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SHEATH STRUCTURE AROUND NEGATIVELY BIASED PROBE IN ELETRONEGATIVE PLASMA

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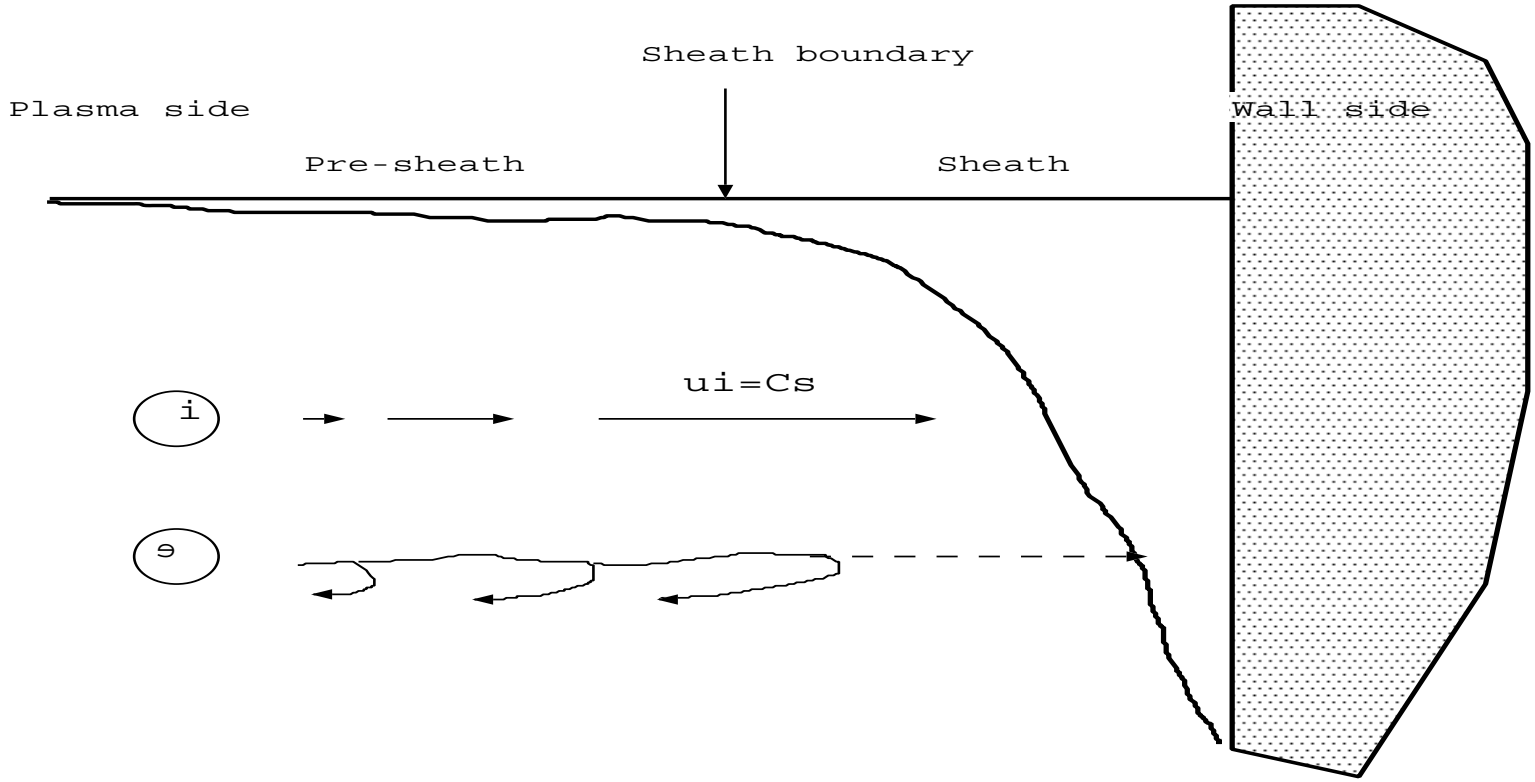
Background

- Langmuir probe method is widely used to determine plasma parameters. Its results is based upon the modeling of sheath potential structure.
  - new type probes (Combined force-Mach-Langmuir probe, Thermal probe) have been also proposed.
- Unconsistency often exists in the modeling of sheath.
  - Sometimes it has been ignored especially in fluid model.
- An instability was observed in PIC simulation of hydrogen negative sheath.
  - Is this real or only numerical phenomena?

Schematic view of fluid model



Ions are accelerated by potential.

- At sheath boundary, they reach at sound velocity.
- Free-fall model is usually assumed.(Zero Ti)

Electrons are reflected by potential

- A few high energy electrons reach at wall boundary.
- Boltzmann relation is usually assumed.

Paradox of fluid model

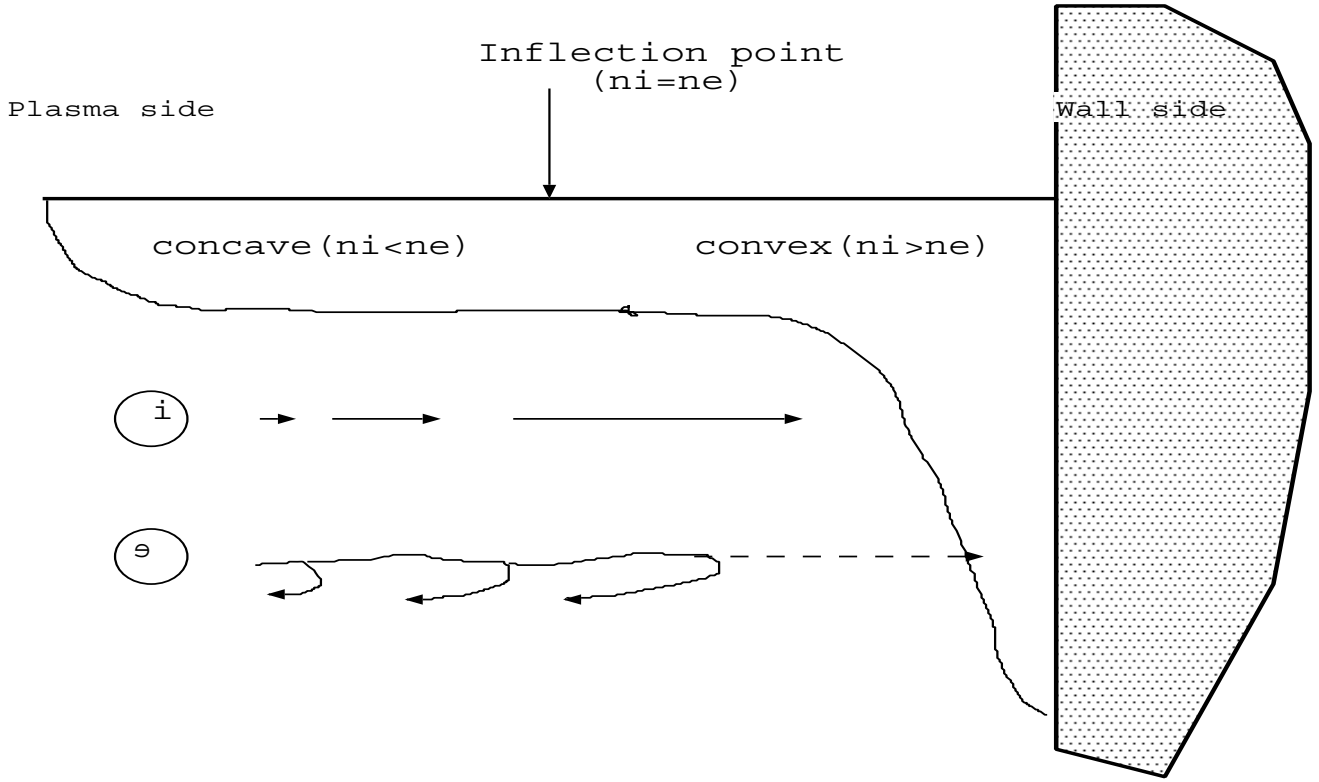
Artificial matching technique at sheath boundary must be introduced. (But it is uncompleted.)

- From the point of presheath modeling
  - length of sheath is infinitely small
  - spatial derivative of ion fluid velocity is infinite.
- From the point of sheath modeling
  - length of presheath is infinitely large
  - spatial derivative of ion fluid velocity is zero.

Moreover, some assumptions (on Ti) are not always available.

- Divertor plasma(Ti > Te)
- Negative ion plasma(T+ ~ T-)

Schematic view of kinetic/PIC model



- 1D in space, stationary.
- no collision, particle source(sink)
- potential is zero at plasma boundary and negatively biased externally at wall boundary.(not difficult to calculate floating case.)
  - ----- R.D.Smirnov; Dr.Thesis,

Solution of Boltzmann equation

1D steady collisionless Boltzmann equation

$$v_x \frac{\partial f_j(x, v_x)}{\partial x} + \frac{-q_j}{m_j} \frac{d\Phi}{dx} \frac{\partial f_j(x, v_x)}{\partial v_x} = 0,$$

can be transferred so that $\epsilon_{jx} = \frac{1}{2} m_j v_x^2 + q_j \Phi$ is used as independent valuable instead of v_x.

$$v_x(x, \epsilon_{jx}) \frac{\partial f_j(x, \epsilon_{jx})}{\partial x} = 0,$$

So energy distribution functions of particle j is the same as those at plasma source boundary.

Boundary condition

Plasma particles(electrons, positive ions, negative ions) are supplied from boundary. In order to simulate the sheath,

- choose particle current intensity(or density) at source boundary so that Debye length is much smaller than geometry size.
- choose current(or density) ratio of positive and negative particles so that potential profile has at least one inflection point(that is perfect neutral point n+ = n-) in the geometry
- Initial velocity distribution is Maxwellian.
- At wall boundaries, ions and electrons are perfectly absorbed.(No reflection/No secondary electrons)

Velocity distribution function

Ion

$$f(v_x) = \begin{cases} n_{is}\sqrt{\frac{m_i}{2\pi T_i}}\exp\left(\frac{-1}{T_i}\left(\frac{1}{2}m_i v_x^2 + e\Phi(x)\right)\right) & \left(v_x < -\sqrt{\frac{2e(\Phi_s - \Phi(x))}{m_i}}\right) \\ 0 & \left(v_x > -\sqrt{\frac{2e(\Phi_s - \Phi(x))}{m_i}}\right) \end{cases}$$

Electron

$$f(v_x) = \begin{cases} 0 & \left(v_x < -\sqrt{\frac{2e(\Phi(x) - \Phi_w)}{m_e}}\right) \\ n_{es}\sqrt{\frac{m_e}{2\pi T_e}}\exp\left(\frac{-1}{T_e}\left(\frac{1}{2}m_e v_x^2 - e\Phi(x)\right)\right) & \left(v_x > -\sqrt{\frac{2e(\Phi(x) - \Phi_w)}{m_e}}\right) \end{cases}$$

Number density

Ion

$$n_i = n_{is} \exp\left(\frac{e}{T_i}\left(\Phi_s - \Phi\right)\right)\mathrm{erfc}\left(\sqrt{\frac{e}{T_i}\left(\Phi_s - \Phi\right)}\right)$$

Electron

$$n_e = n_{es} \exp\left(\frac{-e}{T_e}\left(\Phi_s - \Phi\right)\right)\left\{1 + \mathrm{erf}\left(\sqrt{\frac{e}{T_e}\left(\Phi - \Phi_w\right)}\right)\right\}$$

Inflection point of potential

From normalized Poisson equation

$$-\frac{d^2\phi}{ds^2} = \rho(s) = (n_i - n_e - n_{ni})/n_0,$$

potential profile is convex in the sheath($\rho(s) > 0$).

