# Particle simulation methods for studies of low-pressure plasma sources

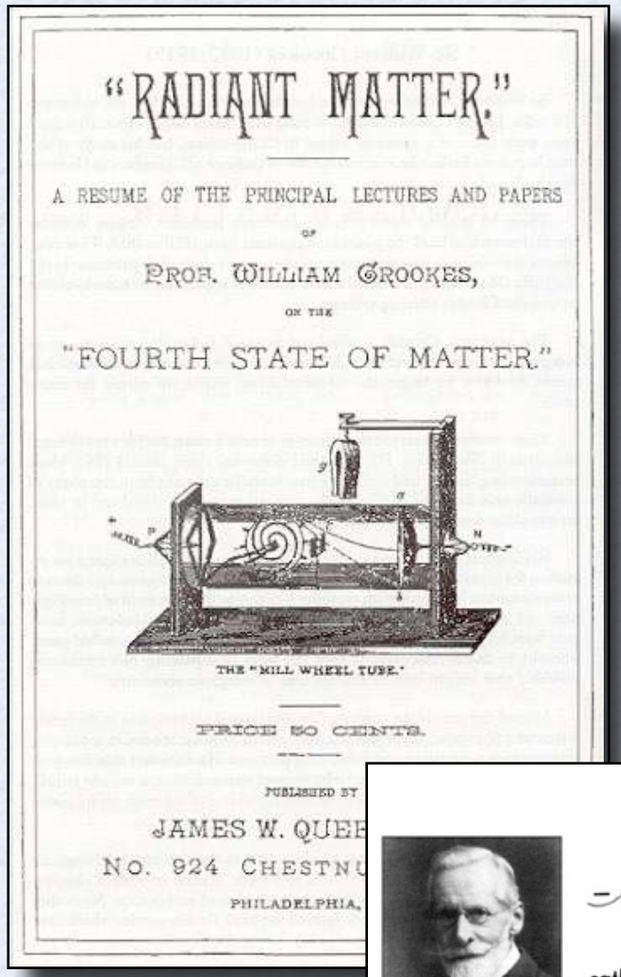
Zoltán Donkó

Electrical Discharges & Plasma Physics Research Group
Research Institute for Solid State Physics and Optics
Hungarian Academy of Sciences, Budapest

W. Crookes Prize lecture

XXth ESCAMPIG - Novi Sad 2010

# Prof. W. Crookes and the 4th state of matter


"RADIANT MATTER."

A RESUME OF THE PRINCIPAL LECTURES AND PAPERS

OF

PROF. WILLIAM CROOKES,

ON THE

"FOURTH STATE OF MATTER."

THE "MILL WHEEL TUBE."

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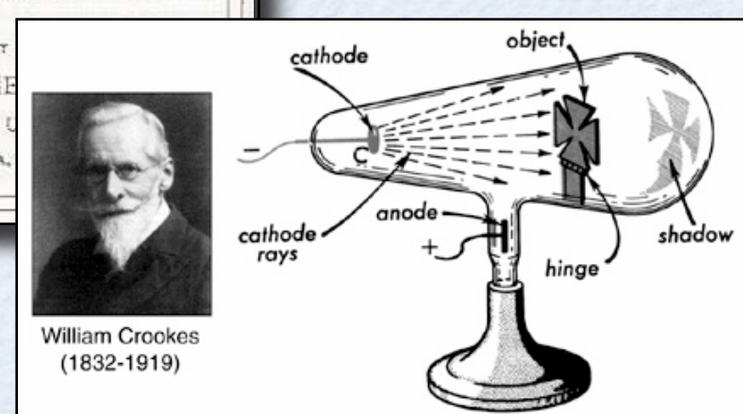
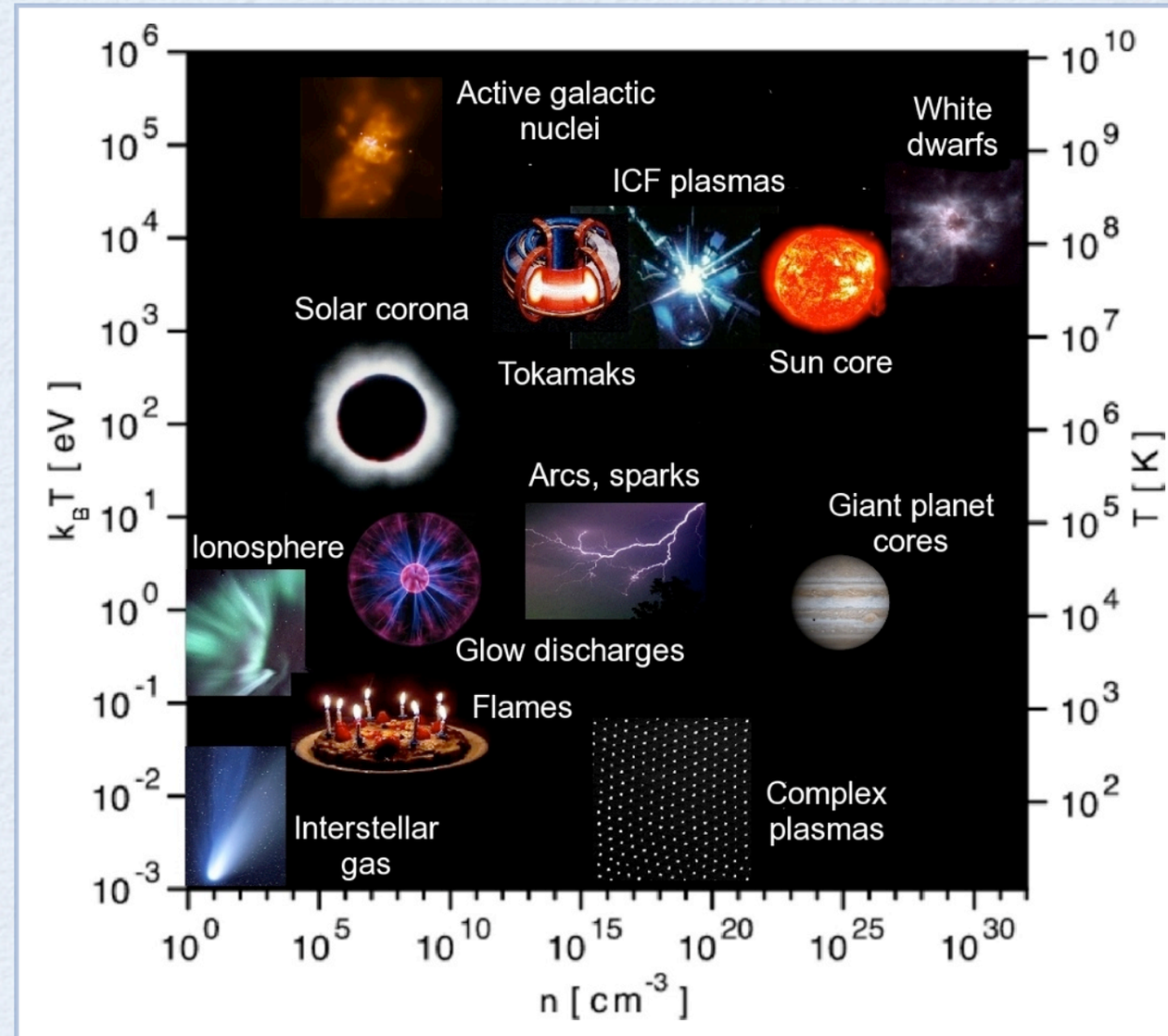



PLASMAS

**Cathode rays**

- carry energy
- move from cathode to anode
- can be deflected by magnetic field
- 4th state of matter, consisting of negatively charged particles

# THANKS : Colleagues, Coworkers & Friends

GLOW DISCHARGE PHYSICS

CHARGED PARTICLE KINETICS

M. Jánossy
G. J. Kalman
K. Rózsa
K. I. Golden
L. C. Pitchford
L. Csillag
B. Nyíri
J. Goree
M. Bonitz
A. V. Phelps
D. Marić
S. Holló
Z. Lj. Petrović
P. Hartmann
A. Derzsi
J. Schulze
G. Malović
J. Karácsony
I. Korolov
A. Bogaerts
H. R. Skullerud
U. Czarnetzki
D. Loffhagen
E. Schüngel
G. Bánó
L. Szalai
A. Gallagher
J. P. Boeuf
K. Kutasi
J. Glosik
K. Wiesemann
F. Gordillo-Vazquez
M. M. Turner
S. Matejčik
F. Sigeneger
P. Simon
L. Tsendin
M. Piheiro
J. Thomán-Forgács
P. Horváth
N. Sadeghi
N. Pinhão
B. Jelenković
D. Luggenhölscher
J. Tóth
E. Sárközi
Gy. Császár
.....

RADIOFREQUENCY DISCHARGES

GAS LASER RESEARCH

PHYSICS OF COMPLEX PLASMAS

# Particle simulation methods for studies of low-pressure plasma sources

MTA SZFKI

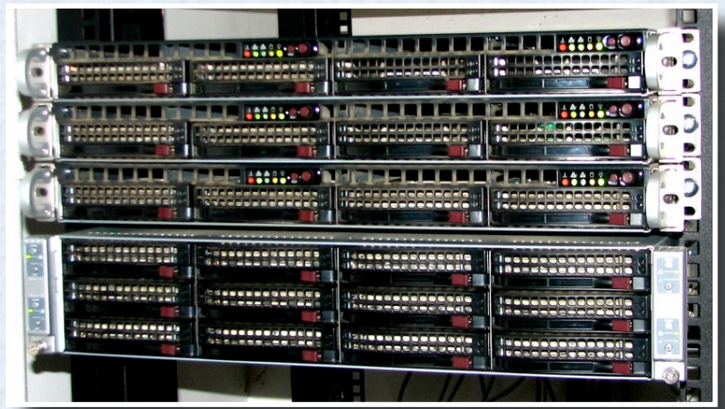
## (Diverse) startup thoughts

- WHAT do we do? - Describe motion and interactions of charged particles - in order to understand the physics of gas discharges
- WHY do we need simulations? - Kinetic level, flexible, visualization
- THIS TALK intends to illustrate the capabilities of particle simulations methods - we start with very elementary examples and proceed towards more complex topics
- “Bloom where you’ve been planted”

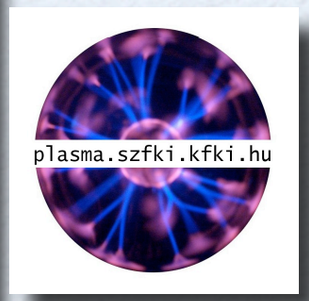
## Topics

- Charged particle kinetics in homogeneous field
- Modeling of cold-cathode glow discharges
- Particle in Cell simulation of radiofrequency discharges

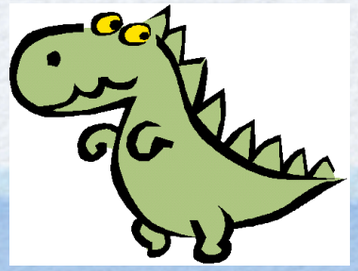
# (Few words about) Computational resources



- Amazing progress of resources [e.g. T. Makabe, ESCAMPIG 2010]
- Strong feedback of plasma science and technology on the development of devices



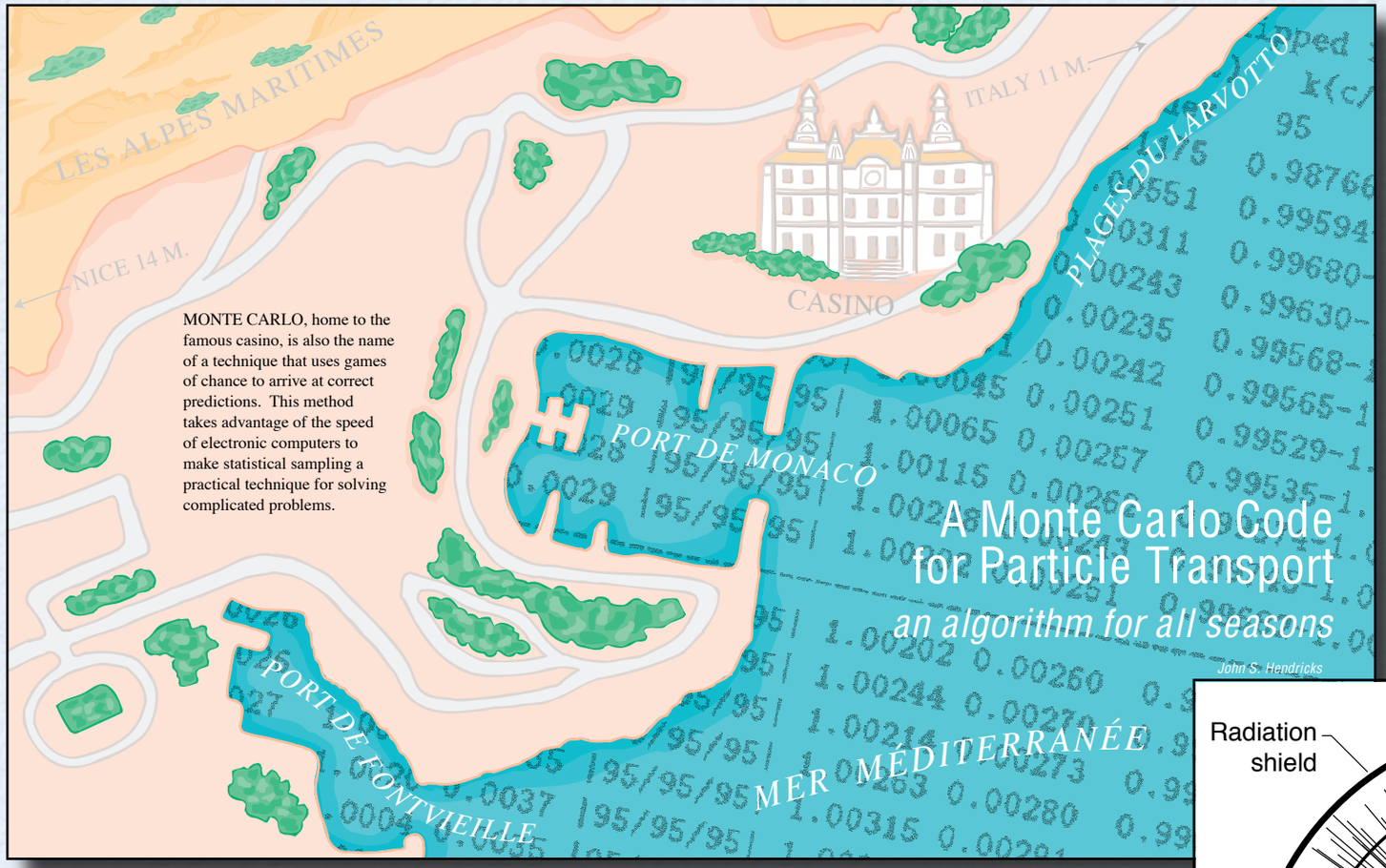

(???)
GPU
Clusters
PCs
PC



# I. Charged particle kinetics

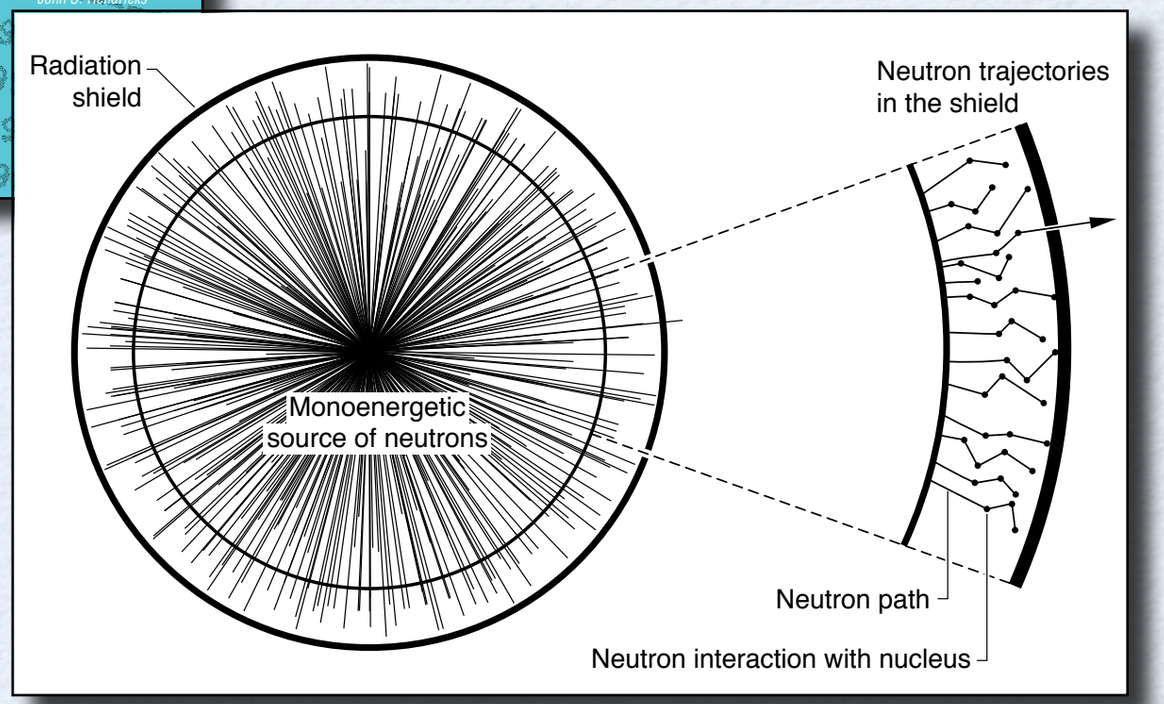
- Basics of Monte Carlo simulation
- Velocity distribution functions and transport parameters in homogeneous field
- Spatio-temporal relaxation of the electron gas
- Gas breakdown

# Monte Carlo methods




Los Alamos Science. No. 22 (1994)

"The Monte Carlo method was first applied on the MANIAC computer at the Laboratory to predict the rate of neutron chain reactions in fission devices..... "

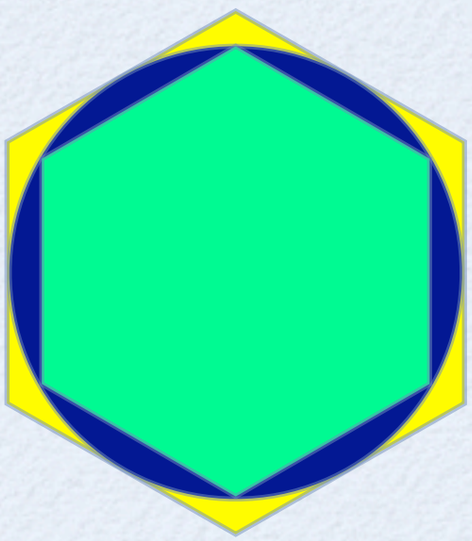



Stanislaw Ulam: statistical sampling
John von Neumann: neutron transport
Nicholas Metropolis: "Monte Carlo"

# Monte Carlo methods: a simple example

**Monte Carlo methods are used in all disciplines of science**

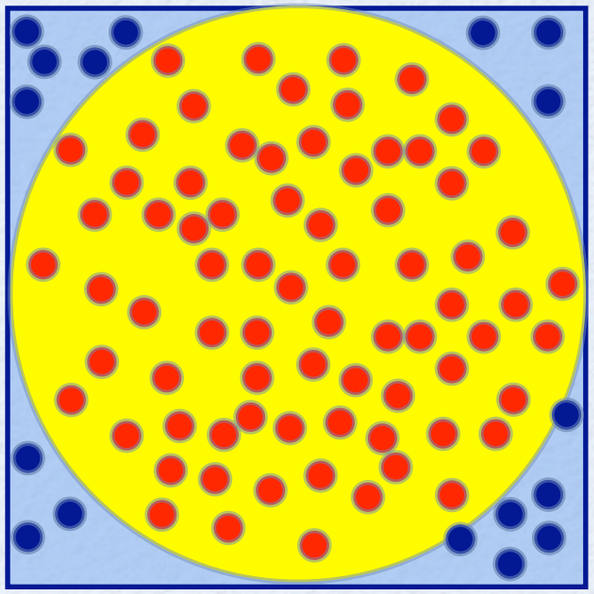
How to approximate $\pi$ ?



.... by the perimeters of polygons inscribed and circumscribed about a given circle (goes back to Archimedes)

Monte Carlo approach:

Throw darts with uniform distribution on a square board



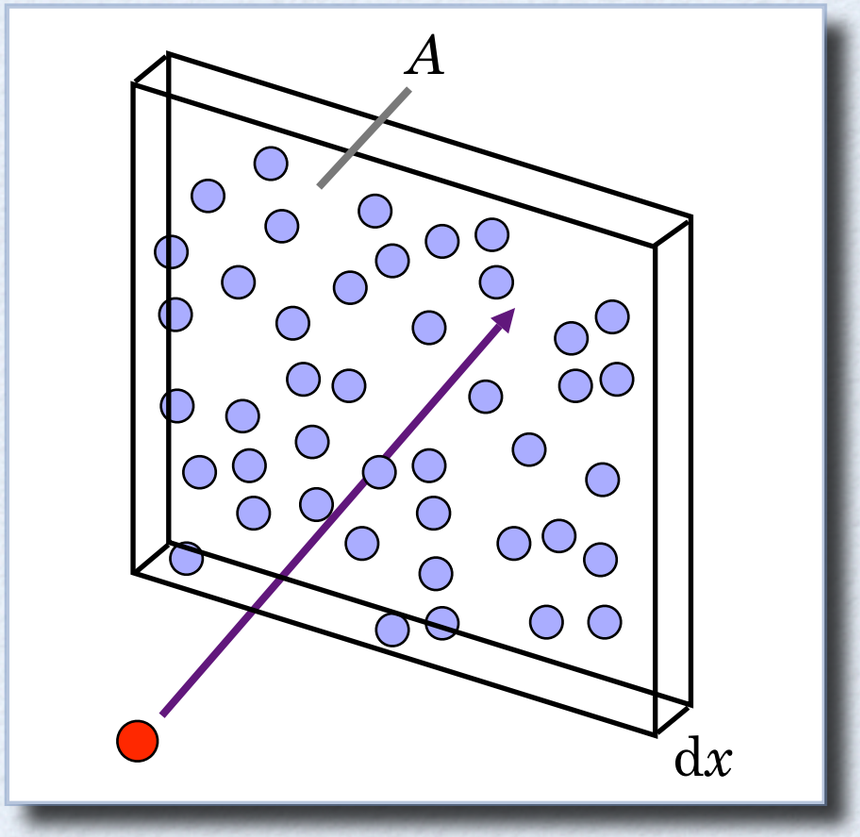
$$\frac{N(\text{red})}{N(\text{all})} \rightarrow \frac{\pi}{4}$$

Efficiency / computing speed

A different way of thinking...

# Monte Carlo method: particle transport

**Transit of a particle through a slab of background gas**




$N$ background gas particles within the slab, each with same cross section

Area occupied by particles: $S = N\sigma$

Total area: $A$

Probability of collision:

$$\mathrm{d}p(x) = \frac{S}{A} = \frac{N\sigma}{A} = \frac{(nA\mathrm{d}x)\sigma}{A} = n\sigma\mathrm{d}x$$

$$\mathrm{d}p(t) = n\sigma v\mathrm{d}t$$

For small time increments:

$$\boxed{p(\Delta t) = n\sigma v\Delta t}$$

$$\Delta t \to 0$$

In general:

$$p(\Delta t) = 1 - \exp\left[-\int_0^{\Delta t} n\sigma[v(t)]v\mathrm{d}t\right]$$

$$p(\Delta s) = 1 - \exp\left[-\int_0^{\Delta s} n\sigma[v(t)]\mathrm{d}s\right]$$

See (much) more, e.g.:
S. Longo, PSST **15**, S181 (2006)

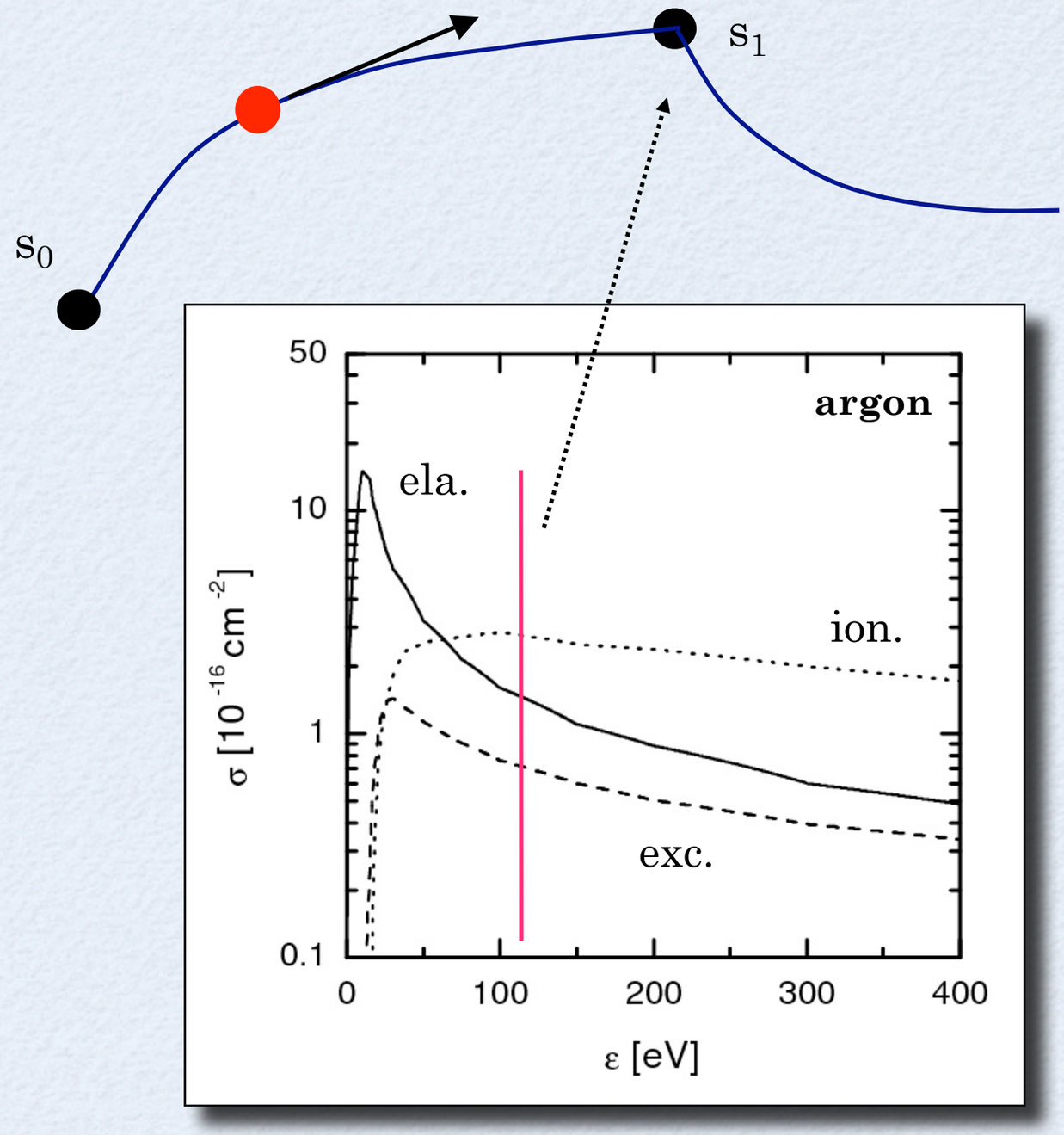
# Monte Carlo method: particle transport

<u>Tracing of individual particles</u>

Equation of motion: $$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = e\mathbf{E}$$

