

# NUMERICAL MODELING OF POWDER PARTICLES LEVITATING IN PLASMA SHEATHS

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## Abstract

Dusty plasmas have received much attention in the last decade, in particular because dust contamination of plasma is a serious problem in industrial applications. We have developed a MATLAB code enabling complex numeric investigations of dust particles levitating above the electrode in rf sheath. Charges, forces, balancing radii and other quantities concerning dust particles are analyzed in dependence on plasma state, position within the sheath and applied mathematical models.

## Introduction

A number of papers concerning experimental and theoretical studies of dusty plasmas appear each year. The permanent interest arises from various applications in astronomy [1,2] and technology [3,4]. Various models were suggested to describe dust charging in plasma bulk and sheath [5-7], forces acting on the individual dust particle [8,9] and collective behavior of dusty clouds [10-13]. We will limit our modeling on particles in radio – frequency (rf) plasma sheath. Our computations will include both the modeling of dust – plasma interactions and rf plasma sheath. The computational scheme partly follows [14].

## 2. Modeling of rf sheath

We suppose a capacitively coupled rf ( $\omega_{\text{rf}} / 2\pi = 13.56$  MHz) discharge in argon plasma with the lower electrode powered. The local potential  $U(t, x)$  in the sheath, with coordinate  $x$  oriented vertically upward from the electrode, will be specified later. At the powered electrode we assume a harmonic potential

$$U(t,0) = U_{\text{dc0}} + U_{\text{rf0}} \sin(\omega_{\text{rf}} t) \quad (1)$$

Here  $U_{\text{dc0}}$  is the dc self bias and  $U_{\text{rf0}}$  is the amplitude of the rf potential oscillations. In capacitively coupled rf discharge the average current to the electrode must be zero:

$$\frac{1}{T} \int_0^T j_e(t) dt + j_i = 0 \quad (2)$$

$T$  is the rf period and  $j_e$  and  $j_i$  are the electron and ion currents, respectively. As this condition couples  $U_{\text{dc0}}$  and  $U_{\text{rf0}}$ , only one of these parameters is optional.

In asymmetric rf discharges, with powered electrode much smaller than the grounded one, the potential oscillations outside the sheath can be neglected [15]. It enables to define the boundary condition at the sheath edge,

$$U(t, L) = 0 \quad (3)$$

where  $L$  is temporarily unknown sheath thickness.

The electrons are assumed to be Maxwellian, although this assumption is not always satisfied in rf discharges. As the rf frequency is for our conditions less than the electron plasma frequency,  $\omega_{rf} < \omega_{pe}$ , the electrons are considered inertialess, i.e. instantaneously following the electric field. Then the electron number density in the sheath and electron current density to the electrode are given by

$$n_e(t, x) = n_s \exp\left(\frac{eU(t, x)}{kT_e}\right) \quad (4)$$

$$j_e(t) = \frac{1}{4} e n_s \exp\left(\frac{eU(t, 0)}{kT_e}\right) v_{me} \quad (5)$$

where  $n_s$  is the electron density at the sheath edge,  $T_e$  is the electron temperature and  $v_{me} = \sqrt{8kT_e/\pi m_e}$  is the mean thermal electron velocity.

The ions are considered cold, i.e. their kinetic energy of drift motion is much greater than their thermal energy. As the plasma ion frequency is lower than the rf frequency,  $\omega_{pi} < \omega_{rf}$ , the ions respond only to the average electric field. The time – averaged equation of ion motion in the sheath is then

$$m_i v_i \frac{dv_i}{dx} = \left\langle -e \frac{\partial U}{\partial x} \right\rangle + n_n \sigma_{in} m_i v_i^2 \quad (6)$$

Angle brackets represent time – averaging,  $v_i(x)$  is the ion drift velocity. The last term on the right hand side of this equation is the friction force due to ion collisions with the neutrals;  $n_n$  is the neutral number density and  $\sigma_{in}$  is the ion – neutral collisional cross section. The corresponding boundary condition is

$$v_i(L) = -v_B \quad (7)$$

where  $L$  is the sheath thickness and  $v_B = (kT_e/m_i)^{1/2}$  is the Bohm velocity [16]. To ensure the ions are accelerated monotonously from the Bohm velocity at the sheath edge, the boundary condition  $dv_i(L)/dx = 0$ , or

$$\left\langle -e \frac{\partial U(t, L)}{\partial x} \right\rangle + n_n \sigma_{in} m_i v_B^2 = 0 \quad (8)$$

is in addition required.

