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A Self-Consistent Open Boundary Model for Particle Simulation in Plasmas

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ABSTRACT

A particle simulation model with open boundary, applicable to a system in which the internal plasma contacts with an external plasma source such as a current generator, is developed. We present this formalism and examine the range of applicability of this procedure. This scheme assures a balance between the outgoing and incoming particle fluxes through the boundaries at each time step. The numerical code developed on this principle is applied to an ion acoustic double layer under the condition that the system is connected to a constant current generator to confirm the soundness and viability of the code.

keywords: particle simulation, open system, constant current generator

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I. INTRODUCTION

Most of the particle simulation studies so far undertaken are compelled to adopt a periodic boundary conditions for elecrons, so that the strict condition of charge nuetrality is maintained. There are some exceptional cases where electrons are injected from one boundary with a very high speed which is far beyond the thermal speed. In these cases, both the electrons flowing out from the upstream boundary and those entering into the system from the downstream boundary are negligibly small, so that the condition of charge nuetrality can be automatically maintained.

The most difficult problem one usually encounters in the construction of an open boundary model for particle simulation, is the matching conditions between the external and internal plasmas. In this paper, we consider for simplicity a simple configuration, which is a one-dimensional electrostatic system. This model can be easily applied to a two-dimensional and three-dimensional configuration. As a list of the number of phenomena tractable by the method of numerical simulation, we can cite formation of an electrostatic potential structure along the magnetic field in the Q-machine, formation of the potential barrier along the divertor magnetic field in the nuclear fusion device, acceleration of auroral particles in space plasmas, etc.

Birdsall and Langdon described a pragmatic method for a system in contact with a cathode and/or an anode in the Q-machine[1]. On the other hand, Sato and Okuda proposed a sophisticated model to deal with the ion-acoustic double layer[2], where an internal plasma connected with an external circuit including a constant voltage source at both ends of the simulation box. The electric potential was solved self-consistently so as to match the applied voltage generator with an internal resistance. A drawback of the model was, however, the imposition of a strictly periodic boundary conditions for the particles, in order to maintain the charge neutrality. Because of this strict periodicity, the electrons largely modified in velocity space (which are accelerated or decelerated by double layers) passing through the downstream/upstream boundary came back to the system through the upstream/downstream boundary. The structure of the generated double layers was destroyed because these electrons modified by double layers were made to circulate in the system. Many researchers have tried to tackle this difficulty; however all of their models were incomplete when judged from the point of view of electrical circuit theory.

In an open system, the source (external) plasma and the bulk plasma are in contact at the upstream and downstream boundaries. On the upstream boundary only the particle with positive velocity can enter into the bulk plasma and the negative velocity particles constitute the backward flow (i.e., they exit from the bulk plasma). On the downstream side the situation is reversed. That means, the positive velocity particles exit from the bulk plasma and negative velocity particles of the external plasma enter into the bulk plasma. For example, a constant flux injection model was proposed[3]. This model ignored the backward flow of the thermal tail (negative velocity side) of the bulk electrons on the upstream and the backward flow of the external plasma through the downstream. Particularly, in the case of ion-acoustic double layers, injected electrons have a drift velocity that is less than the electron thermal velocity. So far there have been no attempts, we believe, to present a simulation model that could self-consistently handle the "outgoing flow" and "incoming flow" through the boundaries, especially through the downstream boundary. We tried to develop a new model that enables us to treat a realistic open system. The boundary condition must be treated as a smooth interface between the bulk and external plasmas.

A new supercomputing system, named as "Advanced Computing System for Complexity Simulation" was introduced at NIFS in March, 1993. This system has enabled us to exploit the practical code for an open boundary particle simulation model.

Our open boundary model has been already applied to a two-dimensional electromagnetic problem. However, using a simple one-dimensional elctrostatic model, we explain our open boundary model as follows. In Section II of this paper, we present the formulation of our model. Next, in Section III, we discuss an application to a constant plasma current case and examine the range of applicability of this procedure. Finally, in Section IV, we demonstrate a physical result in one-dimensional double layer system obtained by using the developed code.

