Extension of collisionless discharge models for application to fusion-relevant and general plasmas

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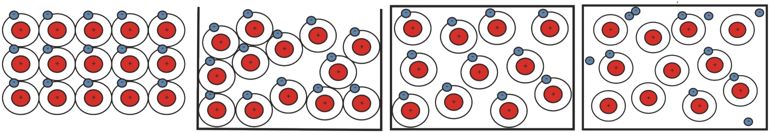
What is plasma?
Fourth state of the matter (fire).



- Solids - have very strong intermolecular bonds.
- Liquid - molecules are tied together by loose strings.
- Gas - atoms bounce around freely in space.
- Plasma - ionized gas, electrons and ions are separately free

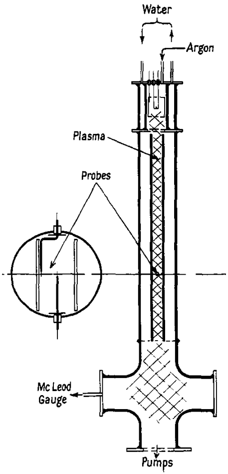
Temperature is the average amount of kinetic energy per atom.

Plasma properties

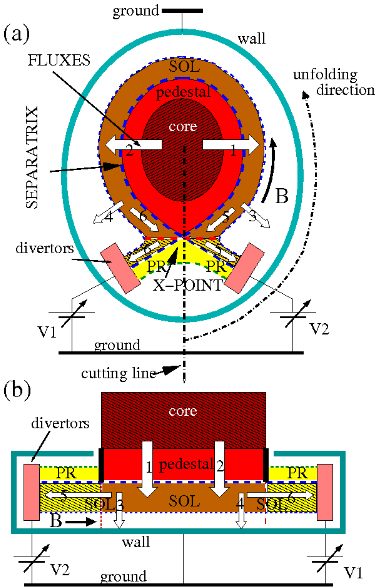
- Quasi-neutral ($n_i = n_e$).
- Thin sheath is observed at the wall ($\lambda_D \ll L$).
- Exhibit collective motion - collisionless.
- Very conductive - can be shaped and confined by electro-magnetic forces.

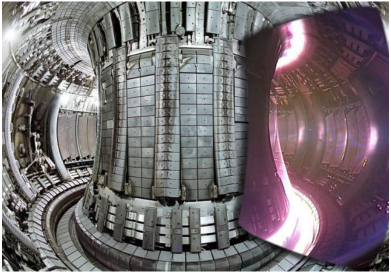
Laboratory plasmas

Aparatus used for producing a plane symmetric positive column in argon showing the position of the probes. [from Harrison-Thompson, 1959]



Fusion
Tokamak - Joint European Torus





Particle tracing developed in LECAD
Toroidal and poloidal magnets

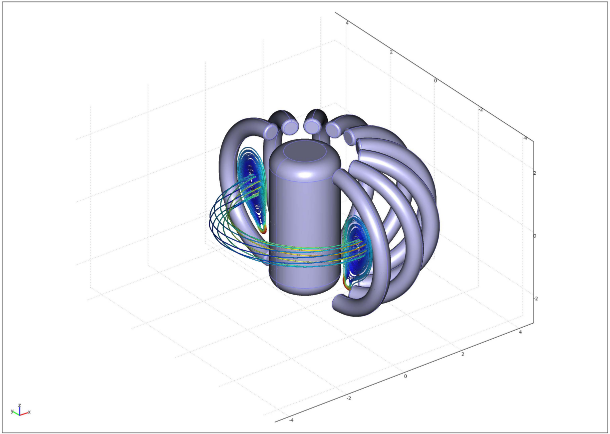
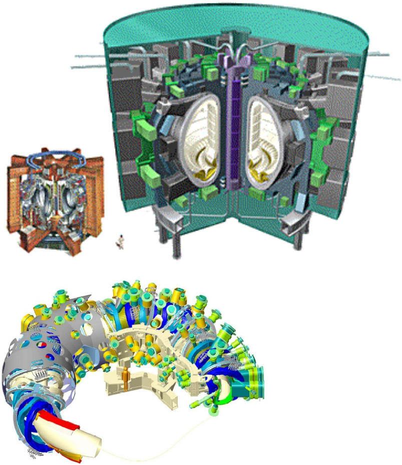


Figure: Particle trajectories by Eržen et al.