Neglecting ionization in the sheath, the ion continuity equation reads

$$n_i(x) v_i(x) = -n_s v_B \quad (9)$$

hence

$$j_i = -e n_s v_B \quad (10)$$

The above equations are completed by the Poisson's equation

$$\frac{\partial^2 U(t, x)}{\partial x^2} = -\frac{e[n_i(x) - n_e(t, x)]}{\epsilon_0} \quad (11)$$

The system of differential equations (6,11) together with boundary conditions (1,3,7,8) and algebraic equations (4,9) is complete, giving  $U(t, x)$ ,  $n_e(t, x)$ ,  $n_i(x)$ ,  $v_i(x)$  and  $L$ .

At the end of this section we shortly outline possible numerical algorithm. The system of three boundary conditions (1,3,8) is seemingly “overdetermined” as the Poisson equation (11) is of the second order. In fact the condition (8), written symbolically as  $f(L) = 0$ , determines the unknown sheath boundary  $L$ . Temporarily we exclude this condition from the solved system and choose some guess  $L = L^{(1)}$  by definition. For this value we solve the system of coupled differential equations (6,11) with boundary conditions (1,3,7). This can be done by simple iterative procedure. At the beginning we suggest an estimation  $U^{(0)}(t, x)$ , e.g. linear or quadratic in variable  $x$  and satisfying boundary conditions (1,3). From its time-average and equations (6,7,9) for the ion motion we find corresponding functions  $v_i^{(1)}(x)$ ,  $n_i^{(1)}(x)$ . The solution  $n_i^{(1)}(x)$  is then substituted in Poisson’s equation (11) with boundary conditions (1,3) to determine  $U^{(1)}(t, x)$ . The successive iterations rapidly converge. We finish this stage by evaluating  $f^{(1)} = f(L^{(1)})$ .

The procedure for value  $L^{(1)}$  is repeated for another value  $L^{(2)}$ . After it the equation  $f(L) = 0$  can be solved, e.g., by secant method,  $L^{(3)} = (f^{(2)}L^{(1)} - f^{(1)}L^{(2)}) / (f^{(2)} - f^{(1)})$ , and so on.

### 3. Modeling of dust particle

#### 3.1 Dust potential

Under usual conditions the particle in the plasma sheath can be approximately considered as a spherical capacitor of the radius  $r_d$ . Hence, its charge  $Q_d$  and potential  $V_d$  relative to the local potential of undisturbed plasma are related by

$$Q_d = 4\pi\epsilon_0 r_d V_d \quad (12)$$

The charge or potential of the particle is a result of electron and ion currents hitting its surface. The electron and ion fluxes reaching the particle are

$$\Gamma_e = \frac{1}{4} n_e v_{me} 4\pi r_d^2 G_e(V_d) \quad (13)$$

$$\Gamma_i = n_s v_B \pi r_d^2 G_i(V_d) \quad (14)$$

Introducing the spreading or focusing factors  $G_e$  and  $G_i$  into these expressions is due to the repulsive or attractive electrostatic interaction between the fluxes and the dust particle. Within the frame of orbital motion limited (OML) theory [17] these factors are

$$G_e(V_d) = \begin{cases} \exp\left(\frac{eV_d}{kT_e}\right), & V_d < 0 \\ 1 + \frac{eV_d}{kT_e}, & V_d > 0 \end{cases} \quad (15)$$

$$G_i(V_d) = \begin{cases} 1 - \frac{2eV_d}{m_i v_i^2}, & eV_d < \frac{m_i v_i^2}{2} \\ 0, & eV_d > \frac{m_i v_i^2}{2} \end{cases} \quad (16)$$

where  $n_e(t, x)$  and  $v_i(x)$  are local values of electron density and ion velocity, respectively.

The simplest model of dust charging in an rf plasma determines the steady value of voltage  $V_{dc} = \langle V_d \rangle$  or charge  $Q_{dc} = \langle Q_d \rangle$  from the equation

$$\langle \Gamma_e - \Gamma_i \rangle = 0 \quad (17)$$

balancing the average electron and ion fluxes impinging the particle. As is shown in [14], the time-averaging can be with high accuracy realized by replacing  $n_e$  with its mean value  $n_{e,dc} = \langle n_e \rangle$ . To simplify the formulas we will not express time-averaging explicitly. For instance,  $\Gamma_e$  and  $V_d$  will represent electron flux and dust potential, respectively, averaged over one rf period.