Though, $\rho(s)$ may be equal to be 0 in presheath of real plasma, we set $\rho(s)$ to be slightly positive (potential is concave) at plasma source boundary so as that inflection point of potential (and flat region around it) exists middle of the simulation geometry.

For example, if $\Phi_w/T_e = 10$ and $R_i = 1.0$, XOOPIC gives us that $-\phi = -\Phi/T_e \sim 1.7$ at the inflection point(In real presheath, $-\phi = 0.5$.), which can confirm by solving collisionless model for $\phi = e\Phi/T_e$

If $n_{is} = n_{es}$, $\phi \sim -1.7$.

Semi-implicit Runge-Kutta method

Kaps-Rentrop-Shapine formula

- T.Watabe et al., "Numerical software by fortran 77",(Maruzen, Tokyo, 1990)[in Japanese].

source code(main)

```
c
      parameter( neq = 2 )
      external rfunc, derf, dfunc
      external fdeni, fdene
      REAL*8 ABSERR,ESTERR,RELERR
      DIMENSION Y(NEQ),YN(NEQ),ESTERR(NEQ)
      DIMENSION WORK1(NEQ),WORK2(NEQ),WORK3(NEQ),WORK4(NEQ,12)
      DIMENSION WORK(NEQ,NEQ),IWORK(NEQ)
c
      common /compar/phiw, denie
c                                                              rkfds option
      ABSERR = 1.0D-6
      RELERR = 0.0D+0
c                                                     phi_w, (ni/ne)_source
      phiw=10.0d0
      denie=1.0d0
c                                                     initial value
      xst = 0.0d0
      y(1) = 0.0d0
      y(2) = 0.7d0
c
      xin = 0.0d0
      do 40 iout = 1,1000
        xout=xin+0.02d0
C
         CALL KRSNAT(NEQ,RFUNC,DFUNC,XIN,XOUT,Y,INIT,RELERR,ABSERR,
     &                YN,ESTERR,IERR,WORK0,WORK1,WORK2,WORK3,WORK4,
     &                WORK,IWORK)
c
        IF ((IERR .EQ. 10000) .OR. (IERR .EQ. 20000) .OR.
     &      (IERR .EQ. 30000) .OR. (IERR .EQ. 40000)) THEN
          WRITE(*,90) IERR
          stop
        end if
c
        if (yn(1).lt.(0.0d0)) then
          write(6,*) '## stop at iout = ',iout
          stop
        end if
        if (yn(1).gt.(phiw*0.98d0)) then
          write(6,*) '## stop at iout = ',iout
          stop
        end if
c
        Y(1)=YN(1)
        Y(2)=YN(2)
        XIN=XOUT
c
  40  continue
  90  format(1x ,'# Error in RKFDS/KRSNAT  IERR=',i7)
c
      stop
c-----------------------------------------------------------------------
      subroutine rfunc (x, y, ydot)
c       sheath potential eqs.
c-----------------------------------------------------------------------
      implicit double precision(a-h,o-z)
      parameter( neq = 2 )
      dimension y(neq), ydot(neq)
      external fdeni, fdene
      common /compar/phiw, denie
c
      phi=y(1)
      ex=y(2)
c
      ydot(1) = ex
c
      call fdeni(phi,deni)
      call fdene(phi,dene)
c
      ydot(2) = denie*deni - dene
c
      return
      end
c
c-----------------------------------------------------------------------
      subroutine dfunc (x, y, dfx,dfy)
c       Jacobian for sheath potential eqs.
c-----------------------------------------------------------------------
      implicit double precision(a-h,o-z)
      parameter( neq = 2 )
      dimension y(neq), dfx(neq), dfy(neq,neq)
      external dfdeni, dfdene
      common /compar/phiw, denie
c
      phi=y(1)
      ex=y(2)
c
(snip)
c
      dfx(1) = 0.0d0
      dfx(2) = 0.0d0
c
      call dfdeni(phi,ddeni)
      call dfdene(phi,ddene)
c
      dfy(1,1) = 0.0d0
      dfy(1,2) = 1.0d0
      dfy(2,1) = denie*ddeni - ddene
      dfy(2,2) = 1.0d0
c
      return
      end
c
```

Input parameters of source boundary

$$\mathrm{phiw}{=}10.0\mathrm{d}0 \Leftarrow \frac{-e\Phi_w}{T_e}$$

$$\mathrm{denie}{=}1.0\mathrm{d}0 \Leftarrow \left(\frac{n_i}{n_e}\right)_s$$

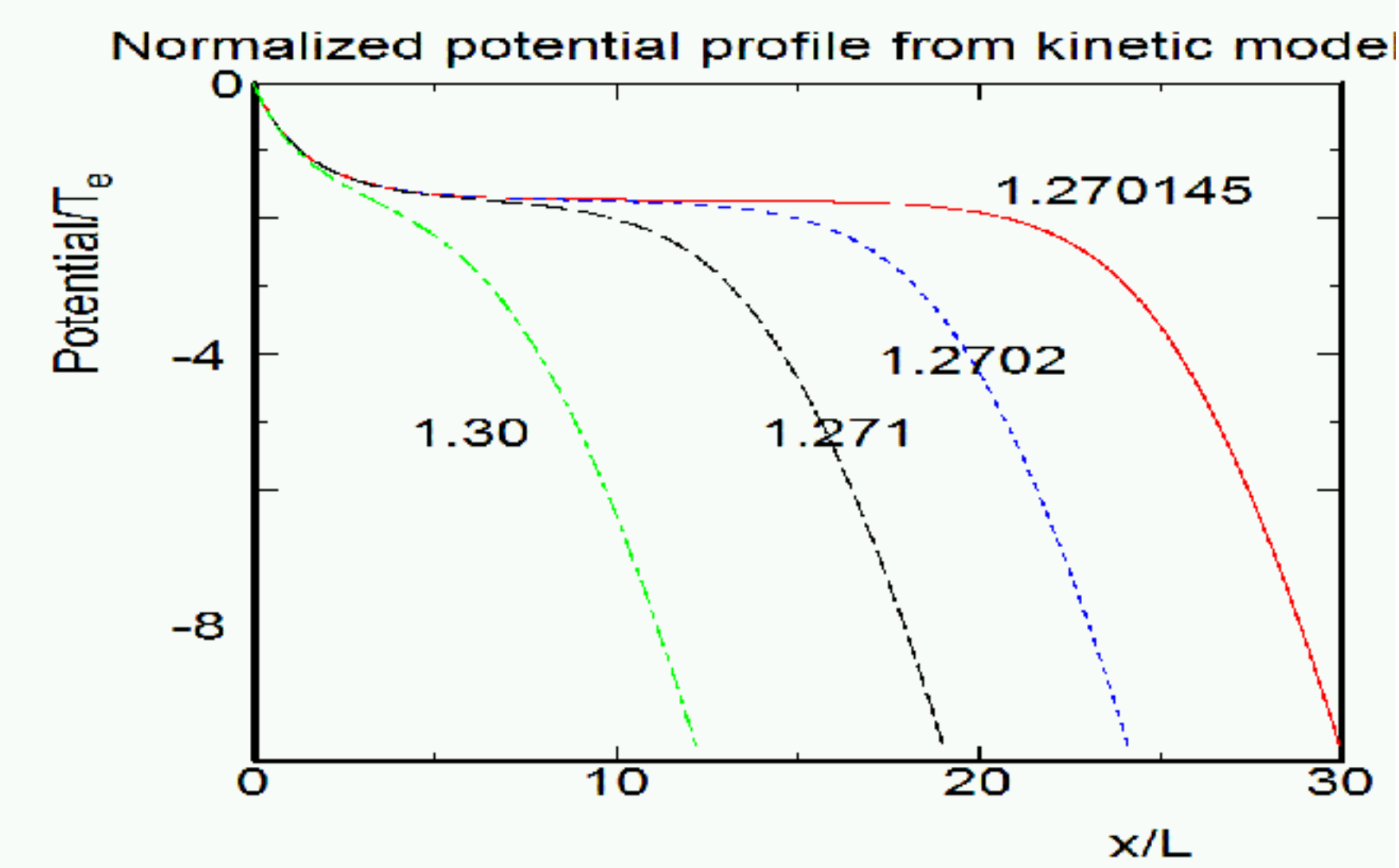
$$\mathrm{xst} = 0.0\mathrm{d}0 \Leftarrow \left(x/\lambda_D\right)_s$$

$$\mathrm{y}(1) = 0.0\mathrm{d}0 \Leftarrow \frac{-e\Phi_s}{T_e}$$

$$\mathrm{y}(2) = 0.7\mathrm{d}0 \Leftarrow \left(-\frac{e\lambda_D}{T_e}\frac{d\Phi}{dx}\right)_s$$

The effect of y(2) is mainly studied.

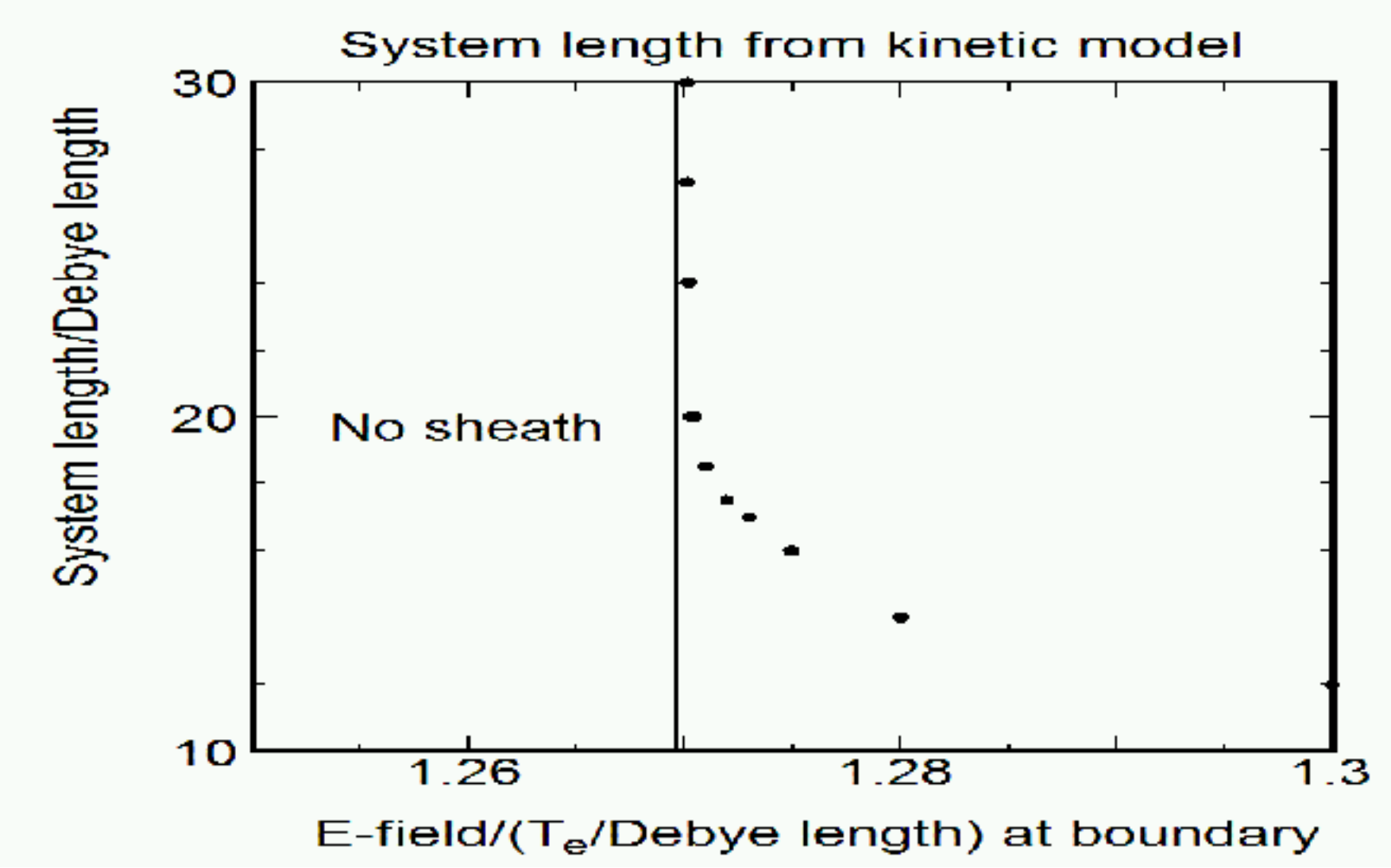
Sheath potential from kinetic model



Distance is normalized with Debye length.