Probability of collision: $$p(\Delta t) = n\sigma v\Delta t$$

total cross section

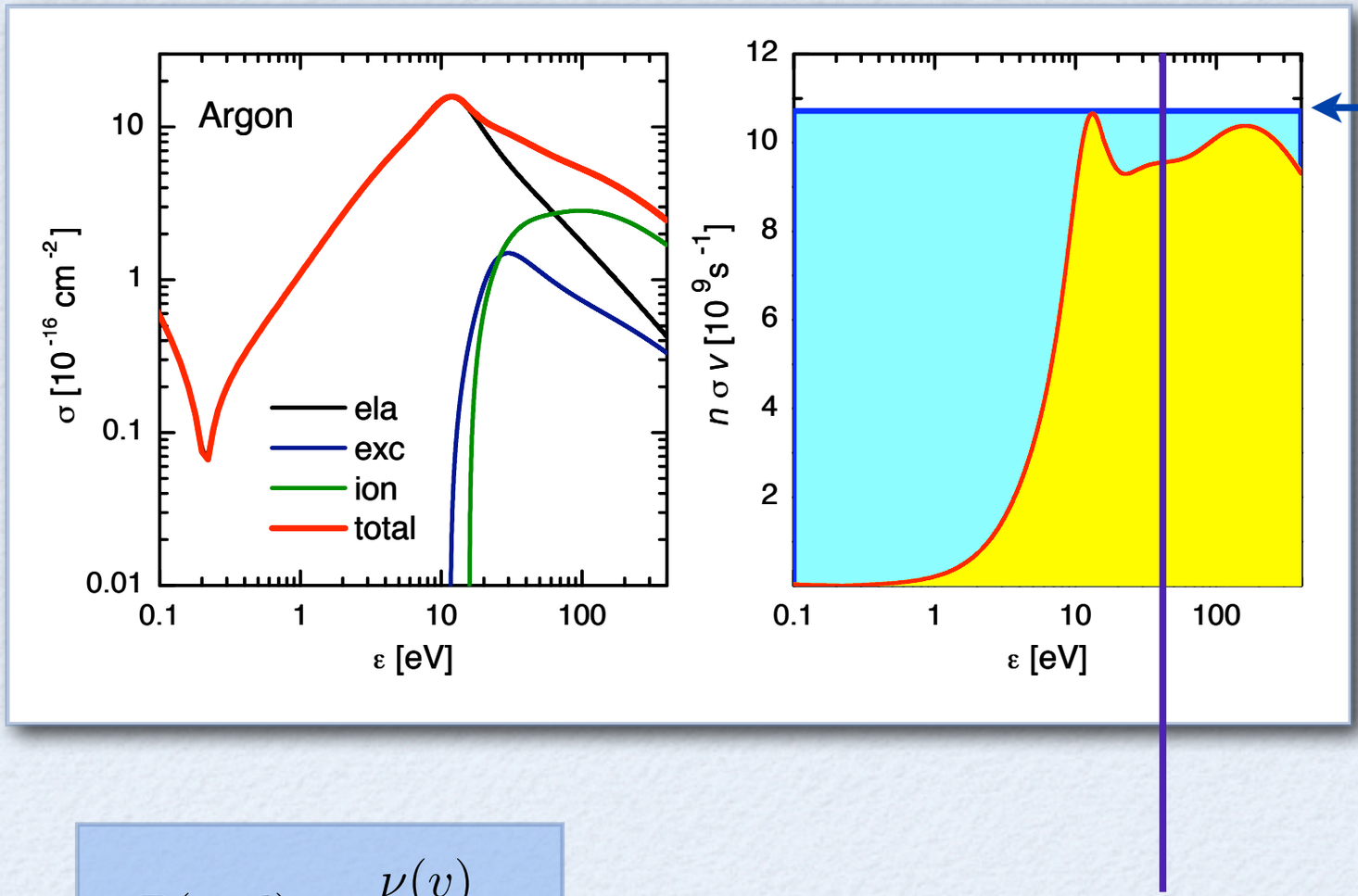



- Processes
  - elastic scattering,
  - electronic excitation,
  - ionization
  - attachment
- Chosen in a probabilistic manner:
  - free path,
  - type of collision,
  - new direction
- 1 particle → avalanche

# Monte Carlo method: particle transport

- *Acceleration techniques - null-collision method* [H. R. Skullerud, J. Phys. D **1**, 1567 (1968)]
- *Rescaling techniques - very strong ionization / attachment* [Y. M. Li, L. C. Pitchford, and T. J. Moratz, Appl. Phys. Lett. **54**, 1403 (1989)]
- *Cold gas approximation (collision partner is at rest)*
  - usually valid for electrons, unless $E/n$ is "very low" [M. Yousfi, A. Hennad, and A. Alkaa, Phys. Rev. E **49**, 3264 (1994)]
  - at very low $E/n$, as well as for simulations of ion transport the collision partner must be chosen from a background gas with Maxwellian velocity distribution
- *Monte Carlo simulation vs. Boltzmann equation*
  - equivalent, both have their advantages [for comparison of different techniques see e.g. N. R. Pinhão, Z. Donkó, D. Loffhagen, M. J. Pinheiro and E. A. Richley, Plasma Sources Sci. Technol. **13**, 719 (2004)].
  - *a lot of progress on BE solution* (multiterm methods, S. Dujko, ESCAMPIG 2010, also Greifswald group, ....)
- *Benchmark your code!* [A. M. Nolan, M. J. Brennan, K. F. Ness and A. B. Wedding, 1997, J. Phys. D **30**, 2865; Z. M. Raspopović, S. Sakadzić, S. A. Bzenić, Z. Lj. Petrović, 1999, IEEE Trans. Plasma Science **27**, 1241.]

# Monte Carlo method - null-collision technique




$$\nu^\star(v) = \nu^\star$$

**The idea:**
introduce an artificial type of collision process (the "null-collision", which makes the total collision frequency constant, independently of the particle velocity

Collision frequency:

$$\nu = n\sigma(v)v$$

Total collision frequency:

$$\nu^\star = n\sigma^\star(v)v$$

$$\nu^\star(v) = \nu(v) + \nu_{\text{null}}(v)$$

We can give the time of free flight:

$$t_{\text{flight}} = -\frac{1}{\nu^\star}\ln(1 - R_{01})$$

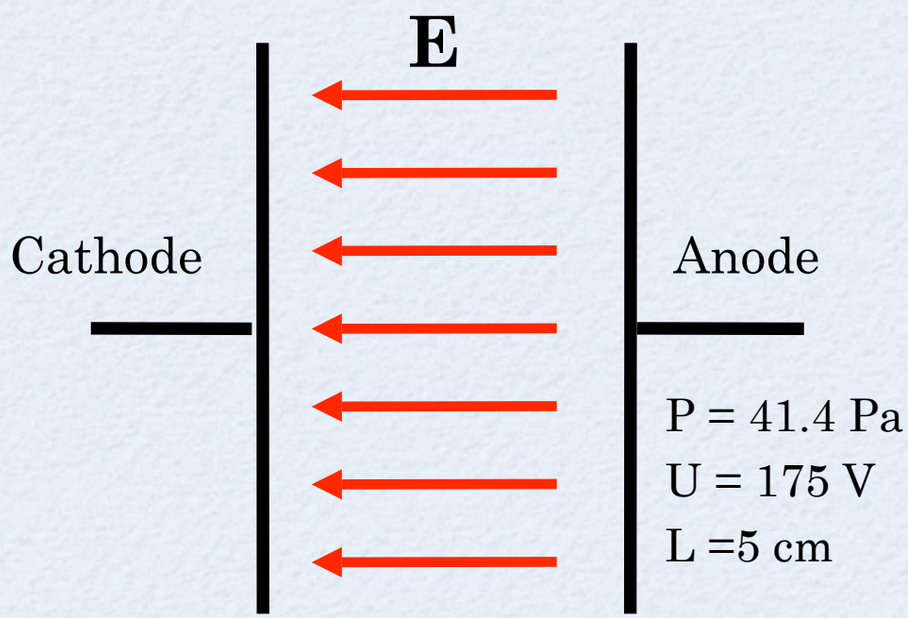
$$P(\text{real}) = \frac{\nu(v)}{\nu^\star(v)}$$

$$P(\text{null}) = \frac{\nu_{\text{null}}(v)}{\nu^\star(v)}$$

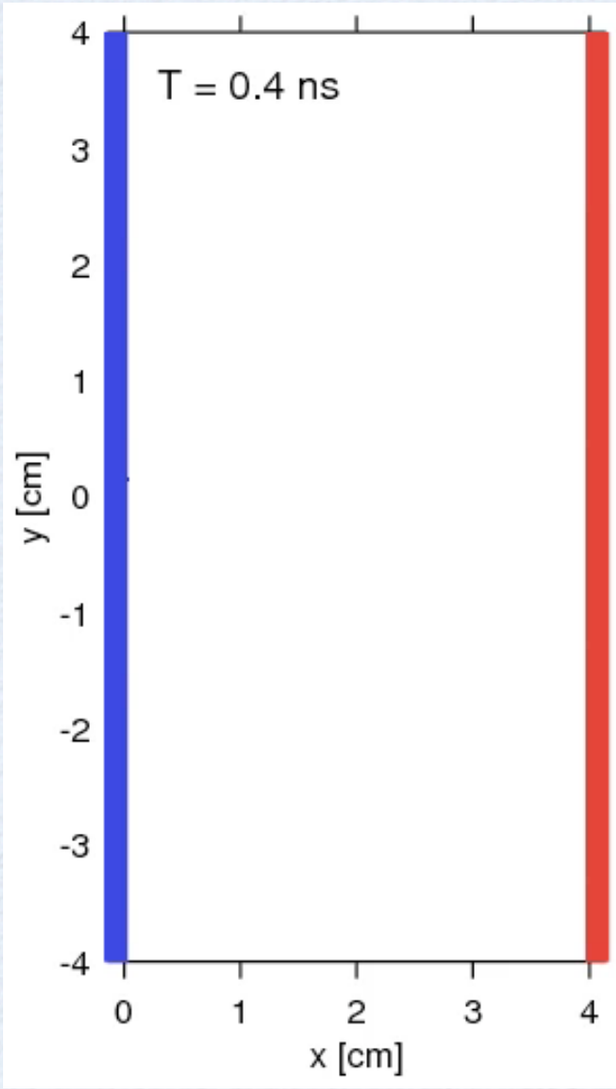
Whenever a collision occurs at a given velocity (energy)

H. R. Skullerud, J. Phys. D: Appl. Phys. 1, 1567 (1968)
"The stochastic computer simulation of ion motion in a gas subjected to a constant electric field"

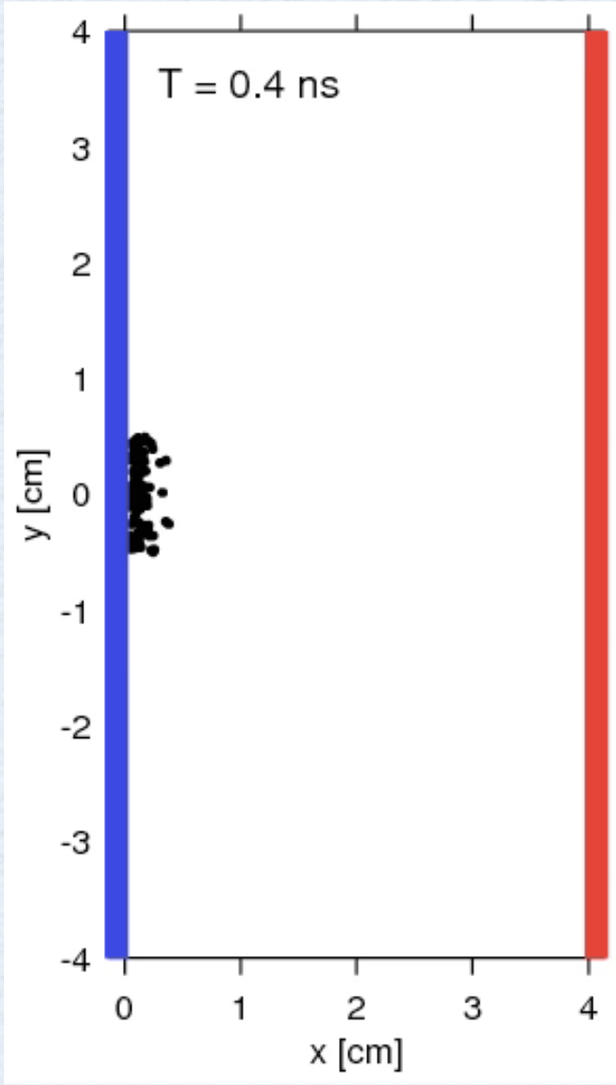
# MC simulation: electron avalanches




Single avalanche

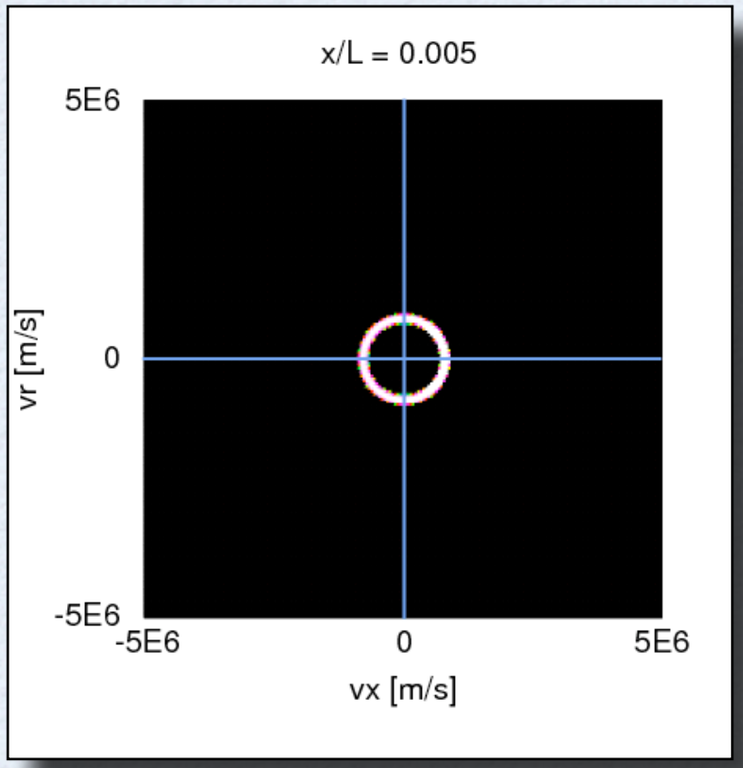


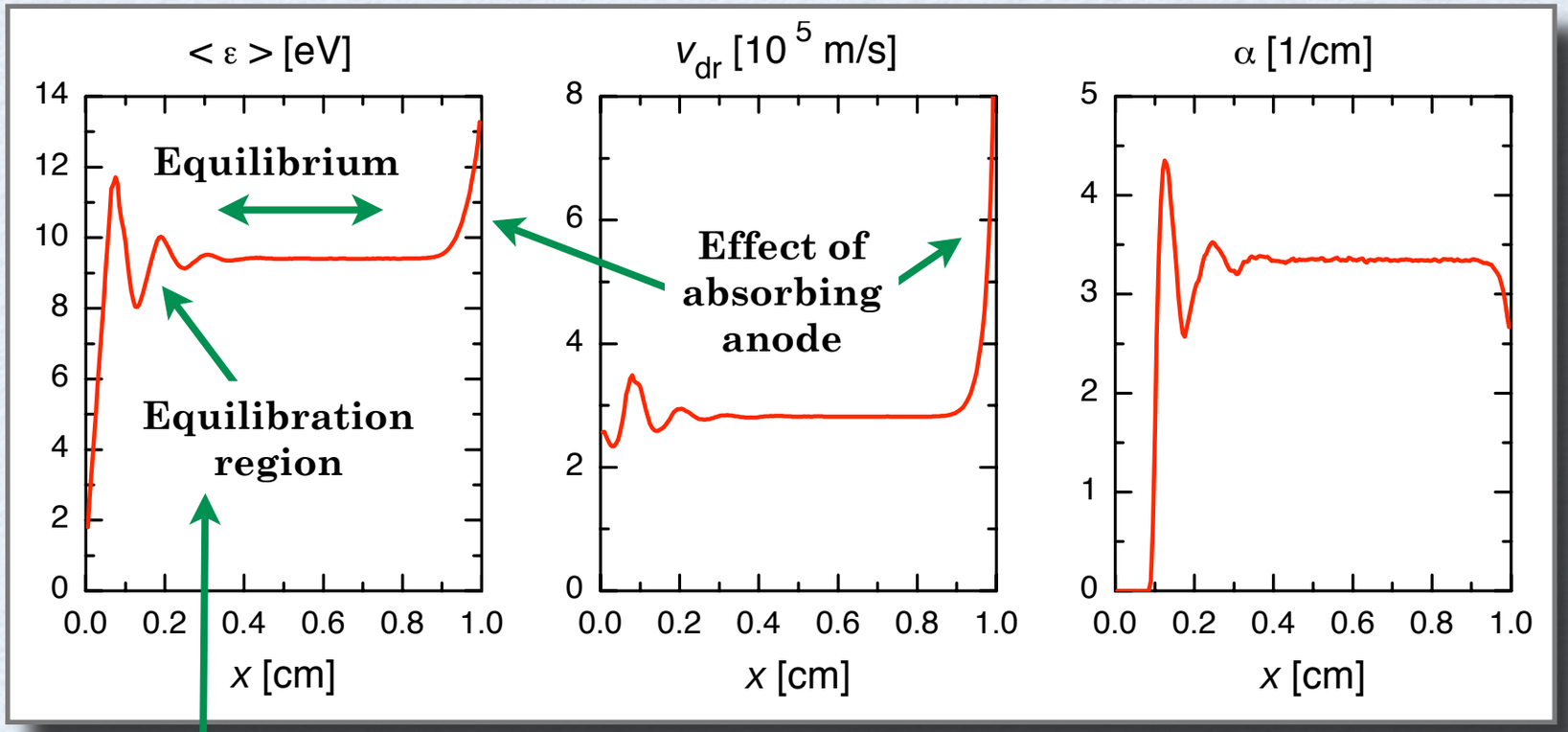

Particle cloud



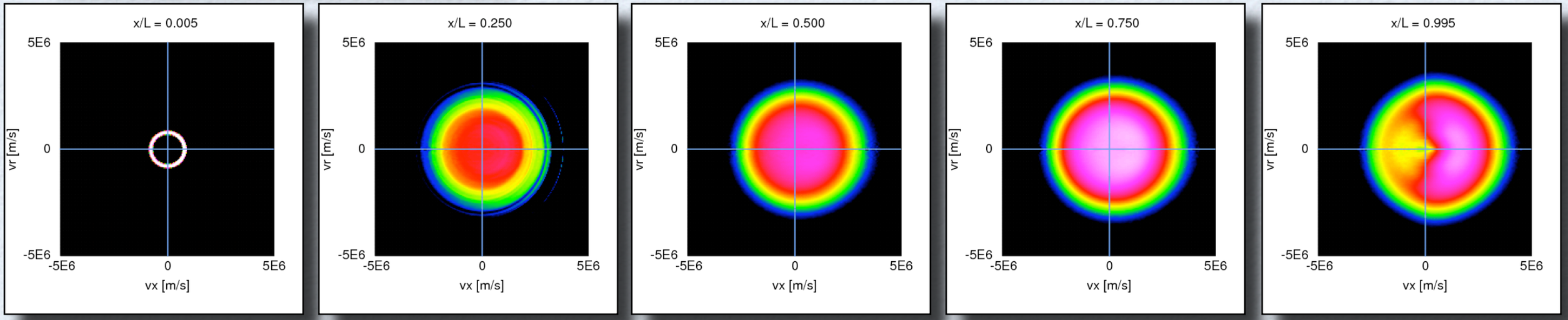
# Electron velocity distribution in homogeneous electric field

***E/n* = 500 Td, *L* = 1 cm, *p* = 1 Torr**



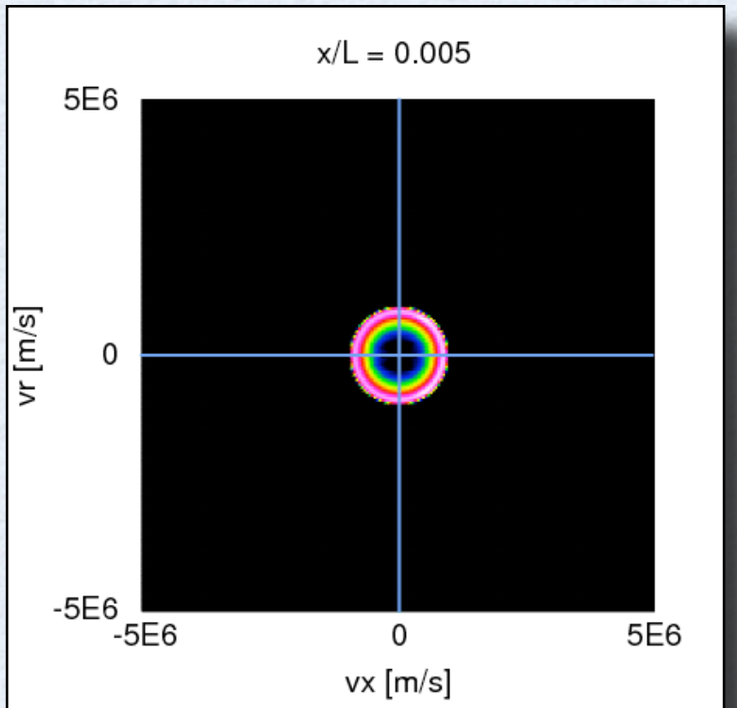



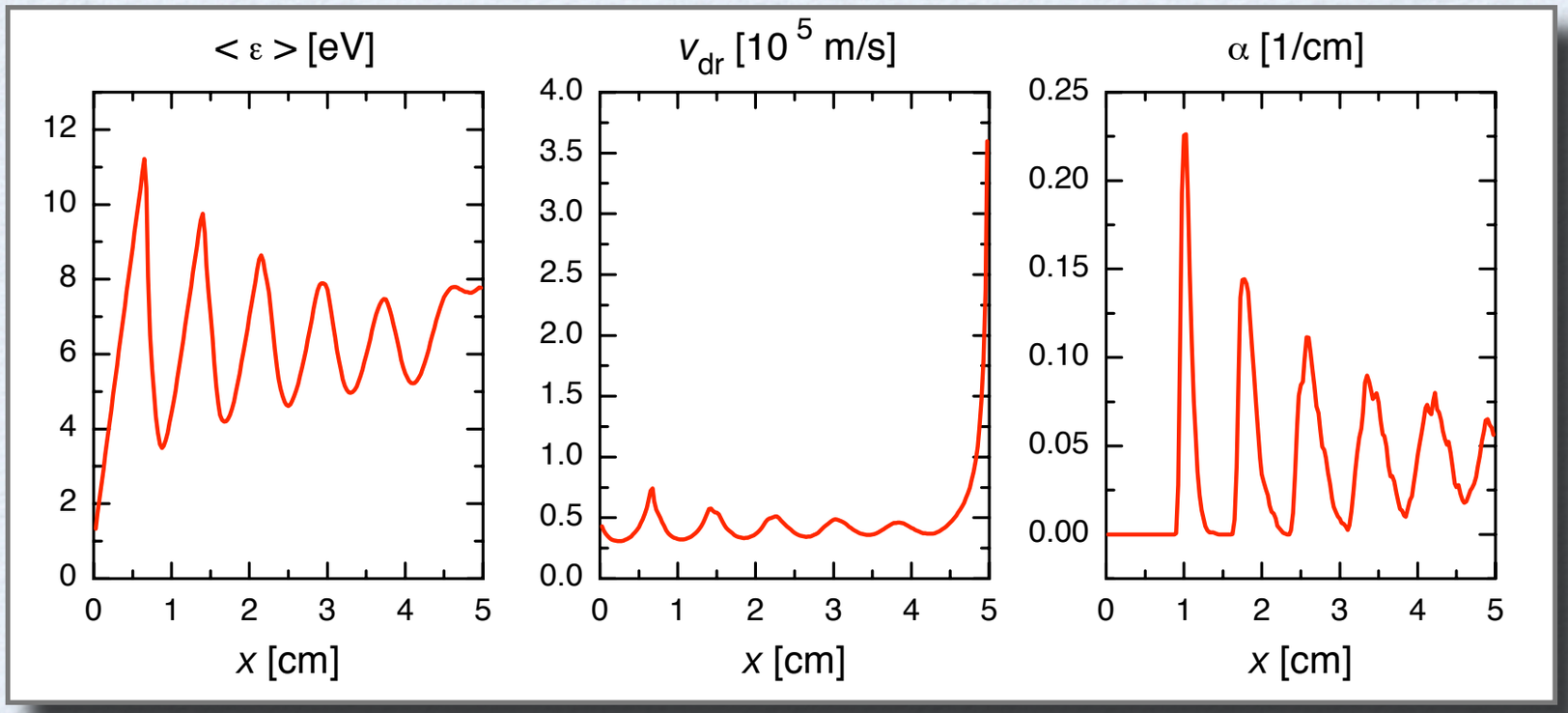

G. Malović, A. Strinić, A. Živanov, D. Marić, and Z. Lj. Petrović, PSST **12,** S1 (2003).



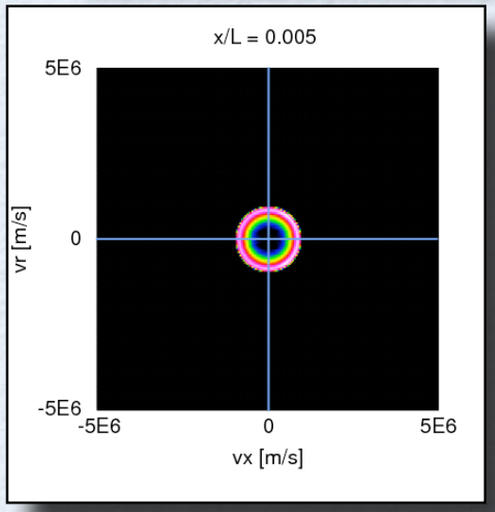
# Electron velocity distribution in homogeneous electric field

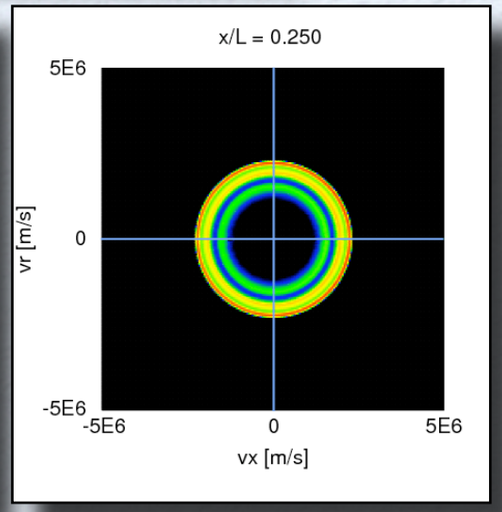
***E/n* = 50 Td, *L* = 5 cm, *p* = 1 Torr**