II. METHODOLOGY

We choose that the left-hand boundary is the upstream boundary and the right-hand boundary is the downstream boundary. Initially, we load particles in the system by mean of a random number generator so as to form a shifted Maxwellian distribution. Figure 1 shows an example of the particle flux distribution that is generated by passing particles through the upstream (left-hand side) boundary during unit time step. The part of the positive distribution ("incoming") represents the injected flux distribution into the system through the upstream boundary and the negative part ("outgoing") does the departing flux distribution through the upstream. The constant flux injection model in the conventional particle simulation assumes that the number of injected particles and the form of the injected flux distribution function are fixed, in spite of the fact that the number of outgoing particles, hence, the outgoing flux, changes with time according to the change of the internal condition of the system. Thus, the balance of the fluxes of electrons and ions between the upstream and downstream boundaries cannot be guaranteed and, hence, an unrealistic phenomena may occur unless the drift speed is much higher than the thermal speed. Such a model may be called "unregulated" open model and, in general, does not guarantee a physically sound result.

Our proposed open boundary model is an essentially different one. In our model, we only assume that the functional form of the incoming particles on both the upstream and downstream boundaries, say, a shifted-Maxwellian, is fixed. The number of injected particles is so adjusted that the net particle flux (difference between the departing flow and the injected flow) through each boundary satisfies a prescribed value. We call this as a "regulated" open boundary model, as distinct from the conventional one.

The shifted Maxwellian $f(v)$ is given by

$$f(v) = \exp[-\frac{(v - v_{drift})^2}{2\, v_{th}^2}], \tag{2.1}$$

where v_{drift} and v_{th} are the drift velocity and the thermal velocity, respectively. The particle flux at the boundary is given by

$$F_b = (n\lambda_D) \int_{-\infty}^{+\infty} \frac{v}{v_{th}} f_b(v)\, dv, \tag{2.2}$$

where n and λ_D are the average number of particles per Debye length, the Debye length, respectively, and f_b represents the distibution function at the boundary. In the actual simulation with the finite descrete time step Δt, the flux cannot be evaluated directly. Therefore, we observe the number of particles passing through the boundary during the finite time step Δt, which is given by

$$(n\lambda_D)\,(\omega_p \Delta t) \int_{-\infty}^{+\infty} \frac{v}{v_{th}} f(v)\, dv, \tag{2.3}$$

where ω_p is the plasma frequency. These relations, Eqs.(2.2) and (2.3), indicate that the particle flux can be known by counting the number of particles passing through the boundary during the time step Δt.

With this preparation, we can proceed towards the actual simulation repeating the following four steps.

Step 1 Observe the number of outgoing particles through the upstream (up) and downstream (down) boundaries in the unit time step Δt, i.e., N_{out}^{up} and N_{out}^{down}.

Step 2 Define the number of injected particles (N_{in}) in the unit time step on both upstream (left-hand) and downstream (right-hand) boundaries according to the following relations:

$$Upstream : N_{in}^{up} = N_{net}^{up} - N_{out}^{up} \tag{2.4}$$

$$Downstream : N_{in}^{down} = N_{out}^{down} - N_{net}^{down}, \tag{2.5}$$

where the net particle fluxes (N_{net}^{up} and N_{net}^{down}) at the upstream and downstream boundaries are prescribed by the given initial conditions of the stream, namely by solving Eq.(2.3) with help of Eq.(2.1).