Plasma diagnostics

JET and ITER



Geometry
One dimensional model

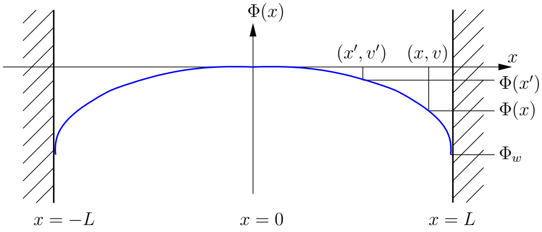


Figure: The geometry and coordinate system.

- Plane–parallel geometry
- Symmetric - we observe only one half
- We normalize problem to $L = 1$.

Motivation

- Provide precise treatment of the sheath region to fluid codes (SOLPS, EDGE2D).
- No analytic-numeric kinetic code available for $T_n > 0$.
- Particle In Cell (PIC) methods are not enough precise and can't simulate $\varepsilon = 0$ case.
- Existing $\varepsilon = 0$ models are limited in temperature range.
- No solution to $\varepsilon > 0$ kinetic model available.
- Can velocity distribution function be obtained from potential curves?

Thesis statement

The problem of a special integro-differential equations should be solved numerically without approximations to achieve an extended solution range applicable to fusion-relevant and general plasmas for an arbitrary ion temperature and arbitrary finite ε.

Methodology

In this thesis the author presents investigations and results with the following assumptions

- The Poisson equation is employed in the whole discharge region.
- A two-scale approximation is obtained just within the limit of the infinitely small Debye length in comparison with the system length.
- The ion-source temperature can take an arbitrary value.
- The electron-neutral impact is considered as a ionization mechanism.

Overview of existing models
Two-scale approximation

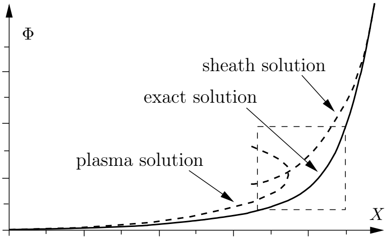


Figure: Symbolic picture illustrating the two-scale approximation.

- Plasma solution - Tonks–Langmuir model
- Sheath solution - Bohm model
- Exact solution - plasma + sheath (Our extended model)

Plasma parameters

1. The macroscopic neutrality $n_e = n_i$
2. Strong electric field is localized to distance λ_D with

$$\lambda_D \ll L \, , \quad \varepsilon \equiv \lambda_D / L \ \ (\ll 1) \, , \tag{1}$$

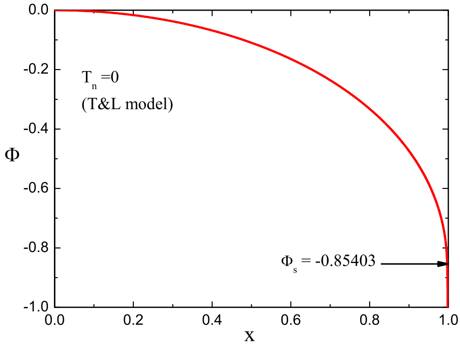
   where

$$\lambda_D = \sqrt{\frac{\epsilon_0 k T_e}{n_0 e^2}} \, , \tag{2}$$

   is the Debye radius.
3. The number of the particles in the Debye sphere is high

$$n \lambda_D^3 \gg 1 \, . \tag{3}$$

Tonks-Langmuir (T&L) model



- Ions are born at rest (cold ion-source case).
- Analytic kinetic solution for $\varepsilon = 0$.
- Beakdown of quasi-neutrality at $\Phi_s = -0.85403$.

Lewi Tonks and Irving Langmuir.
A general theory of the plasma of an arc.
Phys. Rev., 34(6):876–922, Sep 1929.

Bissell-Johnson (B&J) model ($\varepsilon = 0$)

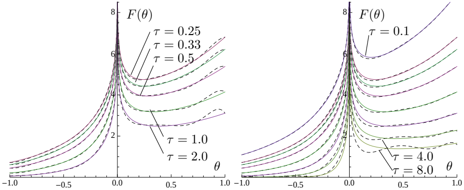


Figure: Kernel $F(\theta)$ B&J equation (left, dashed), our approximation (right, dashed) and the exact kernel (solid).

- Realistic Maxwellian ion-source velocity distribution.
- The Bohm criterion is used as the boundary condition to the quasi-neutrality equation.
- Kernel approximation with 8-th order Chebyshev polynomial and sinh(.) switch function.
- Plasma Eq. with 9-th order polynomial.

R. C. Bissell and P. C. Johnson.
The solution of the plasma equation in plane parallel geometry with a Maxwellian source.
Physics of Fluids, 30(2):779–786, 3 1987.