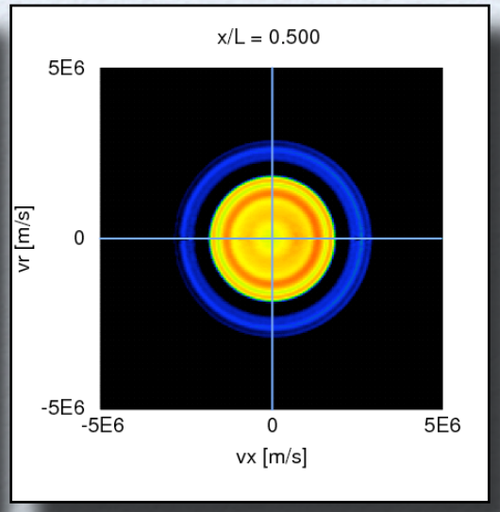


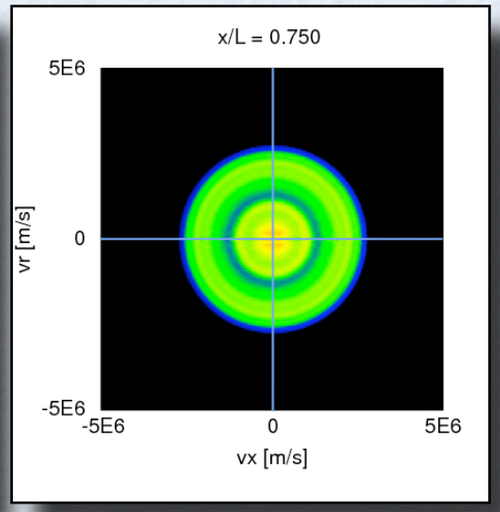



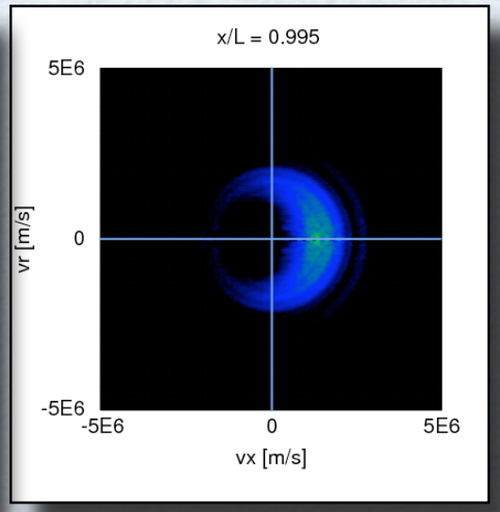

Complete lack of equilibrium region



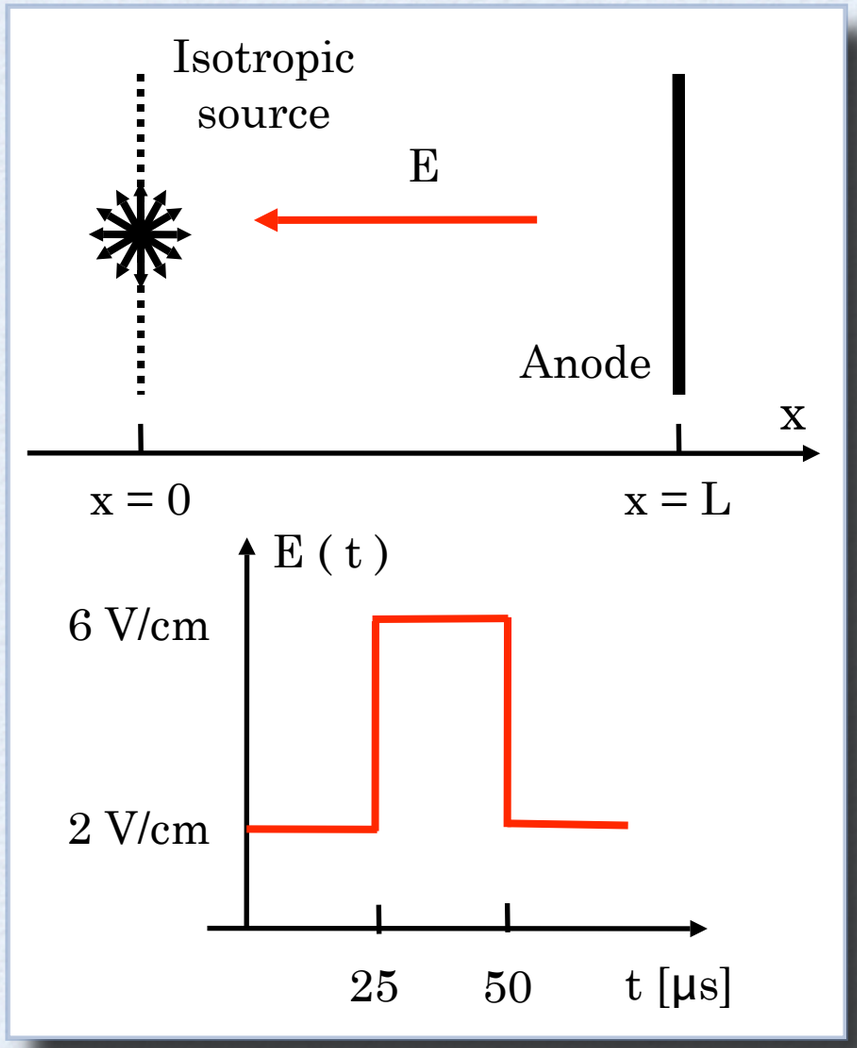



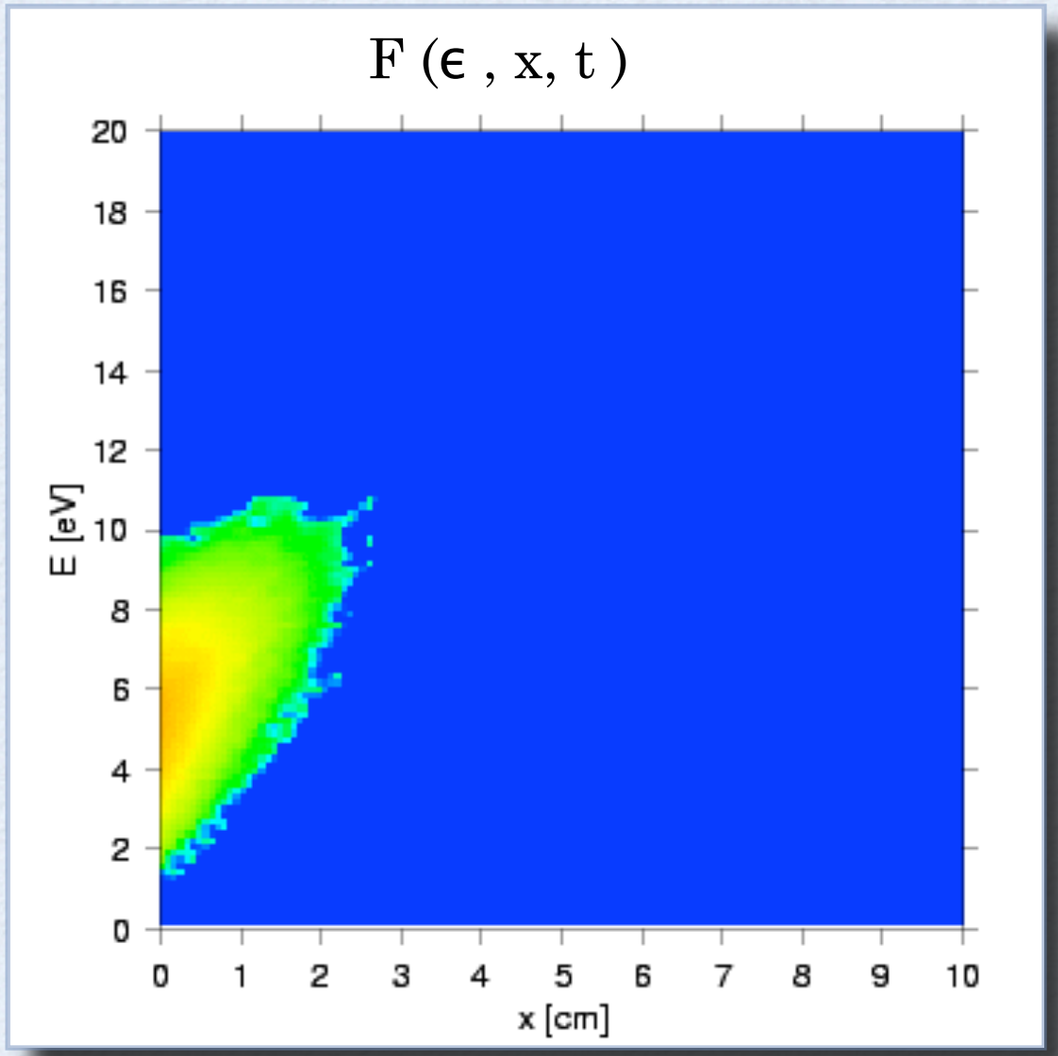



# Spatio-temporal relaxation of an electron swarm



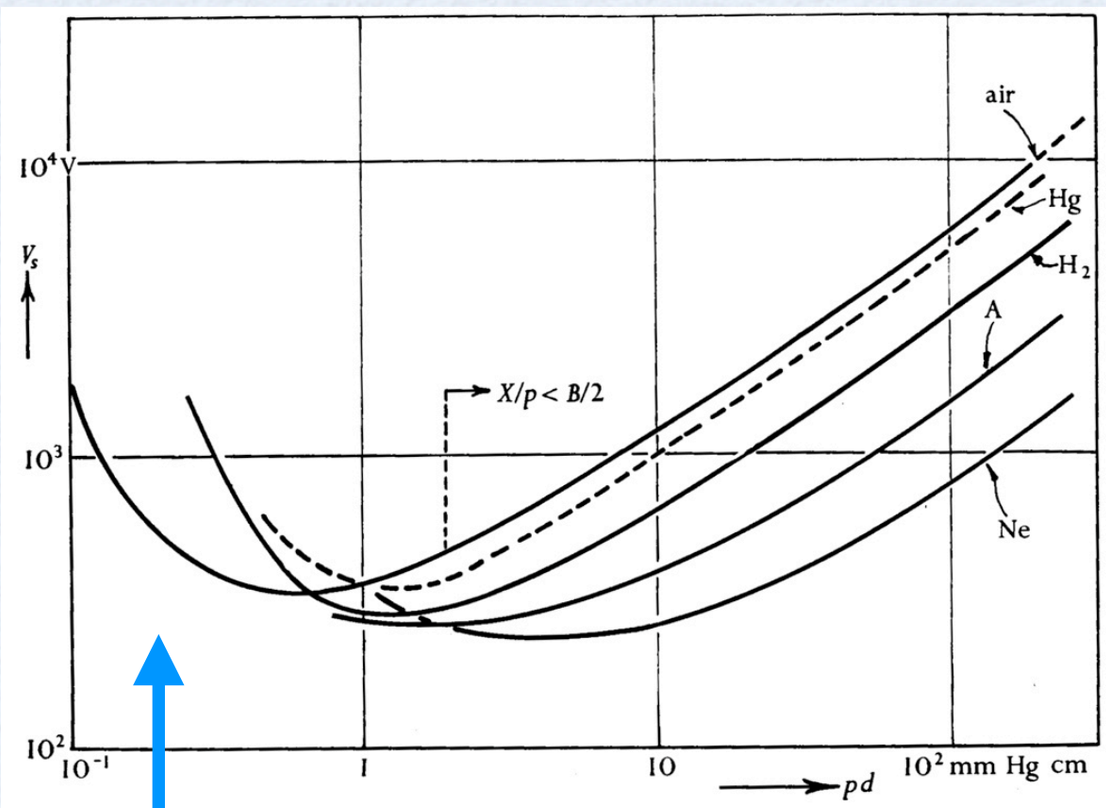




D. Loffhagen, R. Winkler, Z. Donkó, Eur. Phys. J. Appl. Phys. **18**, 189 (2002).

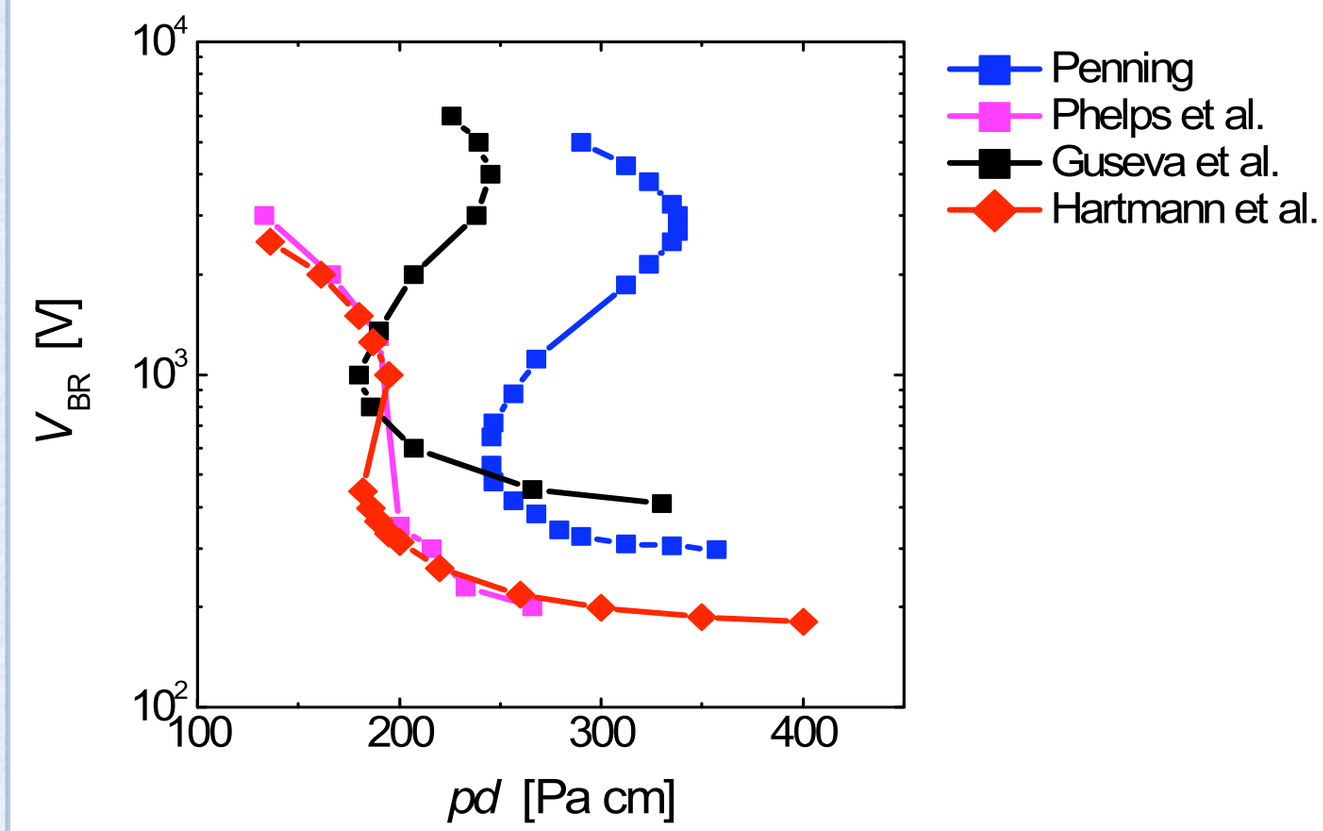
(calculated with both MC simulation and Boltzmann equation)

# Gas breakdown

Paschen curve for Ar, Ne, Hg, ....




Measured breakdown curves for helium gas:




Electron motion at left side of the Paschen curve becomes highly nonlocal → need for kinetic description

What causes the strange shape for Helium ??

P. Hartmann, Z. Donkó, G. Bánó, L. Szalai, K. Rózsa, Plasma Sources Sci. Technol. **9**, 183 (2000).

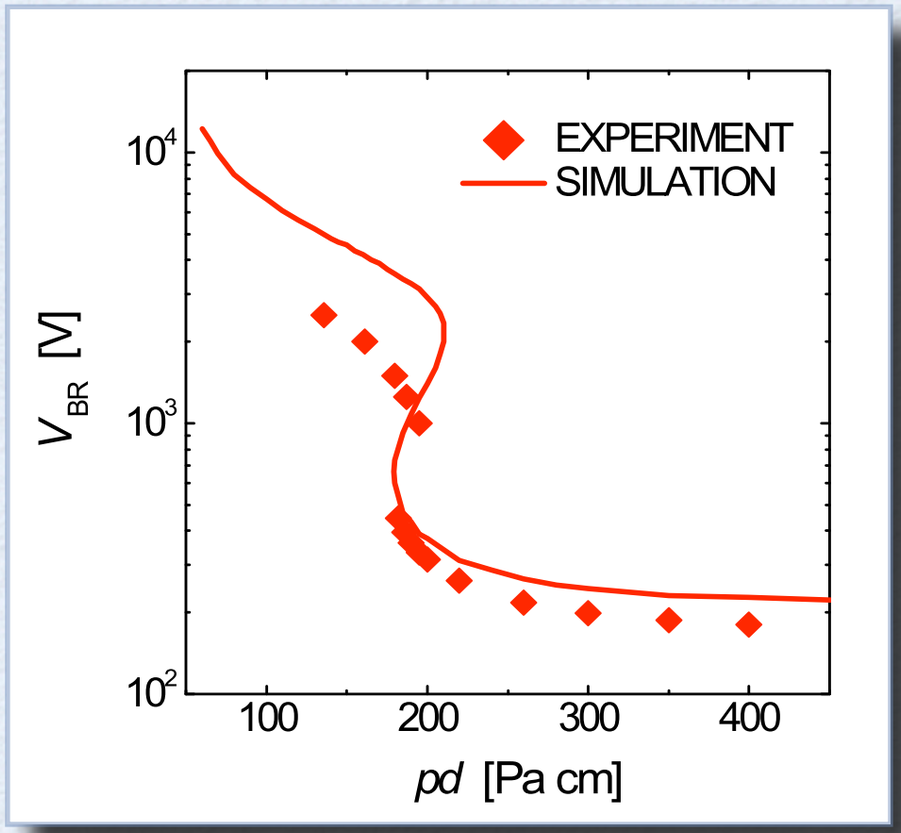
# Paschen curve in helium

Simulation including the Monte Carlo treatment of electrons, ions, as well as fast atoms

| | |
|---|---|
| $e^- + X \rightarrow e^- + X$ | Elastic collision |
| $e^- + X \rightarrow e^- + X^*$ | Excitation |
| $e^- + X \rightarrow 2e^- + X^+$ | Ionization |
| $X^+ + X \rightarrow X^+ + X^F$ | Elastic collision (isotropic part) |
| $X^+ + X \rightarrow X^+ + X^F$ | Elastic collision (backward part) |
| $X^+ + X \rightarrow X^+ + X^*$ | Excitation |
| $X^+ + X \rightarrow 2X^+ + e^-$ | Ionization |
| $X^F + X \rightarrow X^F + X^F$ | Elastic collision |
| $X^F + X \rightarrow X^F + X^*$ | Excitation |
| $X^F + X \rightarrow X^F + X^+ + e^-$ | Ionization |

+ reasonable data for secondary yields for all these species

P. Hartmann, Z. Donkó, G. Bánó, L. Szalai, K. Rózsa, Plasma Sources Sci. Technol. **9**, 183 (2000).




What causes the strange shape for Helium ??

(i) ion-induced ionization,
(ii) secondary electron emission due to fast atoms

# II. Modeling of cold-cathode glow discharges

- Fluid models - how far can we go without kinetic simulations?
- Hybrid models - ionization source calculated at kinetic level
- Heavy-particle hybrid models
- Applications

# Self-consistent gas discharge models: a simple fluid model

- Self-consistent = ???
- What do we need for the mathematical description ?

Continuity equations:

$$\frac{\partial n_\mathrm{i}}{\partial t} + \frac{\partial \phi_\mathrm{i}}{\partial x} = S_\mathrm{i}$$

$$\frac{\partial n_\mathrm{e}}{\partial t} + \frac{\partial \phi_\mathrm{e}}{\partial x} = S_\mathrm{e}$$

Momentum transfer:

$$\phi_\mathrm{i} = \mu_\mathrm{i} n_\mathrm{i} E - \frac{\partial (n_\mathrm{i} D_\mathrm{i})}{\partial x}$$

$$\phi_\mathrm{e} = -\mu_\mathrm{e} n_\mathrm{e} E - \frac{\partial (n_\mathrm{e} D_\mathrm{e})}{\partial x}$$

Poisson equation:

$$\Delta V = -\frac{e}{\varepsilon_0}(n_+ - n_-)$$

Source functions

$$S_- = S_+ = \alpha \Phi_-$$

$$\alpha/n = f(E/n)$$

local field approximation

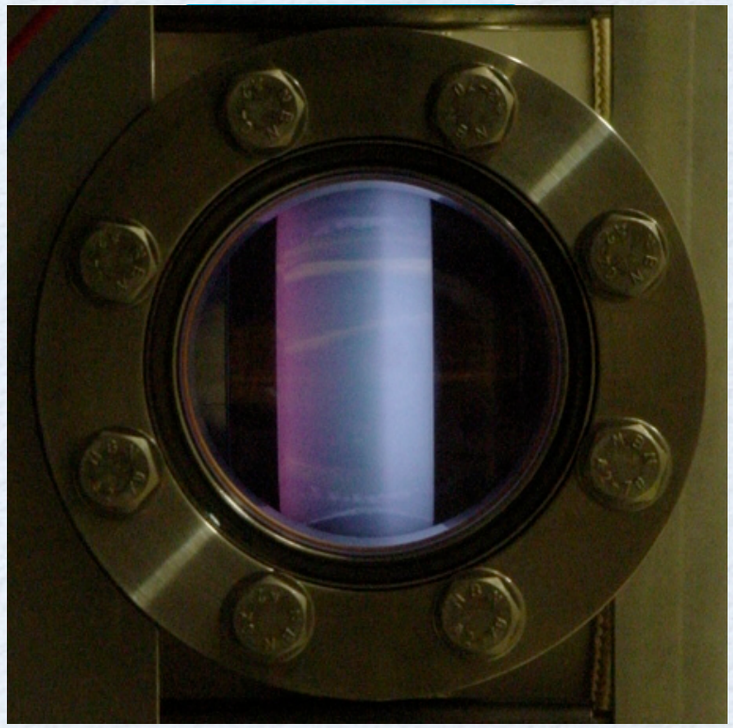
Boundary conditions:

$$V(0) = 0, V(L) = V_0$$

$$\left.\frac{\partial n_\mathrm{i}}{\partial x}\right|_0 = 0 \qquad n_\mathrm{i}(L) = 0$$

$$n_\mathrm{e}(0) v_\mathrm{e}(0) = \gamma n_\mathrm{i}(0) v_\mathrm{i}(0)$$

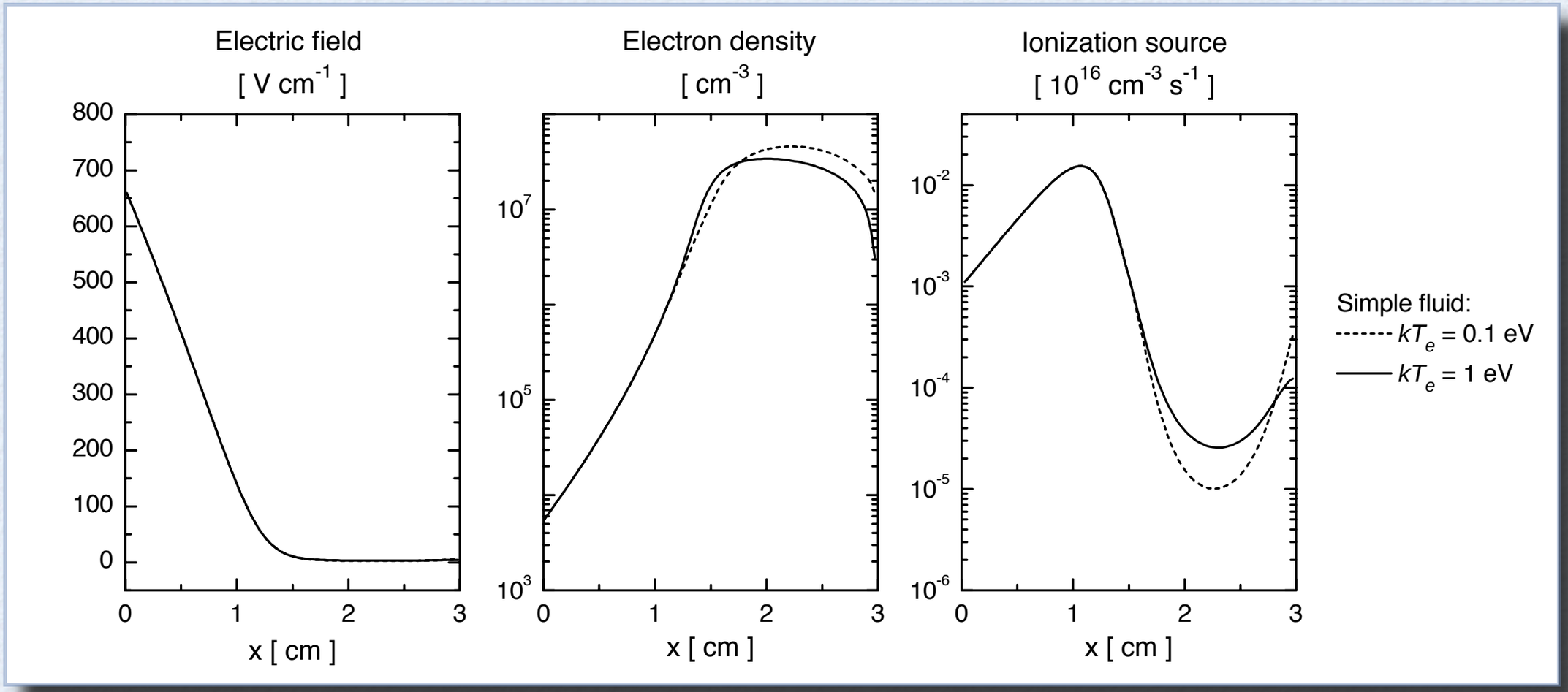
$$n_\mathrm{e}(L) = 0$$



- **Cold-cathode abnormal glow**
- 1 dimension
- "short discharge": D >> L
- Radial losses can be neglected
- 1-dimensional model
- Processes:
  - Drift
  - Diffusion
  - Ionization

# Results: simple fluid model

$p$ = 40 Pa (Ar), $V$ = 441 V, $T_g$ = 300 K, $L$ = 3 cm, $\gamma$ = 0.033




Cathode sheath + negative glow structure reproduced
Using $E/n$-dependent transport parameters is problematic → Can we do better?

Z. Donkó, P. Hartmann, K. Kutasi, Plasma Sources Sci. Technol. **15**, 178 (2006)
W. J. M. Brok, personal communication

# Extended fluid model

**Energy equation & Ionization source**

**Use 3rd moment of BE; equation for energy density ( $n_\varepsilon = n_\mathrm{e}\bar{\varepsilon}$ ):**

$$\frac{\partial n_\varepsilon}{\partial t} + \frac{\partial \phi_\varepsilon}{\partial x} = S_\varepsilon - L_\varepsilon$$

Energy source from field:

$$S_\varepsilon(x) = -E(x)\phi_\mathrm{e} e$$

Energy flux:

$$\phi_\varepsilon = -\mu_\varepsilon n_\varepsilon E - \frac{\partial(n_\varepsilon D_\varepsilon)}{\partial x}$$

Energy loss due to collisions:

$$L_\varepsilon(x) = k_L[\bar{\varepsilon}(x)]n_e(x)$$

**Possibilities to calculate the ionization source:**

Flux - based: $S(x) = \alpha[\bar{\varepsilon}(x)]|\phi_\mathrm{e}(x)|$

Rate coefficient - based: $S(x) = k_\mathrm{i}[\bar{\varepsilon}(x)]n_\mathrm{e}(x)N$

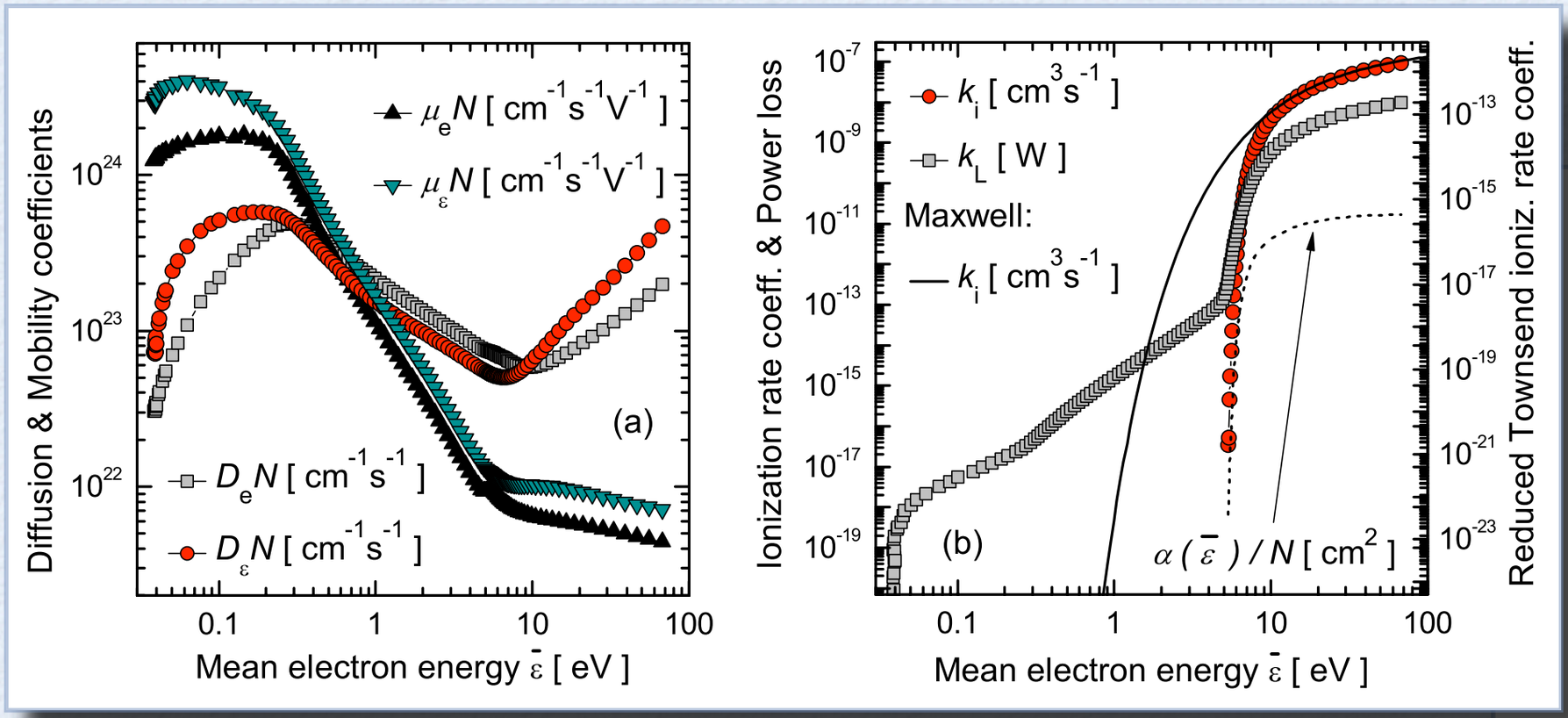
$$k_\mathrm{i}(\bar{\varepsilon}) = \sqrt{\frac{2e}{m}}\int_0^\infty \varepsilon\sigma_\mathrm{i}(\varepsilon)F_0(\varepsilon)\mathrm{d}\varepsilon$$

see e.g. G J M Hagelaar and L C Pitchford, Plasma Sources Sci. Technol. **14,** 722 (2005)