Step 3 Generate the injected particles (N_{in}) in velocity space by using the cumulative distribution function[1]. In order to prevent the numerical defect of depletion of the particle population at v=0 in the phase space, we must expand the domain of integration by Δv which is a cumulative step-size along the velocity axis. Otherwise, the population of particles near v=0 would decrease rapidly and the numerical sheath appears near the boundary. Namely,

$$N_{in}^{up} = (n\lambda_D)\,(\omega_p\Delta t)\int_{0-\frac{1}{2}\Delta v}^{+\infty}\frac{v}{v_{th}}\,f(v)\,dv \tag{2.6}$$

$$N_{in}^{down} = (n\lambda_D)\,(\omega_p\Delta t)\int_{-\infty}^{0+\frac{1}{2}\Delta v}\frac{v}{v_{th}}\,f(v)\,dv. \tag{2.7}$$

Step 4 Load injected particles at positions x = $R_j v_j \Delta t$ ($j = 1, N_{in}$), where R_j is a random number for the j-th particle, thus they can be scattered in the space between x=0 and x=$v_j\Delta t$ [1].

III. CURRENT GENERATOR MODEL

In this section, we apply the above methodology to one important realistic case, namely, to a constant plasma current model. In the current generator case, the numbers of the net particle fluxes at the upstream and downstream boundaries must be the same, i.e., $F^{up} = F^{down}$, which is thus equivalent to

$$N_{net}^{up} = N_{net}^{down} \equiv N_{net} = \text{const}, \tag{3.1}$$

where the electric field at the boundaries of the simulation box is set to zero. With the usage of Eq.(3.1), the integration of the continuity equation over the system length yields that the total number of particles in the simulation box is conserved.

Namely,

$$\frac{\partial N_{total}}{\partial t} = F^{up} - F^{down} = 0, \tag{3.2}$$

where $N_{total} = \int_{up}^{down} ndx$ = total number of particels in the system. This feature that the total number of particles is conserved gives us a great advantage of implementing the simulation code in the sense that the simulation code does not require any superfluous main memory and the size of the required working area for the boundary procedure is at most $n\lambda_D$. This is because the number of particles passing through one boundary under the Particle-in-Cell model per unit time step Δt is limited by $n\lambda_D$.

We shall examine the range of applicability of this procedure. Figure 2 shows the flux distribution function of passing particles through the downstream (right-hand) boundary. Since the outgoing particles through the downstream boundary can change depending on the events evolving in the system, it may happen that the outgoing flux through the downstream boundary becomes $N_{out}^{down} < N_{net}$. This implies from Eq. (2.5) that $N_{in}^{down} < 0$, which is impossible to deal with in a practical simulation.

By changing the drift velocity and the number of particles in unit cell, where $\Delta x = \lambda_D$, we have made numerous test runs up to one plasma period ($2\pi/\omega_p$). The summary of the simulation runs is given in Fig.3. Figure 3 shows the applicable region of our procedure on computer implementation which is denoted by the "green" region. The inapplicable region, which is denoted by "red", is defined when the condition of $N_{in}^{down} < 0$ is met on the way of the test run. The applicable region is the numerically stable region during one plasma period. The "yellow" region satisfies the condition of $N_{in}^{down} > 0$, but N_{in}^{down} becomes quite small so that it may happen that $N_{in}^{down} < 0$ during the nonlinear evolution. The boundary between the "green" region and the "yellow" region is demarcated by whether the root-mean-square of the error between the analytical form and the observation form is less than or greater than 5 % (empirically, $N_{in}^{down} = 100 \sim 150$ particles are required). The boundary between the "red" and the "yellow" region is defined by whether or not $N_{in}^{down} < N_{net}$ is met during one plasma period. A crucial point should be remarked in this figure. Conventional particle simulations use typically 100 particles in one Debye length. Then, N_{in}^{down} is $1 \sim 2$ particles at most, so that the functional form of $vf(v)$ can never be constructed by such a small number of particles. In order to be able to apply the present "regulated" open boundary, therefore, it is definitely required to use a huge number of particles in one Debye length (typically 5000 – 8000) for a small drift velocity such as $v_{drift} \lesssim v_{th}$.