Scheuer-Emmert (S&E) model ($\varepsilon = 0$)

- Better kernel approximation.
- Did not apply any kind of Bohm criterion in advance.
- Dense grid at endpoint singularity.
- Analytic approximation to sub-integrals with a series expansion.
- Different normalization than B&J.
- Ion source temperature range is still limited to non-fusion temperatures.

J. T. Scheuer and G. A. Emmert.
Sheath and presheath in a collisionless plasma with a maxwellian source.
Physics of Fluids, 31(12):3645–3648, 1988.

S&E and our results

What ion-source they employed?

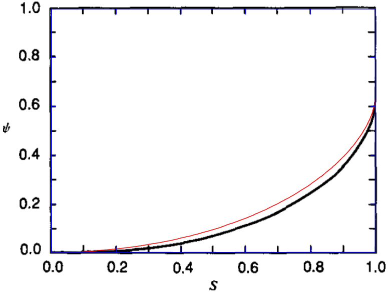


Figure: Comparison of the potential profile with S&E for $T_i = T_e$. The original scan is overlayed with our potential profile and axis box.

OUR FUNDAMENTAL WORK

1. Analytic-numerical method ($\varepsilon = 0$) for wide temp. range
2. Extension of the theoretical model ($\varepsilon > 0$)

L. Kos, N. Jelić, S. Kuhn, and J. Duhovnik.
Extension of the Bissel-Johnson plasma-sheath model for application to fusion-relevant and general plasmas.
Physics of Plasmas, 16(9):093503, 2009.

L. Kos, N. Jelić, and J. Duhovnik.
Modelling the plasma-sheath boundary for plasmas with warm-ion sources.
In *Proceedings of the International Conference Nuclear Energy for New Europe*, pages 807.1–807.8, 2008.

L. Kos, J. Duhovnik, and N. Jelić.
Extension of collisionless discharge models for application to fusion-relevant and general plasmas, In *NENE 2009*, pages 820.1–820.10. 2009.

N. Jelić, L. Kos, and D. D. Tskhakaya (sr.).
The ionization length in plasmas with finite temperature ion sources.
Physics of Plasmas, 2009. (under review).

M. Haefele, L. Kos, P. Navaro, and E. Sonnendrücker.
Euforia integrated visualization.
In *PDP 2010* , Pisa, Italy, 2010. (accepted).

F. Castejón Maga na, L. Kos, et al.
EUFORIA: Grid and high performance computing at the service of fusion modelling.
Ibergrid. Grid Infrastructure Conference Proceedings, 12-14 May 2008, Porto, Portugal

Analytic-Numerical method

Dimensionless quasi-neutrality equation

We are solving special integral equation in normalized form

$$\frac{1}{B} = \int_0^1 dx' \exp\left[\left(\vartheta + \frac{1}{2T_n}\right)\Phi(x') - \left(1 + \frac{1}{2T_n}\right)\Phi(x)\right] \times \mathrm{K}_0\left(\frac{1}{2T_n}|\Phi(x') - \Phi(x)|\right) \tag{4}$$

- $\Phi(x)$ is the unknown electrostatic potential
- B is the unknown constant which we fix by chooosing $\Phi(0) = 0$.
- $\mathrm{K}_0(z)$ is the modified Bessel function with logarithmic singularity at $|z| = 0$.
- T_n (neutral-gas temp.) and ϑ (ionization mechanism) are free parameters.

Computational domain in 1-D

We introduce the following node positions for N points of the system

$$x_i = \left[1 - [1 - i/(N-1)]^{\lambda_2}\right]^{\lambda_1} \quad , \qquad i = 0, 1, \ldots, N-1 \ , \qquad (5)$$

where λ_1 and λ_2 control the density at each boundary.

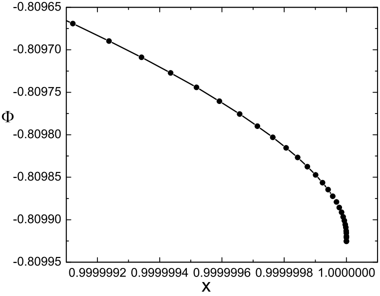


Figure: Last 28 points of the potential profile for $T_n = 0.1$, $\vartheta = 1$ with $N = 2401$ points and grid density $\lambda_1 = 1$, $\lambda_2 = 2.4$.

