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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.
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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

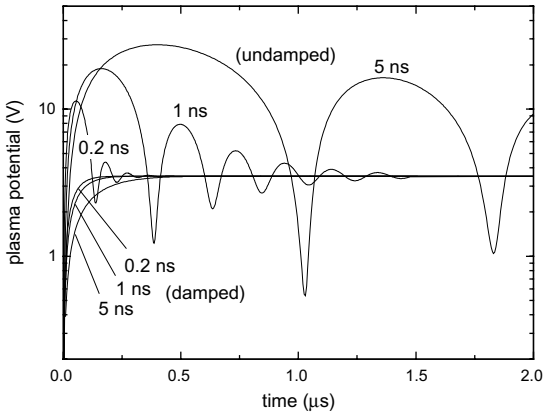

Fig. 1. Time evolution of the plasma potential (log scale) during the formation of the plasma sheath (see text), obtained using Eq. (9) (oscillating curves) and Eq. (19) (monotonous curves) for different numerical time steps.

small. An example is shown in Fig. 1. On closer inspection, it appears that this is a fundamental problem, related to the global nature of the Boltzmann relation, which cannot be solved by rewriting the equations in terms of current conservation or reference potential. This problem strongly complicates and limits the use of the Boltzmann relation in transient plasma models. Most of the models cited above circumvent the problem by additional assumptions on n_0, i.e. they do not calculate n_0 self-consistently at risk of physical errors and artefacts.

The present paper proposes a simple scheme to prevent numerical oscillations due to the calculation of n_0 by a slight modification of Eq. (9) such as to obtain critical oscillation damping. This makes it possible to calculate n_0 self-consistently in transient plasma models without additional time step conditions. In the following sections, we analyse the origin of the oscillations, describe and explain our scheme, and show simulation results demonstrating its efficacy.

2. Analysis

To see why Eq. (9) causes numerical oscillations and to find out what we can do about it, we need to understand how the electric potential reacts to changes in n_0. Due to the implicit updating of the Boltzmann factor $\exp(\Phi/T_e)$ in Poisson's equation, the potential tends to compensate for any change in n_0 such as to keep the electron density constant in most of the plasma volume, i.e. the product $n_0 p$ is kept approximately constant. Let us investigate this behaviour more in detail.

Subtracting Poisson's Eq. (2) at two subsequent time iterations and integrating over the plasma volume, we obtain

$$-\frac{\varepsilon_0}{e}\iint_{\text{surface}} \Delta E_\perp \mathrm{d}A = n_0\Delta p + p\Delta n_0 - \Delta N_i, \tag{10}$$

where Δ symbolizes the change between the iterations, $E_\perp$ is the electric field towards the wall, and N_i is the total number of ions in the volume. We now wish to estimate the left-hand side of this equation. We know from plasma physics that the potential is relatively constant in the bulk of the plasma and then suddenly drops to the wall potential within a narrow sheath region in front of the wall. The average potential drop across the sheath is approximately $T_e\ln(p/V) - T_e\ln(q/A) = T_e\ln(p/q\Lambda)$, where V is the total plasma volume, A is the total wall surface, and $\Lambda = V/A$ is the effective plasma radius. The ion density in the sheath is of the order of the average plasma density $n_0 p/V$. Integrating Poisson's equation across the sheath, we find for the electric field at the wall

$$E_\perp \approx \frac{T_e}{\lambda_D}\sqrt{2\ln(p/q\Lambda)}, \tag{11}$$

where $\lambda_D = (\varepsilon_0 T_e V/en_0 p)^{1/2}$ is the average Debye length. The left-hand side of Eq. (10) becomes

$$-\frac{\varepsilon_0}{e}\iint_{\text{surface}} \Delta E_\perp \mathrm{d}A \approx -\alpha n_0 \Delta p \tag{12}$$

where $\alpha = (\lambda_D/\Lambda)(2\ln(p/q\Lambda))^{-1/2}$ is a small parameter of the order of the ratio of the Debye length to the plasma radius. Substituting this expression into Eq. (10) and neglecting the ion density term, we find the following estimate for the change Δp due to a change Δn_0

$$\frac{\Delta p}{p} \approx -(1-\alpha)\frac{\Delta n_0}{n_0}. \tag{13}$$

Let us now use this result to analyse the behaviour of n_0 from Eq. (9). Applied to the time step from $k-1$ to k, Eq. (13) yields

$$\frac{p^{k-1}}{p^k} \approx 2 - \alpha - (1-\alpha)\frac{n_0^{k-1}}{n_0^k}. \tag{14}$$