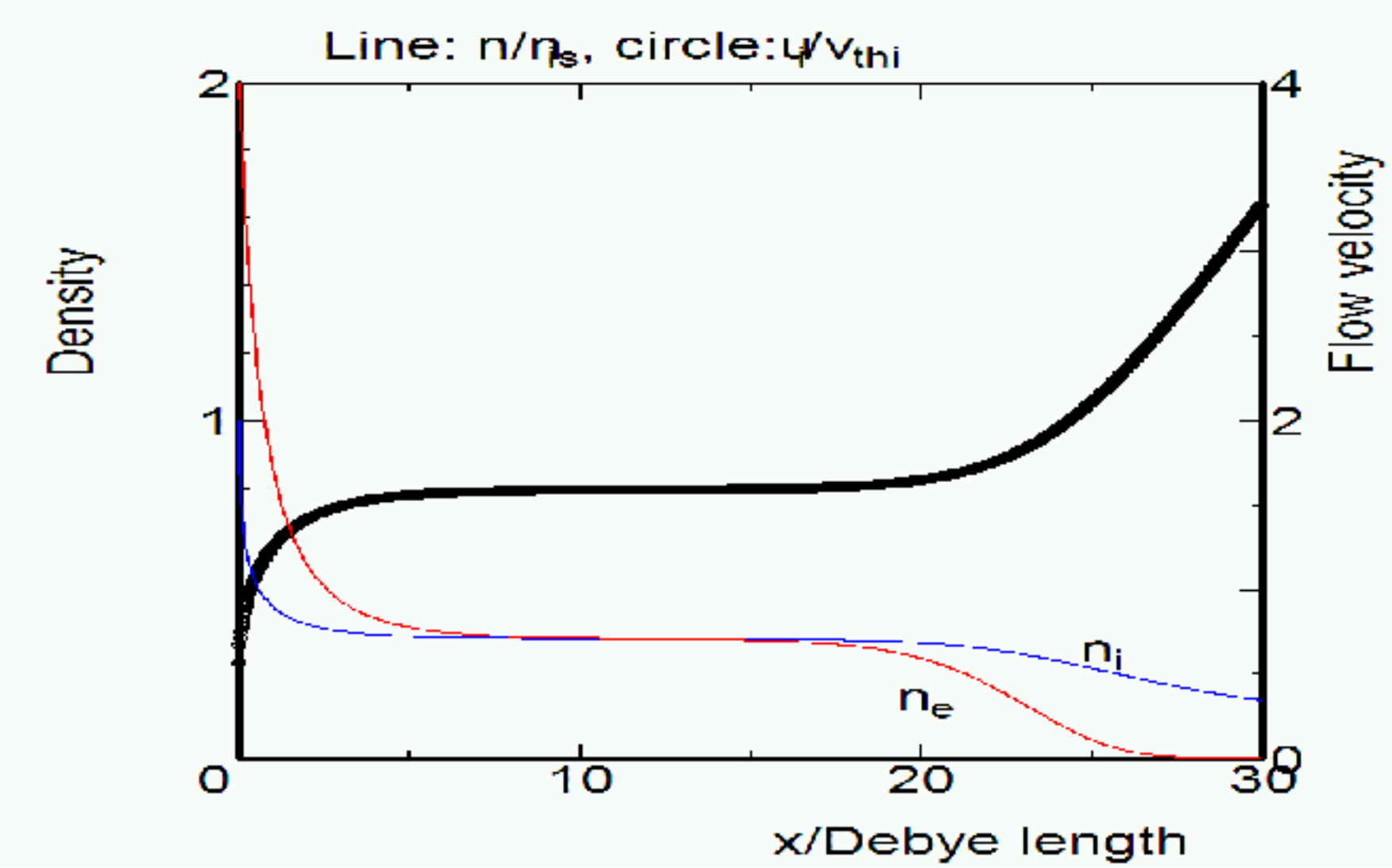
The legends are the normalized electric field(y(2))at source boundary.

Condition for sheath establishment



Absolute value of electric field at source boundary must exceed the critical value. The long flat potential is obtain for lower electric field.

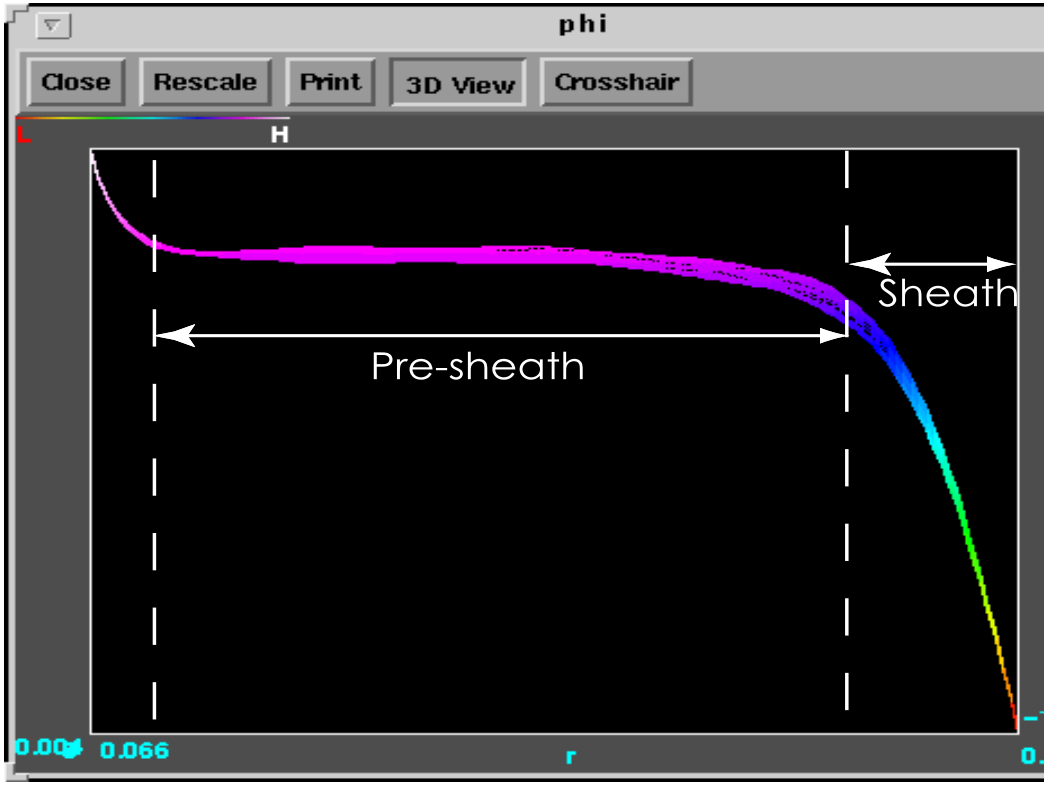
density and flow velocity



So called bohm condition is not so clear in the kinetic model, since definition of Mach number is not clear for finite Ti.

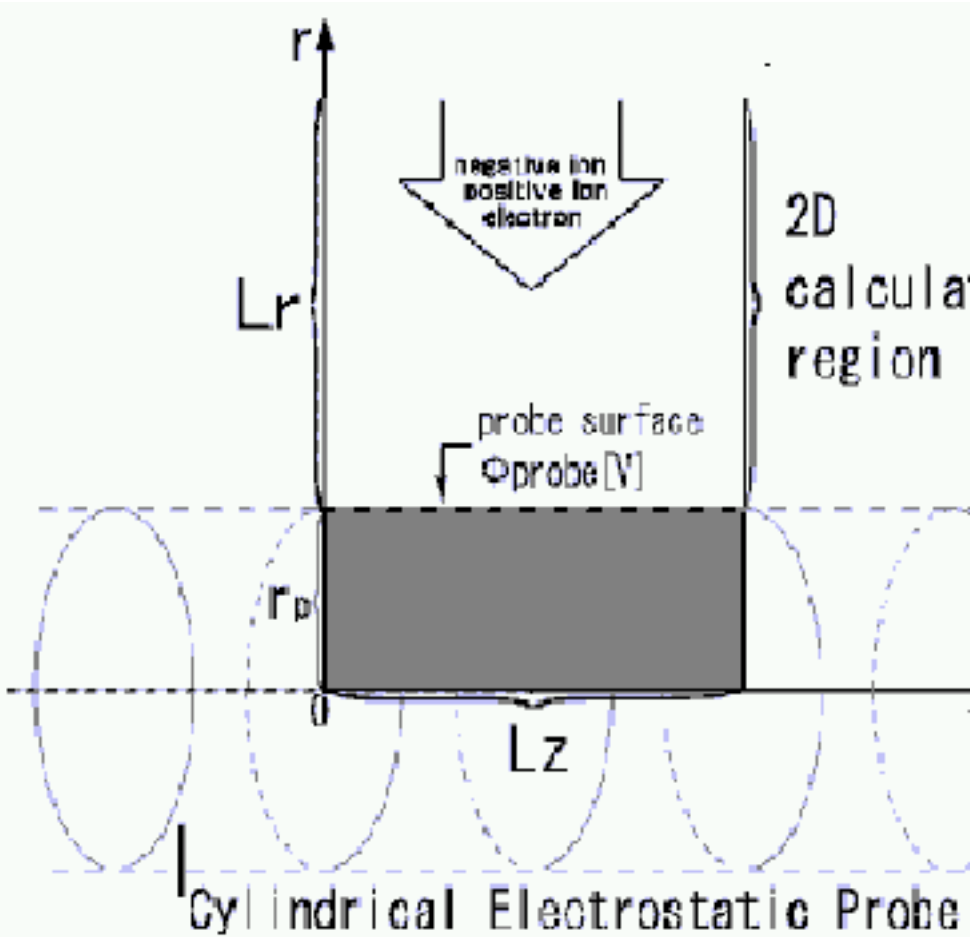
Berkeley code(XOOPIC)

- 2-Dimensional PIC code developed and distributed by PTSG group(Prof. C. K. Birdsall)
  - J.P.Verboncoeur et al.;Comp.Phys.Comm.,87(1995)199-211.
  - http://ptsg.eecs.Berkeley.edu/