Discretized version suitable for iteration

$$\exp\left[(1+\frac{1}{2T_n})V_k\right] = B\sum_{i=0}^{N-1}\int_{x_i}^{x_{i+1}} dx' \exp[(\vartheta + \frac{1}{2T_n})V(x')] \times \mathrm{K}_0\left(\frac{1}{2T_n}|V(x') - V_k|\right) . \quad (6)$$

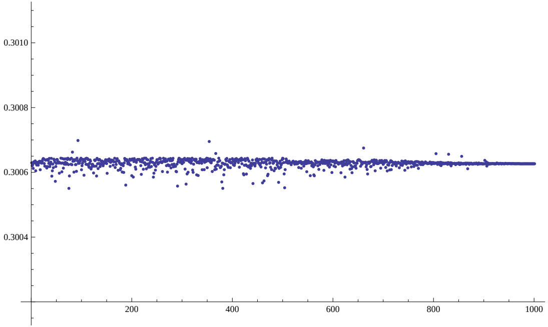
Iterative formula (7) that evaluates to new V_k is mathematically exact, but can only be applied when all V_k are perfectly accurate.

$$V_k = \frac{1}{1+\frac{1}{2T_n}} \ln(B\sum_{i=0}^{N-1} L_i), \quad (7)$$

What about eigenvalue B?

Only one equation (4) and two unknowns $\Phi(x)$ and B!

- B appears to be a true eigenvalue of the system.
- B contributes to shift only.
- B can be calculated at any position like Eq. (7) during iterations.



Iterate using soft (time) step

$$V_k^{new} = V_k + \alpha(V_l - V_k) \tag{8}$$

- With sufficiently low α Eq. (6) converges!
- α averages many previous solutions.
- Practical values in range [0.0001, 0.1]
- Consequence - huge number of iteration steps required

Can we speedup convergence somehow?

Yes, with parabolic interpolation near $x = 0$!

$$
\begin{aligned}
V_k &= a x_k^2 + b x_k + c\ , \quad k = 0, 1, \ldots, m \qquad (9)\\
a &= \frac{V_l - V_m}{x_l^2 - x_m^2}\ , \quad b = 0\ , \quad c = \frac{x_l^2 V_m - x_m^2 V_l}{x_l^2 - x_m^2}\ ,
\end{aligned}
$$

where mesh point x_l is chosen at $l = 3/4m$.

- Practical value for the length of rewrite is from 1% to 10%.
- Completely disable it when approaching saturated solution.

Solution smoothing
What is this good for?

A simple Laplacian-like smoothing technique with smooth-step parameter β

$$V_k^{new} = V_k + \beta \left[\frac{V_{k-1} + V_{k+1}}{2} - V_k \right], \quad k = N-1, N-2, \ldots, 1\,. \tag{10}$$

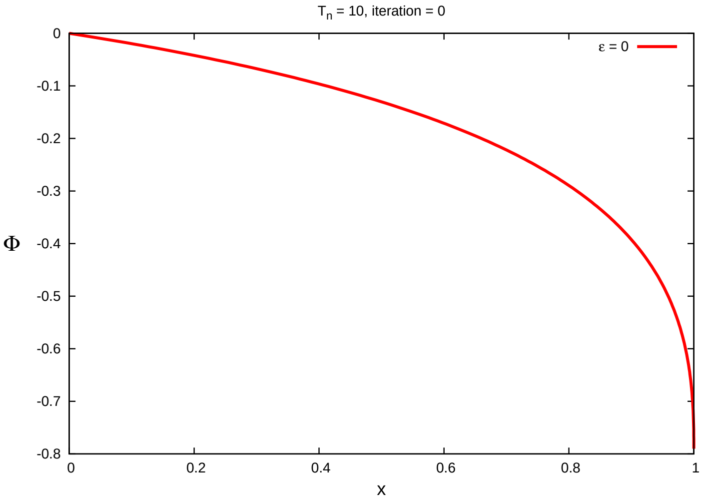
- Prevents low frequency oscillations of the solution.
- Helpful for $T_n \leq 0.05$.
- Practical range [0, 1].
- Should vanish for the final solution.