An alternative model of dust charging was proposed in [7]. This model includes elementary processes at the dust surface: adsorption and desorption of incoming charge carriers and their recombination on the surface. The balance equations for electrons and ions are

$$P_e \gamma_e(V_d) - \frac{\sigma_e}{\tau_e} - \alpha_R \sigma_e \sigma_i = 0 \quad (18)$$

$$P_i \gamma_i(V_d) - \frac{\sigma_i}{\tau_i} - \alpha_R \sigma_e \sigma_i = 0 \quad (19)$$

where  $\gamma_{e,i} = \Gamma_{e,i} / 4\pi r_d^2$  are the electron and ion fluxes per unit area of the particle surface,  $P_{e,i}$  are the sticking probabilities for impinging electrons and ions,  $\sigma_{e,i}$  are electron and ion surface densities,  $\tau_{e,i}$  are their residence times and  $\alpha_R$  is the coefficient for recombination. A more detailed structure of these coefficients as well as their relevant numerical estimations are given in [7]. Formulas (18,19) together with the capacitor formula (12) rewritten as

$$4\pi r_d^2 e(\sigma_i - \sigma_e) - 4\pi \epsilon_0 r_d V_d = 0 \quad (20)$$

represent three algebraic equations for three unknowns  $V_d$ ,  $\sigma_e$ ,  $\sigma_i$ .

### 3.2. Forces

A dust particle in a plasma sheath experiences various forces [14]. The most common are gravity and electrostatic interaction, but in some conditions other types of forces can be important, e.g. ion drag force, neutral gas friction or thermophoretic force. The charged dust particles levitate above the electrode at the position where the resulting force is zero.

The gravitation force is given by

$$F_g = -m_d g = -\frac{4}{3} \pi r_d^3 \rho_d g \quad (21)$$

where  $m_d$  is the mass of the particle, and  $\rho_d$  is the mass density. A negative sign means that the force is oriented downwards to the lower electrode.

The electric force is given by

$$F_E = Q_d E \quad (22)$$

where  $E(x) = -\langle \partial U(t, x) / \partial x \rangle$  is the local electric field averaged over rf oscillations.

The ion drag force, depending on the mechanism of momentum transfer from ions to the dust particle, consists of two components [9,14],

$$F_i = F_{i,\text{coll}} + F_{i,\text{Coul}} \quad (23)$$

The collection part is given by ions directly collected on the particle surface,

$$F_{i,\text{coll}} = -n_i m_i v_i^2 \pi r_d^2 G_i(V_d) \quad (24)$$

with the electrostatic focusing term  $G_i$  defined in (16). The Coulomb part is due to the momentum transfer from scattered ions not sticking to the surface,

$$F_{i,\text{Coul}} = -n_i \frac{2(eV_d)^2}{m_i v_i^2} \pi r_d^2 \ln \Lambda \quad (25)$$

where  $\ln \Lambda$  is the Coulomb logarithm with

$$\Lambda = \frac{\frac{\epsilon_0 k T_e}{n_e e^2 r_d^2} + \left( \frac{eV_d}{m_i v_i^2} \right)^2}{G_i(V_d) + \left( \frac{eV_d}{m_i v_i^2} \right)^2} \quad (26)$$

If the dust particle moves in the gas, the gas friction force appears. The expression depends on the nature of reflection of neutrals from the dust surface – if it is specular or diffuse [18]. For diffuse reflection we have

$$F_f = -2m_d b v_d \quad (27)$$

where  $v_d$  is the velocity of the dust grain relatively to the gas and  $b$  is the damping constant,

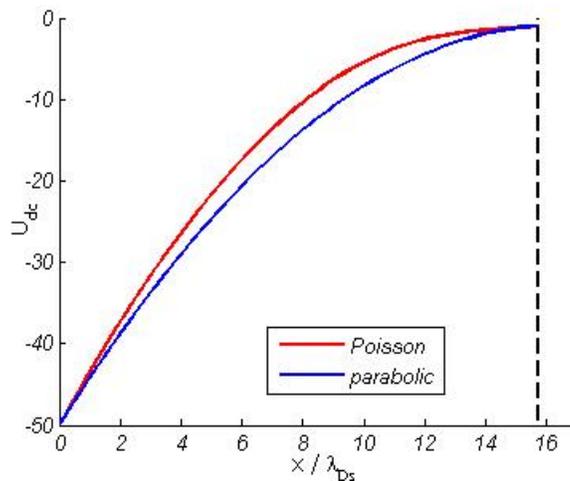
$$b = \frac{16}{3m_d} \left( 1 + \frac{\pi}{8} \right) \frac{p_g}{v_{\text{mg}}} r_d^2. \quad (28)$$