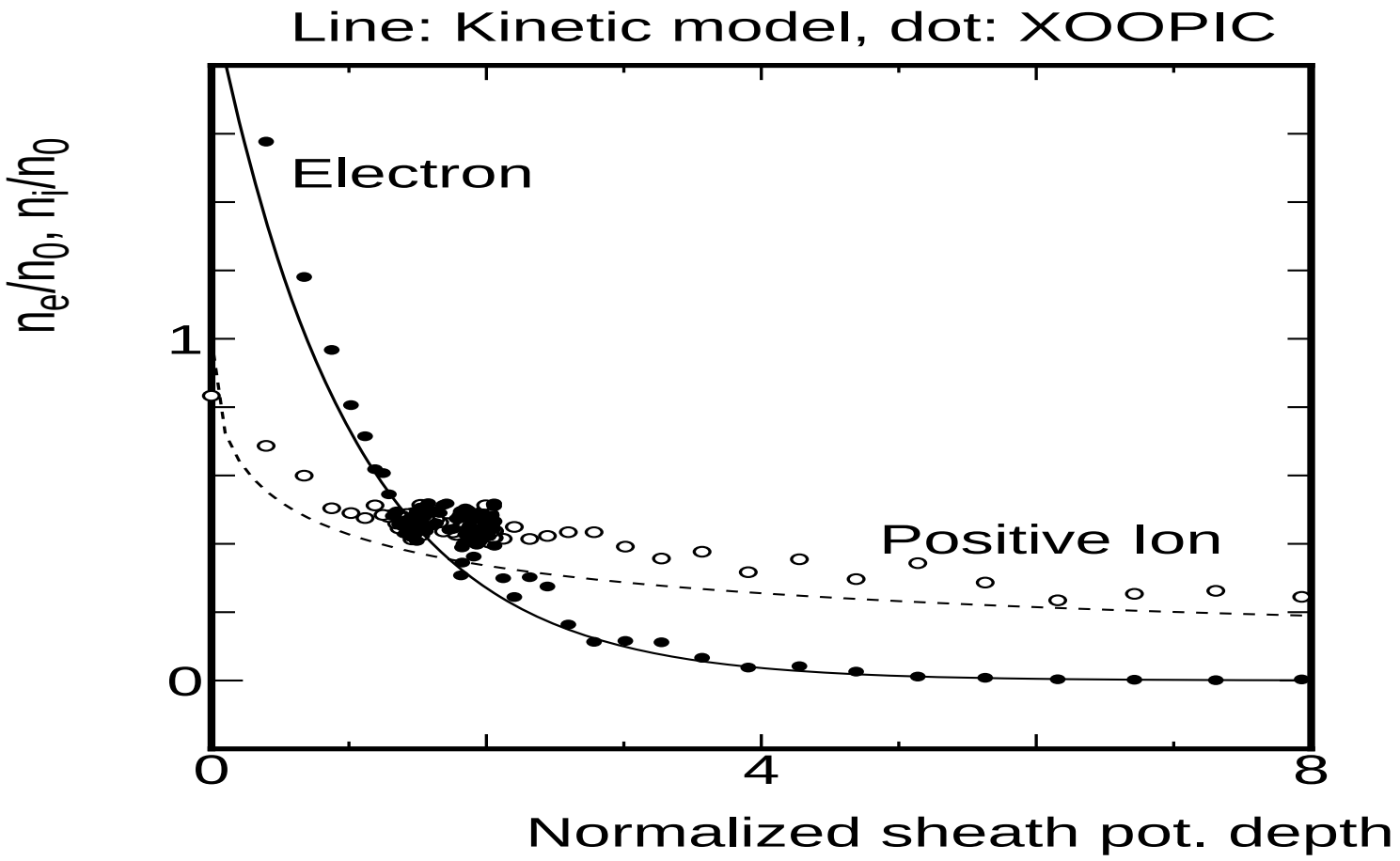


Simulation condition

geometry size : L_r	$6.0 \times 10^{-3}[m]$
: L_z	$4.0 \times 10^{-3}[m]$
Probe radius : r_p	$6.0 \times 10^{-2}[m]$
mesh size r	120
z	40
time stepΔt	$2.0 \times 10^{-11}[s]$
particle weight : g	2.0×10^{5}
Source current : I	$10[A]$
Ion	H^+ and H^-
Neutral	Ar
Boundary condition	
: left & right	Perfect absorbing dielectric
: top	Plasma source(and Exit) with $\Phi = 0$[V]
: bottom	Probe surface with $\Phi = -100$[V]

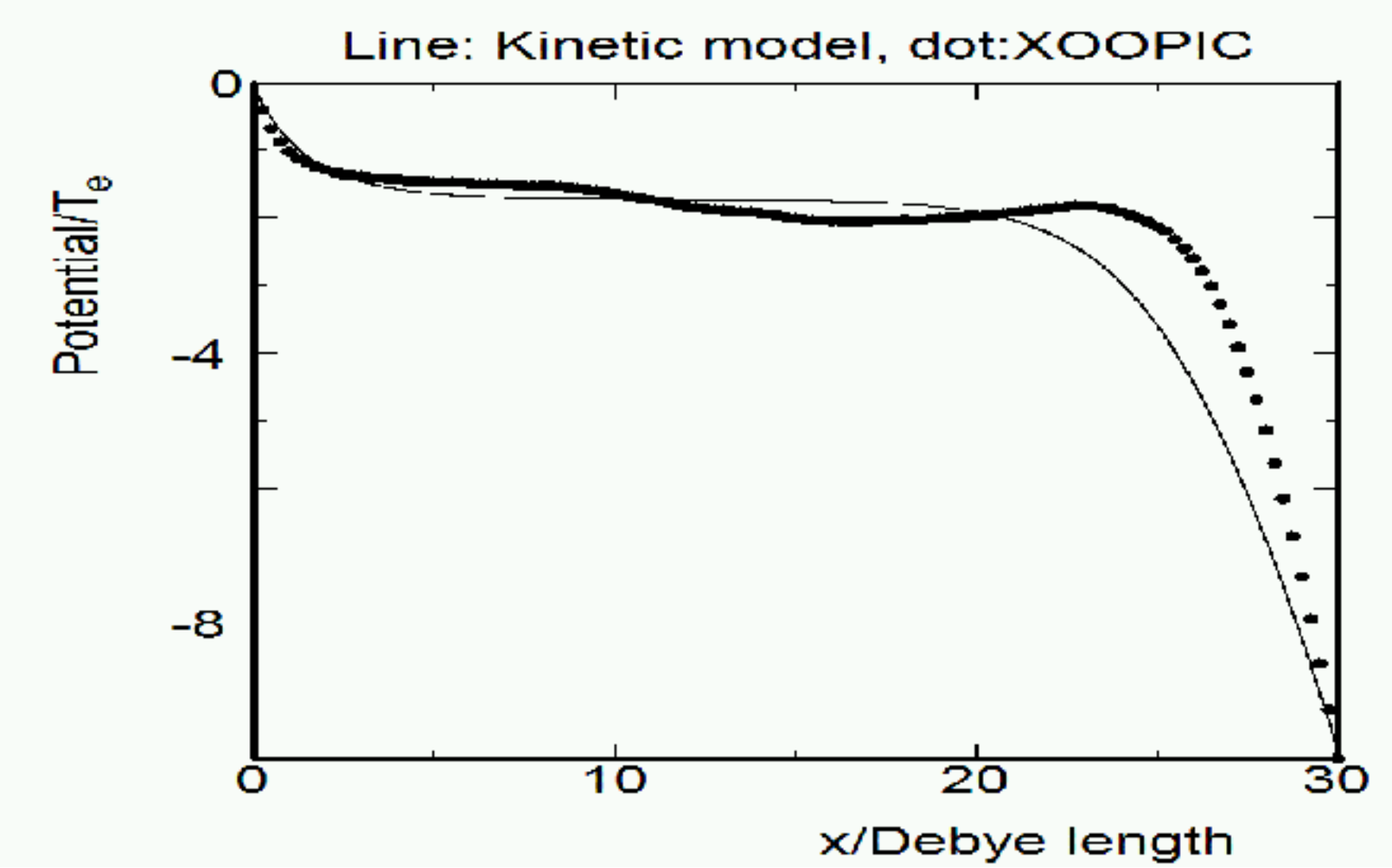


Comparison of kinetic model and PIC



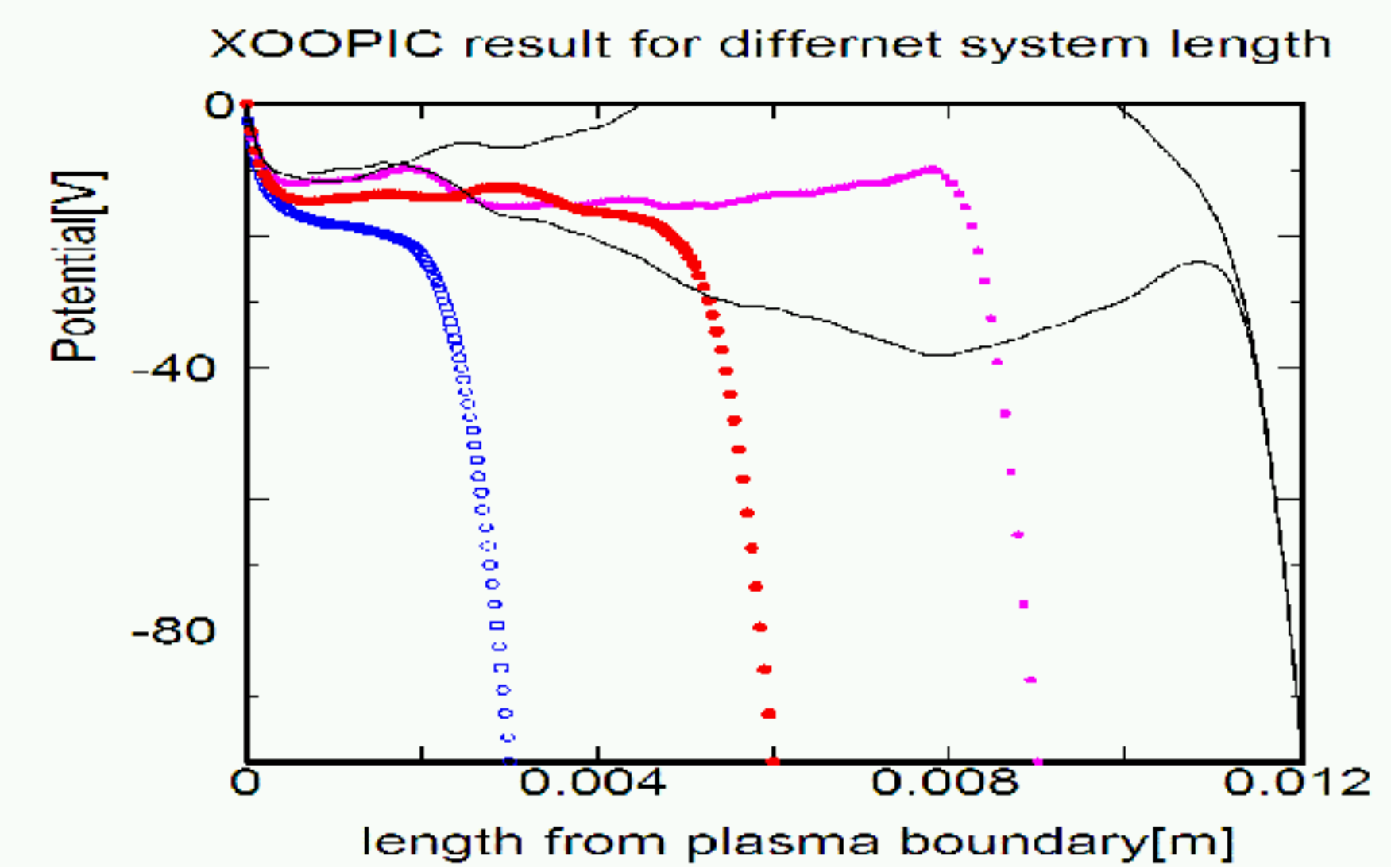
Density dependence on potential is well interpreted with the kinetic model.