Implementation aspects

- Direct integration using adaptive quadrature (QAG, QAGS)
- We extended Gnu Scientific Library (GSL) integration routines to 128 bit `long double` for improved accuracy.
- Parallelization using OpenMP standard
- Employment of XML schema for input
- Dump files for restarting
- Regrid for faster convergence from scratch

Convergence demonstration for $\varepsilon = 0$

$T_n = 10$, iteration steps $= 139000$



Extended model requires?
Simultaneous solving of

- Boltzmann's kinetic equation

$$v\frac{\partial f_i}{\partial x} - \frac{e}{m_i}\frac{d\Phi}{dx}\frac{\partial f_i}{\partial v} = S_i(x, v) \ , \tag{11}$$

with the ion-source term $S_i(x, v)$

$$S_i(v, x) = Rn_n n_e(x) f_n\left(\frac{v}{v_{T_n}}\right) \ , \tag{12}$$

- and Poisson's equation

$$-\frac{d^2\Phi}{dx^2} = \frac{e}{\varepsilon_0}(n_i - n_e) \ . \tag{13}$$

Extension of the theoretical model

Target equation for $\varepsilon > 0$

We are solving a special non-linear integro-differential equation with a singular kernel

$$\frac{1}{B} = \frac{1}{1 - \exp(-\Phi)\varepsilon^2 \dfrac{d^2\Phi}{dx^2}} \times \int_0^1 dx' \exp\left[\left(\vartheta + \frac{1}{2T_n}\right)\Phi(x') - \left(1 + \frac{1}{2T_n}\right)\Phi(x)\right] \times \mathrm{K}_0\left(\frac{1}{2T_n}|\Phi(x') - \Phi(x)|\right) \tag{14}$$

Numerical method for $\varepsilon > 0$

- Converted to relaxation method with
- Initial floating wall potential

$$\Phi[i] = \frac{\Phi_w}{1 - \exp(1)} \left[1 - \exp\left(\frac{i}{N}\right) \right] \,, \qquad (15)$$

from $\varepsilon = 0$ case

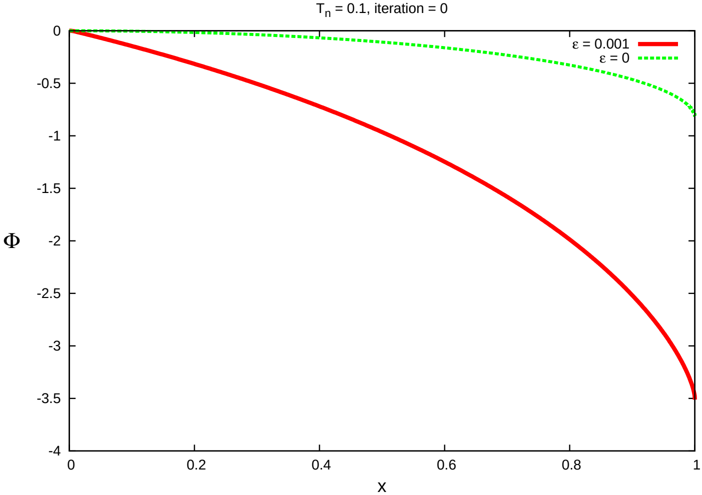
- Floating wall condition

$$\exp(\Phi_w) = 2\pi \sqrt{\frac{m_e}{m_i}} \sqrt{\frac{T_n}{T_e}} B \int_0^1 dx' \exp[\Phi(x')] \,, \qquad (16)$$

is smoothly adjusted after converged state is reached.

Convergence demonstration for finite ε

$T_n = 0.1$, $\varepsilon = 0.001$, iteration steps $= 172000$



Potential profiles for $\varepsilon = 0$

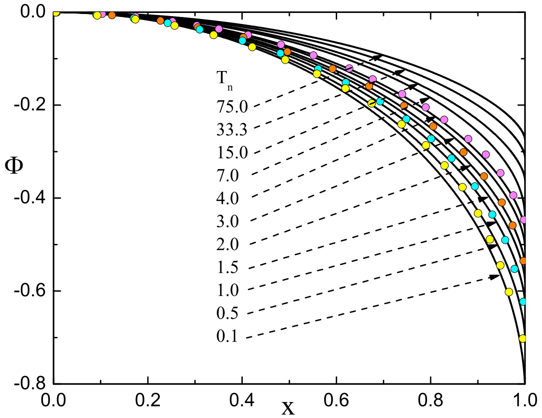
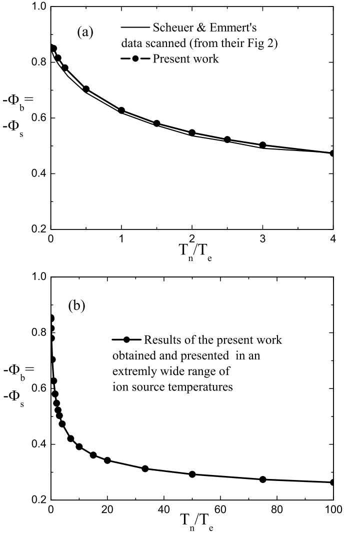