# Extended fluid model

**Transport coefficients & rates**

To obtain these data: (1) carry out swarm calculations (MC) for a series of E/n values, and (2) organize the data as a function of the electron mean energy




$$\phi_{\rm i} = \mu_{\rm i} n_{\rm i} E - \frac{\partial(n_{\rm i} D_{\rm i})}{\partial x}$$

$$\phi_{\rm e} = -\mu_{\rm e} n_{\rm e} E - \frac{\partial(n_{\rm e} D_{\rm e})}{\partial x}$$

$$\phi_\varepsilon = -\mu_\varepsilon n_\varepsilon E - \frac{\partial(n_\varepsilon D_\varepsilon)}{\partial x}$$

$$L_\varepsilon(x) = k_L[\bar{\varepsilon}(x)] n_e(x)$$

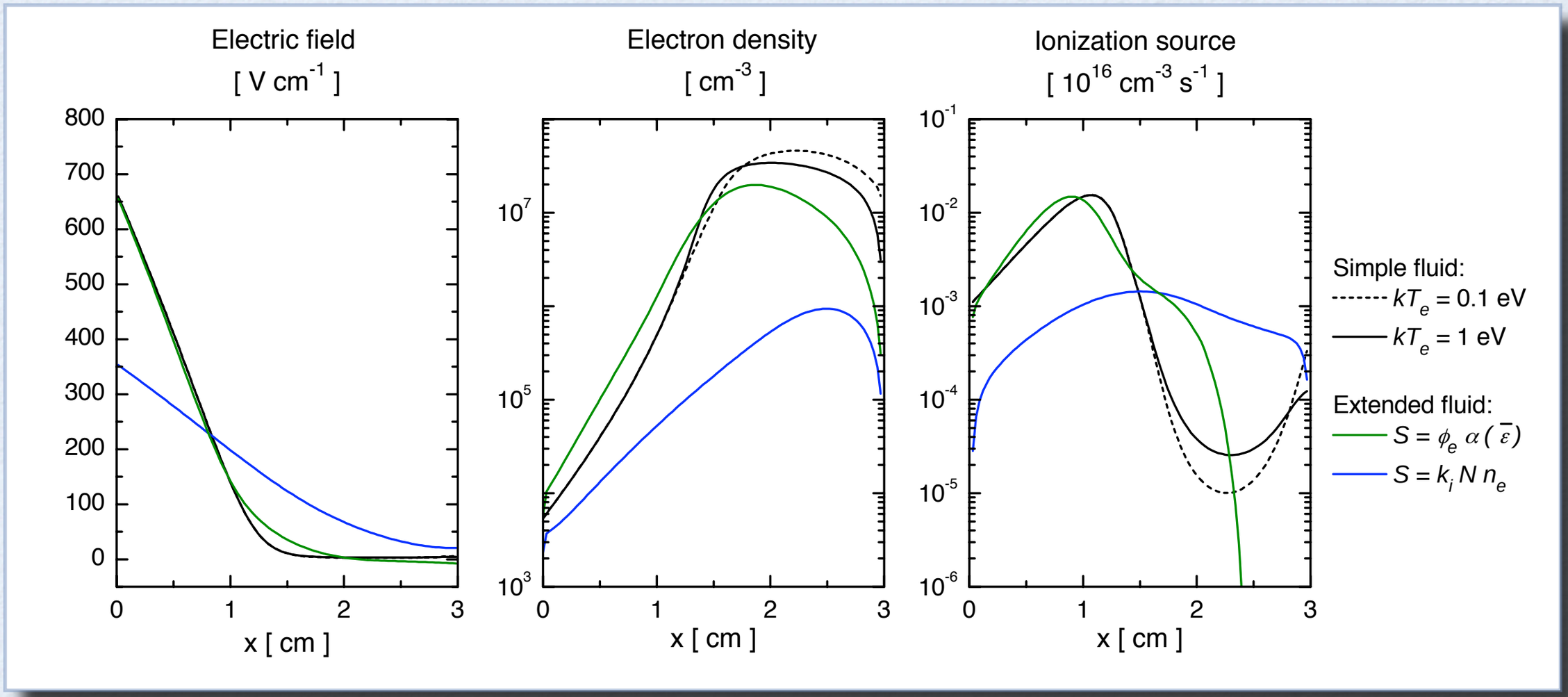
$$k_{\rm i}(\bar{\varepsilon}) = \sqrt{\frac{2e}{m}} \int_0^\infty \varepsilon \sigma_{\rm i}(\varepsilon) F_0(\varepsilon) {\rm d}\varepsilon$$

A. Derzsi, P. Hartmann, I. Korolov, J. Karácsony, G. Bánó, and Z Donkó, J. Phys. D: Appl. Phys. **42,** 225204 (2009)

M. M. Becker, D. Loffhagen, and W. Schmidt, Comput. Phys. Commun. **180**, 1230 (2009), .... and many groups before...

# Extended fluid model : results

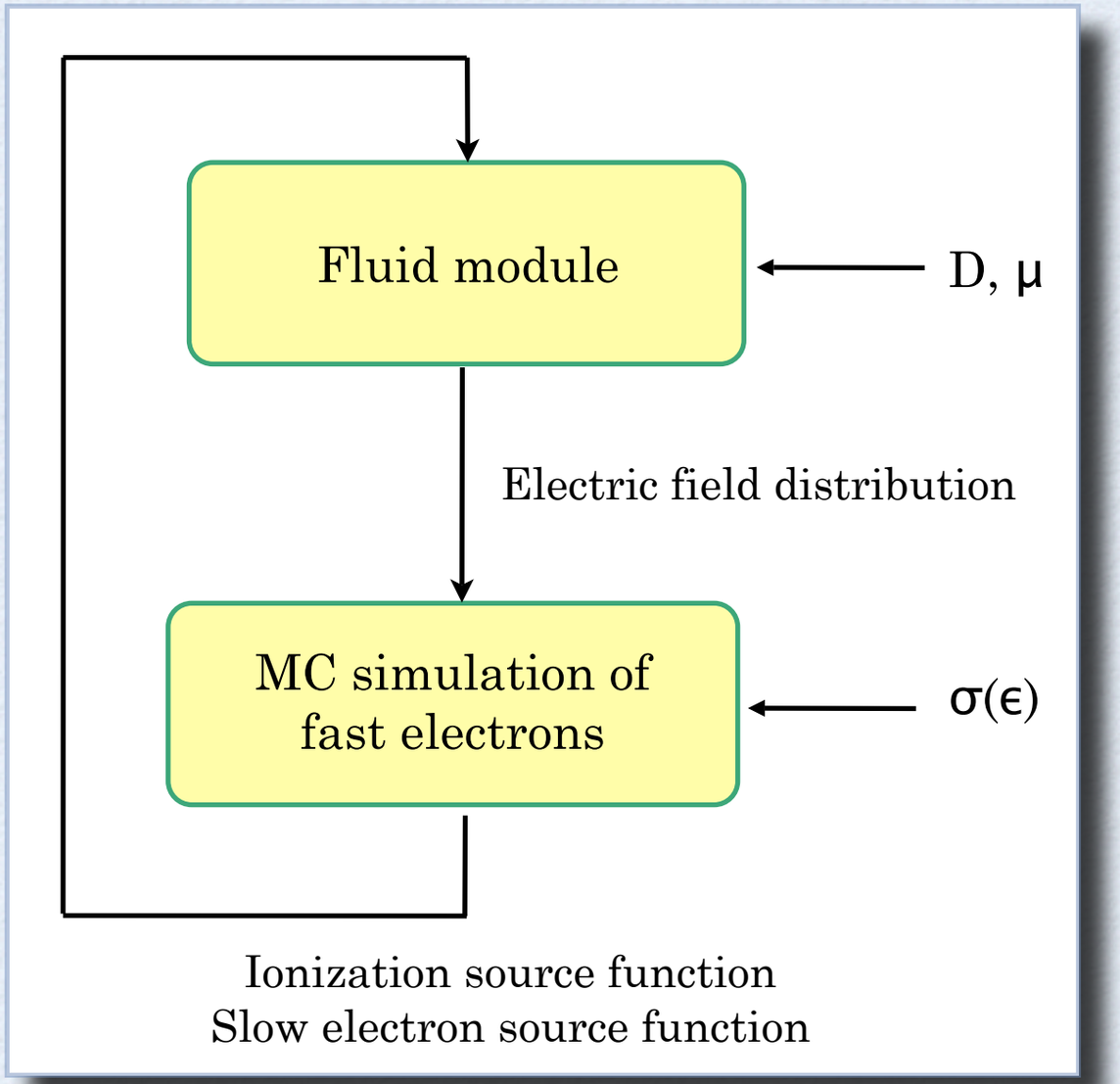
$p$ = 40 Pa (Ar), $V$ = 441 V, $T_g$ = 300 K, $L$ = 3 cm, $\gamma$ = 0.033




Most of the results are close to those of "simple" fluid models
Extended fluid model with flux-based source calculation predicts a field reversal

BUT: still large differences between the results of different models → Can we do better?

# Hybrid model




**The idea:**

calculate the ionization source from kinetic simulation of fast electrons

Monte Carlo simulation - becomes inefficient for slow electrons - treat slow electrons as fluid


M. Surendra, D. B. Graves, and G. M. Jellum, Phys. Rev. A **41**, 1112 (1990).

J. P. Boeuf and L. C. Pitchford, IEEE Trans. Plasma Sci. **19**, 286 (1991).

A. Fiala, L. C. Pitchford, and J. P. Boeuf, Phys. Rev. E **49**, 5607 (1994).

A. Bogaerts, R. Gijbels, and W. J. Goedheer, J. Appl. Phys. **78**, 2233 (1995).

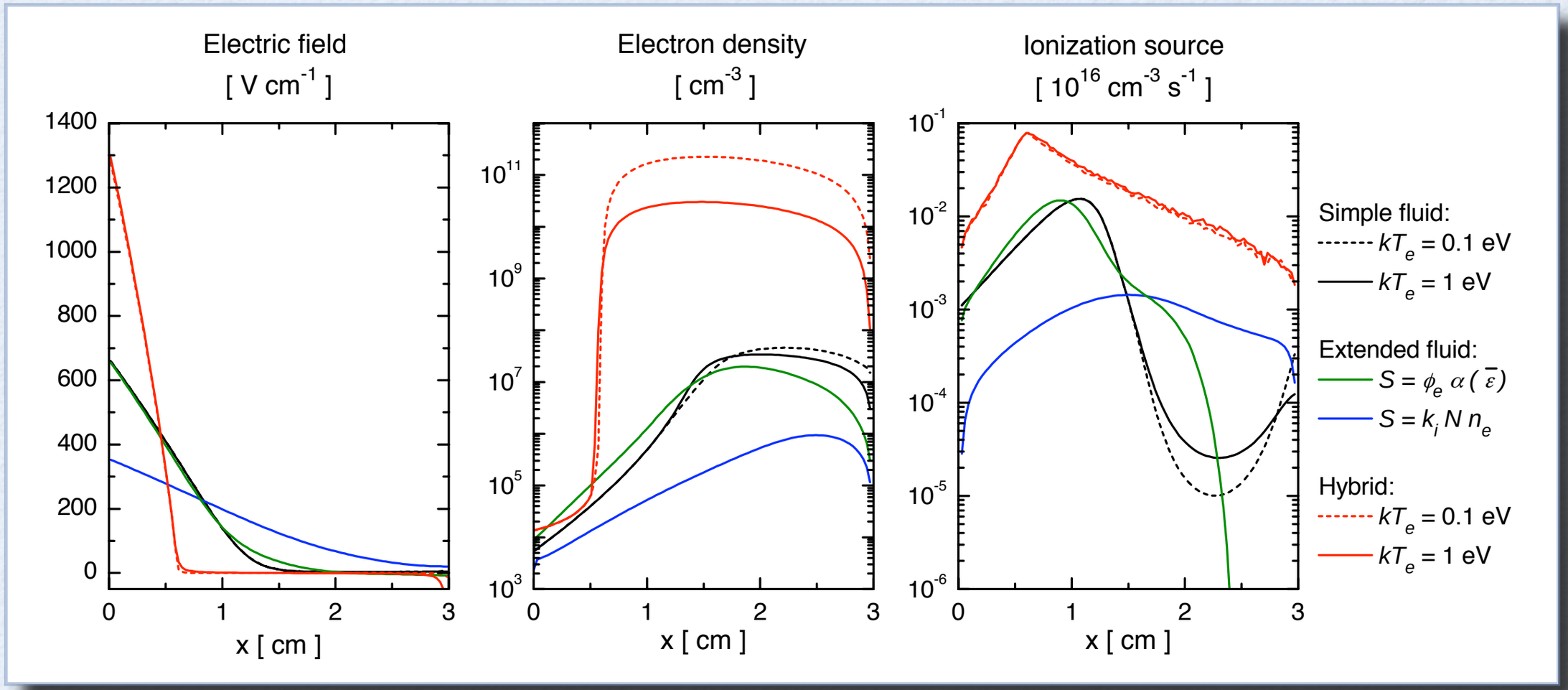

$$S_{\mathrm{i,e}}(x) = \frac{j}{e(1+1/\gamma)\Delta x}\frac{N_{\mathrm{i,e}}(x)}{N_0^{\mathrm{MC}}}$$

$$\frac{\partial n_{\mathrm{i}}}{\partial t} + \frac{\partial \phi_{\mathrm{i}}}{\partial x} = S_{\mathrm{i}}$$

$$\frac{\partial n_{\mathrm{e}}}{\partial t} + \frac{\partial \phi_{\mathrm{e}}}{\partial x} = S_{\mathrm{e}}$$

# Hybrid model : results

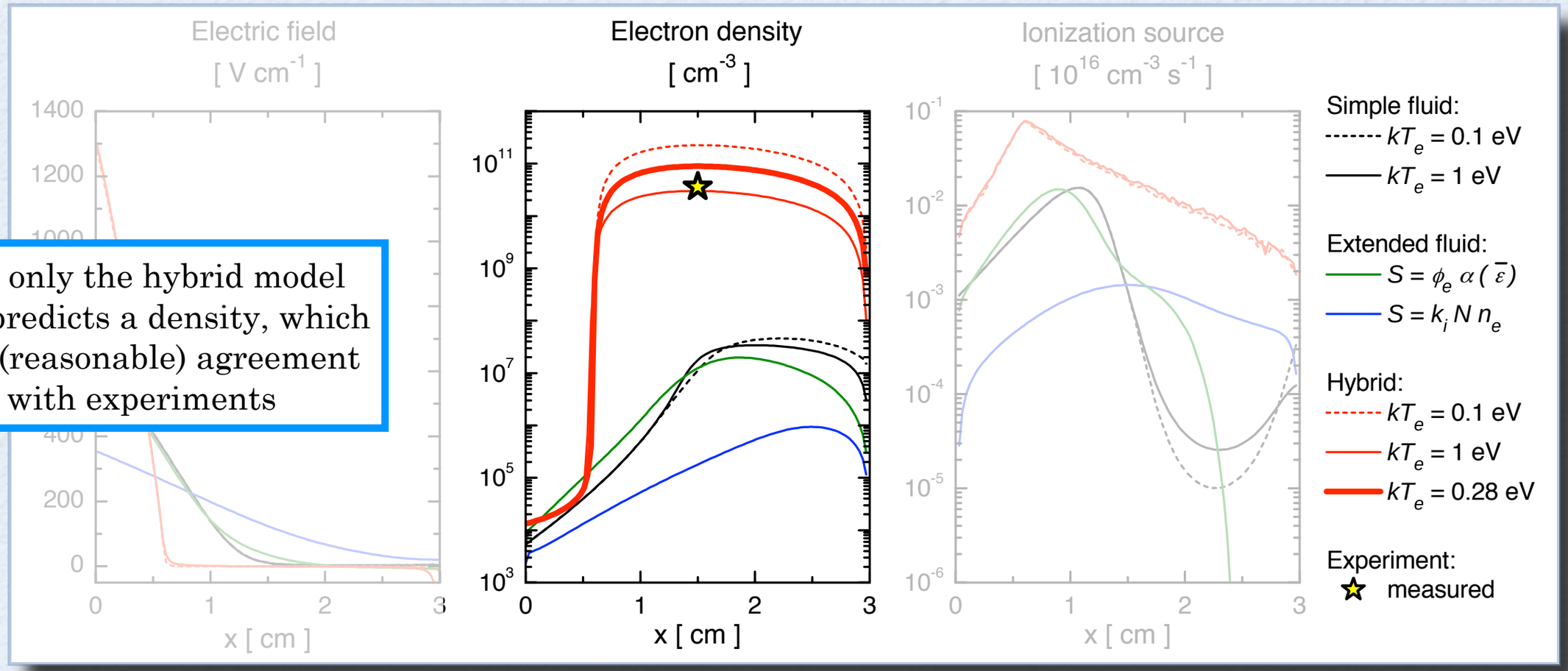
$p$ = 40 Pa (Ar), $V$ = 441 V, $T_g$ = 300 K, $L$ = 3 cm, $\gamma$ = 0.033




Significant differences: e.g. orders of magnitude difference between the charge densities

"On the accuracy and limitations of fluid models of the cathode region of dc glow discharges"
A. Derzsi, P. Hartmann, I. Korolov, J. Karácsony, G. Bánó, and Z Donkó, J. Phys. D: Appl. Phys. **42,** 225204 (2009)

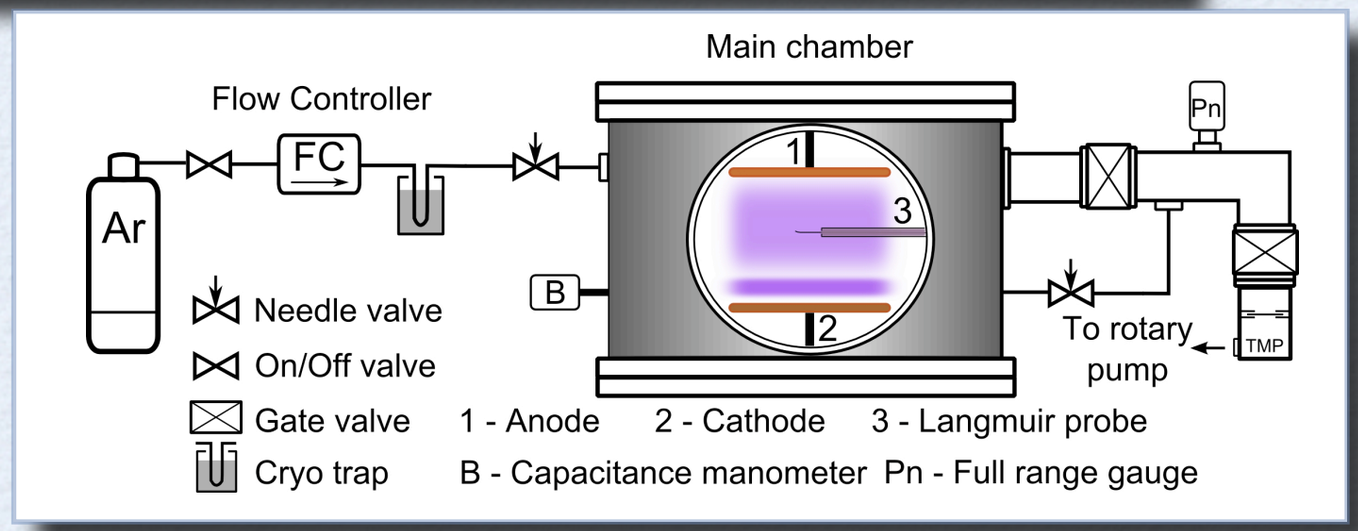
# Hybrid model : consistency (1)




It is only the hybrid model that predicts a density, which is in (reasonable) agreement with experiments

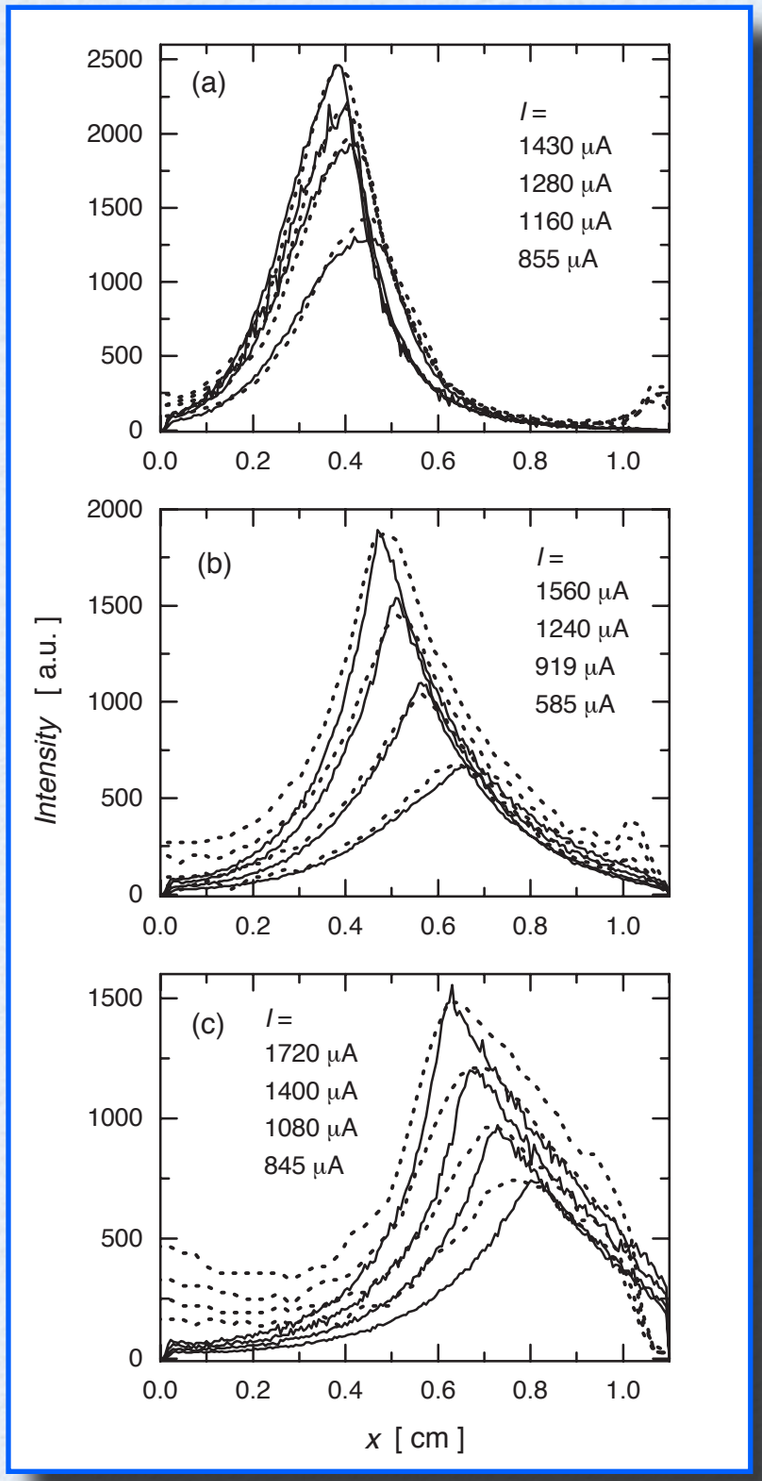
$p$ = 40 Pa (Ar),
$V$ = 441 V,
$T_g$ = 300 K,
$L$ = 3 cm,
$\gamma$ = 0.033

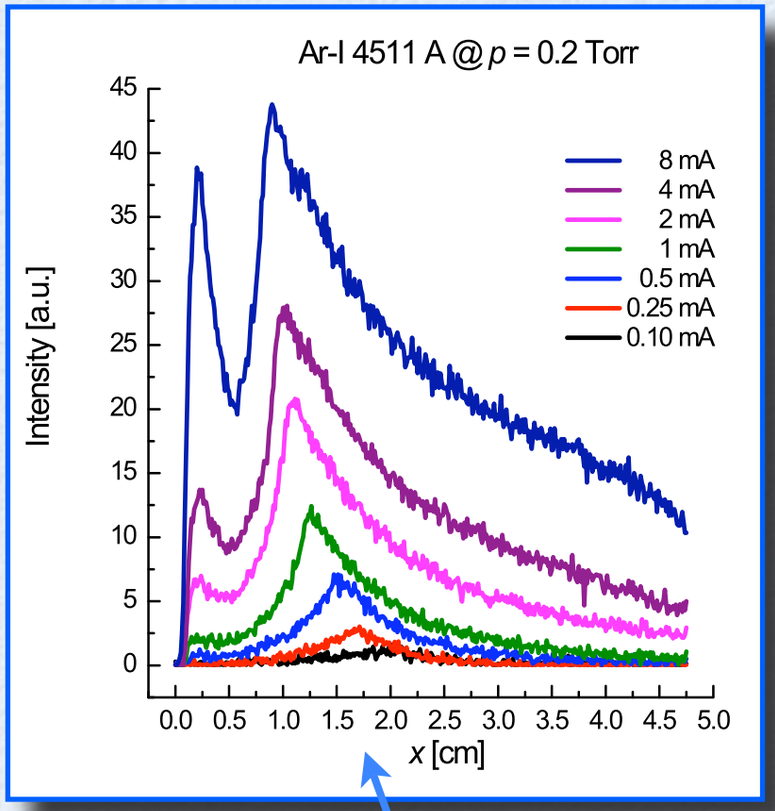
Measurements with Langmuir probe (poster of Ihor Korolov *et al.*)

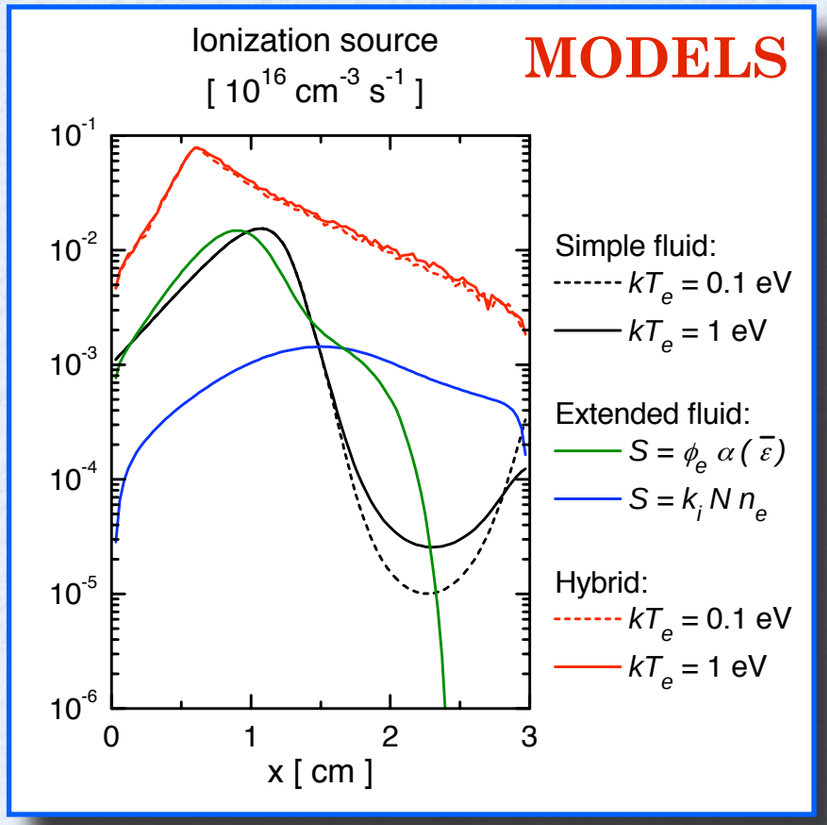



A. Derzsi, P. Hartmann, I. Korolov, J. Karácsony, G. Bánó, and Z Donkó, J. Phys. D: Appl. Phys. **42,** 225204 (2009)

# Hybrid model : consistency (2)




K. Rózsa, A. Gallagher and Z. Donkó: "Excitation of Ar lines in the cathode region of a DC discharge", Physical Review E **52**, 913-918 (1995)