Comparison of kinetic model and PIC



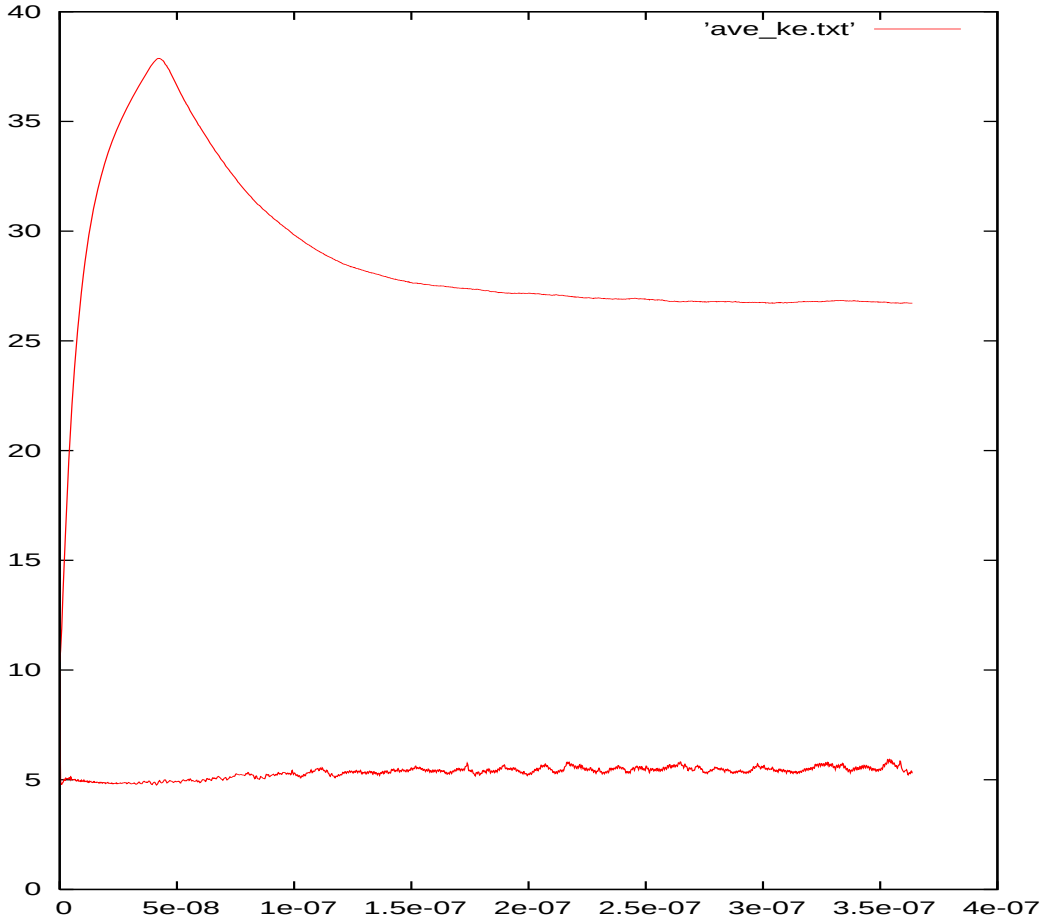
There is an infraction point around x= 10--15.
PIC model shows somehow high potential at X > 20.

Sheath potential from XOOPIC

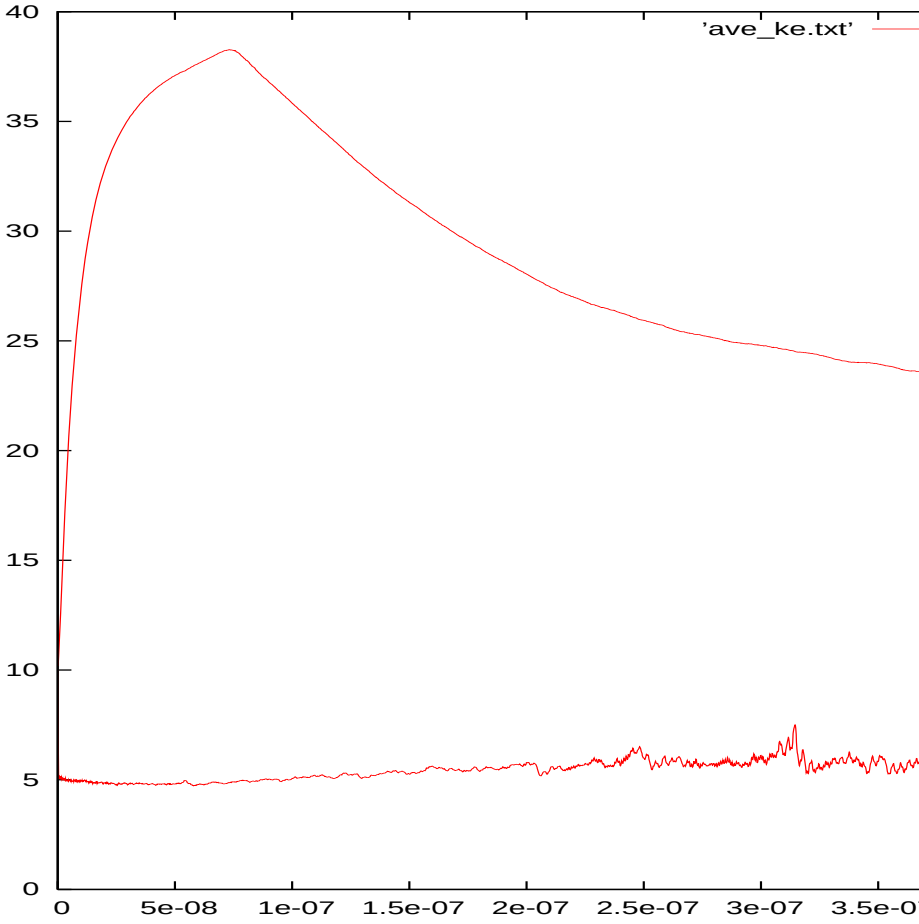


If system size becomes too large, the simulation becomes unstable due to plasma oscillation.

Average energy from XOOPIC



L=0.006[m]



L=0.012[m]

In case of right figure, though potential profile oscillates with large amplitude, no effect on ion energy is observed.

Hydrogen negative sheath

Hydrogen negative ion(H-) is important in recent NBI source plasma and detached divertor plasma with Molecular Activated Recombination(MAR).

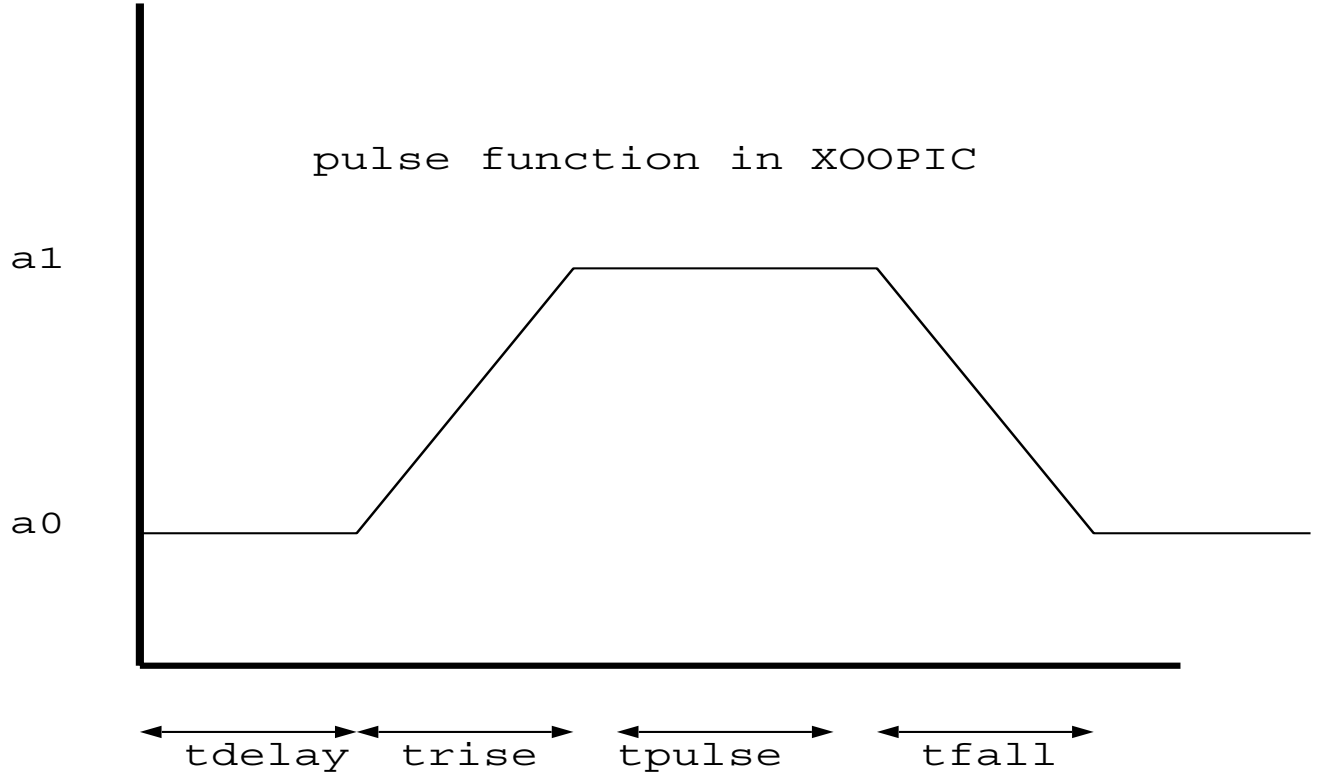
In conventional sheath model, many assumptions, which may break in some kind of plasma, are used without checking.

So the analytical results such as famous formula $\frac{eV_f}{kT_e} = 0.5 \ln\left(\left(2\pi \frac{m_e}{m_i}\right)\left(1 + \frac{T_i}{T_e}\right)\right)$ can not be applied to electronegative plasma only by setting $m_e \rightarrow m_i$.

In XOOPIC simulation, by changing electrons with hydrogen negative ions, the simulation becomes unstable and numbers of hydrogen positive/ negative ion in the calculation geometry oscillates with time much slower than plasma oscillation period.

Pulse function of XOOPIC

Source current intensity in XOOPIC can be controlled with six parameters (a0, a1, tdelay, trise, tpulse, tfall).