IV. APPLICATION

In order to testify the validity and usefulness of our open boundary procedure, we have applied the one-dimensional electrostatic particle simulation code to the evolutions of the electrons and ions for the ion-acoustic double layer formation where fresh particles are continuously supplied through the boundaries to conserve the net current. The system length is 1023 λ_D, where λ_D is the initial electron Debye length that is equal to the computational mesh size. Initially the system is filled uniformly with the drifting Maxwellian electrons and the low temperature Maxwellian ions. The electron drift velocity, the ion drift velocity, the initial temperature ratio, the mass ratio and time step are $v^e_{drift}/v^e_{th} = 0.6$, $v^i_{drift}/v^e_{th} = 0.0$, $T_e/T_i = 20$, $m_e/m_i = 1/100$, and $\omega_{pe}\Delta t = 0.16$, respectively. The number of electrons in one grid space (Debye length) is 8000, namely, $n\lambda_D = 8000$. The electrostatic potential inside the system is calculated directly from the electrostatic field, where the potential value at the upstream boundary is set to be zero.

Figure 4 shows the time evolution of the spatial profile of the electrostatic potential, where the electrostatic potential is averaged over the period of $10\pi/\omega_{pe}$. In the early phase of evolution, a stairs-like ("normal") potential structure is formed where the ordinary weak ion acoustic double layers are formed with spatial intervals of the order of 200 - 500 λ_D. The potential jump ϕ_{DL} across a single double layer is approximately $e\phi_{DL}/k_BT_e \sim 1$. This feature is in good agreement with the previous simulation by Sato and Okuda[2] except that the structure is extremely noiseless because of the usage of a huge number of particles in one grid cell ($n\lambda_D = 8000$ in contrast with $n\lambda_D = 100$ in Sato and Okuda). This stairs-like structure is destroyed by emitting ion acoustic solitons. Thereafter, another stairs-like weak potential structure reappears. They are closely resembling the double layers developed in the first stage. After a few recurrent processes of creation and destruction of the structure, a single but gigantic double layer is generated of which the peak potential can exceed ten times of the thermal potential. We call this huge double layer as a "super" ion acoustic double layer. This "super" double layer is generated by either of the electron-electron two-stream instability or the electron-ion two-stream instability, the condition of which happens to be locally satisfied by strong nonlinear deformations of particle distributions due to the preexisting weak ion acoustic double layers[4]. This super double layer exhibits a recurrent appearance and disappearance but with a longer duration time.

This new finding illustrates that the development of an open boundary model for particle simulation is of practical importance and opens the possibility of wide applications in plasma kinetics.