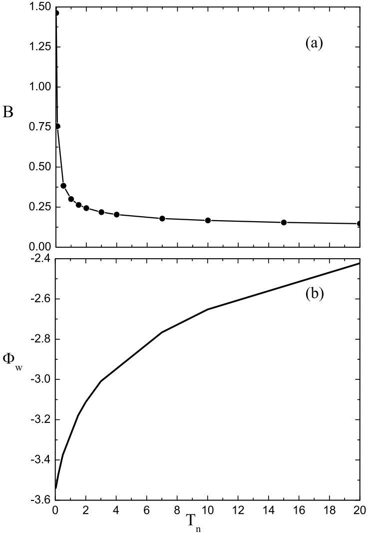
Figure: Potential profiles for various ion-source temperatures as obtained by us with the exact kernel (solid lines) and by Bissell and Johnson with their approximate kernel (scattered).

Plasma sheath boundary potential Φ_s



The plasma sheath boundary potential in a limited range of ion source temperatures, where the S&E approximate kernel is valid, in comparison with our results (a), and in a wide range of of the ion source temperatures (b), where we employed the exact kernel.

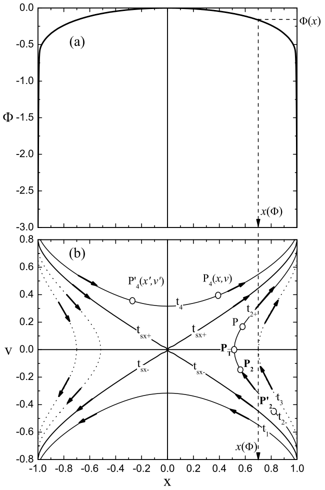
Wall potential Φ_w

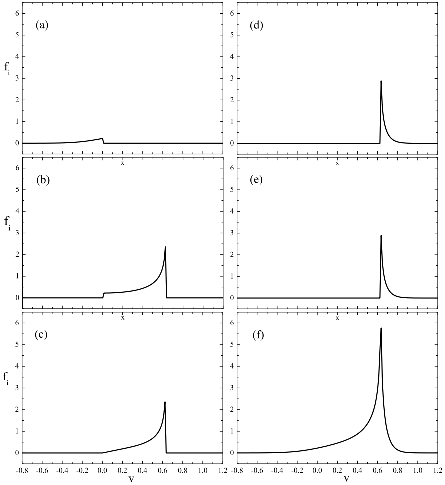


The dependence of B (a) and of the wall potential (b) on the ion source temperature.

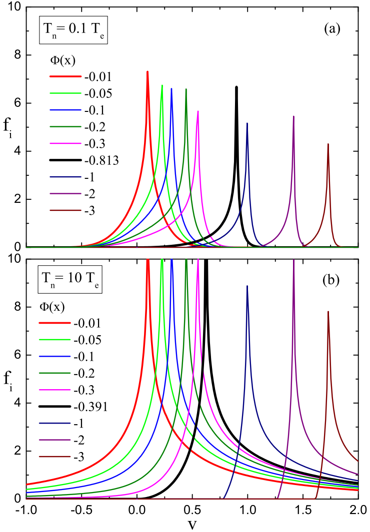
Trajectory method

Method of characteristics for Velocity Distribution Function $f_i(\Phi(x), v)$



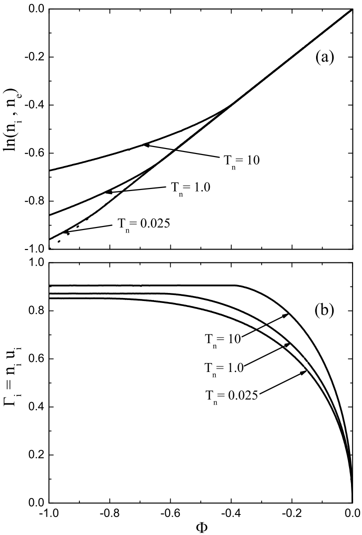


Velocity distributions



Velocity distributions for (a) $T_n = 0.1$, and (b) $T_n = 10$.