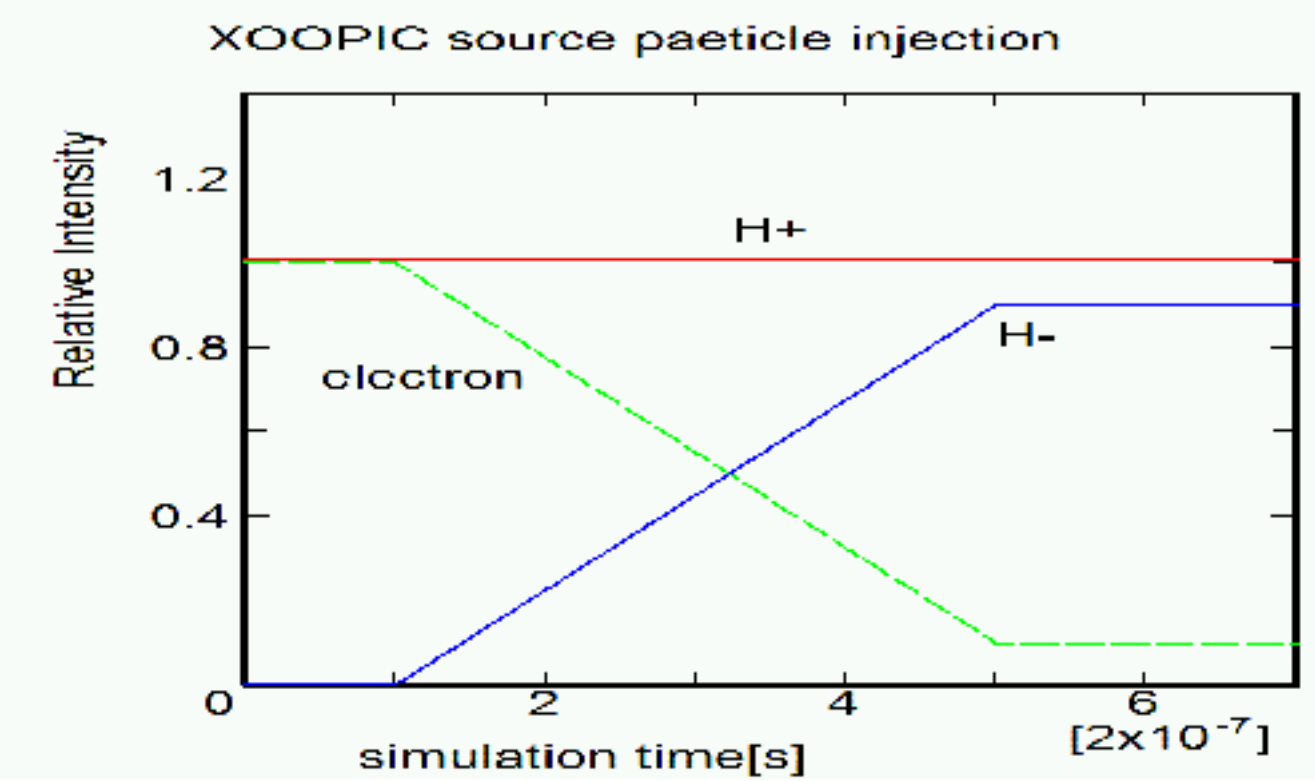


	electron	H
a0	0	0
a1	1	1
tdelay	0	1e
trise	0	1e
tpulse	1e-7	1e
tfall	1e-7	1e

Time dependent boundary

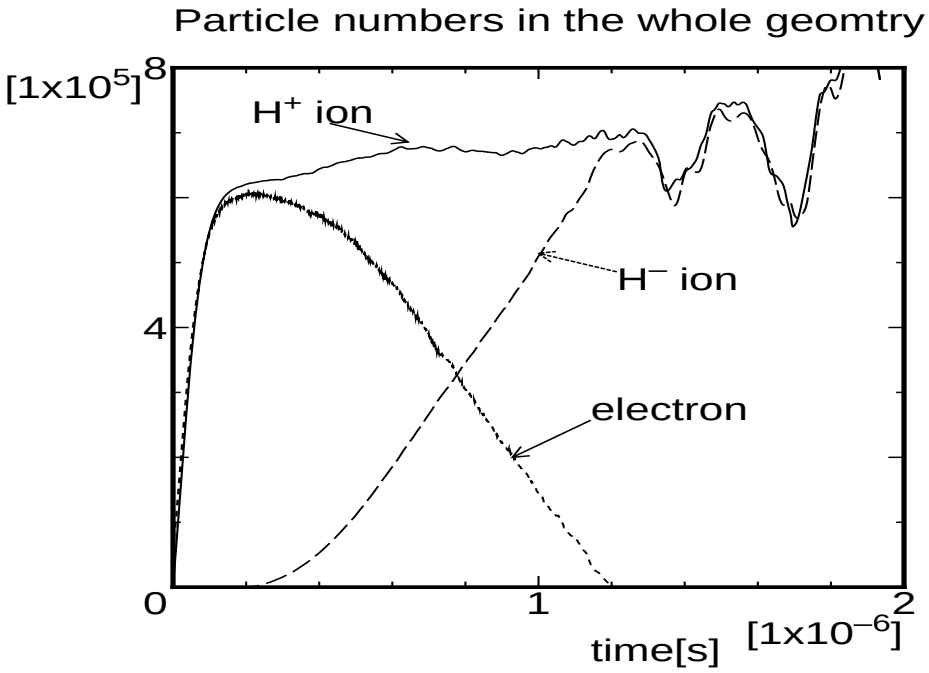
$$I_e = I \times (1 - R_{ni}) f_e(t), I_i = I \times \sqrt{\frac{T_i m_e}{T_e m_i}} \times R_i f_i(t), I_{ni} = I \times \sqrt{\frac{T_{ni} m_e}{T_e m_{ni}}} \times R_{ni} f_{ni}(t),$$

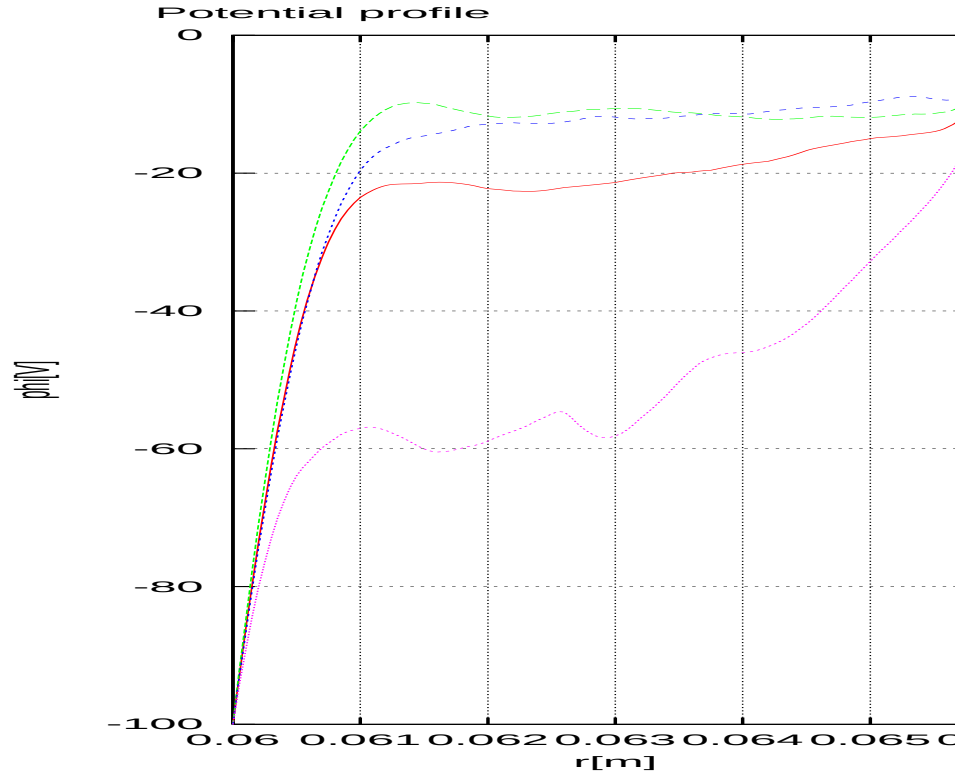
electron(green), H^+(red), H^-(blue),



After t=0.2e-6[s], electron injection decreases gradually and negative ion starts to be injected to keep charge neutrality.

Potential profile (n-/n+ => 1.00)





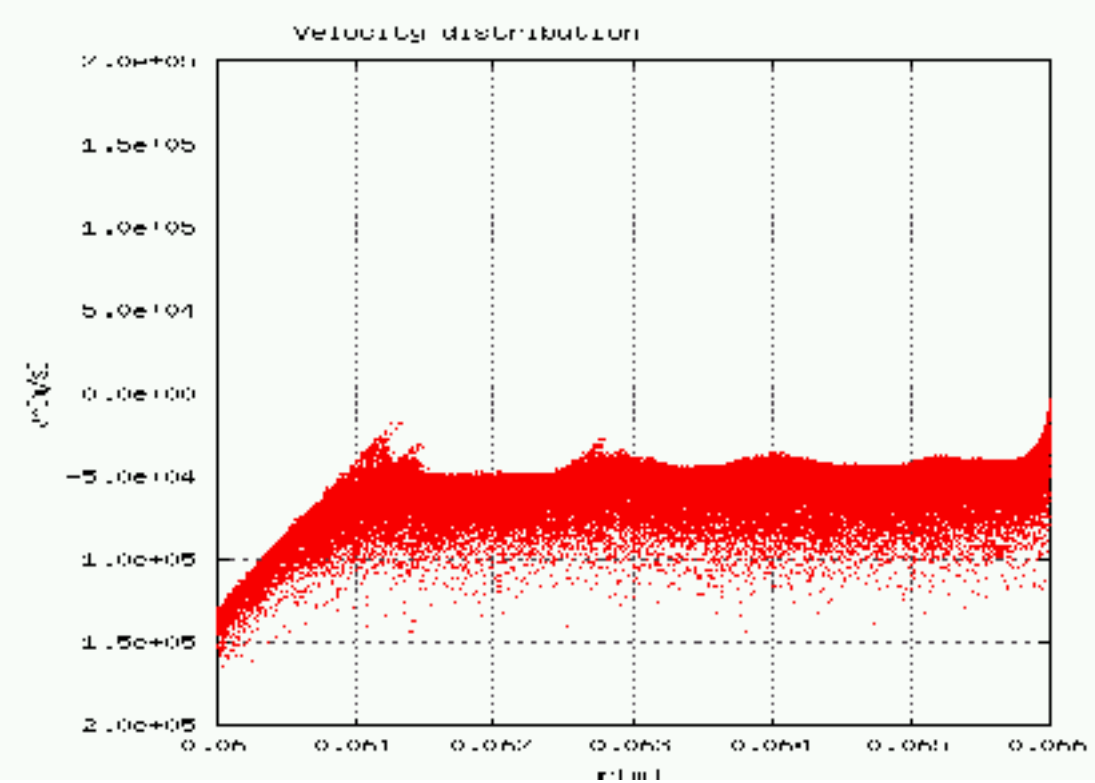
Red: t=0.31e-6[s], Blue: 1.2e-6[s

Orange: 1.9e-6[s

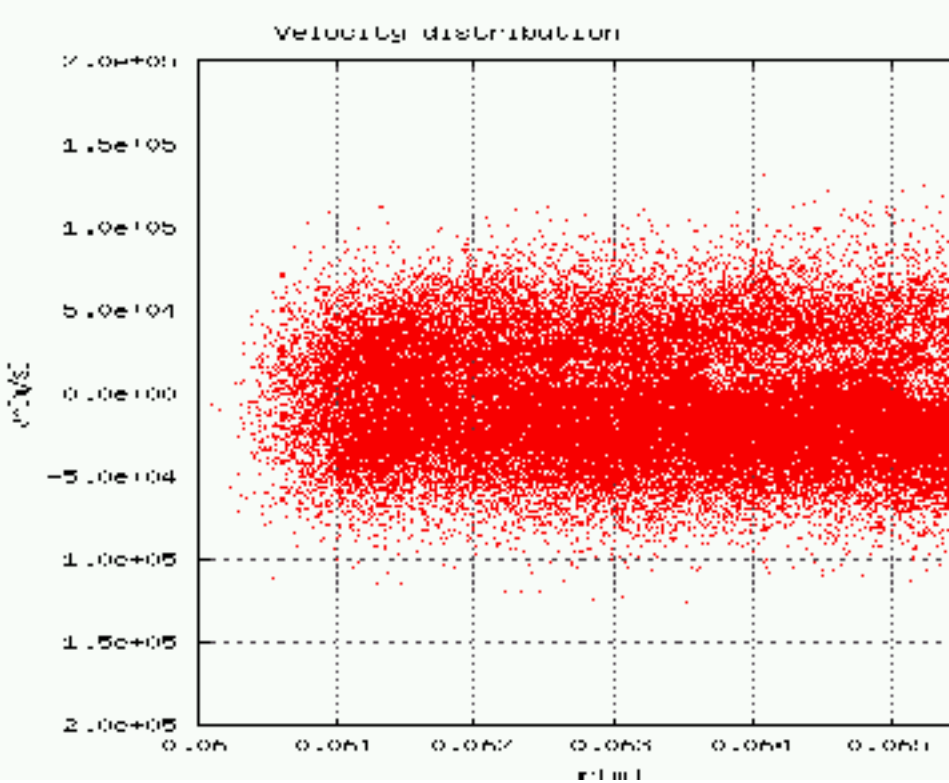
After t=0.2e-6[s], electron injection decreases gradually and negative ion starts to be injected to keep charge neutrality.