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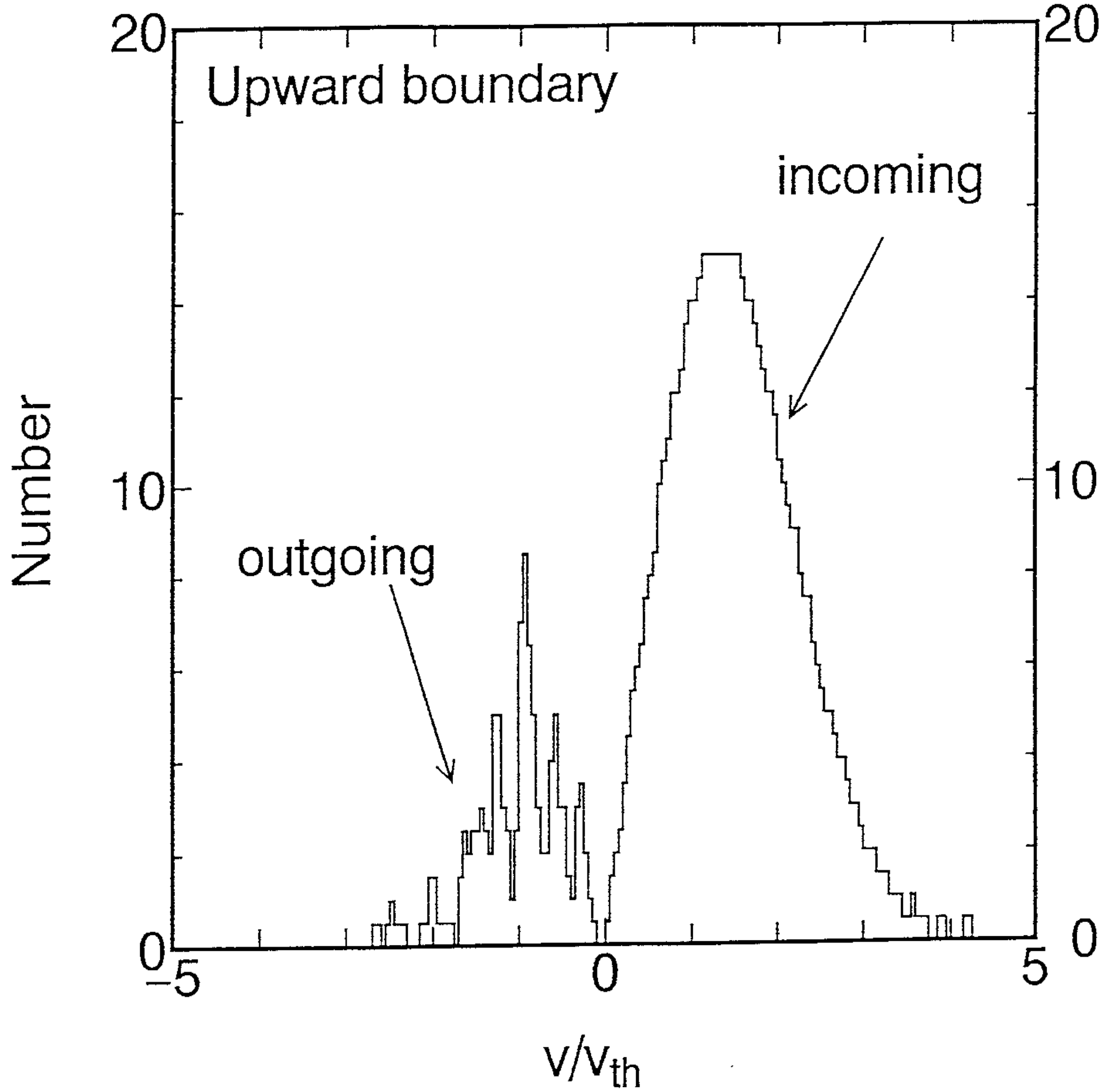
FIGURE CAPTION

Fig.1. An example of the distribution functions of incoming and outgoing particles through the upstream (left-side hand) boundary during unit time step Δt, when 5000 particles are loaded per unit grid space (Debye length).

Fig.2. Same as Fig.1 but for the distributions of the outgoing and incoming particles through the downstream (right-hand side) boundary.

Fig.3. The range of applicability of the proposed open boundary model in the number - drift domain of the particles. Applicable and inapplicable regions are denoted by "green" and "red" regions, respectively. The "yellow" region satisfies the condition for $N_{in}^{down} > 0$, but N_{in}^{down} becomes quite small so that it may happen that $N_{in}^{down} < 0$ during the nonlinear evolution, where N_{in}^{down} is the number of injected particle on the downstream boundary in the unit time step.

Fig.4. An example of simulation performed by one-dimensional electrostatic particle code based on the proposed open boundary model. The system is connected with a current (electron stream) generator which has an ability of generating a shifted Maxwellian electron stream with the drift speed of 0.6 V_{th}^{e}. A gigantic, or "super", ion acoustic double layer (lower panel) is observed to be formed after a few times repetition of generation and disappearance of the weak ("normal") ion acoustic double layers (upper panel).



