, and $\lambda_e = \bar{Z}\lambda_{ei}$.

We can try to find an approximate solution while using the first term of expansion in λ_e and μ as

$$\tilde{f}(z, v, \mu) = f^0(z, v) + f^1(z, v)\lambda_{ei}\mu. \tag{15}$$

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\boldsymbol{B}} = \tilde{B}_z \boldsymbol{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z}\boldsymbol{e}_z$ and appropriately $\tilde{\boldsymbol{E}} = \tilde{E}_z \boldsymbol{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\boldsymbol{E}}\cdot\boldsymbol{n} = \tilde{E}_z\cos(\phi) = \mu$ and $\tilde{\boldsymbol{E}}\cdot\boldsymbol{e}_\phi = -\tilde{E}_z\sin(\phi)$. As a result, the analyzed AWBS equation reads

$$\begin{aligned}\mu\frac{\partial}{\partial z}\left(f^0 + f^1\lambda_{ei}\mu\right) + \frac{1}{v}\left[\tilde{E}_z\mu\frac{\partial}{\partial v}\left(f^0 + f^1\lambda_{ei}\mu\right) - \frac{\tilde{E}_z\sin(\phi)}{v}\frac{\partial}{\partial\phi}\left(f^0 + f^1\lambda_{ei}\mu\right)\right] = \\ \frac{v}{\lambda_e}\frac{\partial}{\partial v}\left(\left(f^0 + f^1\lambda_{ei}\mu\right) - f_M\right) + \frac{\bar{Z}+1}{2\lambda_{ei}\bar{Z}}\frac{\partial}{\partial\mu}\left((1-\mu^2)\frac{\partial}{\partial\mu}\left(f^0 + f^1\lambda_{ei}\mu\right)\right),\end{aligned} \tag{16}$$

$$\begin{aligned}\mu\frac{\partial f^0}{\partial z} + \mu^2\frac{\partial}{\partial z}\left(f^1\lambda_{ei}\right) + \frac{\tilde{E}_z}{v}\left[\mu\frac{\partial f^0}{\partial v} + \mu^2\frac{\partial}{\partial v}\left(f^1\lambda_{ei}\right) + \frac{1-\mu^2}{v}f^1\lambda_{ei}\right] = \\ \frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial}{\partial v}\left(f^0 - f_M\right) + \mu\frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial(f^1\lambda_{ei})}{\partial v} - \mu\frac{\bar{Z}+1}{\bar{Z}}f^1,\end{aligned} \tag{17}$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, ...$ equations

$$\begin{aligned}\frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial}{\partial v}\left(f^0 - f_M\right) &= \frac{\tilde{E}_z}{v^2}f^1\lambda_{ei}, \\ \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v} &= \frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial(f^1\lambda_{ei})}{\partial v} - \frac{\bar{Z}+1}{\bar{Z}}f^1, \\ \frac{\partial}{\partial z}\left(f^1\lambda_{ei}\right) + \frac{\tilde{E}_z}{v}\left[\frac{\partial}{\partial v}\left(f^1\lambda_{ei}\right) - \frac{1}{v}f^1\lambda_{ei}\right] &= 0,\end{aligned}$$

which lead to the definitions

$$
\begin{aligned}
\frac{\partial}{\partial v}\left(f^0 - f_M\right) &= \frac{1}{v^2} f^1 \bar{Z}\lambda_{ei}^2, \qquad (18)\\
\frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial (f^1\lambda_{ei})}{\partial v} - \frac{\bar{Z}+1}{\bar{Z}} f^1 &= \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v}\\
\frac{v}{\bar{Z}}\frac{\partial f^1}{\partial v} + \frac{4}{\bar{Z}} f^1 - \frac{\bar{Z}+1}{\bar{Z}} f^1 &= \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v}\\
\frac{\partial f^1}{\partial v} + \frac{1}{v}(3-\bar{Z}) f^1 &= \frac{\bar{Z}}{v}\left(\frac{1}{\rho}\frac{\partial \rho}{\partial z} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial z} - \frac{\tilde{E}_z}{v_{th}^2}\right) f_M. \qquad (19)
\end{aligned}
$$