$p_g$  is the gas pressure and  $v_{mg}$  is the mean velocity of gas atoms,  $v_{mg} = \sqrt{8kT_g/\pi m_g}$ .

#### 4. Numerical results

Previous formulas have been incorporated into set of several codes, written in MATLAB. The codes enable complex investigation of particle behavior in the rf plasma sheath depending on the chosen model and parameters. Till now two models of rf plasma sheath have been realized. The first model is based on the coupled equations (6,11) for electric field and ion motion. We will call it here as Poissons's model. The second one comes out from the indication that the sheath potential may be very closely approximated with a parabola [19]. This approximation enables to solve equations (6,9) and (4) for ion velocity, ion density and electron density in the sheath analytically. Computations in the parabolic approximation are very fast and quantitatively correspond to more sophisticated Poissons's model, but, contrary to it, the parabolic model does not predict the sheath thickness  $L$ .

Input parameters of presented rf sheath models were chosen as follows: electron temperature  $T_e = 2\text{ eV}$ , plasma bulk density  $n_0 = 1 \times 10^{16} \text{ m}^{-3}$ , dc self bias at the electrode relatively to the plasma bulk  $U_{dc0} = -50 \text{ V}$  and self bias at the sheath boundary  $U_{dcL} = -kT_e/2e = -1 \text{ V}$  (Bohm theory). As a working gas was argon at the pressure  $p_g = 13.3 \text{ Pa}$  and temperature  $T_g = 300 \text{ K}$ .



**Fig. 1**

In figure 1 time-averaged potentials  $U_{dc}(x) = \langle U(t, x) \rangle$  from both models are compared. The distance  $x$  from the electrode is normalized by electron Debye length  $\lambda_{Ds} = (\epsilon_0 kT_e / n_s e^2)^{1/2}$  taken at the sheath edge. The sheath thickness in the parabolic model was adopted from the Poissons's model. For our data  $L = 15.7 \times \lambda_{Ds}$ . The sheath boundary is depicted by the vertical dashed line.

In dust modeling particles made of melamine formaldehyde of mass density  $\rho = 1.5 \times 10^3 \text{ kg/m}^3$  and of radius 10 micrometers have been considered. Both dust charging models (17) and (18-20) were realized. As is seen in figure 2, their predictions of dust charge are quite different. The absolute value of dust charge in microscopic model is much lower in comparison to the value obtained by equating electron and ion currents.

Figure 3 depicts the total force acting on the dust in both models. The microscopic model gives two equilibrium positions: The equilibrium point closer to the electrode is unstable while the outer is stable. The macroscopic model gives one stable equilibrium in this case.