Substituting this into Eq. (9), we find

$$n_0^{k+1} = (2-\alpha)n_0^k - (1-\alpha)n_0^{k-1} - n_0^k \frac{v_e q^k \Delta t}{4p^k} + \frac{r^k \Delta t}{p^k}, \tag{15}$$

which can be identified with the finite difference discretization of

$$\Delta t^2 \frac{\mathrm{d}^2 n_0}{\mathrm{d}t^2} + \alpha \Delta t \frac{\mathrm{d}n_0}{\mathrm{d}t} + \frac{v_e q \Delta t}{4p} n_0 = \frac{r\Delta t}{p}. \tag{16}$$

Most coefficients in this equation are more or less constant, except for p which is inversely proportional to n_0 to first order. However, substituting $p \sim 1/n_0$ and linearizing around the steady state solution $n_0 = 4r/qv_e$, we recover exactly the same equation. Eq. (16) can therefore be considered as a linear differential equation with constant coefficients. Posing $n_0(t) = a\exp(\Omega t) + b$, we find the solution

$$\Omega = \frac{-1}{2\Delta t}(\alpha \pm \sqrt{\alpha^2 - v_e q \Delta t/p}). \tag{17}$$

Oscillations can appear in case the square root is imaginary and are damped only weakly on a time scale $2\Delta t/\alpha$. To avoid oscillations, it is necessary to restrict the time step to

$$\Delta t < \frac{\alpha^2 p}{v_e q}. \tag{18}$$

This condition is generally much more severe than other time step conditions related to ion transport and accuracy, and is, therefore, very limiting for the overall simulation speed. Note that due to the crude approximations of our analysis, Eq. (18) is no more than an order-of-magnitude estimate and should not be taken too literally.

3. Proposed numerical scheme

Based on the above analysis, we propose to modify Eq. (9) as follows

$$n_0^{k+1} = n_0^k\left((1-f)\frac{p^{k-1}}{p^k} + f\right) - n_0^k \frac{v_e q^k \Delta t}{4p^k} + \frac{r^k \Delta t}{p^k}, \tag{19}$$

where f is a small parameter and the change in p is slightly under-relaxed by a factor $(1-f)$. Upon substitution of Eq. (14), the parameter f adds directly to α, and therefore, relieves the time step condition (18). Rather than restricting the time step, we propose to adjust f such as to obtain critical damping, i.e. to make the square root in Eq. (17) vanish

$$f = \sqrt{v_e q \Delta t/p} - \alpha \approx \sqrt{v_e q \Delta t/p}, \tag{20}$$

where we prefer to altogether neglect the negative contribution from α in view of the crude approximations necessary to estimate this parameter. (Note that the purpose of Eq. (19) is to be able to use large time steps for which α is negligibly small.) With these modifications the time advancement scheme becomes:

(1) calculate the ion density n_i^{k+1} using Φ^k;
(2) calculate the reference density n_0^{k+1} from Eq. (19) using $f = (v_e q^k \Delta t/p^k)^{1/2}$;
(3) solve the potential Φ^{k+1} from Eq. (2) using n_i^{k+1} and n_0^{k+1};
(4) calculate the coefficients p^{k+1}, q^{k+1} and r^{k+1} from Eqs. (5)–(7) using Φ^{k+1}.

This scheme leads to smooth simulation results for any time step small enough to resolve the ion transport. However, the under-relaxation of Δp in Eq. (19) is not justified by physical reasons and can be expected to cause physical errors in the time evolution, and increasingly so as Δt and hence f are larger. From Eq. (17), we expect evolution errors on a time scale $2\Delta t/f = 2(p\Delta t/v_e q)^{1/2}$. Time step restrictions could be necessary to ensure accuracy.

4. Test results

We tested the above numerical scheme for a one-dimensional model and the following conditions: uniform numerical grid of 200 cells, domain size $d = 0.01$ m, electron temperature $T_e = 1$ eV, fixed potential at the boundaries $\Phi(0) = \Phi(d) = 0$ V. Two test cases were investigated: (1) formation of the plasma sheath; and (2) plasma decay.

In the first test case, we fixed a uniform ion density of 10^{16} m^{-3} and a uniform ionisation source term of 10^{22} m^{-3} s^{-1}. Ion transport was not simulated. As an initial condition, we set the electron density equal to the ion density, i.e. $\Phi(x) = 0$ V and $n_0 = 10^{16}$ m^{-3}, and simulated the relaxation to steady state, i.e. the formation of the plasma sheath. We tested both Eqs. (9) and (8) for different time steps. Fig. 1 shows the time evolution of the potential in the centre of the plasma $\Phi(d/2)$. In agreement with the above analysis, Eq. (9) causes numerical oscillations which are slowly damped on a time scale proportional to Δt. Using Eq. (19) the oscillations are completely damped out but the relaxation to steady state is slowed down for larger time steps. To assess whether this slow-down is acceptable and determine an appropriate time step, one should realize that it is not physically meaningful to resolve the time evolution of the problem on the electron transport time scale $4d/v_e$ ($\approx$0.1 μs) since the electron Maxwell–Boltzmann distribution is valid only for much longer time scales. The important thing is to properly describe the ion transport time scale. This was investigated in our second test.