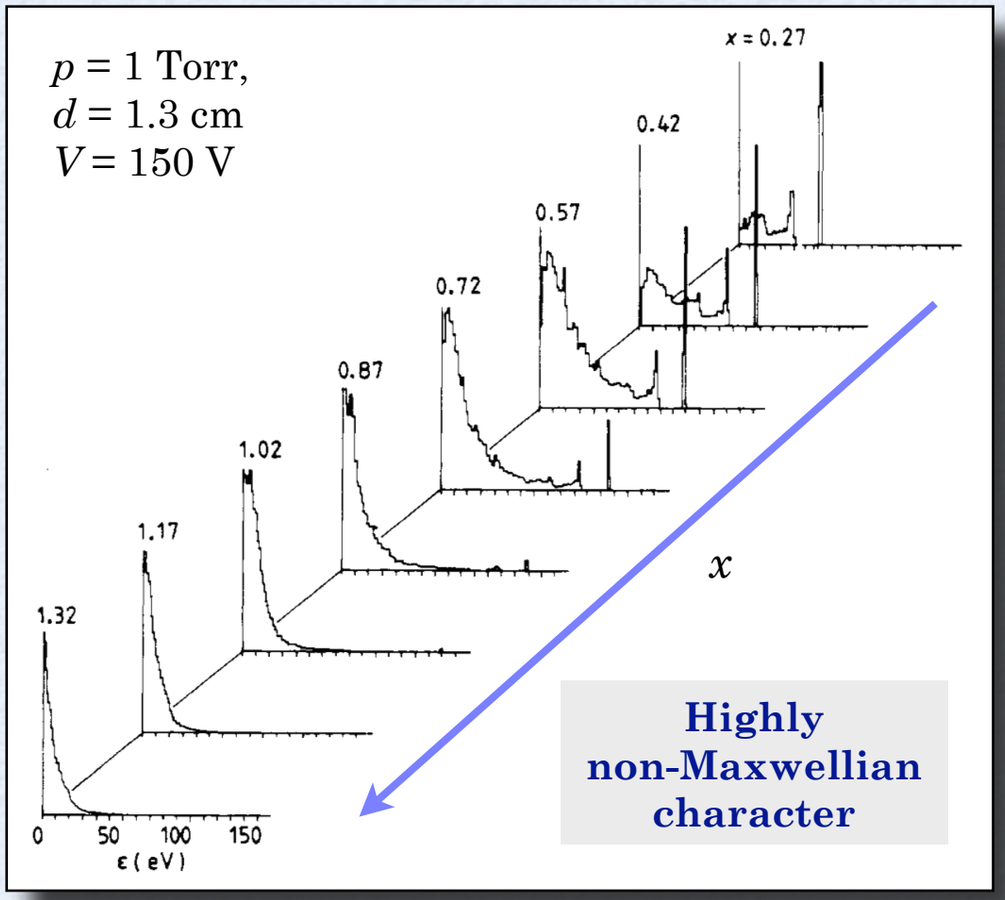
It is only the hybrid model that predicts an exponentially falling ionization (and excitation) source beyond the sheath-glow boundary

**EXPERIMENTS**

D. Marić, K. Kutasi, G. Malović, Z. Donkó and Z. Lj. Petrović: "Axial emission profiles and apparent secondary electron yield in abnormal glow discharges in argon", Eur. Phys. J D **21**, 73 (2002)

# Analysis of the distribution functions in the DC glow sheath

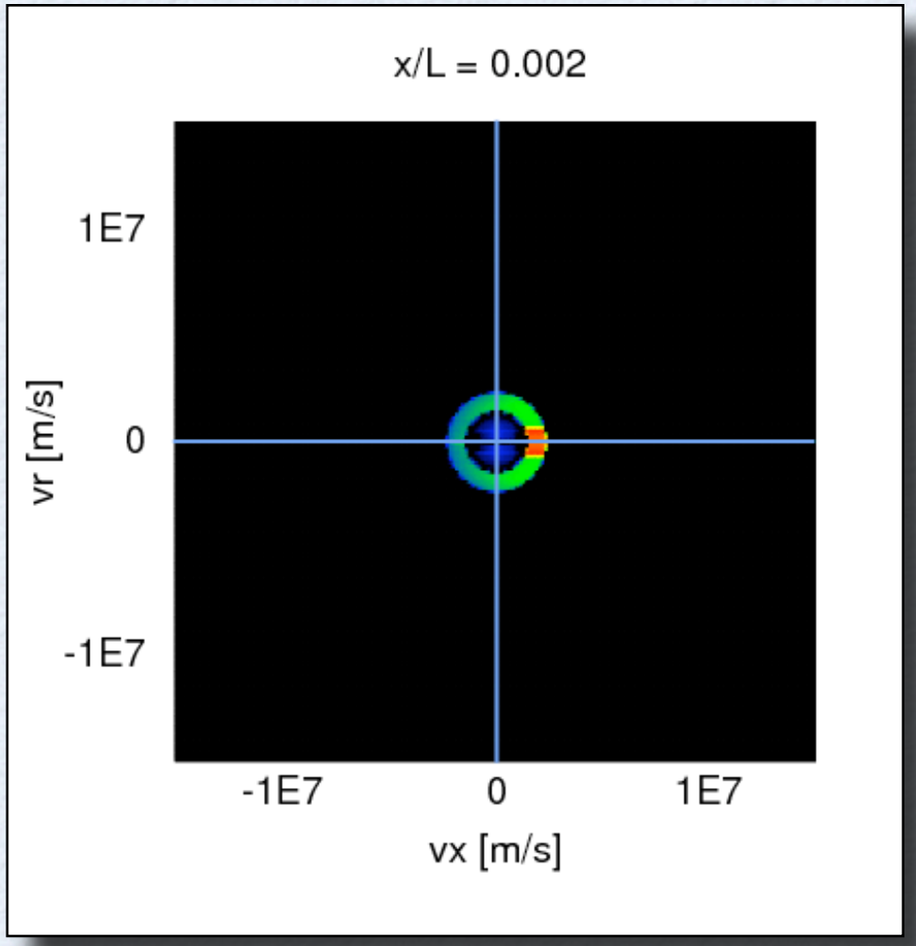
The spatial variation of the distribution function in the cathode sheath



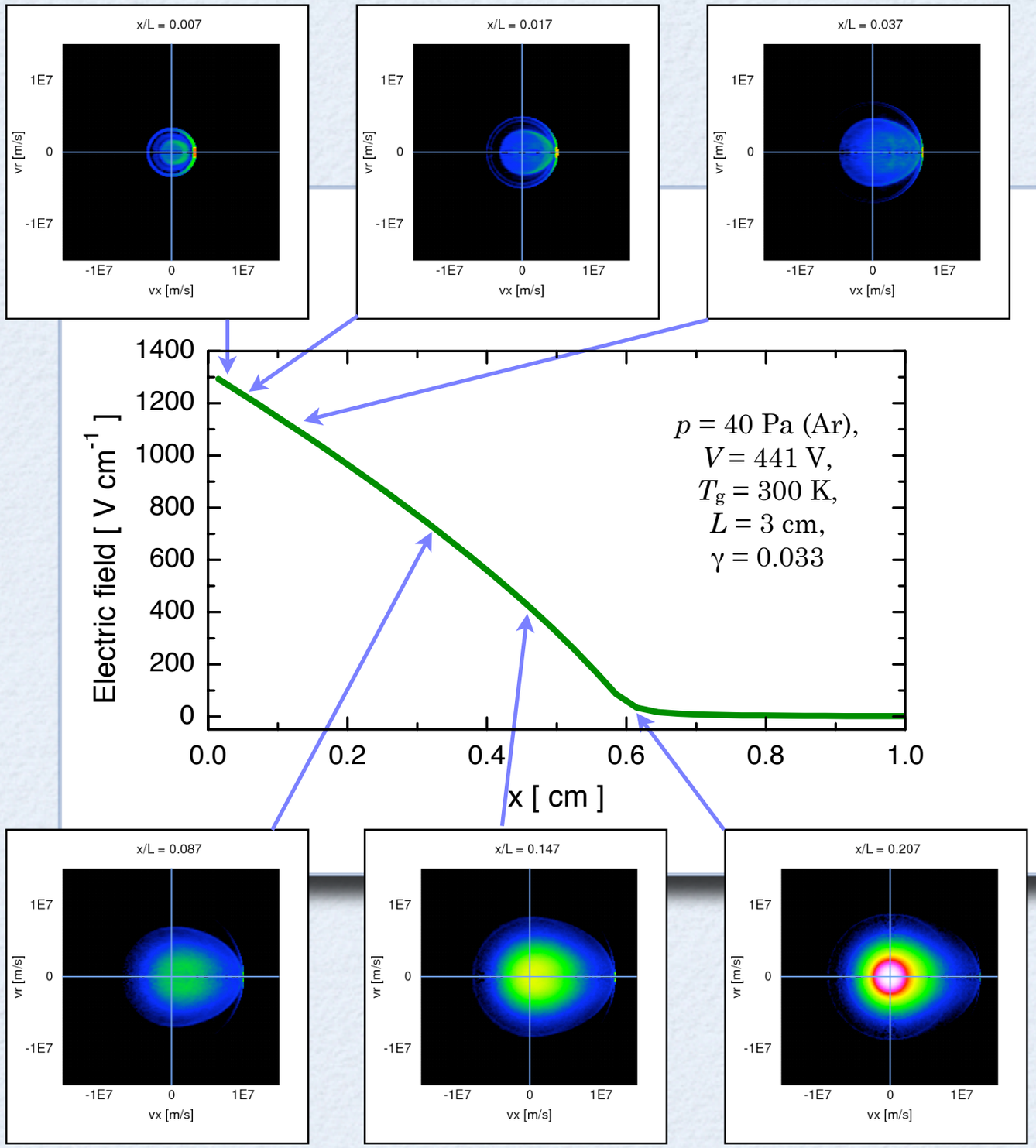

J. P. Boeuf and E. Marode J. Phys. D **15** 2169 (1982)
"A Monte Carlo analysis of an electron swarm in nonuniform field: the cathode region of a glow discharge in helium"

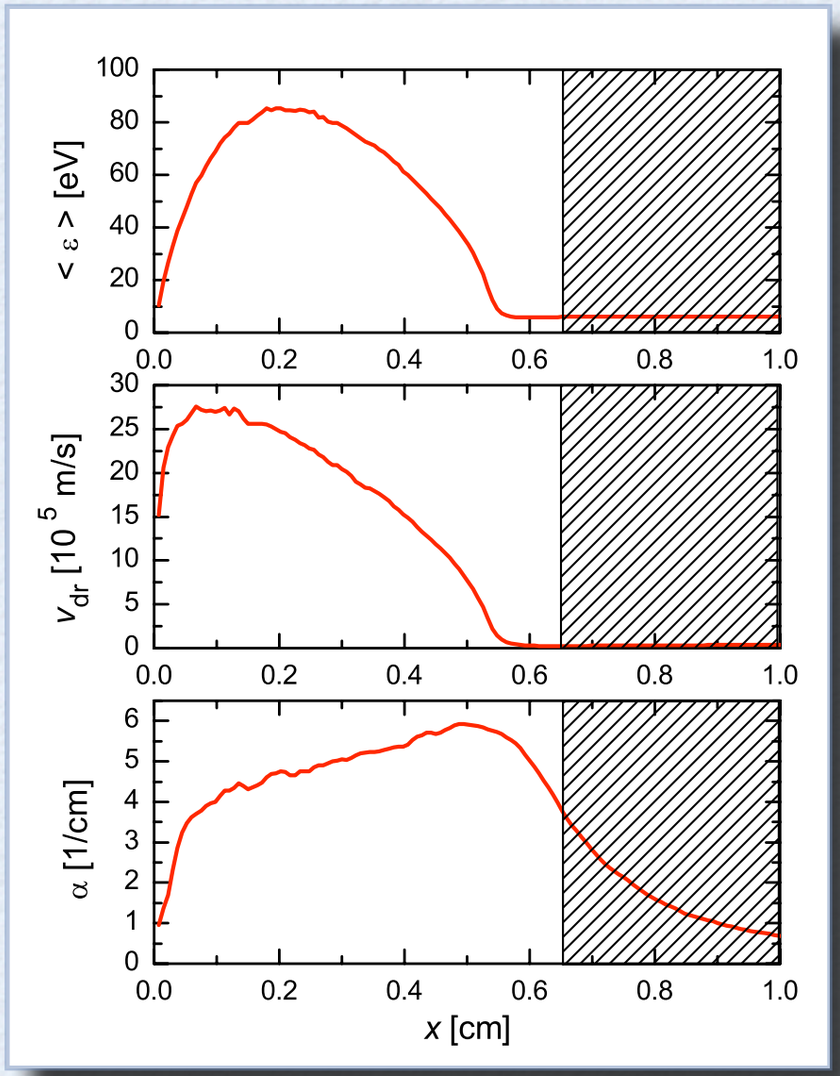
The VDF:

$p$ = 40 Pa (Ar), $V$ = 441 V, $T_g$ = 300 K,
$L$ = 3 cm, $\gamma$ = 0.033



# Analysis of the VDF in the DC glow sheath



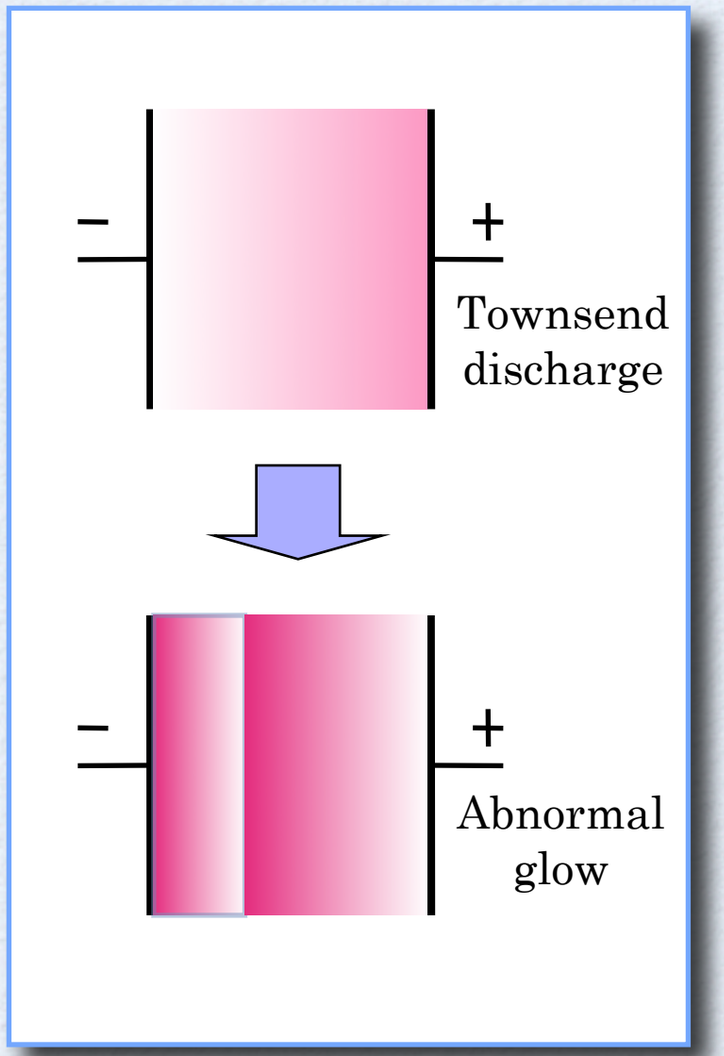



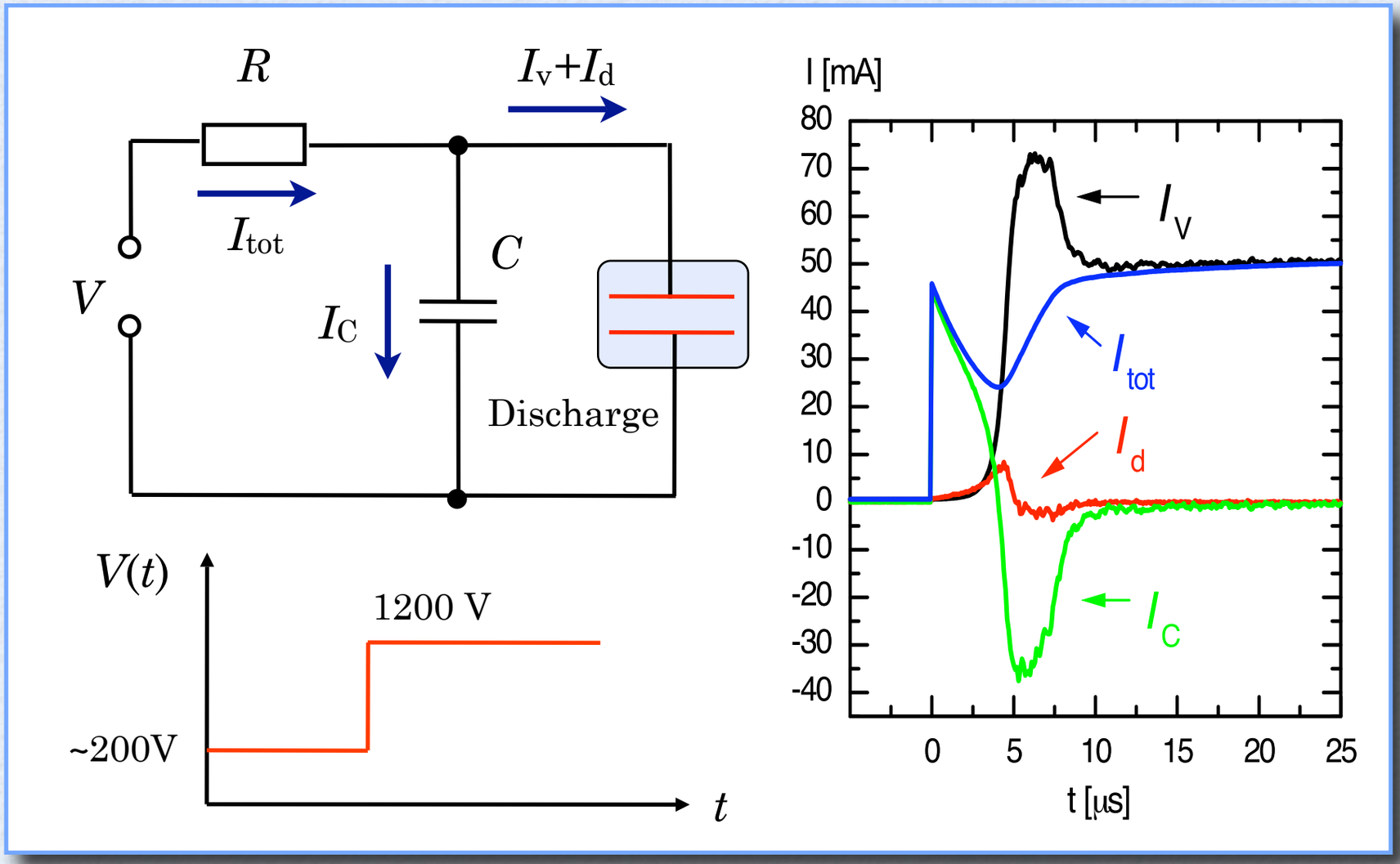

Conclusion: characteristic features captured by kinetic description only

# Application of hybrid models: (1) Townsend discharge – abnormal glow transition

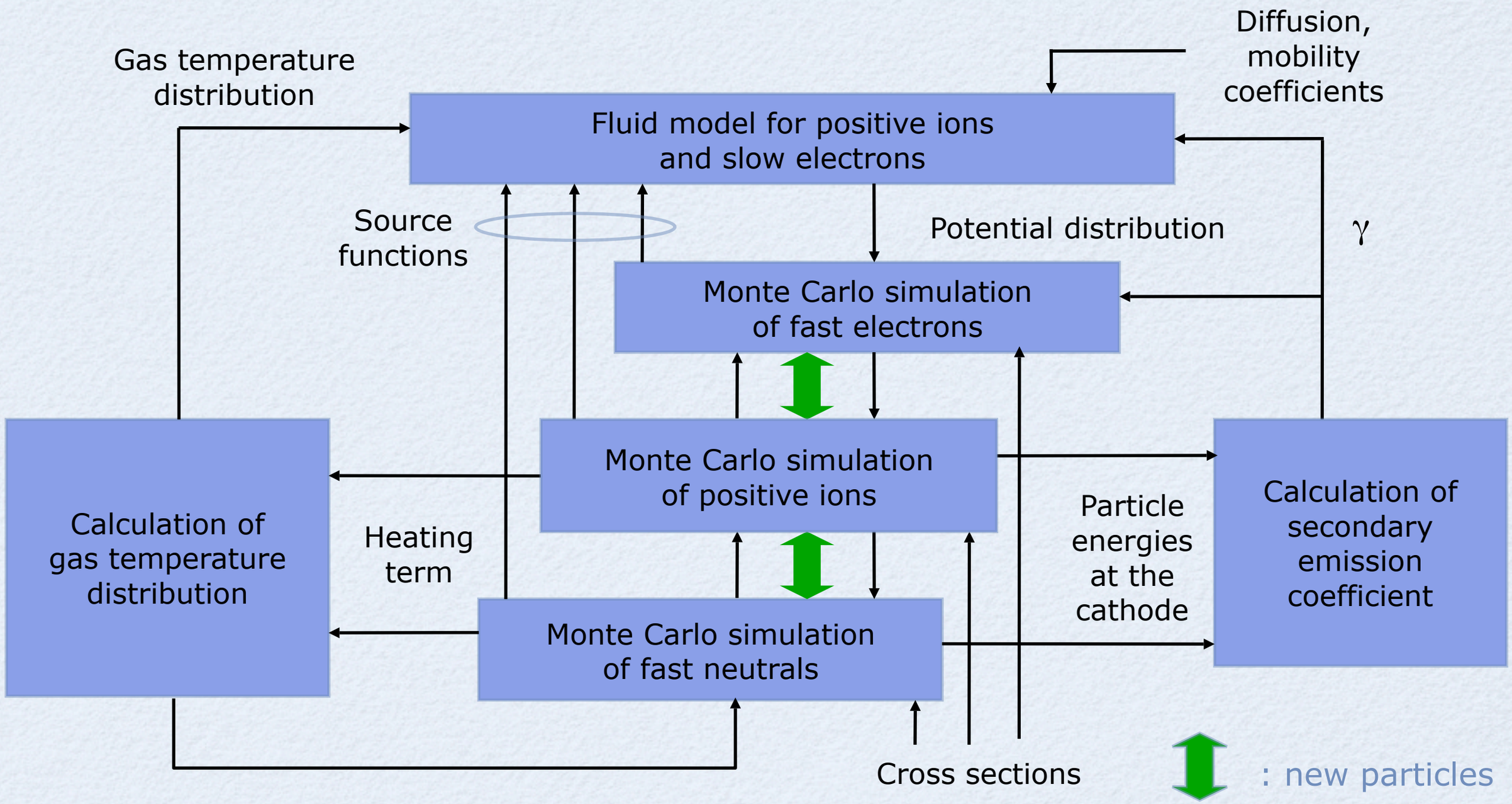
Experiments:
B. M. Jelenković and A. V. Phelps,
J. Appl. Phys. **85**, 7089 (1999)

Heavy particle hybrid model:
Monte Carlo simulation of *fast electrons*,
*fast positive ions* and *fast neutrals*