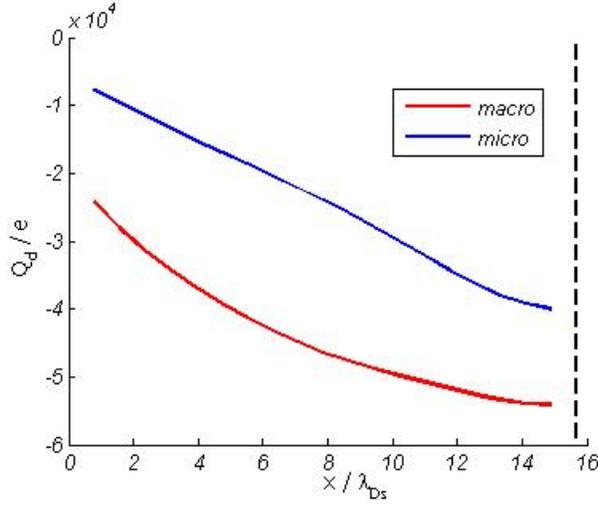


Fig. 2

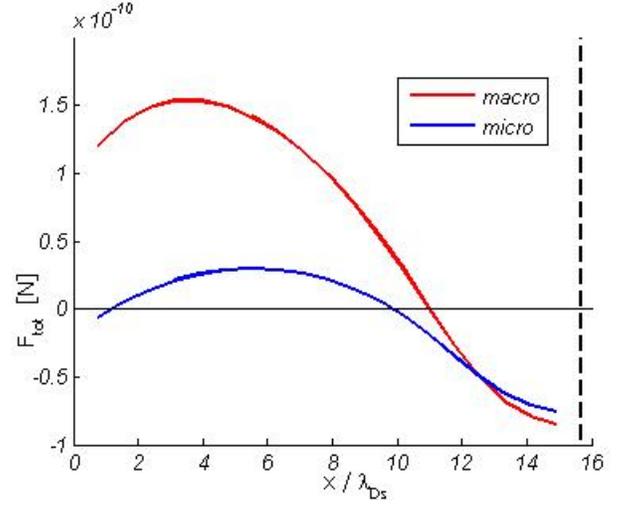


Fig. 3

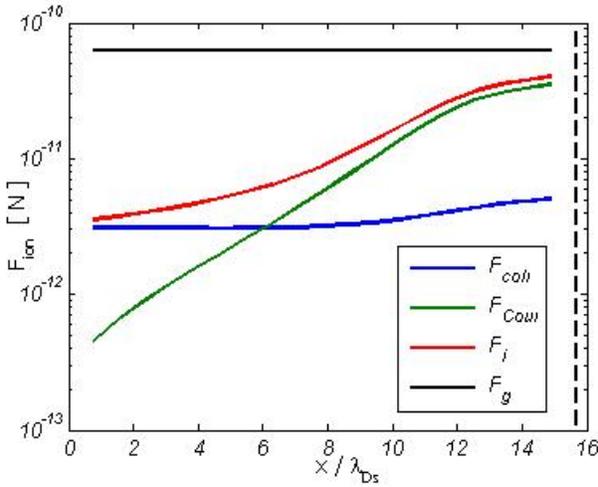


Fig. 4

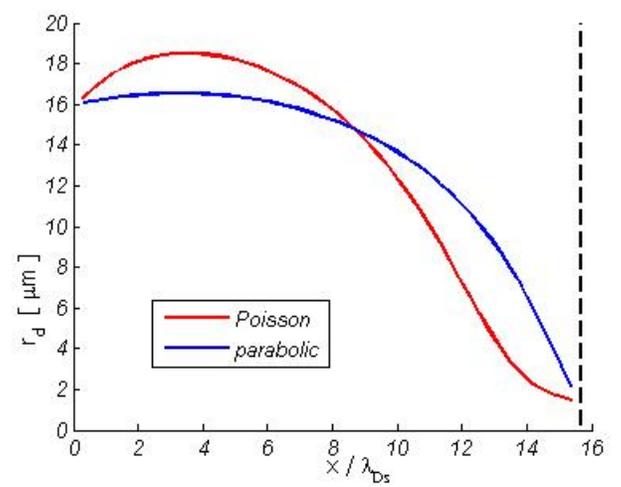


Fig. 5

As is shown in figure 4, the ion drag force  $F_i$  becomes insignificant in the inner part of the sheath. The collection and Coulomb components of the ion force are shown separately. For comparison the gravitational force is added.

Figure 5 shows the radii of levitating particles versus normalized distances from the lower electrode. The radius at each position is obtained by equating the local value of total force to zero. Both models of rf sheath give similar results. The particles with radius greater than about 19  $\mu\text{m}$  will fall down on the electrode.

The particles may serve as a fine diagnostic tool for the study of electric field in the sheath. Neglecting ion and neutral drag forces, the field strength  $E$  at the stable position  $x$  of trapped particle satisfies  $m_d g + Q_d(x) E(x) = 0$ . The unknown field strength in this formula is multiplied by the dust

charge, which is not satisfactorily theoretically predicted (Fig. 2). This obstacle is also met in more elaborated dynamical methods [20]. The equation of motion of a dust particle is

$$m_d \frac{d^2 x}{dt^2} = F_{\text{tot}} - 2m_d b \frac{dx}{dt} \quad (29)$$

where  $F_{\text{tot}} = F_g + F_E + F_i$  is the total static force and  $b$  is defined in (28). For small oscillations about the equilibrium point  $x_0$  we get

$$F_{\text{tot}}(x) \approx \frac{dF_{\text{tot}}(x_0)}{dx} (x - x_0) \quad (30)$$