Occurrence of instability is observed after most electrons are lost.

Velocity distribution(n-/n+=0.80)



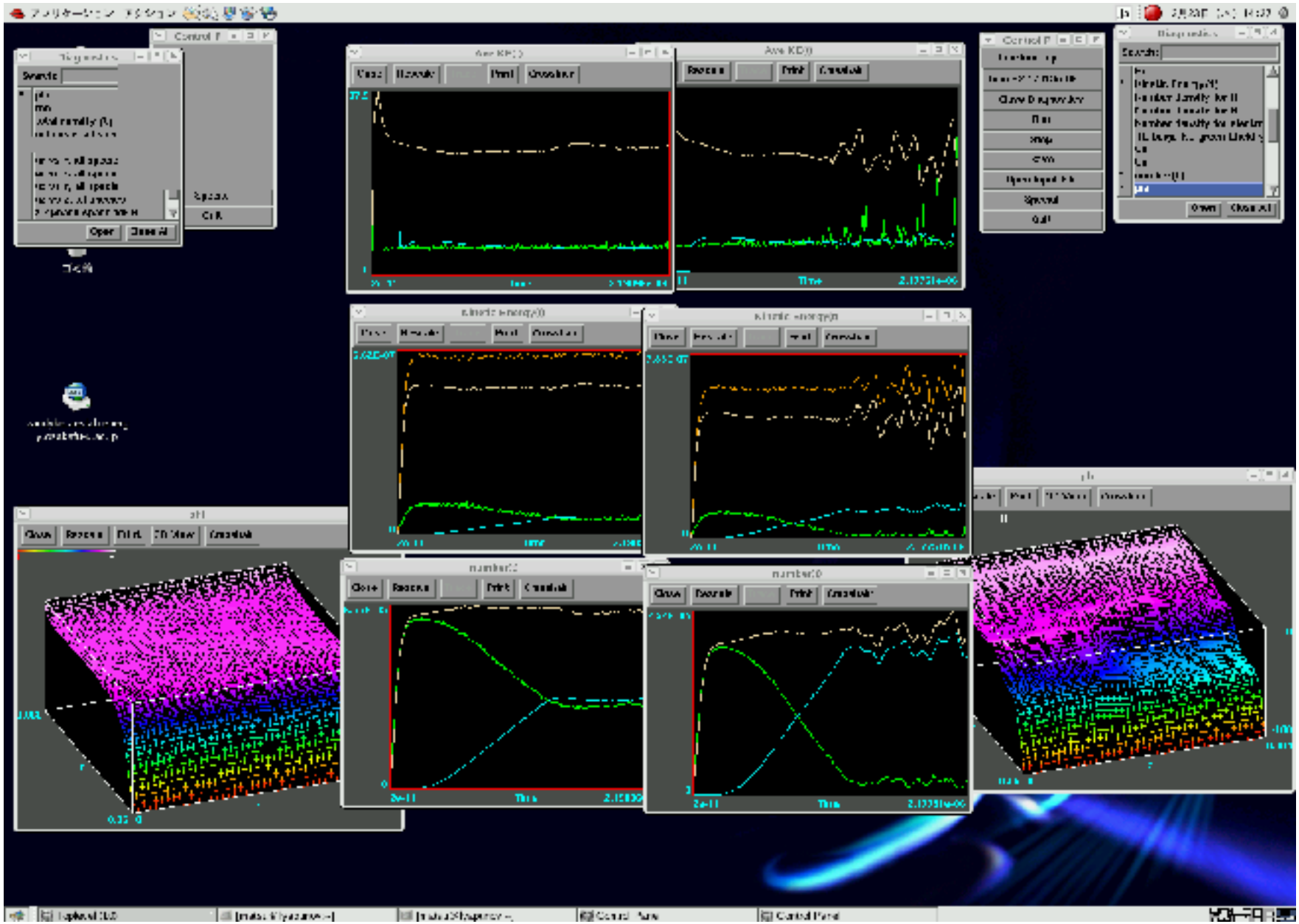
Positive ion



Negative ion

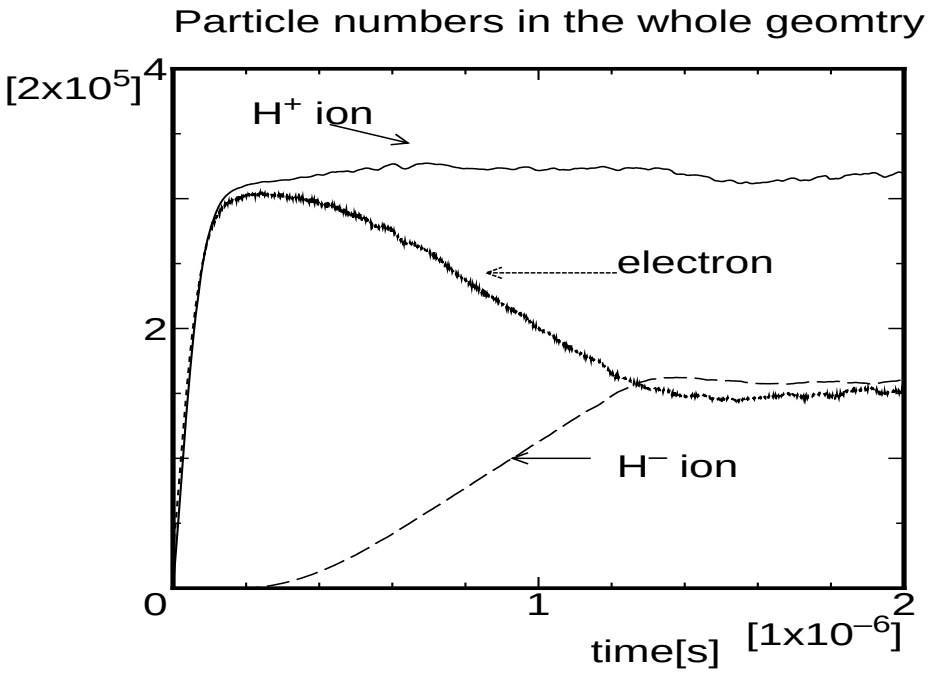
80 percent electrons are exchanged with Hydrogen negative ions. Sheath structure is still stable. (t=1.2e-6[s])

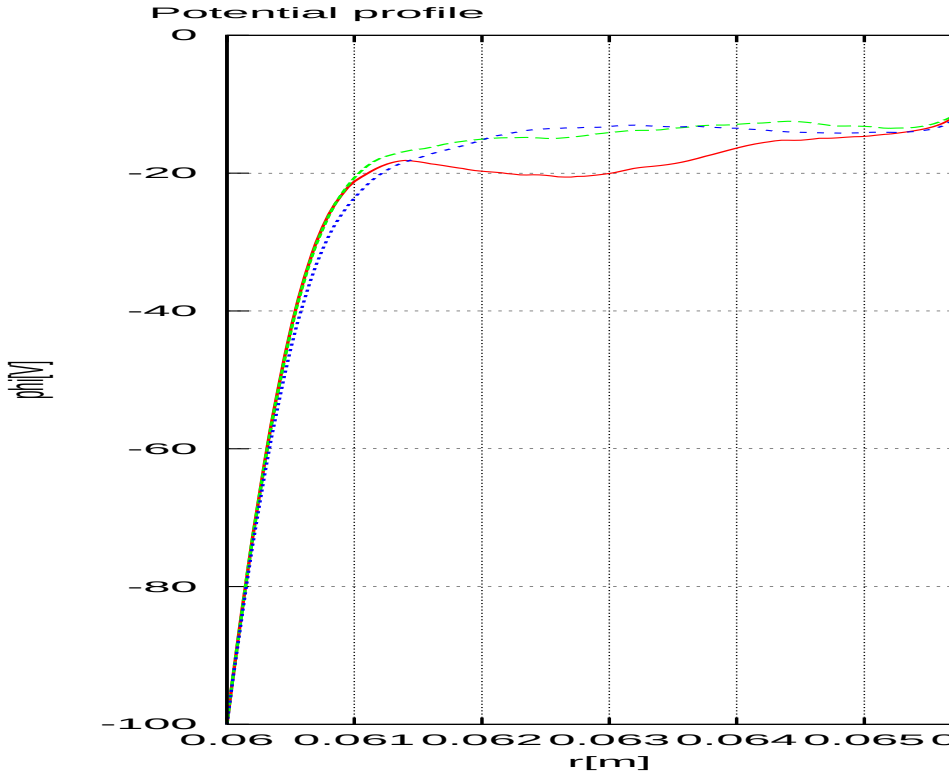
Snap (n-/n+ => 0.50 and 0.90)



n-/n+=0.50 0.90

Potential profile (n-/n+ => 0.50)