Moments



(a) Ion and electron densities

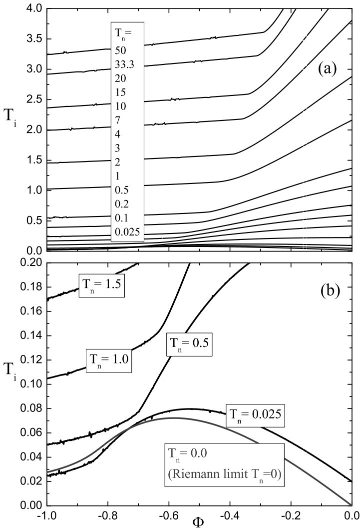
$$n_i(\Phi(x)) = \int_{-\infty}^{\infty} f_i(v)dv$$

in a logarithmic presentation as a function of local potential $\Phi(x)$.
(b)The ion flux

$$\Gamma_i(\Phi(x)) = \int_{-\infty}^{\infty} vf_i(v)dv$$

as a function of $\Phi(x)$.

Effective ion (final) temperature T_i



Profiles of the ion temperature T_i for various ion source temperatures. The ion total energy:

$$K_i(\Phi(x))) = \frac{1}{n_i}\int_{-\infty}^{\infty} v^2 f_i(v)dv$$

Ion directional velocity:

$$u_i(\Phi(x)) = \frac{1}{n_i(\Phi)}\Gamma_i(\Phi)$$

The ion temperature:

$$T_i(\Phi(x)) = K_i(\Phi) - u_i^2(\Phi)$$

Ion temperature at the center and at the edge

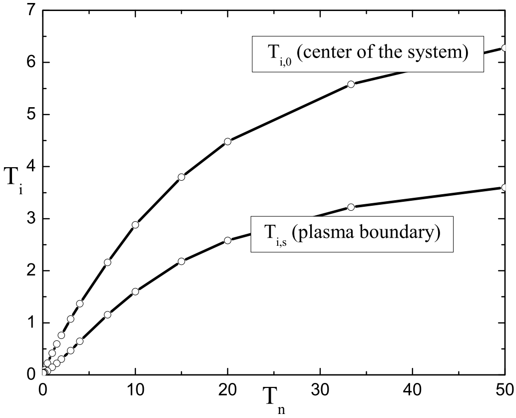


Figure: The ion temperature at the center and the edge of plasma for various ion source neutral temperatures.

Ionization length

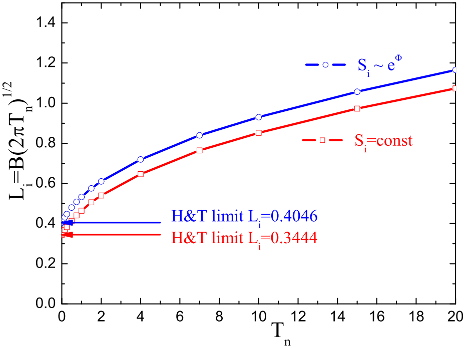
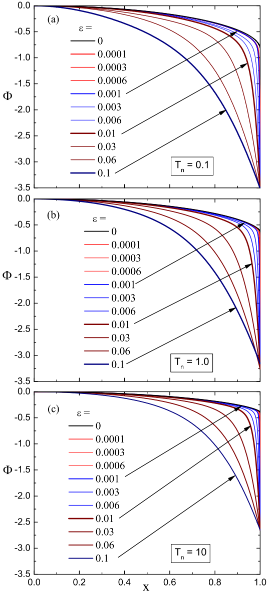


Figure: Ionization lengths of the Maxwellian-source and flat-source ionization mechanisms as defined by H&T.

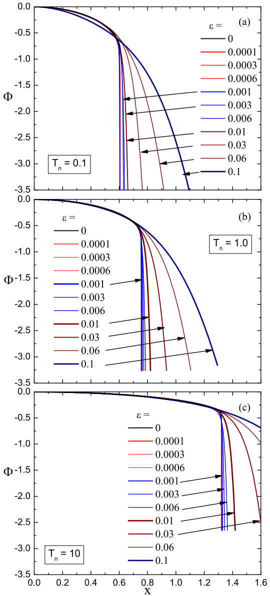
E. R. Harrison and W. B. Thompson.
The low pressure plane symmetric discharge.
Proceedings of the Physical Society, 74(2):145–152, 1959.

Potential profiles for various ε



Potential profiles for various ε and
(a) $T_n = 0.1$,
(b) $T_n = 1.0$,
(c) $T_n = 10.0$.
Our results obtained with the fixed system length $L = 1$.
Wall potential Φ_w is dependent on T_n.
Hydrogen was used for this simulation.