3.3. The Fokker-Planck diffusive electron transport

$$v_{2th} = \sqrt{\frac{2k_B T}{m_e}} = 1/j,$$

$$
\begin{aligned}
A &= -\frac{m_e^2 v_{2th}^2 \tilde{\boldsymbol{E}}}{2\pi e^4 n_e \ln\Lambda} = -\frac{mE}{2\pi j^2 e^3 n_e \ln\Lambda},\\
B &= \frac{m_e^2 v_{2th}^4 |\nabla T|}{2\pi e^4 n_e \ln\Lambda T} = \frac{2k_B^2 T|\nabla T|}{\pi e^4 n_e \ln\Lambda},
\end{aligned}
$$

$$\frac{A}{B} = -\frac{|\tilde{\boldsymbol{E}}|T}{v_{2th}^2 |\nabla T|},$$

$$\tilde{\boldsymbol{E}} = -\frac{3}{2}\frac{v_{2th}^2}{2}\frac{\gamma_T}{\gamma_E}\frac{\nabla T}{T},$$

From Eq. (24) CSR, we can write the form of f_1 including both ∇T and $\tilde{\boldsymbol{E}}$ effects as

$$f_1(v,\theta) = \cos(\theta)\frac{B}{\bar{Z}}\left(d_T(v/v_{2th}) + \frac{A}{B} d_E(v/v_{2th})\right) f_M(v),$$

where in the case of vanishing current one gets

$$\frac{A}{B} = \frac{3}{2}\frac{\gamma_T}{2\gamma_E},$$

i.e.

$$f_1(v,\theta) = \cos(\theta)\frac{m_e^2}{4\pi e^4 \ln\Lambda}\frac{v_{2th}^4}{\bar{Z}}\left(2d_T(v/v_{2th}) + \frac{3}{2}\frac{\gamma_T}{\gamma_E}d_E(v/v_{2th})\right)\frac{f_M(v)}{n_e}\frac{\nabla T}{T}, \tag{20}$$

where $d_T(x) = \bar{Z}D_T(x)/B$ and $d_E(x) = \bar{Z}D_E(x)/A$ are represented by numerical values in TABLE I and TABLE II in [5], respectively. In the case of high $\bar{Z}$ limit, $\gamma_T \to 1$, $\gamma_E \to 1$, $d_E(x) = x^4$, and $d_T(x) = x^4(2.5 - x^2)/2$ [5], which leads to the standard Lorentz gas model

$$f_1(v,\theta) = \cos(\theta)\frac{m_e^2}{4\pi e^4 \ln\Lambda}\frac{v^4}{\bar{Z}}\left(4 - \frac{v^2}{v_{2th}^2}\right)\frac{f_M(v)}{n_e}\frac{\nabla T}{T}, \tag{21}$$

[2], [3], [4]