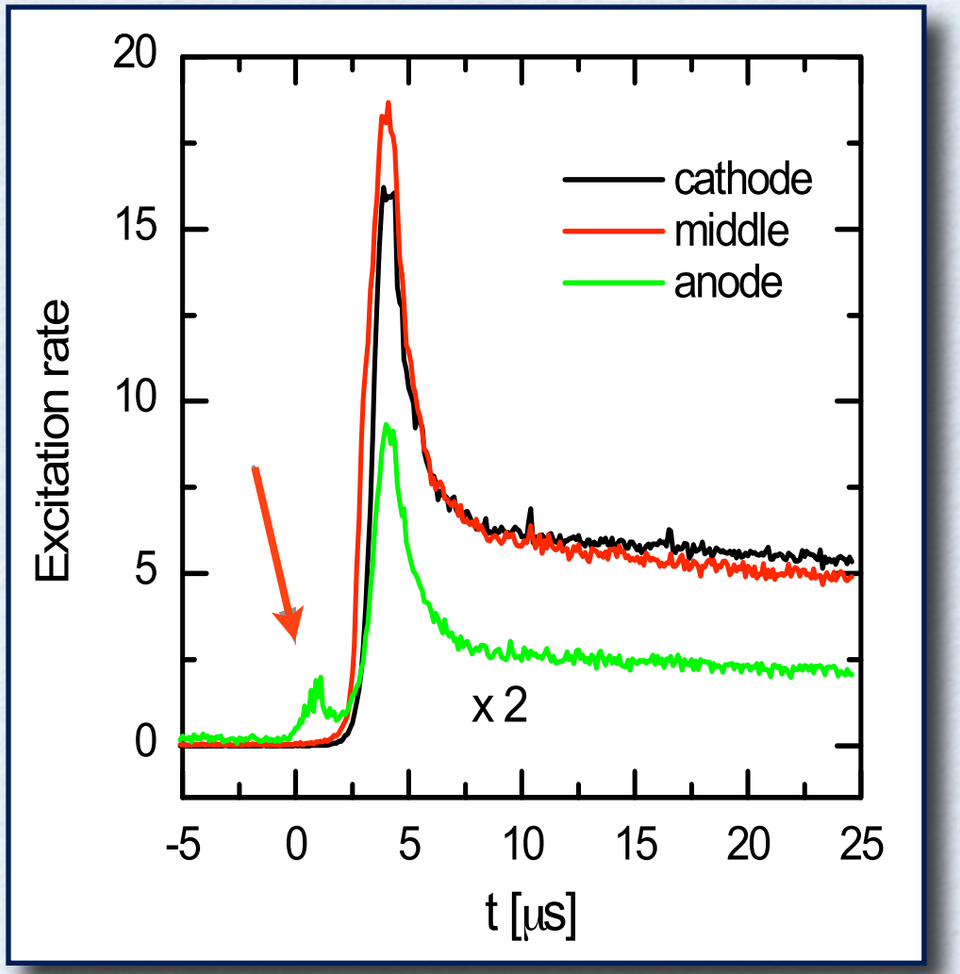
# Heavy-particle hybrid model



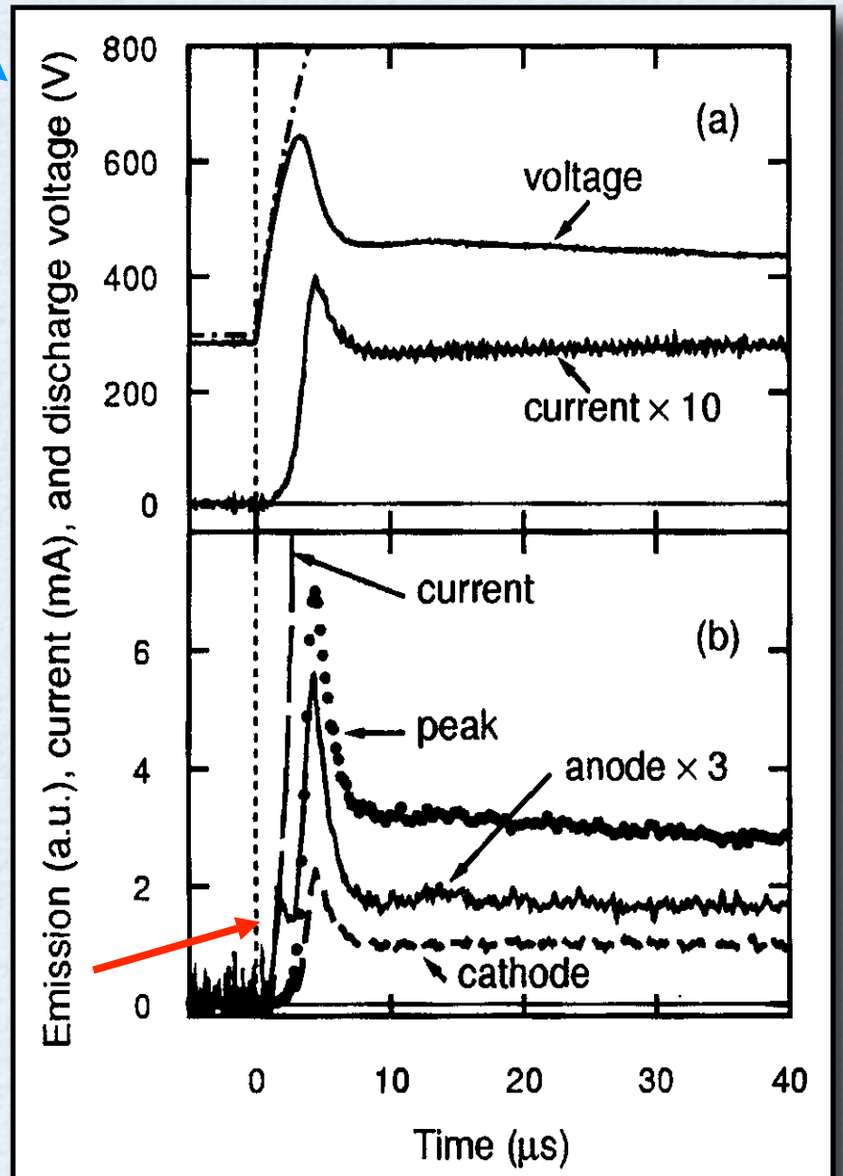

Z. Donkó, Phys. Rev. E **64**, 026401 (2001).

# Discharge transient: temporal changes of light intensity

Simulations




Measurement



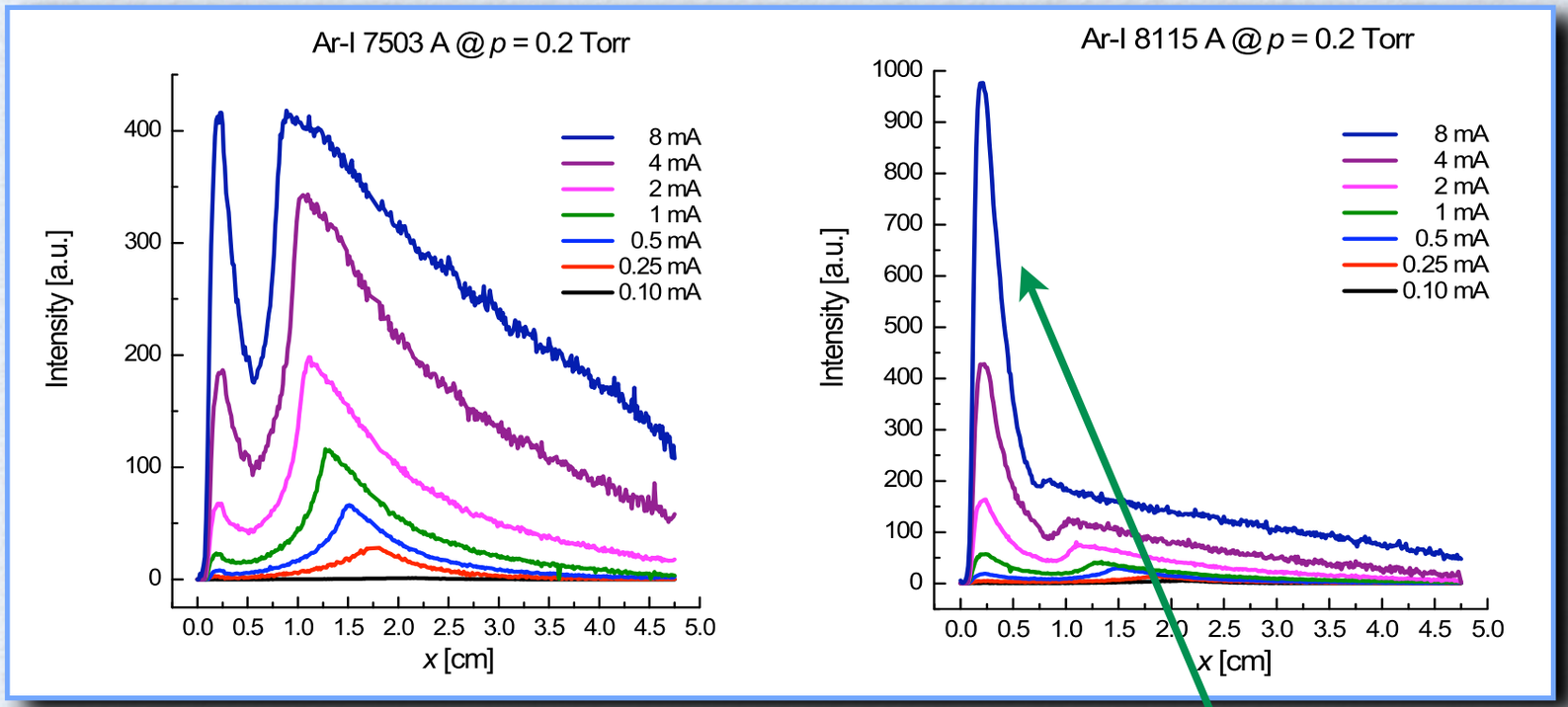

Z. Donkó, J. Appl. Phys. 88, 2226 (2000)

B. M. Jelenković and A. V. Phelps, J. Appl. Phys. 85, 7089 (1999)

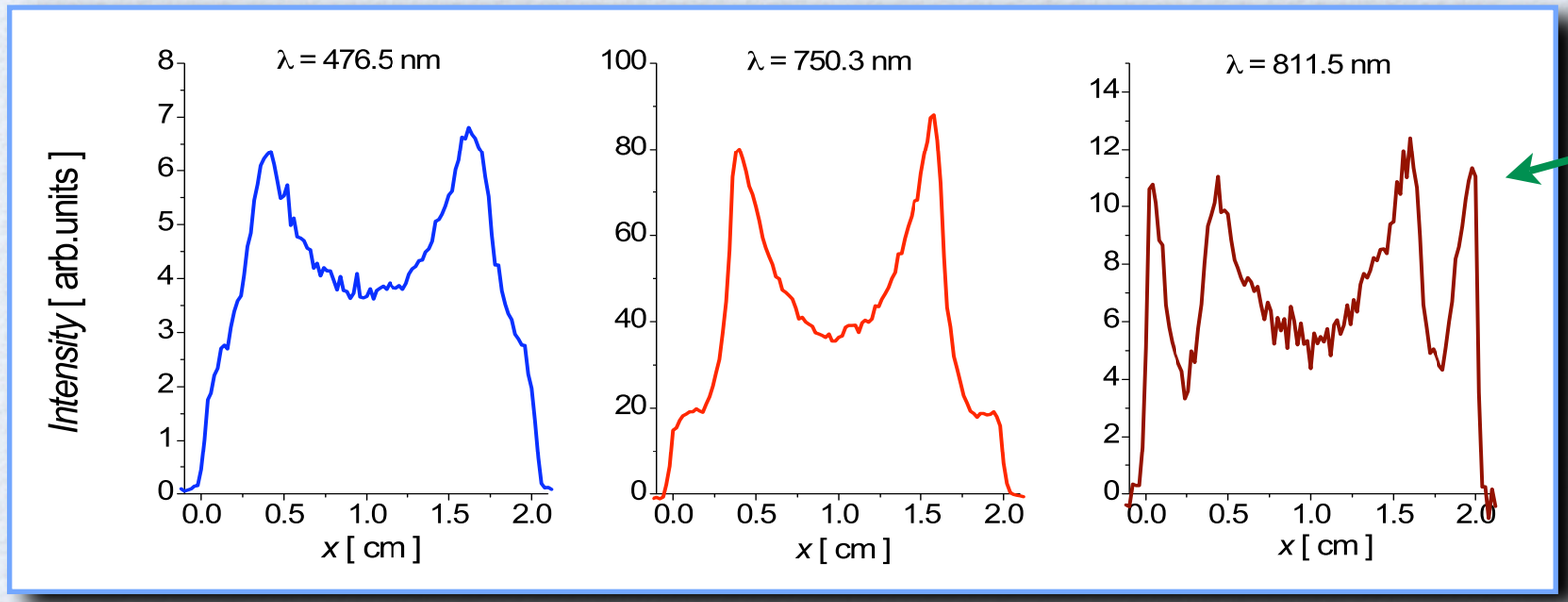
# Application of hybrid models:
# (2) Heavy-particle excitation in the cathode region

Spatial distributions of spectral line intensities over a plane cathode

K. Rózsa, A. Gallagher, Z. Donkó, Phys. Rev. E 52, 913 (1995).




Especially sensitive to heavy-particle excitation



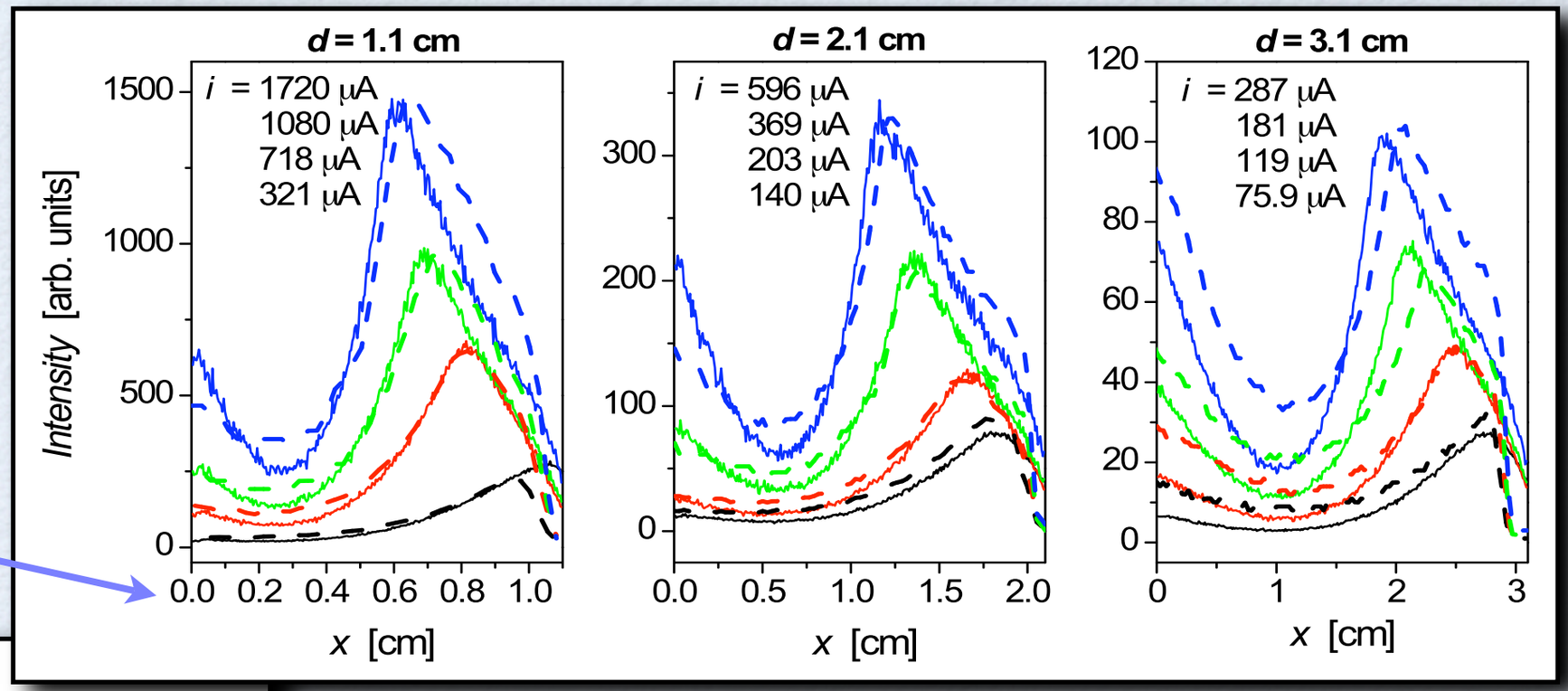

Line intensities in a hollow cathode discharge with plane & parallel cathodes

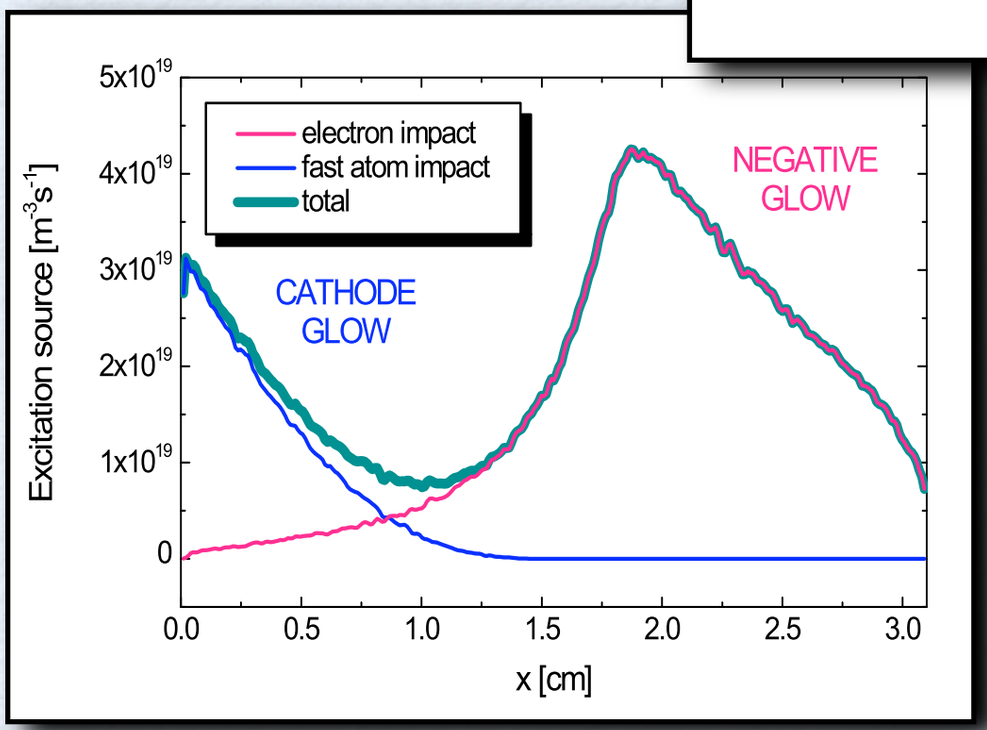
K. Kutasi and Z. Donkó, J. Phys. D. **33**, 1081 (2000).

# Application of hybrid models:
# (2) Heavy-particle excitation in the cathode region

Intensity distributions at
$pd$ = 45 Pa cm
(Solid lines: measurements,
dashed lines: simulations)

cathode at $x = 0$




The source of excitation can easily be decomposed in the simulation

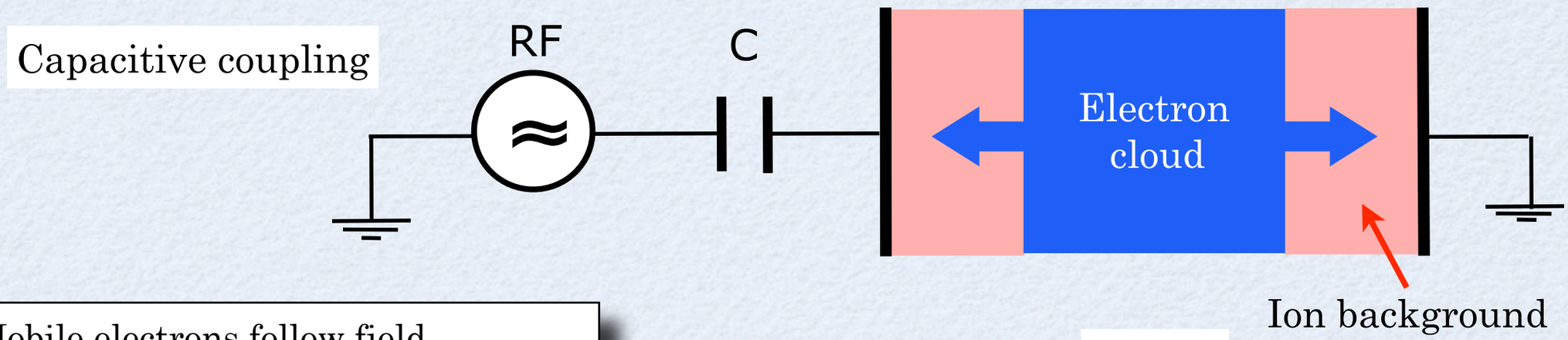
NEGATIVE GLOW: electron impact
CATHODE GLOW: fast atom impact

D. Marić, P. Hartmann, G. Malović, Z. Donkó, Z. Lj. Petrović, J. Phys. D **36**, 2639 (2003).

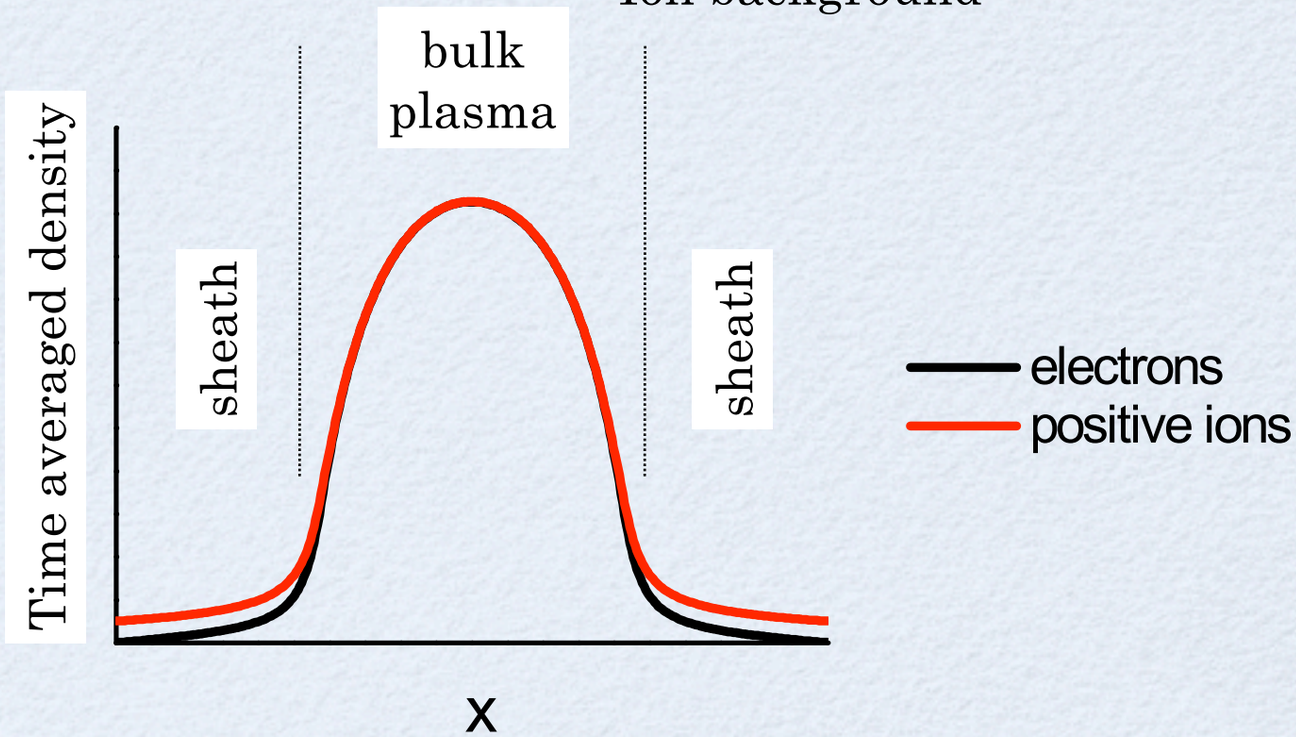
# III. Radiofrequency discharges

- Modeling - basics of Particle-in-Cell method
- Flux-energy distribution of ions at the electrodes
- Independent control of ion properties

# Radiofrequency discharges




- Mobile electrons follow field variation → ionization
- Ions "feel" the time-averaged electric field
- Sheath + bulk structure develops
- Symmetric / asymmetric configurations
- Mathematical description:
  - fluid
  - hybrid
  - Particle-in-Cell



# Bounded plasma PIC simulation with Monte Carlo collisions (PIC/MCC)

The IDEA:

Due to the huge number of particles in real plasmas considering all pairwise interactions is hopeless

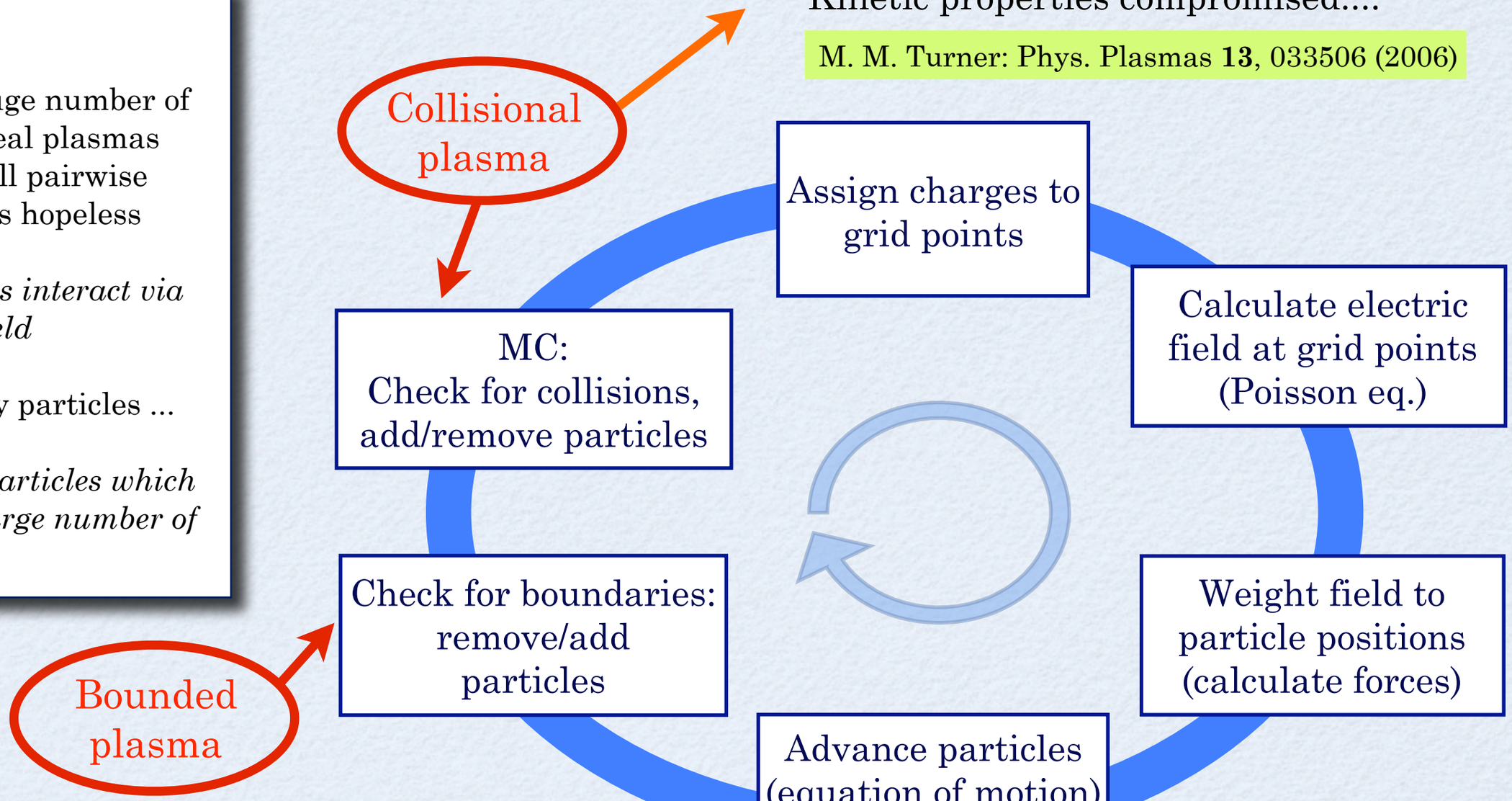
→ *let particles interact via the electric field*

Still too many particles ...

→ *use superparticles which represent a large number of real particles*

Kinetic properties compromised....

M. M. Turner: Phys. Plasmas **13**, 033506 (2006)

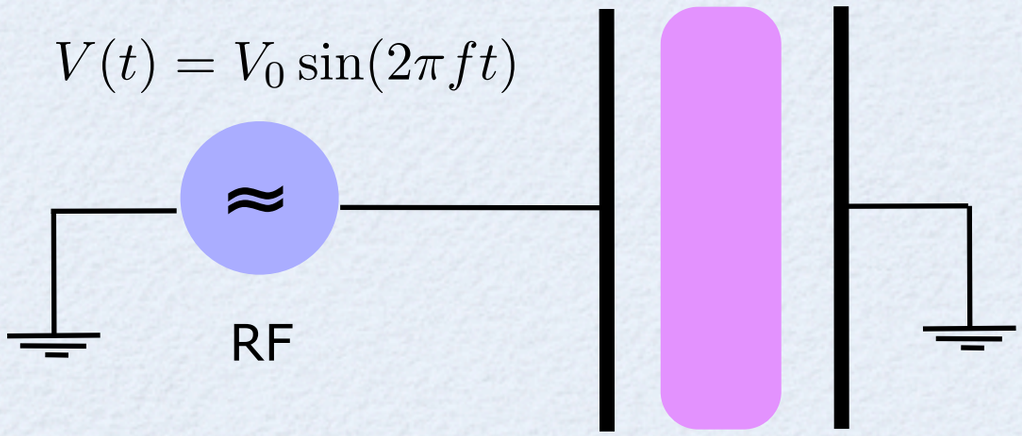



e.g. C. K. Birdsall, IEEE Trans. Plasma Sci, **19** (1991).
[Berkeley Plasma Theory and Simulation Group (PTSG)]

J. P. Verboncoeur, Plasma Phys. Control. Fusion 47 (2005) A231–A260
Particle simulation of plasmas: review and advances

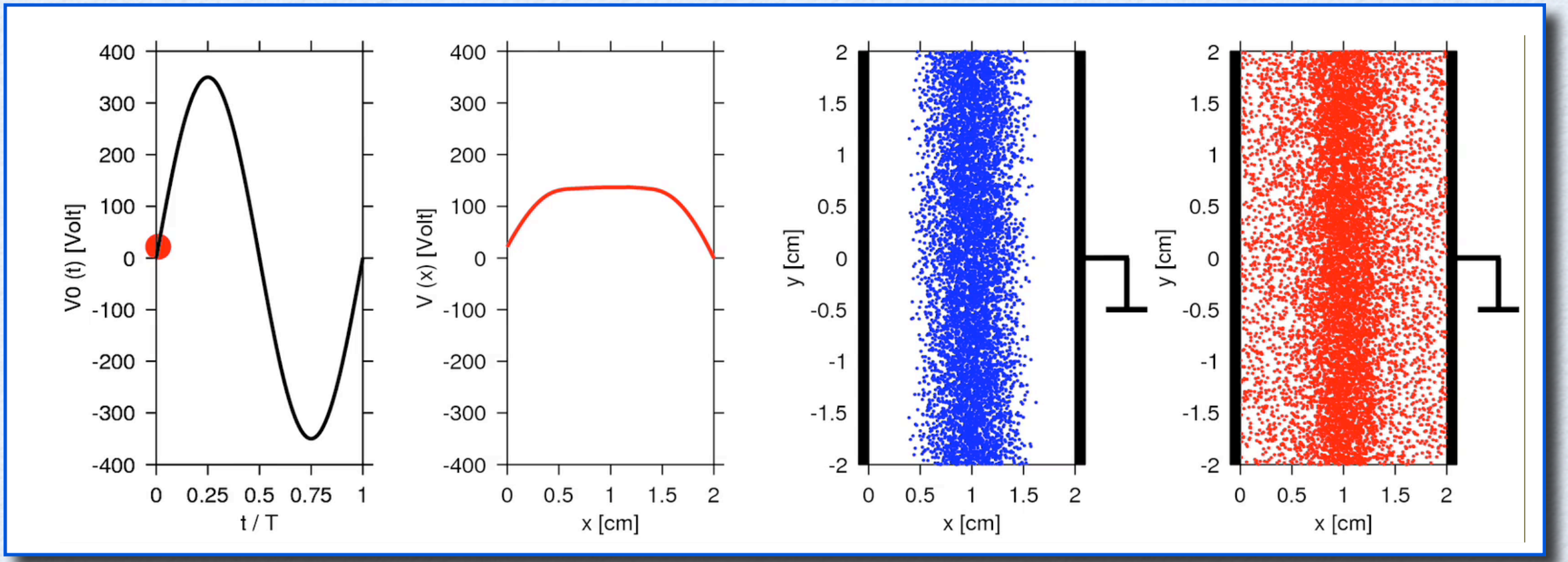
Electrostatic
1D
"HOME MADE"