Rescaled potential profiles for various ε



Potential profiles for various ε and

(a) $T_n = 0.1$,
(b) $T_n = 1.0$,
(c) $T_n = 10.0$.

Rescaled results according to $x_s = \sqrt{2\pi}\sqrt{T_n}B$.

From (b) it can be observed that wall potential Φ_w also changes with ε.

K.-U. Riemann.
Plasma-sheath transition in the kinetic Tonks-Langmuir model.
Physics of Plasmas, 13(6):063508, 2006.

Zoom of the potential profiles

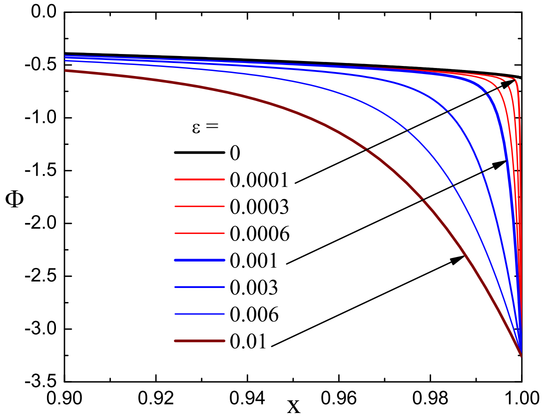


Figure: Potential profiles for various ε and $T_n = 1$ with a zoomed x range shows high precision results with $\varepsilon \leq 0.0006$.

Dependence on T_n

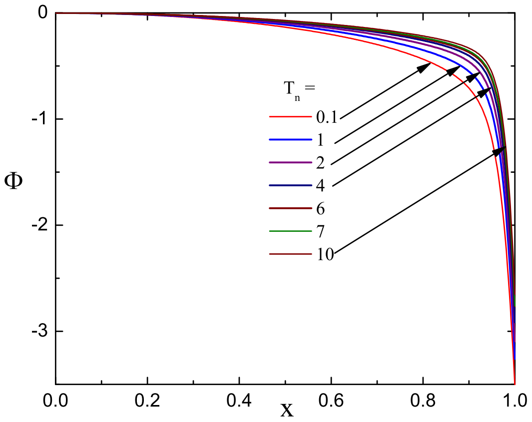
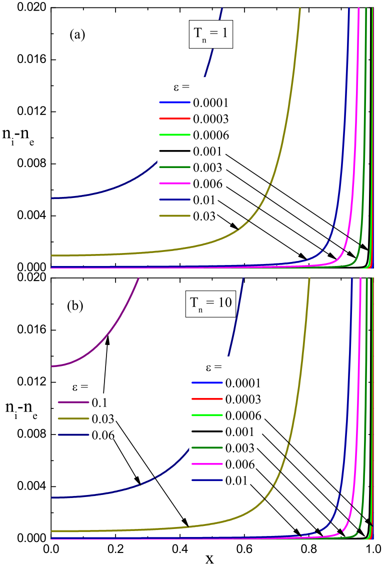


Figure: Potential profiles for various ion-source temperatures and fixed $\varepsilon = 0.01$.

Charge imbalance



Charge imbalance for
(a) $T_n = 1$,
(b) $T_n = 10$

Our contributions

- Extended temperature range with exact kernel.
- Derived quantities obtained from velocity distribution with direct integration.
- Extension to the case of finite ε.

- Future work
  - Precise investigation of the sheath edge singularity.
  - Definition of PWT on the basis of VDF for $\varepsilon > 0$.
  - Parallelization with MPI.
  - Continuation of work in EUFORIA project.

Singularity form for $\varepsilon = 0$ (preliminary results)

Finding power of α with fitting $(\Phi_s - \Phi) \to C(x_s - x)^{\alpha}$

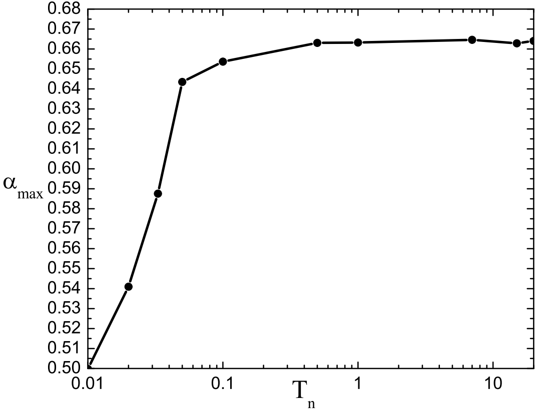


Figure: Dependence of α_{max} on the ion-source temperature for logarithmic scale of T_n.