3.4. Summary of BGK, AWBS, and Fokker-Planck diffusion

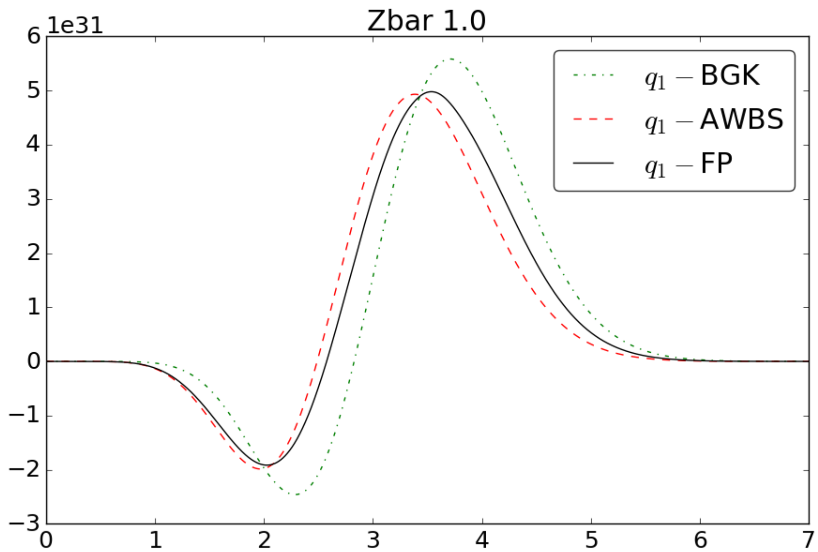

Figure 1: The flux velocity moment of the anisotropic part of the electron distribution function in low Z plasmas in diffusive regime.

	$\bar{Z}=1$	$\bar{Z}=2$	$\bar{Z}=4$	$\bar{Z}=16$	$\bar{Z}\to\infty$
$error(\boldsymbol{q}_{AWBS})$	0.057	0.004	0.038	0.049	0.000

Table 1: Relative $error(\boldsymbol{q}_{AWBS}) = |\boldsymbol{q}_{AWBS} - \boldsymbol{q}_{SH}|/\boldsymbol{q}_{SH}$ of the AWBS kinetic model equation (1) showing the discrepancy (maximum around 5%) with respect to the original solution of the heat flux given by Spitzer and Harm [5].

4. Benchmarking the AWBS nonlocal transport model

4.1. Review of simulation codes

4.1.1. C7

4.1.2. ALADIN

4.1.3. IMPACT

4.1.4. CALDER

4.2. Simulation results

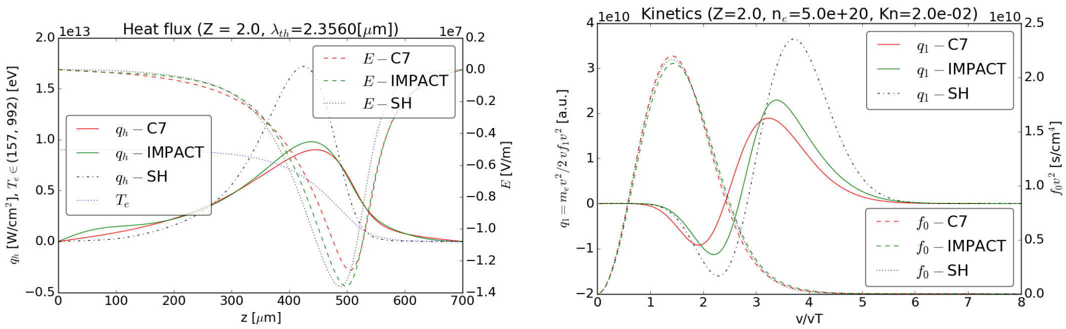

Figure 2: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles by IMPACT.

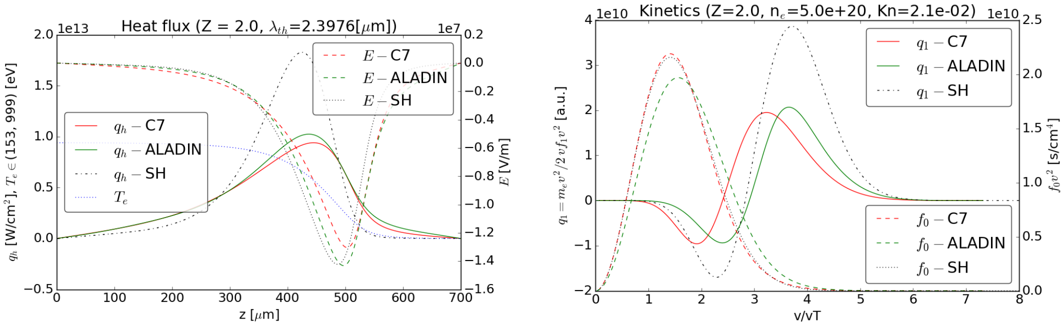

Figure 3: Snapshot 12 ps. Left: correct steady solution. Right: time and point to be precised by ALADIN.