# Particle-in-Cell simulation of RF discharges



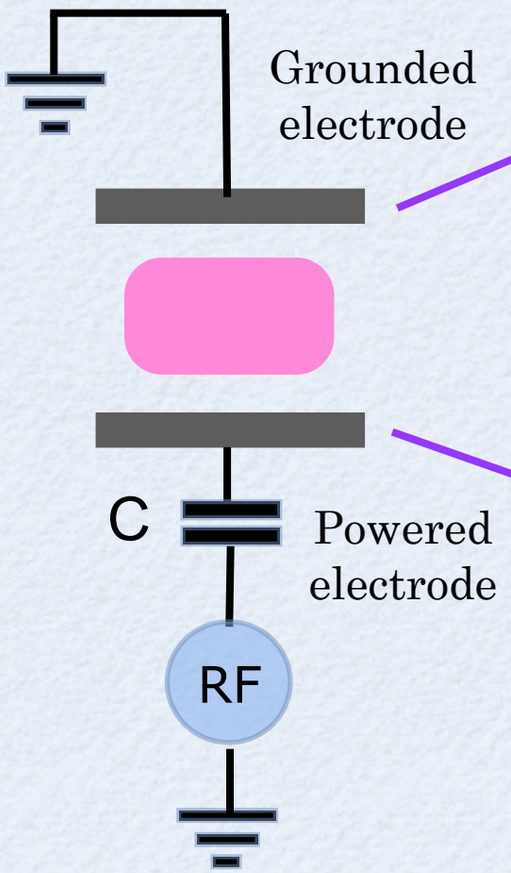

- Particles: electrons and $Ar^+$ ions
- Processes:
  - electrons: elastic collisions, excitation and ionization
  - ions: elastic w/ isotropic and backward scattering

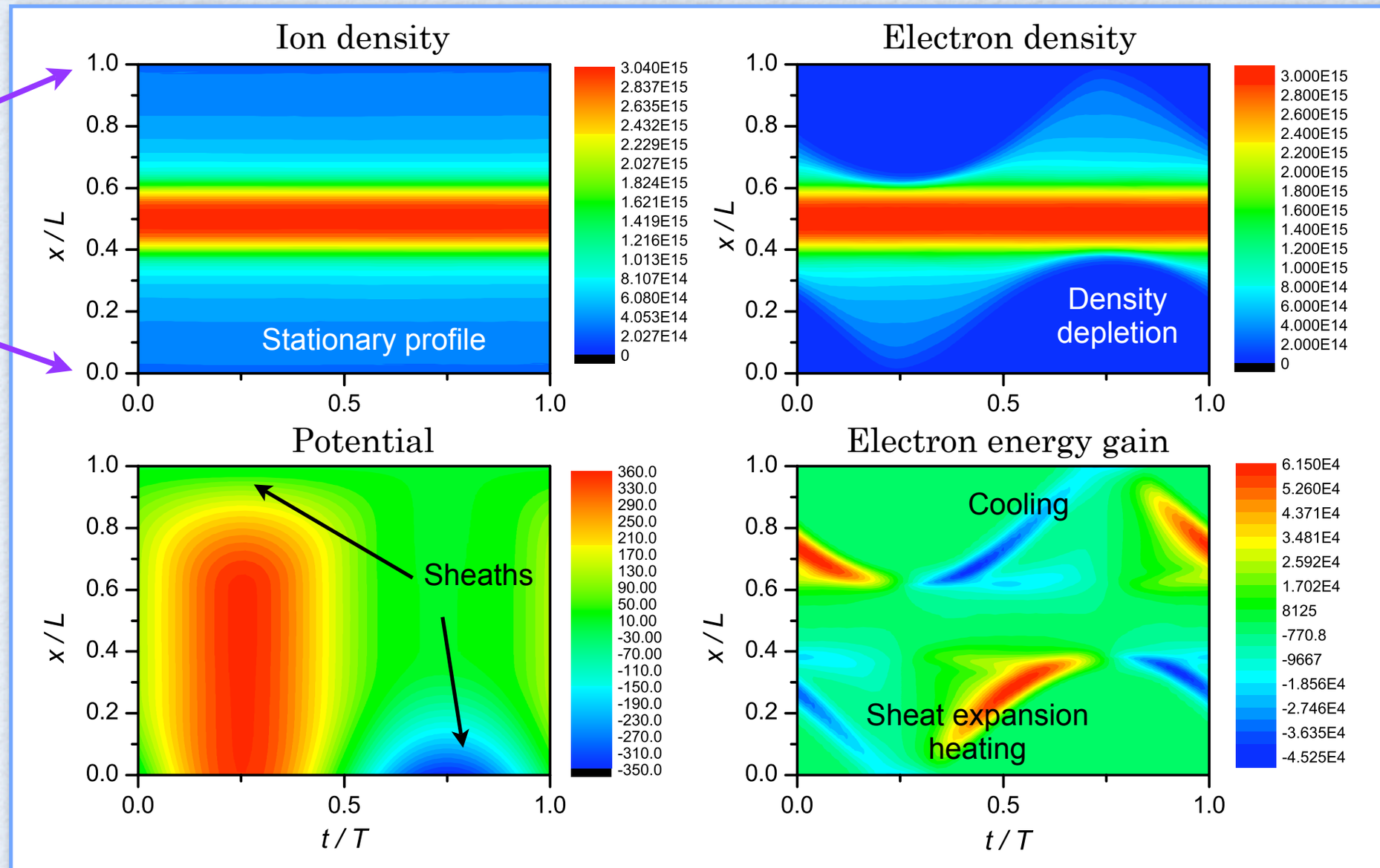
Ar @ p = 50 mTorr, f = 13.56 MHz, V = 350 V



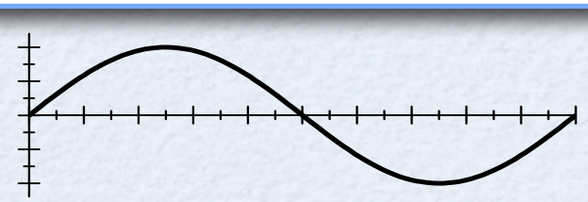
# Particle-in-Cell simulation of RF discharges

Ar @ p = 50 mTorr, f = 13.56 MHz, V = 350 V



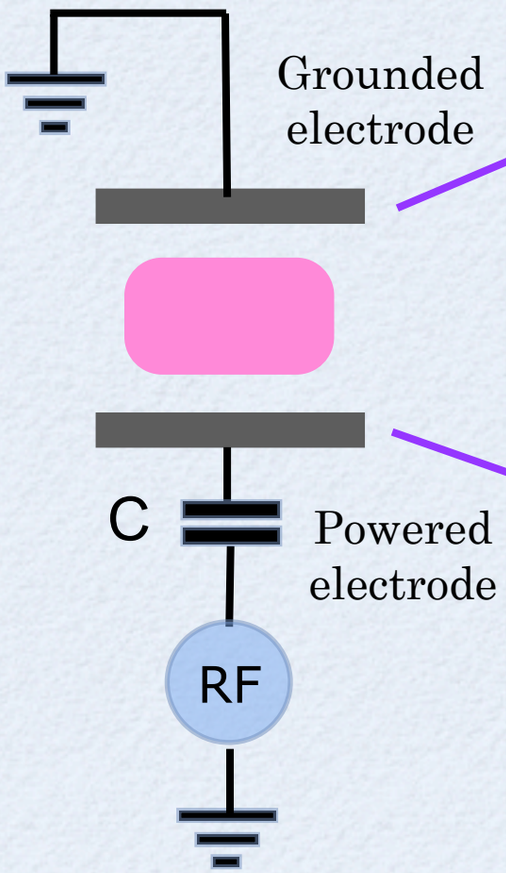

$$V(t) = V_0 \sin(2\pi f t)$$

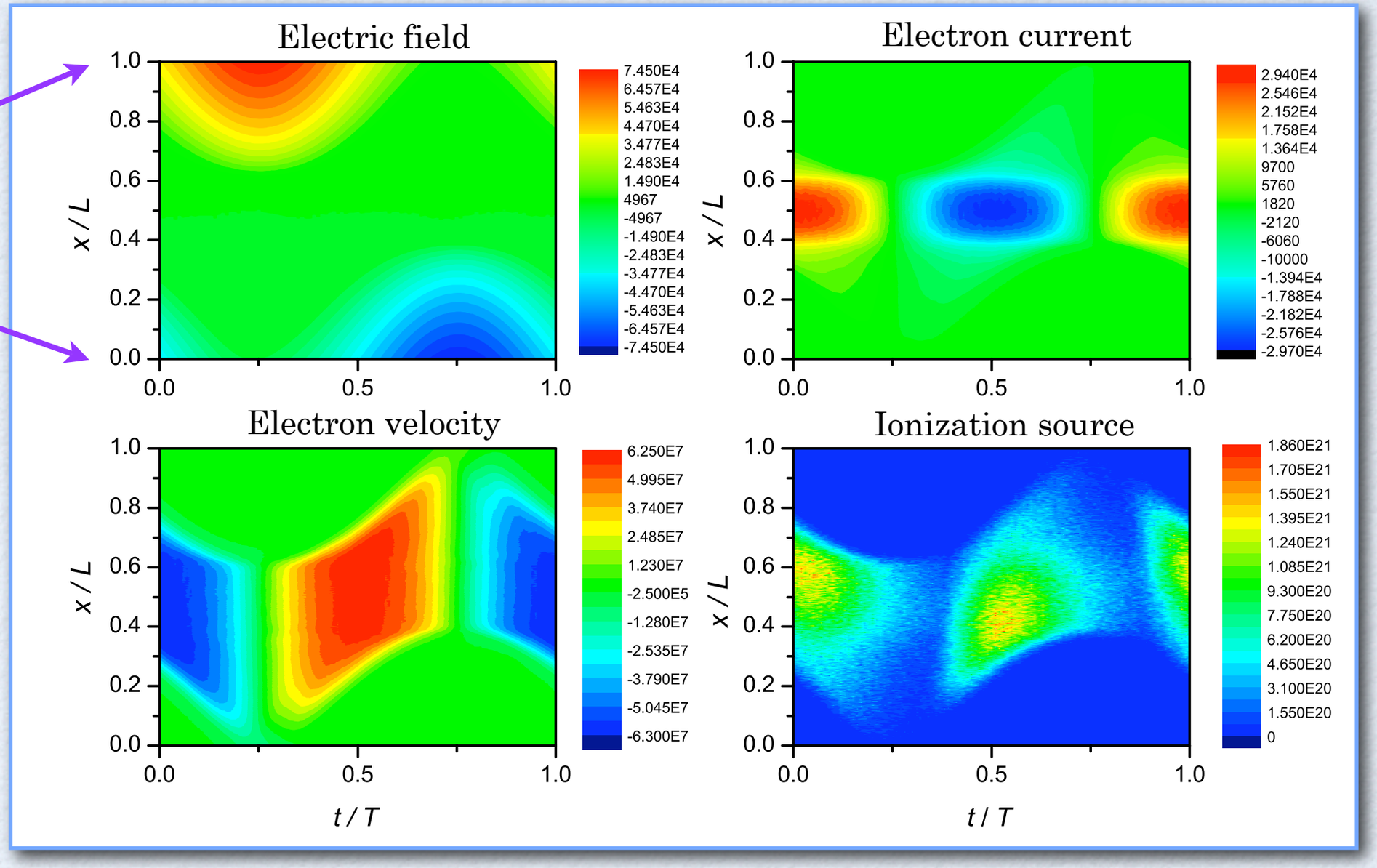


units in SI

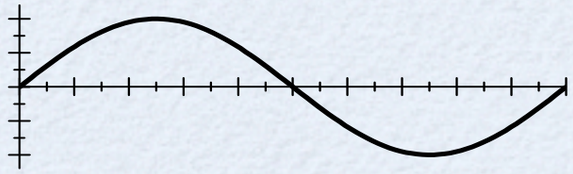
# Particle-in-Cell simulation of RF discharges

Ar @ p = 50 mTorr, f = 13.56 MHz, V = 350 V



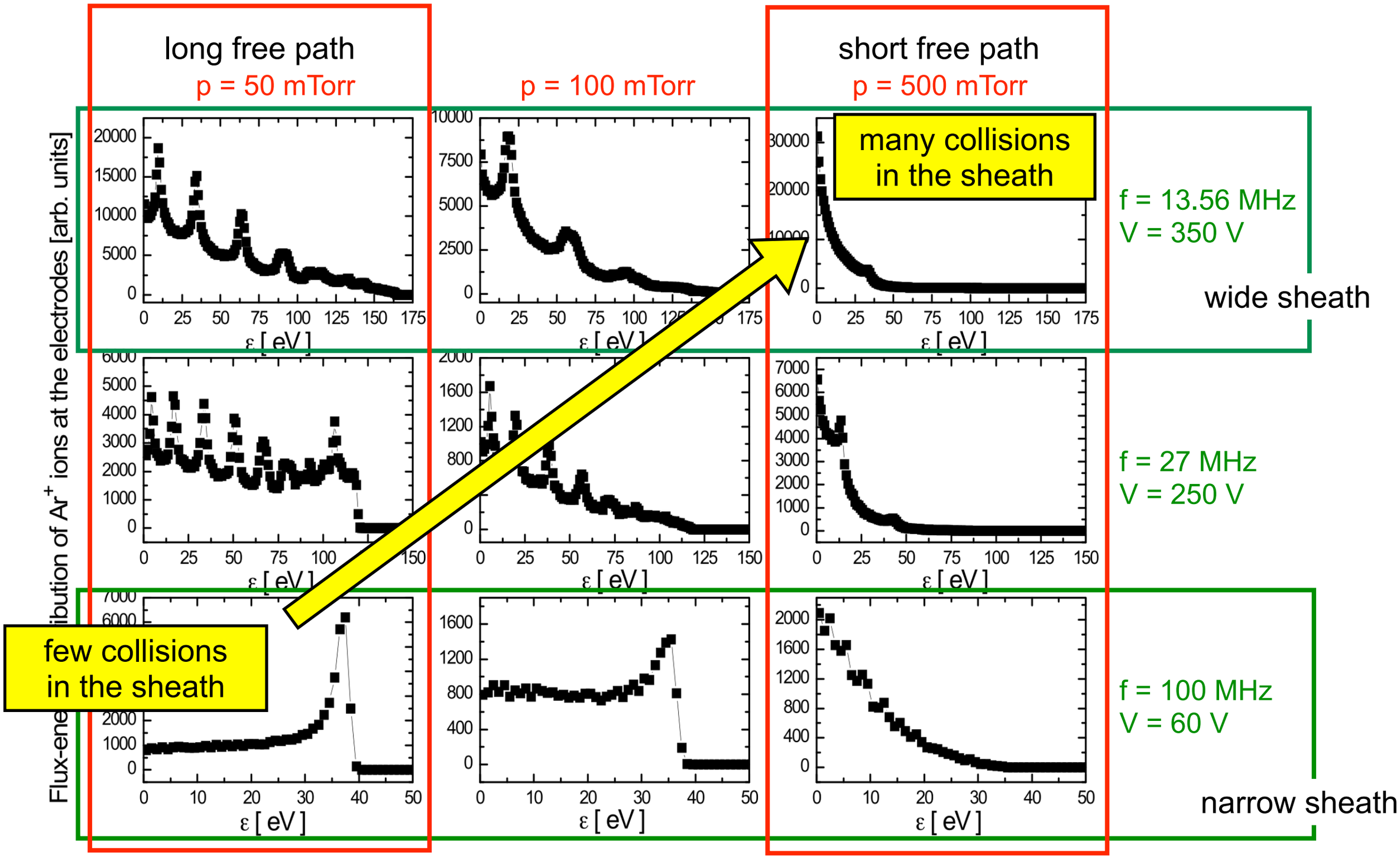




$$V(t) = V_0 \sin(2\pi f t)$$



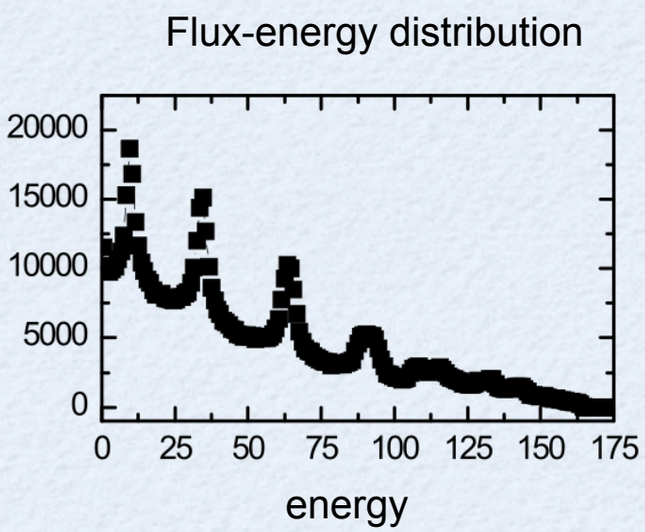
units in SI

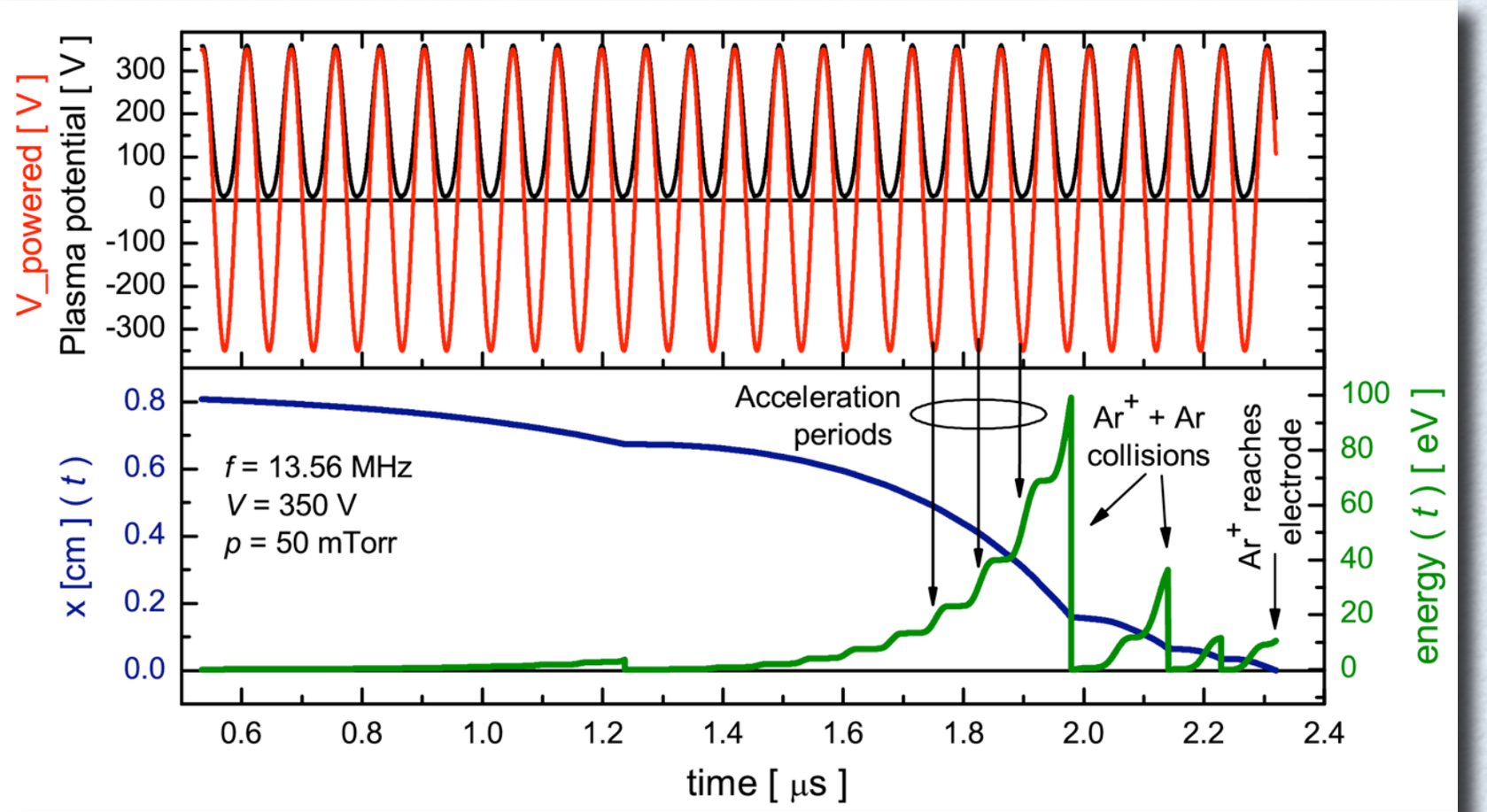
# Flux-energy distributions of ions reaching the electrodes



# Formation of ion energy distribution (single ion trajectories)

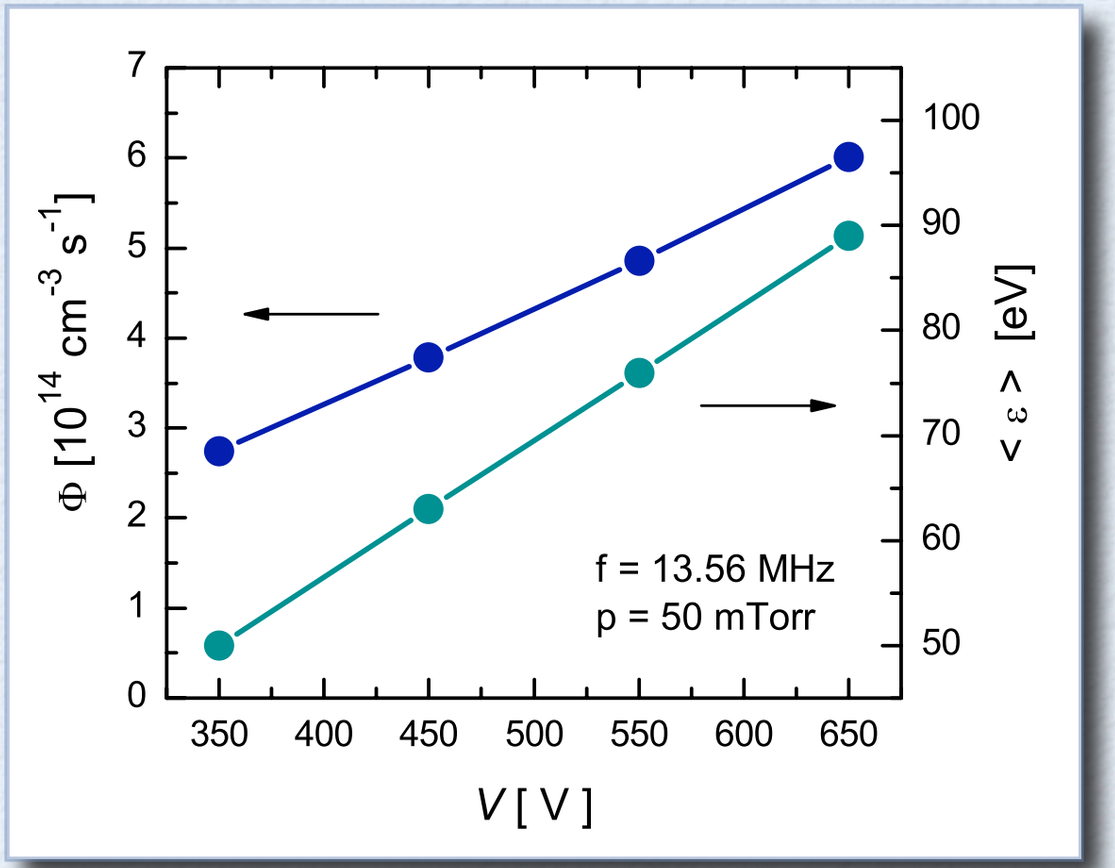
- Ar discharge
- f = 13.56 MHz
- p = 50 mTorr
- V = 350 V




- Ion transit time τ >> T → ions feel the average electric field
- Periodic acceleration in the sheath
- Effect of charge exchange collisions

# Control of ion properties (flux and energy)




In a single-frequency discharge the driving voltage influences both the ion flux and the ion energy

Is it possible to control these properties independently of each other?

**DUAL FREQUENCY DISCHARGE**

$$V(t) = V_{\mathrm{HF}} \sin(2\pi f_{\mathrm{HF}} t) + V_{\mathrm{LF}} \sin(2\pi f_{\mathrm{LF}} t)$$

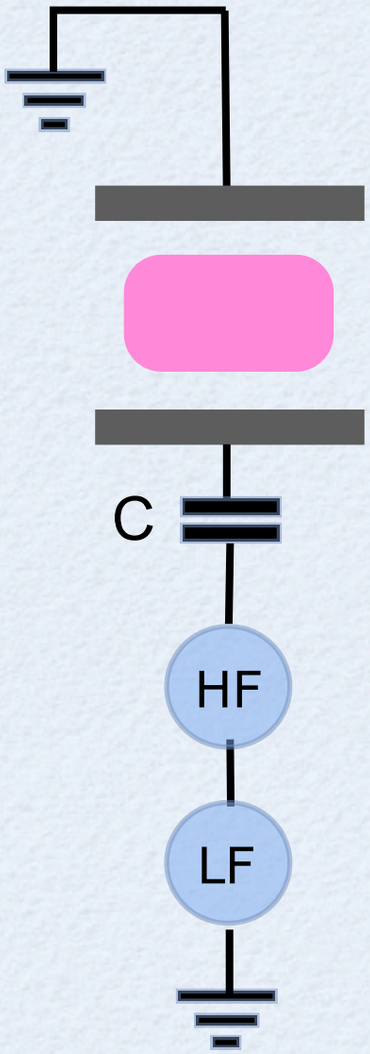
**Heating: density & flux**

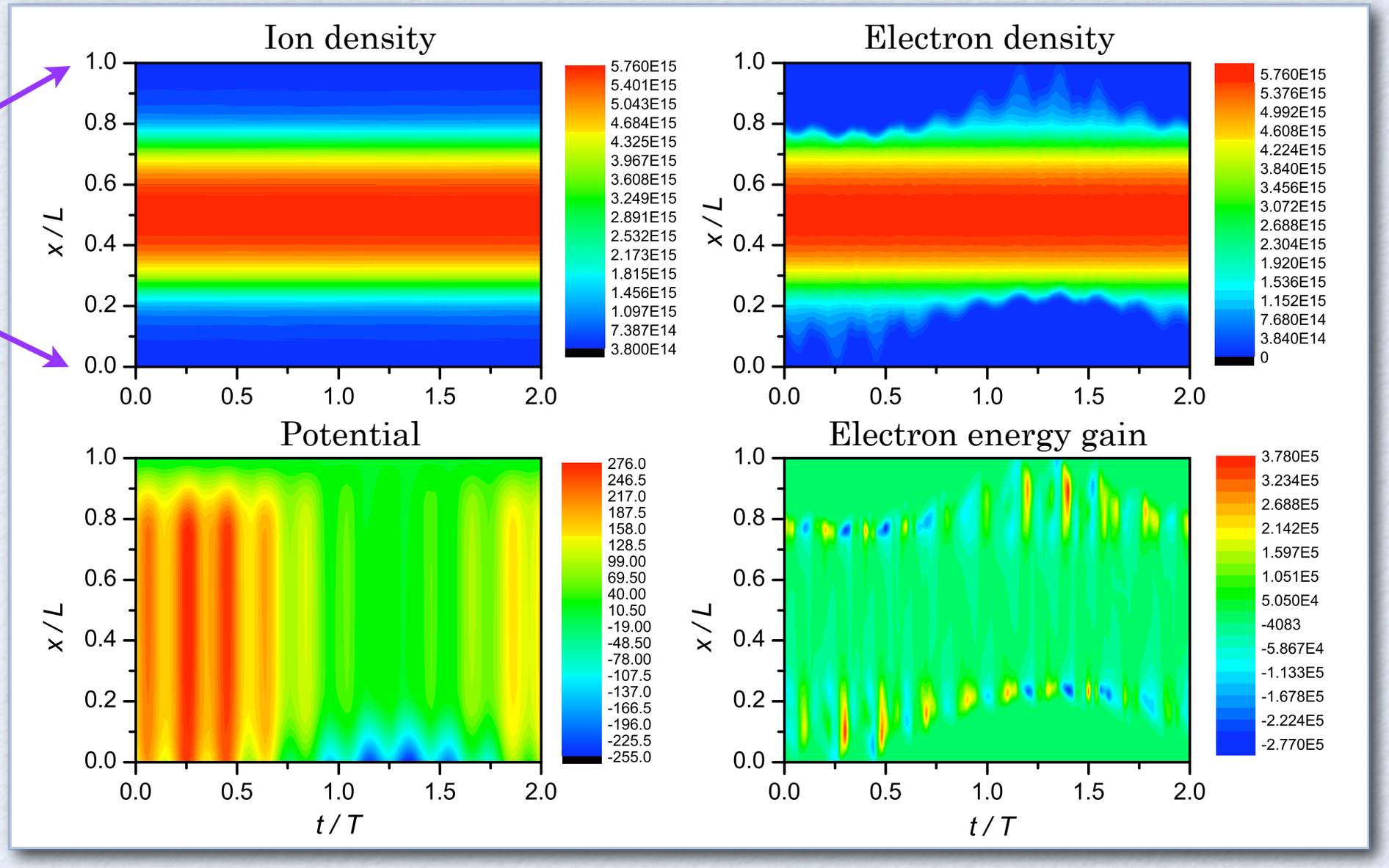
**Acceleration: energy**

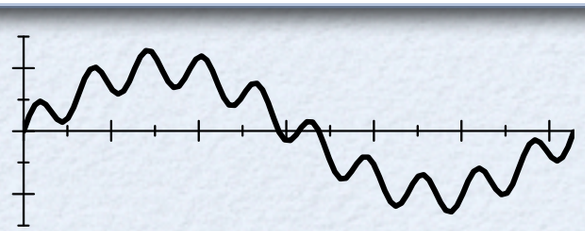

P. C. Boyle, A. R. Ellingboe and M. M. Turner, Plasma Sources Sci. Technol. **13,** 493-503, J. Phys. D. **37,** 697 (2004)
T. Kitajima, Y. Takeo, Z. Lj. Petrovic and T. Makabe, Appl. Phys. Lett. **77,** 489 (2000)
J. K. Lee, O. V. Manuilenko, N. Yu. Babaeva, H. C. Kim and J. W. Shon, Plasma Sources Sci. Technol. **14,** 89 (2005).
E. Kawamura, M. A. Lieberman and A. J. Lichtenberg, Phys. Plasmas **13** 053506 (2006)
M. M. Turner and P. Chabert, Phys. Rev. Lett. **96,** 205001 (2006)
T. Gans, J. Schulze, D. O'Connell, U. Czarnetzki, R. Faulkner, A. R. Ellingboe and M. M. Turner, Appl. Phys. Lett. **89,** 261502 (2006)
J. Schulze, Z. Donkó, D. Luggenhölscher and U. Czarnetzki, Plasma Sources Sci. Technol. **18,**, 034011 (2009)
E. Semmler, P. Awakowicz and A. von Keudell, Plasma Sources Sci. Technol. **16,** 839 (2007)
A. Salabas and R. P. Brinkmann, Plasma Sources Sci. Technol. **14,** 2 53 (2005)
V. Georgieva and A. Bogaerts, Plasma Sources Sci. Technol., **15**, 368 (2006)
Z. Donkó and Z. Lj. Petrović, Jpn. J. Appl. Phys. **45**, 8151 (2006)