The linearized equation describes damped oscillations with the oscillation frequency

$$\omega = \sqrt{-\frac{1}{m_d} F'_{\text{tot}}(x_0) - b^2} \quad (31)$$

Stable equilibrium satisfies  $F'_{\text{tot}} < 0$ . Neglecting ion drag and damping, the last equation is reduced to

$$\omega \approx \sqrt{-g \frac{(Q_d E)'}{Q_d E}} \approx \sqrt{-g \frac{E'}{E}} \quad (32)$$

The second equality was obtained under assumption that the charge remains constant during particle motion [21],  $Q_d(x) \approx \text{const}$ .

The measurement of frequencies for dust particles of various radii oscillating in various distances above the electrode gives the function  $\omega(x)$  experimentally. The last formula then represents a simple differential equation for field strength  $E(x)$ . Unfortunately, our computations show that the charge changes during particle oscillations cannot be neglected. It is clearly demonstrated in figure 6, in which frequencies computed from formulas (31) and (32) are compared. Neglecting charge changes during oscillations noticeable overestimates the resonance frequencies.

For applied models we have also tested their sensitivity to optional input parameters. As a measure of sensitivity of an output parameter  $A$  on an input parameter  $b$  we have taken the ratio of their relative changes,

$$s(A, b) = \frac{b}{A} \frac{\partial A}{\partial b} \quad (34)$$

Figure 7 depicts the sensitivity of the balancing dust radius on the self bias at the electrode for each position in the sheath. For the model described by equations (18-20) the sensitivities of the dust potential  $V_d$  on electron sticking probability  $P_e$ , electron residence time  $\tau_e$  and recombination coefficient  $\alpha_R$  are  $s(V_d, P_e) = 0.4$ ,  $s(V_d, \tau_e) = 0.3$  and  $s(V_d, \alpha_R) = 2 \times 10^{-4}$ , respectively. The model is therefore insensitive to the exact value of  $\alpha_R$ . The sensitivities of the sheath thickness  $L$  on the electron temperature  $T_e$  and dc self bias  $U_{\text{dc0}}$  are  $s(L, T_e) = -2 \times 10^{-2}$  and  $s(L, U_{\text{dc0}}) = 0.6$ , respectively.

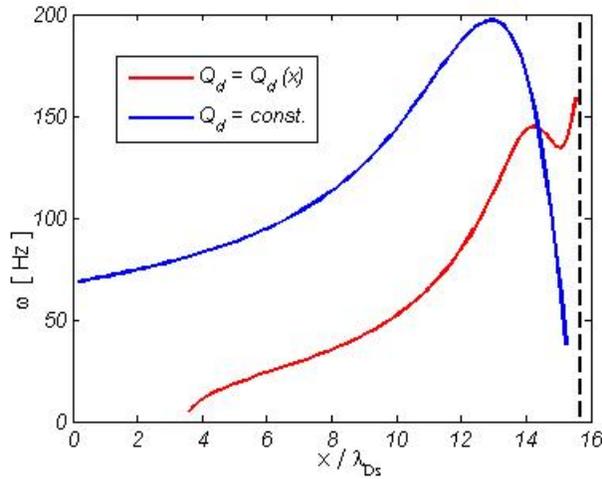


Fig. 6

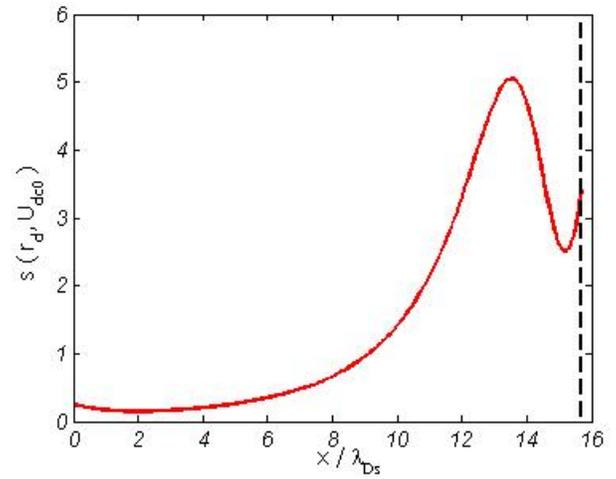


Fig. 7

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