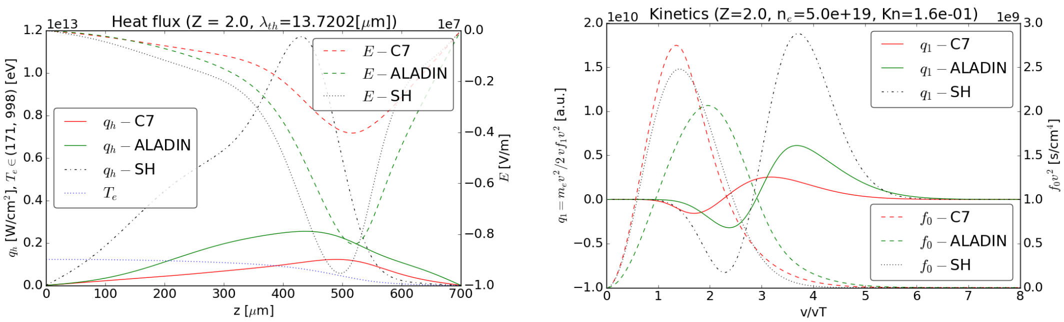

Figure 4: Snapshot 12 ps. Left: Does not look as steady solution. Right: time and point to be precised by ALADIN.

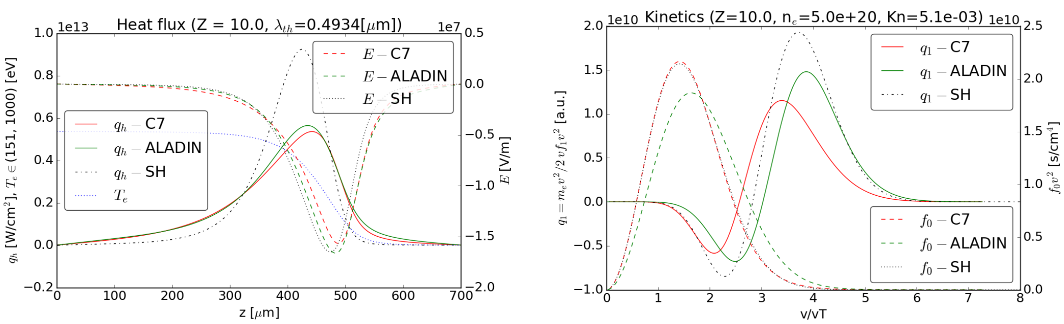

Figure 5: Snapshot 12 ps. Left: correct steady solution. Right: time and point to be precised by ALADIN.

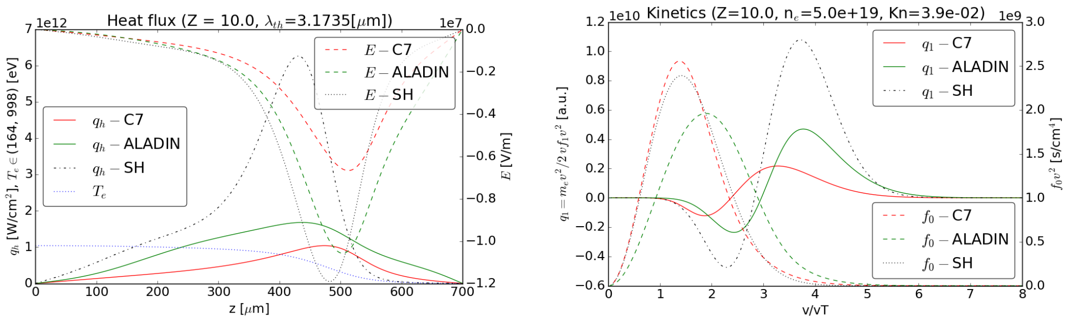

Figure 6: Snapshot 12 ps. Left: Does not look as steady solution. Right: time and point to be precised by ALADIN.

5. Conclusions

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