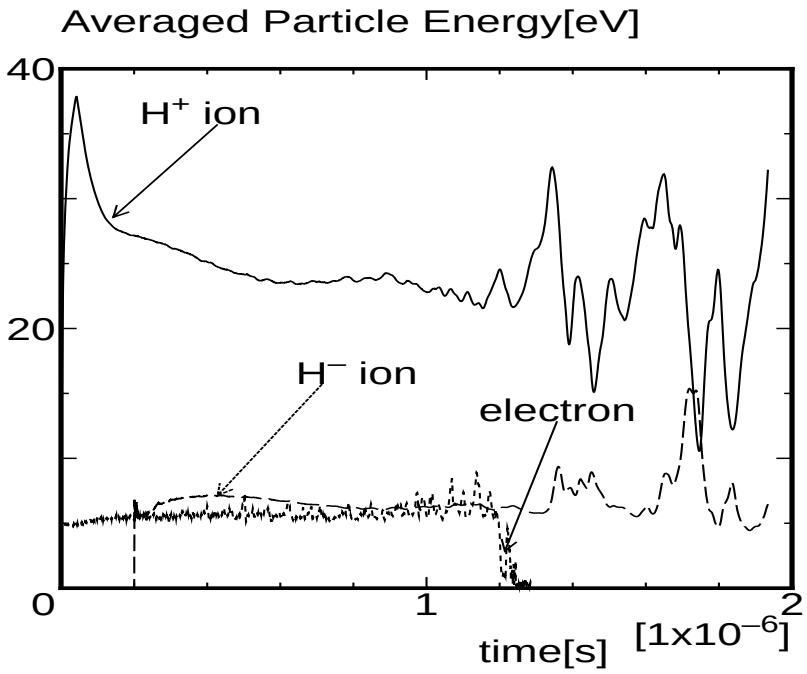


Red: t=0.23e-6[s], Blue: 1.2e-6[s

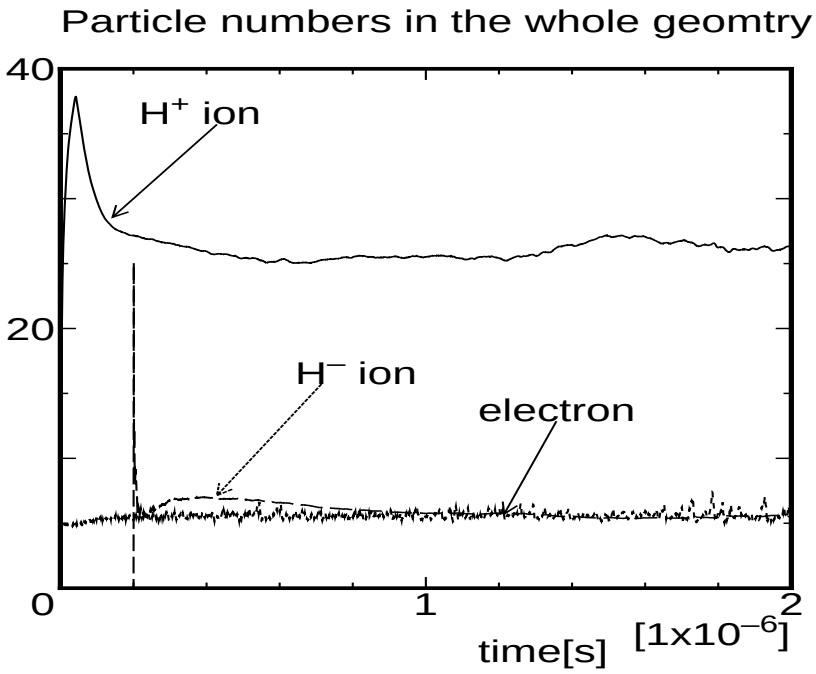
Green: 2.2e-6[s

In the case where 50 percent electrons are retained, no instability was observed.

Average kinetic energy(n-/n+=1.00, 0.50)



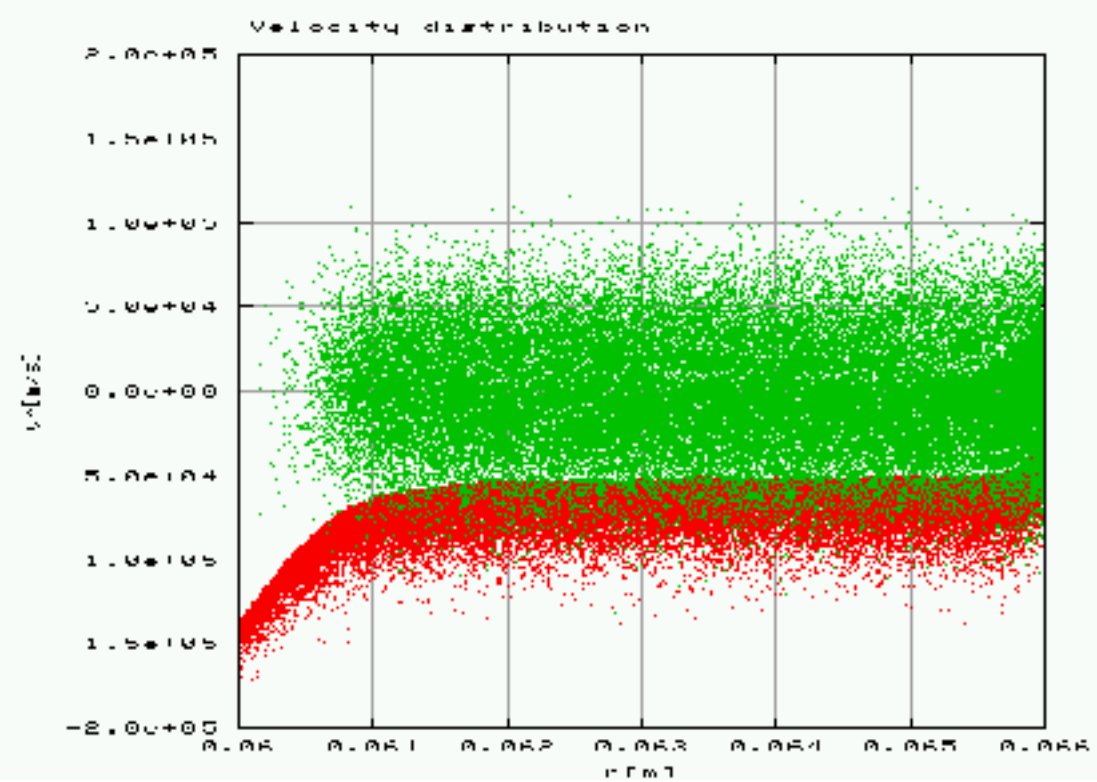
n-/n+=1.00

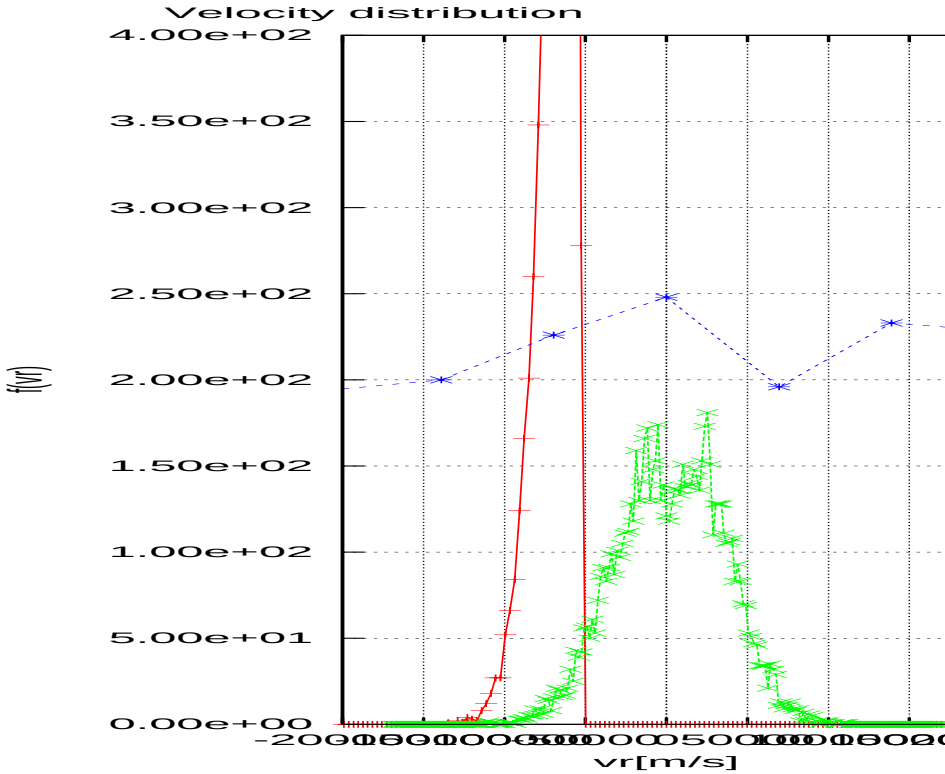


n-/n+=0.50

As long as there exit electrons, average kinetic energy of ions is kept constant. Collision with electrons (and also neutral gas) must have some dumping effect on instability growth.

Velocity distribution(n-/n+=0.50)

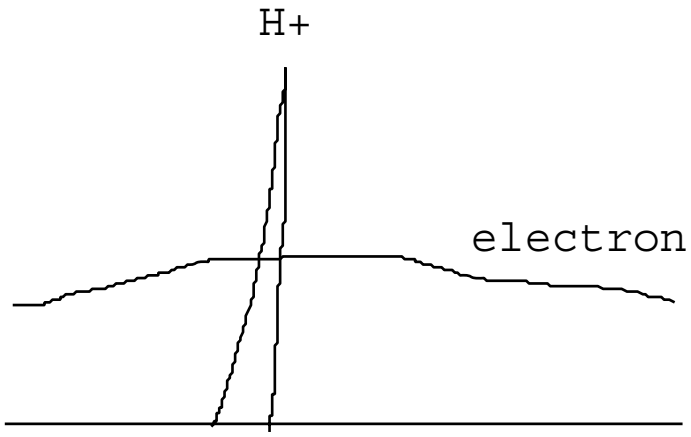




Red: H+, Green:

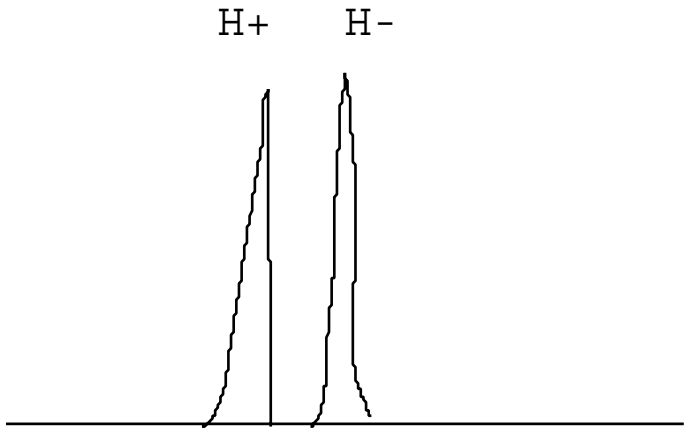
Positive and negative ion shows two peak distribution, but electron covers these peaks.

Two stream instability



H+ peak is inside of
electron distribution.

Stable



H+ peak is separated
from H- peak.

Unstable

If we can approximate velocity distribution as zero temperature beam, instability onset condition for pure negative ion plasma is

$$\frac{kV_0}{\omega_{p-}} < 2\sqrt{2}.$$

where $k \sim \frac{1}{L}$ is wave number, V_0 is peak separation of ion distribution functions, ω_{p-} is H^- plasma frequency.

Characteristic parameters in XOOPIC

density at sheath edge 1.5e+16[1/m^3]

electron plasma freq. 6.9e+9[1/s]
Its period 0.91e-9[s]
ion plasma freq. 1.6e+8[1/s]
Its period 3.9e-8[s]

electron thermal velo. 1.3e+6[m/s]
transition time 4.6e-9[s]
ion thermal velo. 3.1e+4[m/s]
transition time 1.9e-7[s]
Debye length 1.9e-4[m]

Time step of PIC 2e-11[s]
Instability period(?) (1-2)e-7[s] --- H+ - H-
5e-9[s] --- ele. - pos.

Conclusions

- A kinetic sheath model was developed with Boltzmann - PoissonEquations and confirmed XOOPIC results with it.
- In order to model sheath, the choice of source boundary parametersuch as electric field and charge neutrality (ni/ne) is important.
- The length of potential plateau (presheath) in simulation is determined by boundary conditions.
- PIC simulation is applied to Hydrogen negative plasma sheath. When negative ions increase, PIC simulation shows unstable behavior. This was unexpected from analytical sheath model.

Conclusions(cont.)

- We must consider kinetic interaction between positive/ negative ions. (Two stream instability ?)
  - There exist beam components in distribution function of electronegative plasma.

- If there are some dumping channel with interaction with electrons or heavy gas molecules, fluctuation of positive ions does not develop. But pure H- plasma must be lack o such a channel.

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