In the second test, case we used a particle description of the ions as in [3–7], where we set the ion mass equal to 6.64×10^{-26} kg (argon), and we turned off the ionisation source term. As an initial condition, we distributed

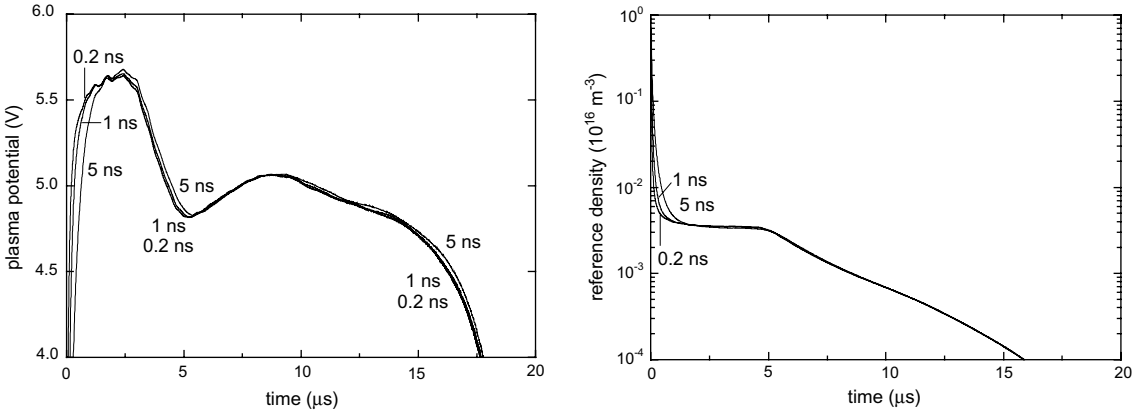

Fig. 2. Time evolution of the plasma potential and the reference density n_0 during the decay of a plasma in the absence of ionisation (see text), obtained using Eq. (19) for different numerical time steps.

10^5 macro-ions of weight 10^9 m^{-2} uniformly over the domain at a Maxwellian temperature of 300 K and set the electron density equal to the ion density of 10^{16} m^{-3}. We then simulated the formation of the plasma sheath (as in the previous test) and the decay of the plasma using Eq. (19) for different time steps. Fig. 2 shows again the time evolution of the potential in the centre of the plasma and also that of n_0. Note that the ion simulation imposes a maximum time step of the order of 5 ns due to the CFL condition. Simulation results are very similar for any of the time steps, although a slight delay can be observed for $\Delta t = 5$ ns. These results confirm that our scheme is appropriate to simulate the overall plasma evolution.

5. Concluding remarks

Proper normalization of the Maxwell–Boltzmann electron distribution in transient plasma models requires the self-consistent calculation of the reference density n_0 from global electron conservation. This calculation tends to produce numerical oscillations in the time evolution of the plasma, in particular during the formation of the plasma sheath. We propose a simple numerical scheme to prevent these oscillations by slight under-relaxation of the plasma potential such as to obtain critical damping. The numerical errors due to the under-relaxation appear to have no significant effect on the time evolution of the plasma on the ion transport time scale, although some slight delay can be observed for larger time steps. We conclude that our scheme is appropriate to simulate transient plasma phenomena without electron-related time step conditions.

A final remark concerns the definition of the electric potential. Contrary to Maxwell's equations, the Boltzmann relation involves the absolute value of the potential and therefore depends on the definition of the potential reference. For example, simultaneously changing all electrode potentials by the same amount (i.e. changing the potential reference) requires readjustment of the reference density n_0, which is taken care of by our numerical scheme, but not instantaneously, and causes errors depending the time step. This issue can become problematic in case a time-dependent voltage is applied across the plasma. Additional time step restriction can then be necessary to limit errors. We recommend to define the potential with respect to the anode (i.e. keep $\Phi = 0$ at the anode) and change only the cathode potential: since the plasma potential follows the anode rather than the cathode this leads to easier readjustment of n_0 and smaller errors. In any case we recommend to test several time steps and check that they yield the same results.

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