20
20
Upward boundary
incoming
Number
10
10
outgoing
0
0
-5
0
5
v/v_th

Fig.1

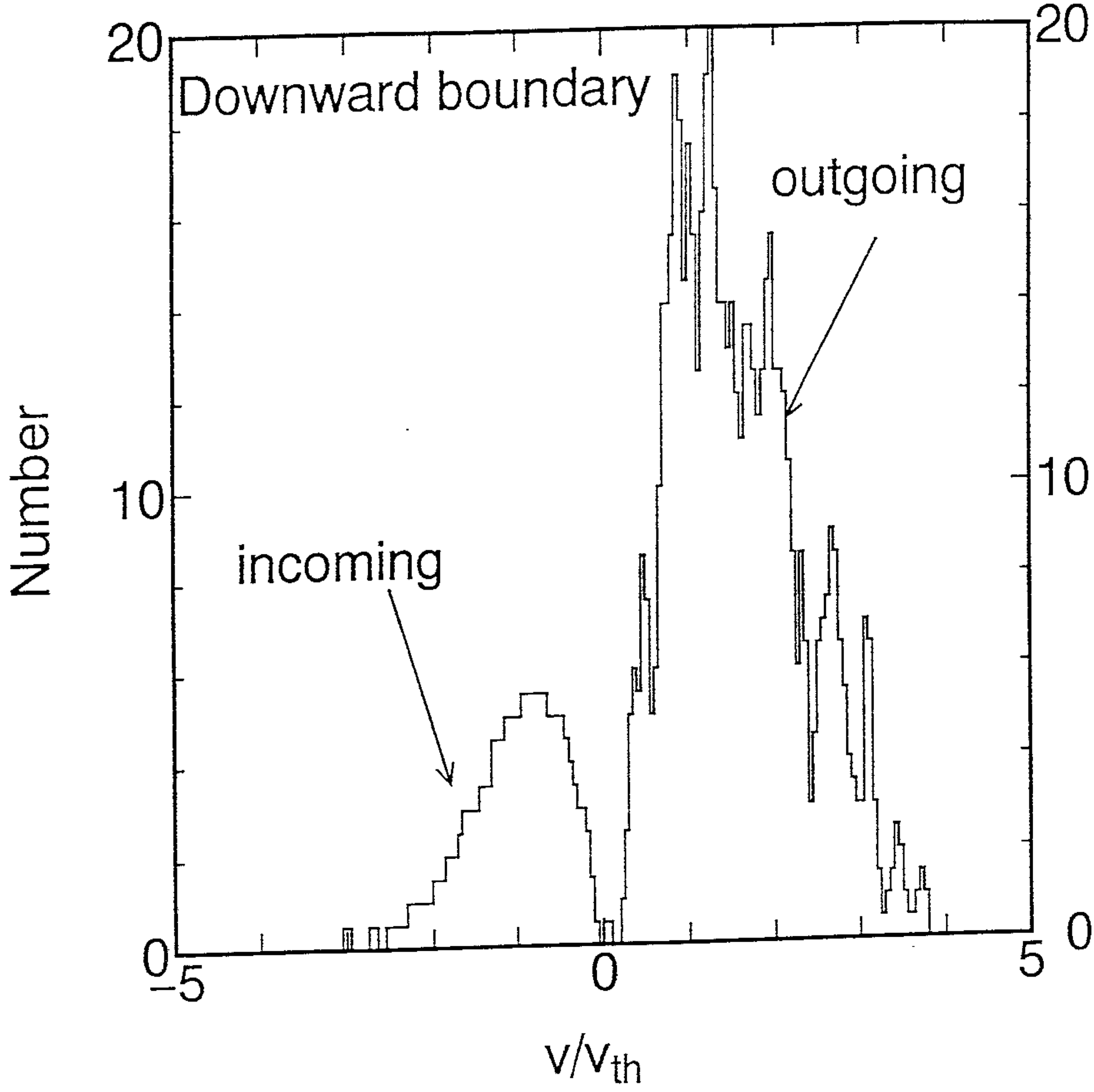

20
20
Downward boundary
outgoing
Number
10
10
incoming
0
0
-5
0
5
v/v_th

Fig.2

