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Short Note

How to normalize Maxwell–Boltzmann electrons in transient plasma models

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Abstract

Proper normalization of a Maxwell–Boltzmann electron distribution in transient plasma models requires the self-consistent calculation of a reference density from a global electron conservation equation. This calculation tends to produce numerical oscillations in the time evolution of the plasma, in particular during the formation of the plasma sheath. The present paper proposes a simple numerical scheme to prevent these oscillations by artificial critical damping, which makes it possible to simulate transient plasma phenomena without electron-related time step conditions.

Keywords: Plasma sheath models; Plasma simulations; Maxwell–Boltzmann distribution; Boltzmann relation; Boltzmann reference density; Time advancement; Numerical methods; Critical damping

1. Introduction and problem definition

A ubiquitous approximation in elementary plasma theory is to assume a Maxwell–Boltzmann equilibrium-distribution of electrons:

$$n_e(\mathbf{x}) = n_0 \exp(\Phi(\mathbf{x})/T_e), \tag{1}$$

where $\mathbf{x}$ are the space coordinates, n_e is the electron number density, Φ is the electric potential, T_e is the electron temperature in eV which is constant and given, and n_0 is a reference density corresponding to $\Phi = 0$. This approximation is used in particular to study phenomena where the electron collision length is large compared to the length scale of interest, such as the space charge sheath on the plasma edge, and is at the basis of plasma sheath theory, probe theory, the Bohm criterion, etc. Eq. (1) is then usually coupled to an ion transport equation and Poisson's equation to obtain the potential in a self-consistent manner.

Elementary theory can be generalized to multidimensional or transient problems by numerical models. The literature reports numerical models for ion extraction through metal grids [1], ion implantation sheaths [2,3],

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vacuum circuit breakers [4], electro-negative plasma sheaths [5,6], etc., all based on the electron Boltzmann relation shown in Eq. (1). Most of these models are transient in the sense that they describe time evolution on the time scale of the ion transport. The numerical time advancement scheme of these models is as follows. Consider that all quantities are known at time t^k and are to be calculated at time $t^{k+1} = t^k + \Delta t$. First, the new ion density n_i^{k+1} is calculated from an ion transport equation or an ion particle simulation using the electric potential Φ^k. Subsequently the new potential Φ^{k+1} is solved from Poisson's equation

$$\begin{aligned}\varepsilon_0 \nabla^2 \Phi^{k+1} &= e n_0 \exp(\Phi^{k+1}/T_e) - e n_i^{k+1} \\ &\approx e n_0 \exp(\Phi^k/T_e)(1 + (\Phi^{k+1} - \Phi^k)/T_e) - e n_i^{k+1},\end{aligned} \tag{2}$$

where Eq. (1) has been substituted for the electron density, e is the elementary charge, and ε_0 is the permittivity of free space. The potential in the Boltzmann factor on the right hand side of Eq. (2) must be implicit to avoid severe time step conditions of the type $\omega_{pe}\Delta t < 0.2$, where $\omega_{pe} = (e^2 n_e/\varepsilon_0 m_e)^{1/2}$ is the electron plasma frequency. [2] In order to solve Eq. (2) it is usually linearized by a Newton–Raphson iteration as shown in the third member.

The problem with the above model scheme is that the electron reference density n_0 is not known a priori but has to be calculated self-consistently from electron conservation [7] and that this calculation leads to numerical difficulties. The global electron conservation equation is

$$\frac{\partial}{\partial t}\iiint_{\text{volume}} n_e \mathrm{d}V + \iint_{\text{surface}} \frac{1}{4} v_e n_e \mathrm{d}A = \iiint_{\text{volume}} S \mathrm{d}V, \tag{3}$$

where $v_e = (8eT_e/\pi m_e)^{1/2}$ is the Maxwellian thermal speed and S is the source term, accounting for bulk ionisation, recombination, and attachment. Substituting Eq. (1) into Eq. (3), we find the following equation for n_0

$$\frac{\partial(n_0 p)}{\partial t} + \frac{1}{4} v_e n_0 q = r, \tag{4}$$

where

$$p = \iiint_{\text{volume}} \exp(\Phi/T_e)\mathrm{d}V \tag{5}$$

$$q = \iint_{\text{surface}} \exp(\Phi/T_e)\mathrm{d}A \tag{6}$$

$$r = \iiint_{\text{volume}} S \mathrm{d}V. \tag{7}$$

Alternatively one can obtain n_0 from a global current conservation equation or work with a reference potential $\Phi_0 = -T_e \ln(n_0)$ rather than n_0 but this eventually comes all down to the same. In stationary problems Eq. (4) reduces to $n_0 = 4r/qv_e$ which is readily evaluated especially if the total volume source term S is a fixed model parameter. In transient problems, however, n_0 changes in time and is directly related to the potential everywhere in space through the integral p shown in Eq. (5). Discretizing the time derivative in Eq. (4), we obtain

$$n_0^{k+1} = n_0^k \frac{p^k}{p^{k+1}} - n_0 \frac{v_e q \Delta t}{4p^{k+1}} + \frac{r\Delta t}{p^{k+1}}. \tag{8}$$

The last two terms on the right account for electron loss and production and determine the steady state value of n_0. The first term compensates for changes in the plasma potential and is important (often dominant) during transient phenomena. Because p^{k+1} is to be calculated from Φ^{k+1}, the value of n_0^{k+1} from Eq. (8) is not available when solving Poisson's Eq. (2) at time t^{k+1} and it is necessary to approximate Eq. (8). Extrapolating from previous time steps, we try

$$n_0^{k+1} = n_0^k \frac{p^{k-1}}{p^k} - n_0^k \frac{v_e q^k \Delta t}{4p^k} + \frac{r^k \Delta t}{p^k}. \tag{9}$$

Unfortunately, it turns out that this causes strong oscillations in the time evolution of the plasma during rapid transient phenomena, in particular during the formation of the plasma sheath, unless the time step Δt is very