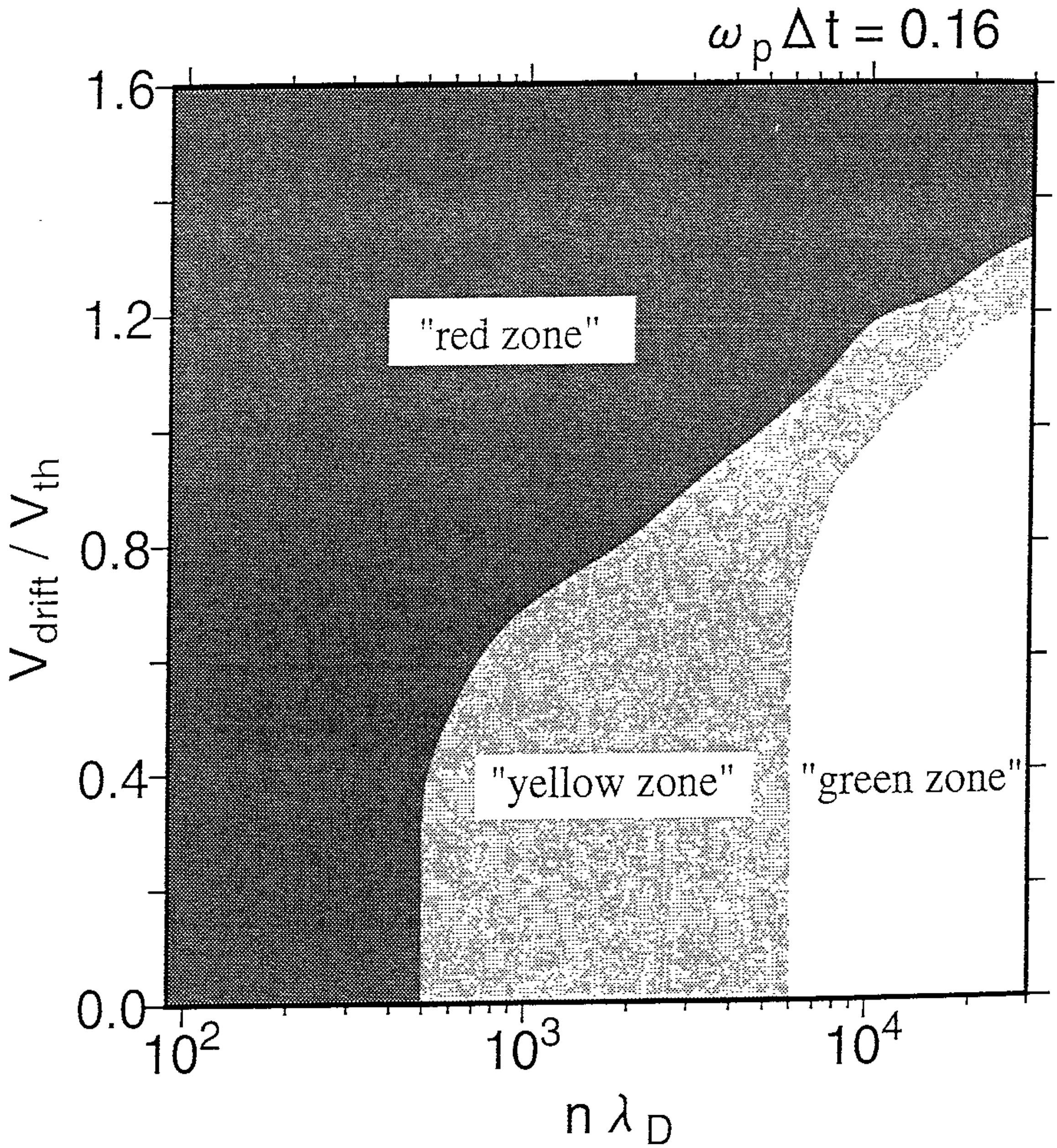
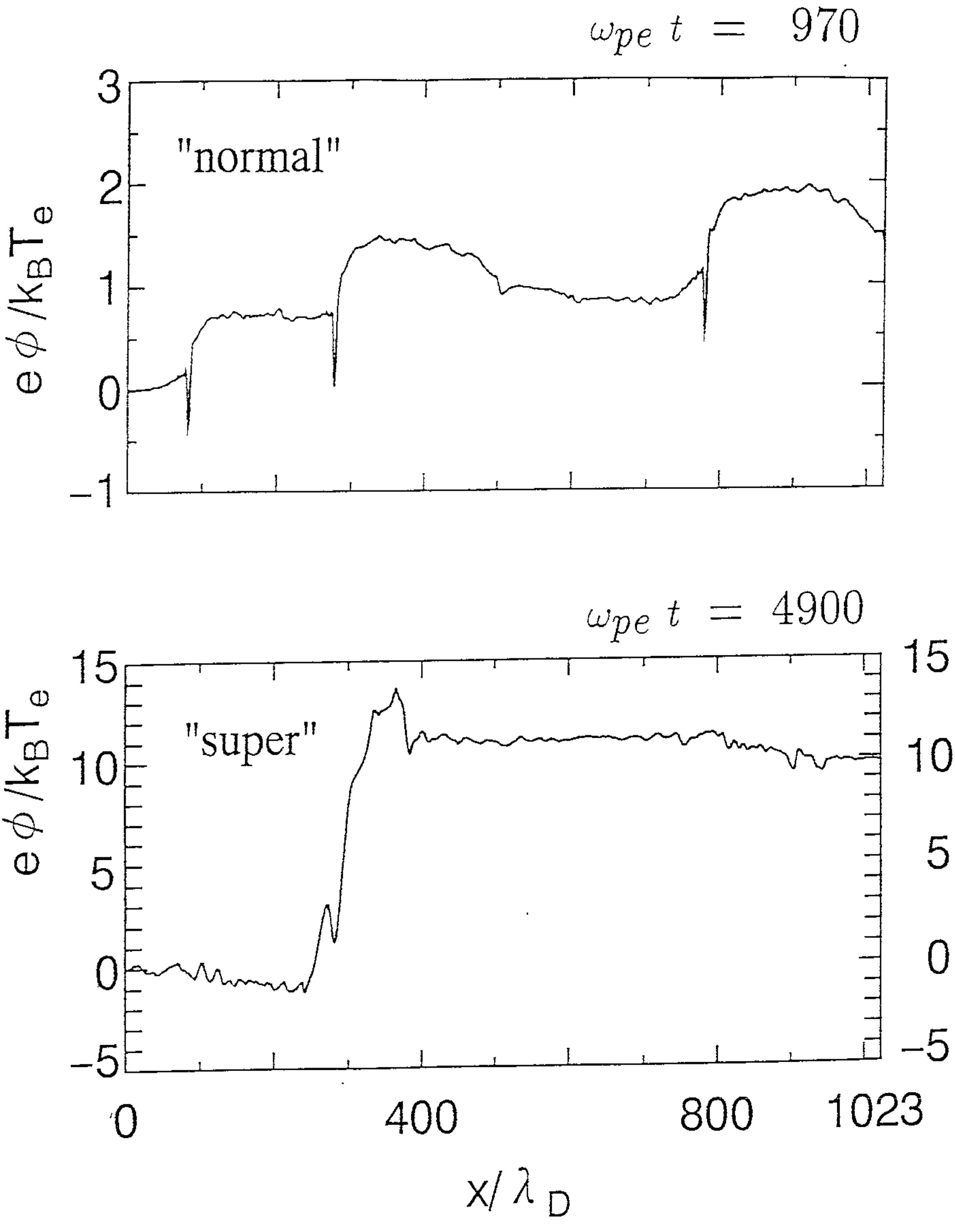

ω p Δ t = 0.16
1.6
1.2
0.8
0.4
0.0
V drift / V th
"red zone"
"yellow zone"
"green zone"
10^2
10^3
10^4
n λ D

Fig.3



$\omega_{pe}\, t\ =\ 970$
"normal"
$e\phi/k_BT_e$
3
2
1
0
−1
$\omega_{pe}\, t\ =\ 4900$
"super"
$e\phi/k_BT_e$
15
10
5
0
−5
0
400
800
1023
x/λ_D

Fig.4

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