# Dual-frequency excitation: PIC results

Ar @ p = 25 mTorr, L = 2 cm
HF = 60 V @ 100 MHz / LF = 200 V @ 10 MHz



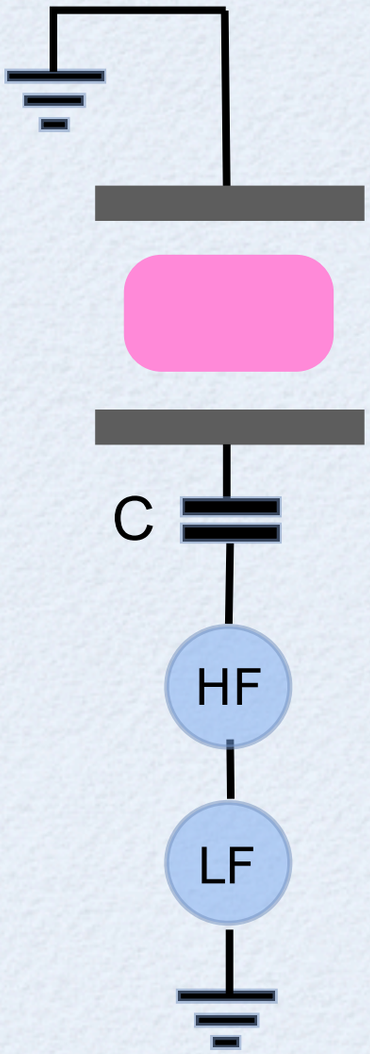



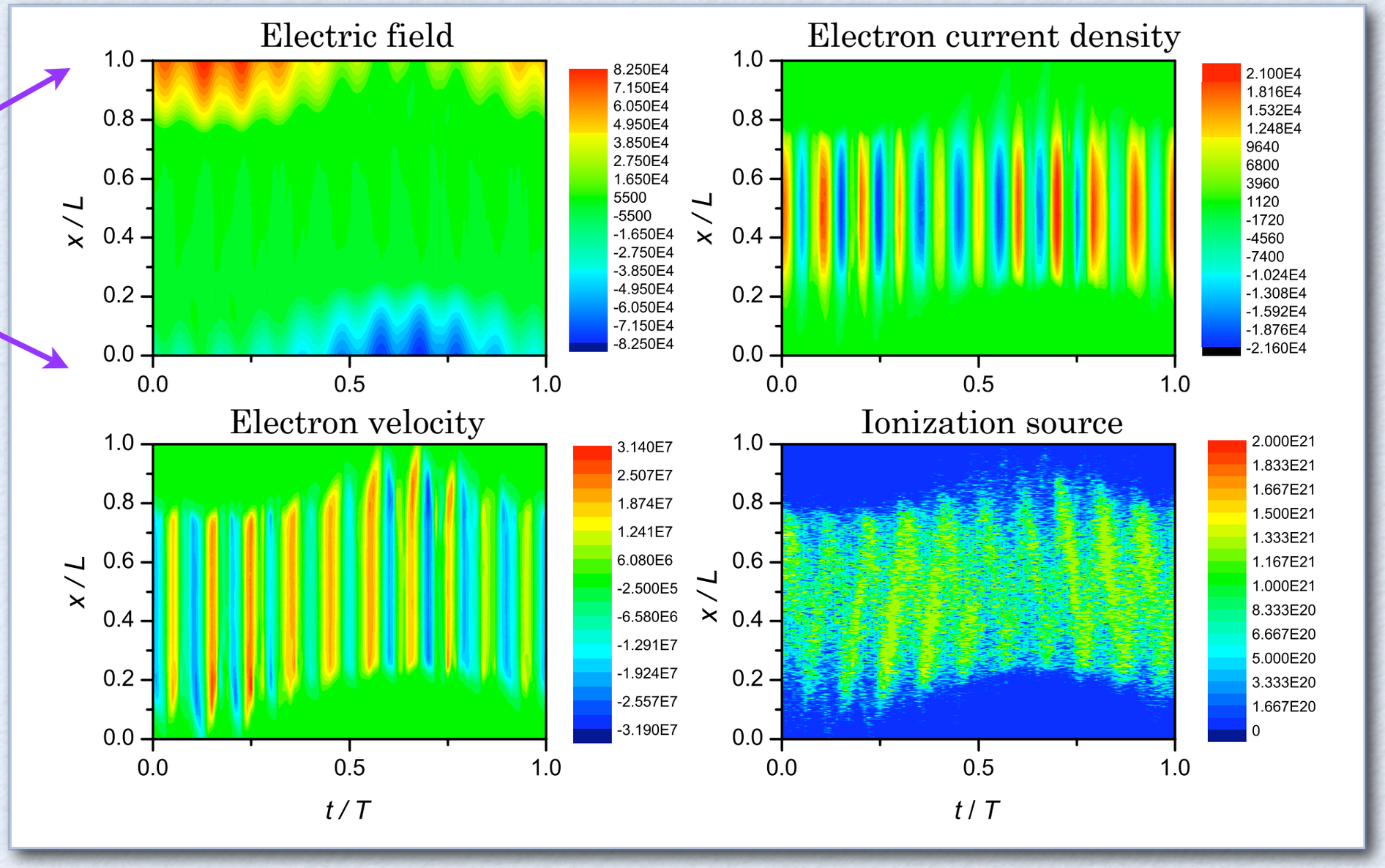



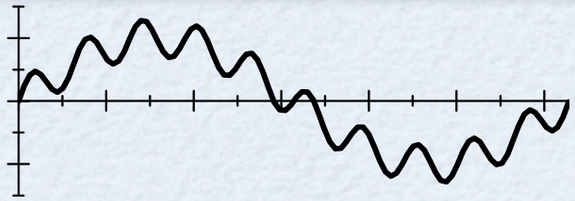
$$V(t) = V_{\mathrm{HF}} \sin(2\pi f_{\mathrm{HF}} t) + V_{\mathrm{LF}} \sin(2\pi f_{\mathrm{LF}} t)$$

# Dual-frequency excitation: PIC results

Ar @ p = 25 mTorr, L = 2 cm
HF = 60 V @ 100 MHz / LF = 200 V @ 10 MHz



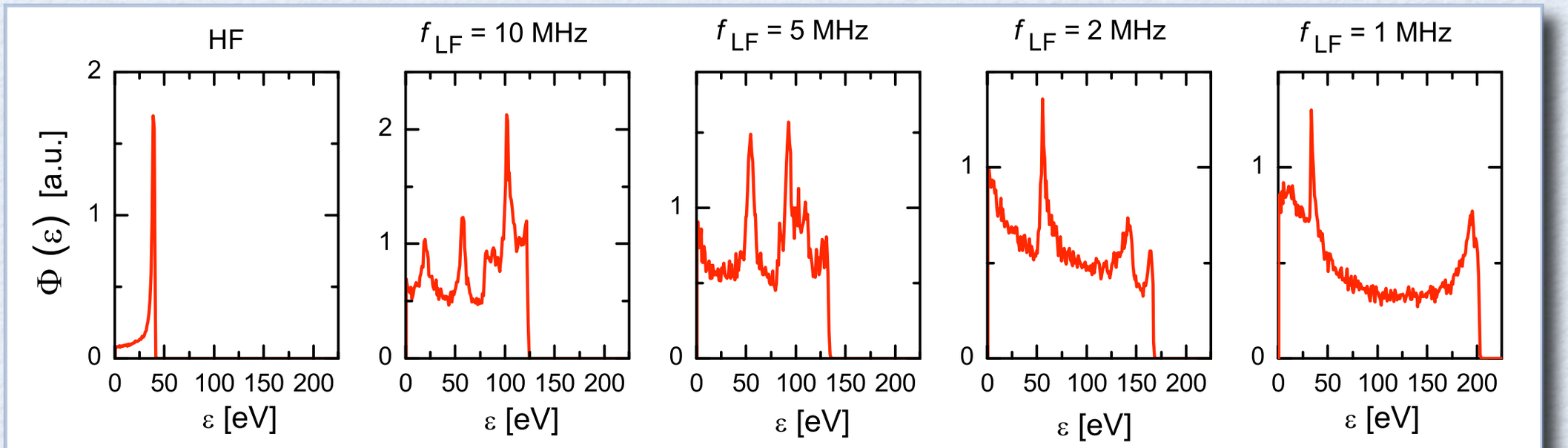



$$V(t) = V_{\mathrm{HF}} \sin(2\pi f_{\mathrm{HF}} t) + V_{\mathrm{LF}} \sin(2\pi f_{\mathrm{LF}} t)$$

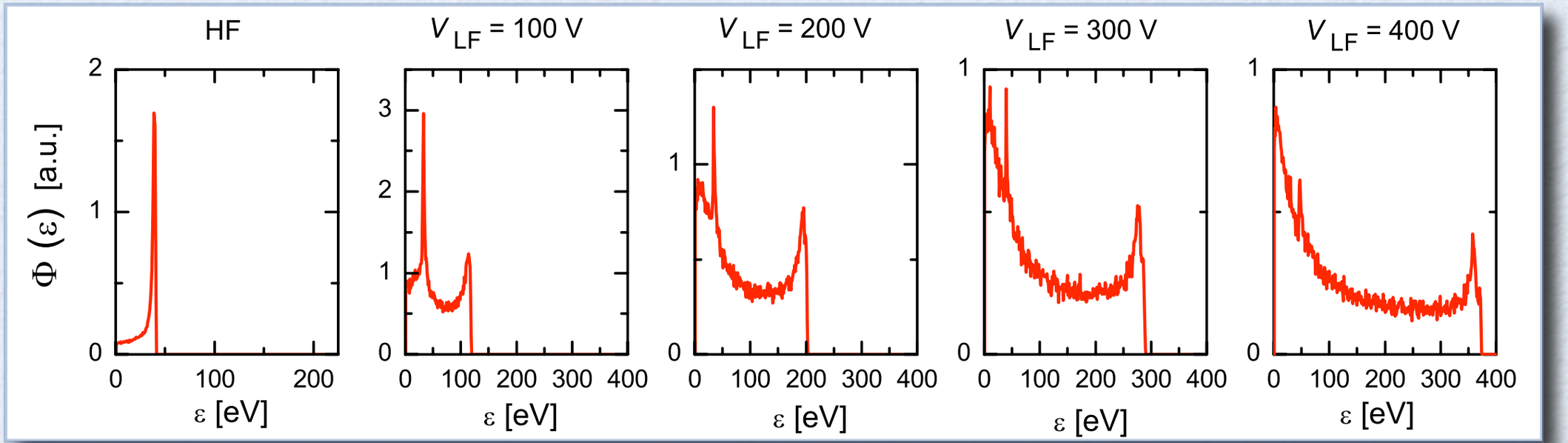
# Dual-frequency excitation: ion flux-energy distributions

Argon, $V_{HF}$ = 60 V, $f_{HF}$ = 100 MHz , L = 2 cm, 25 mTorr

effect of LF at $V_{LF}$ = 200V

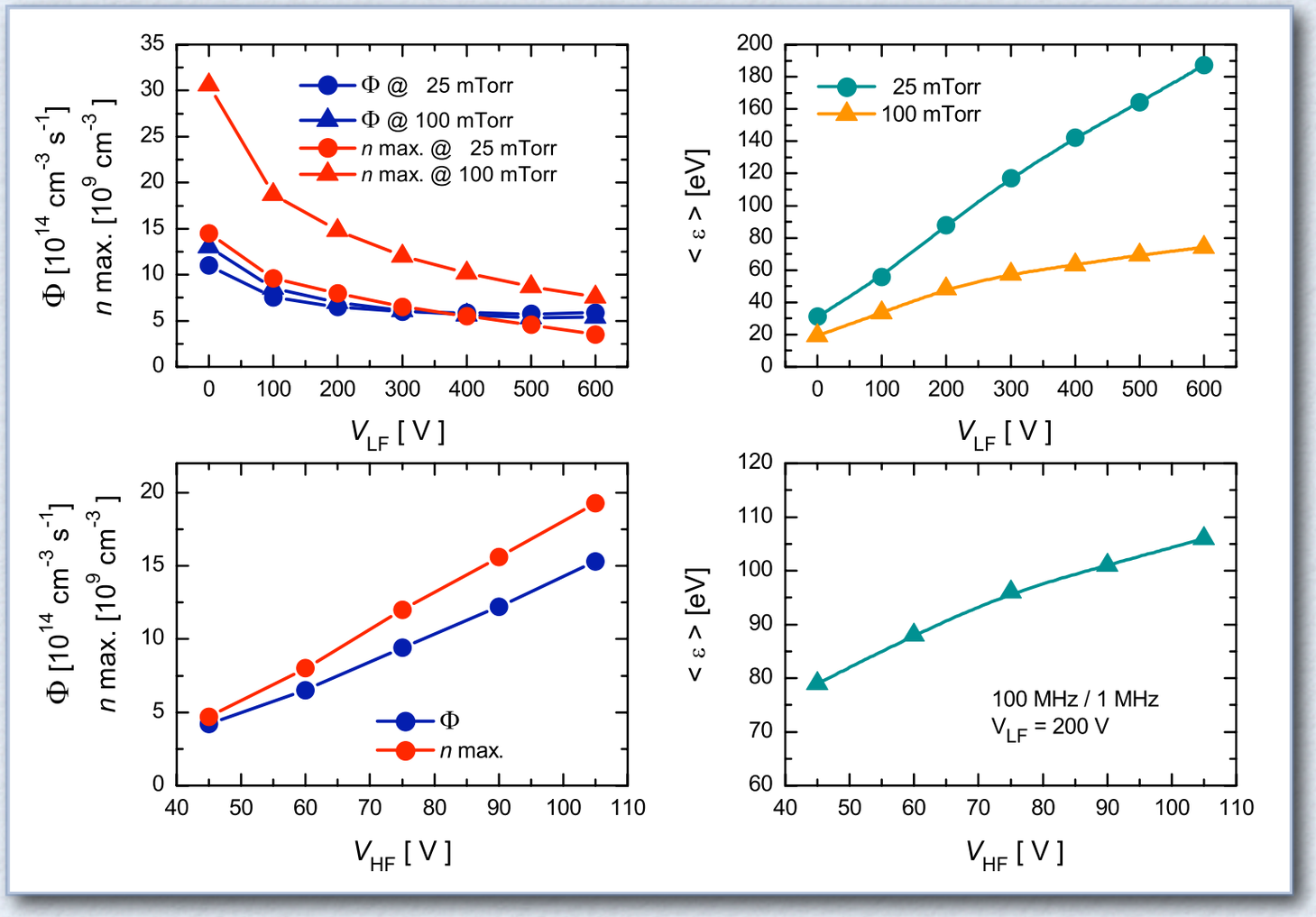



effect of $V_{LF}$ at $f_{LF}$ =1 MHZ

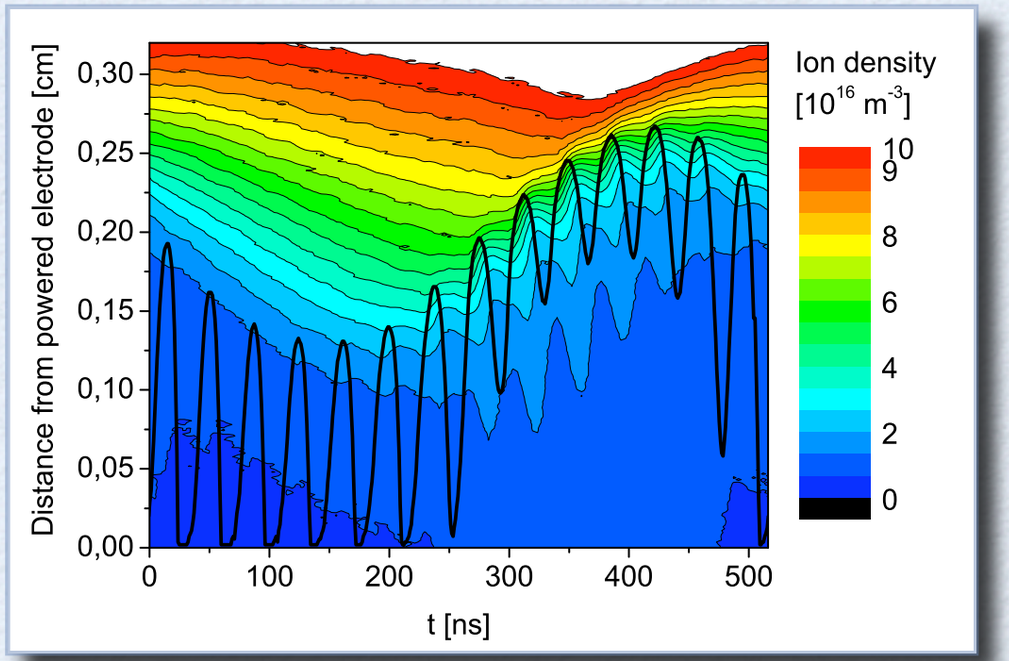


# Dual-frequency excitation: independent (?) control of ion properties

Ar @ p = 25 mTorr, L = 2 cm
$V_{HF}$ = 60 V @ 100 MHz / $V_{LF}$ = 200 V @ 10 MHz




He @ p = 65 Pa, L = 1.2 cm, T = 400K, $\gamma$ = 0.45
$V_{HF}$ = 550 V @ 27.118 MHz
$V_{LF}$ = 800 V @ 1.937 MHz




**FREQUENCY COUPLING:**
HF sheath is pushed away from electrode, which results in less efficient heating

The GOAL: ion flux is controlled by $V_{HF}$ and ion energy is controlled by $V_{LF}$

The REALITY: ion flux depends on some extent on $V_{LF}$ , ion energy is somewhat influenced by $V_{HF}$

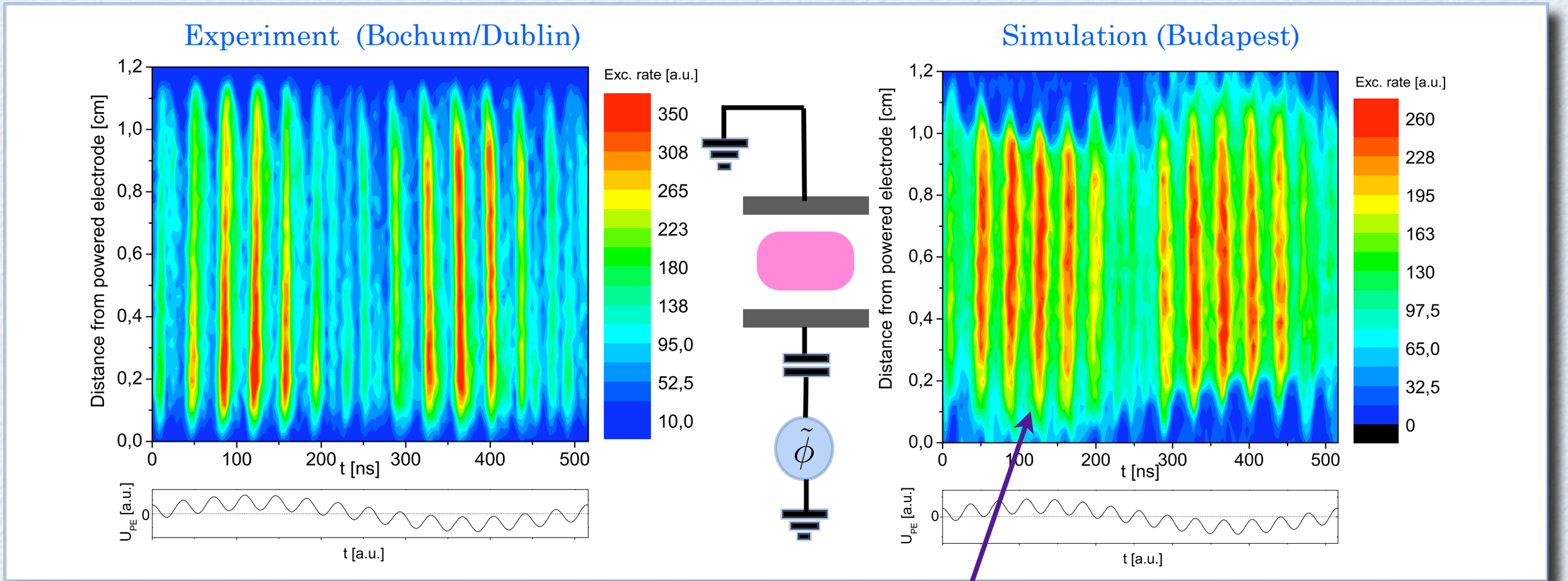

M. M. Turner and P. Chabert 2006 Phys. Rev. Lett. **96** 205001

T. Gans, J. Schulze, D. O'Connell, U. Czarnetzki, R. Faulkner, A. R. Ellingboe and M. M. Turner 2006 Appl. Phys. Lett. **89** 261502

J. Schulze, Z. Donkó, D. Luggenhölscher and U. Czarnetzki 2009 PSST **18**, 034011

# PIC vs. experiment

**Spatio-temporal distribution of electron impact excitation**




J. Schulze, T. Gans, D. O'Connell, U. Czarnetzki, A. R. Ellingboe, and M. M. Turner, J. Phys. D **40** 7008 (2007).

Electron beams

He @ 65 Pa
$f_{HF}$ = 27.118 MHz
$f_{LF}$ = 1.937 MHz (= $f_{HF}$/14)

not science fiction!

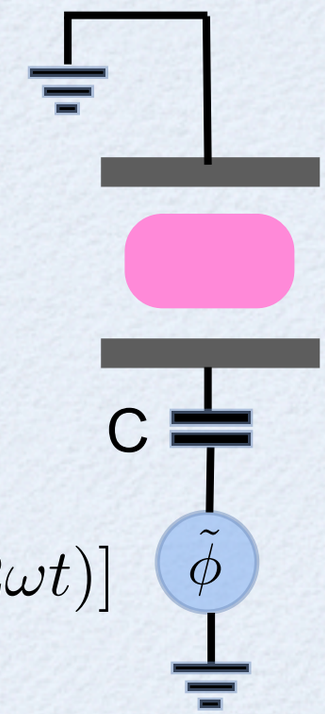
J. Schulze, Z. Donkó, D. Luggenhölscher and U. Czarnetzki, Plasma Sources Sci. Technol. **18**, 034011 (2009).

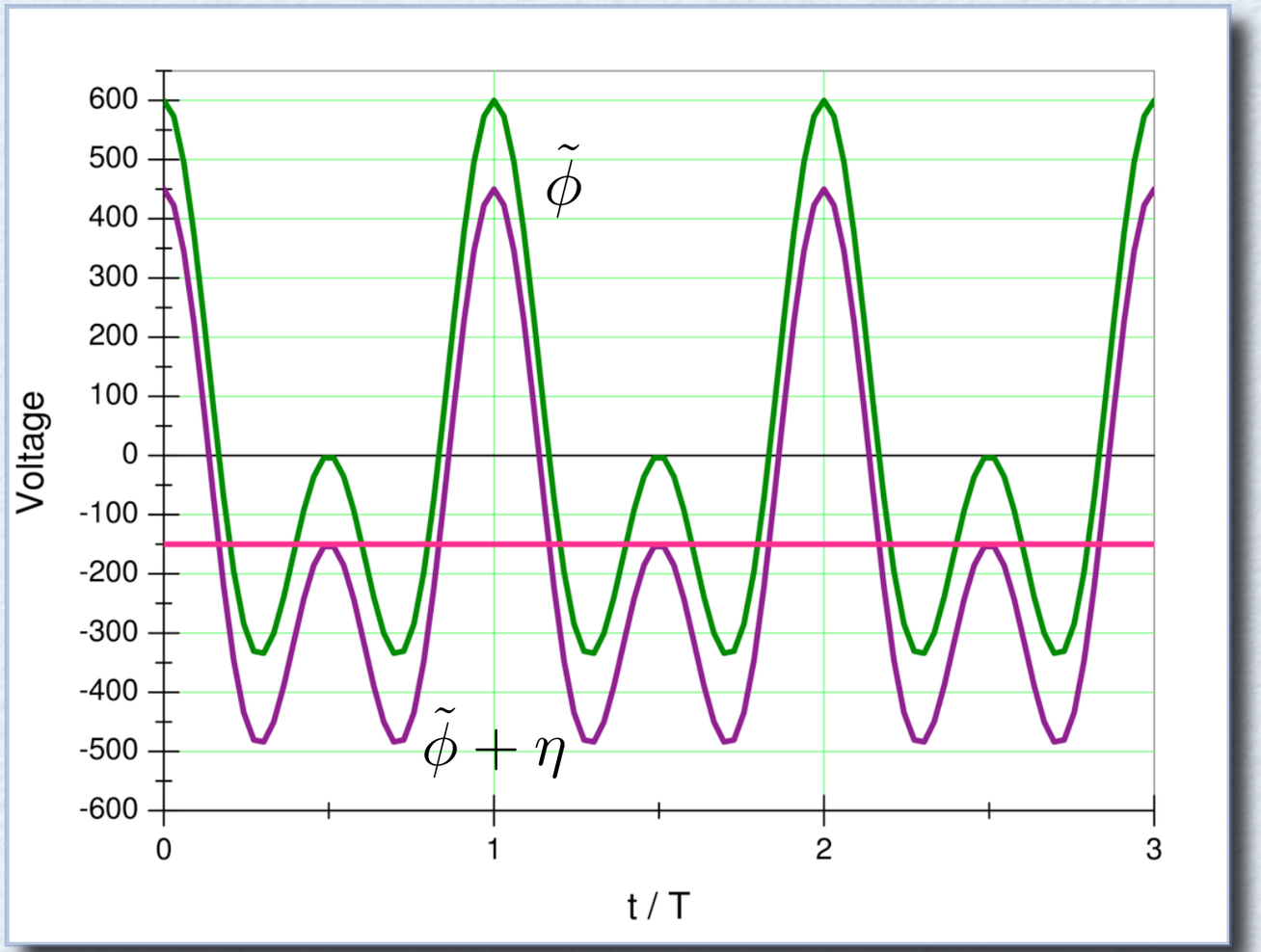
# Alternative method: Electrical Asymmetry Effect

B. G. Heil, J. Schulze, T. Mussenbrock, R. P. Brinkmann and U. Czarnetzki 2008 IEEE Trans. Plasma Sci. **36** 1404

B. G. Heil, U. Czarnetzki, R. P. Brinkmann and T. Mussenbrock, 2008 J. Phys. D **41** 165202

$$\tilde{\phi} = V_0[\cos(\omega t + \theta) + \cos(2\omega t)]$$

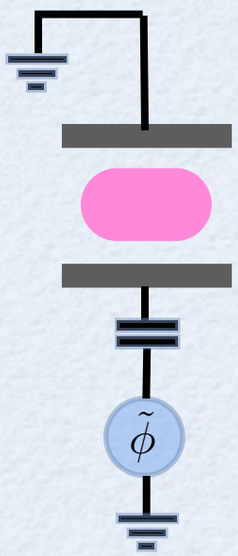



In geometrically symmetrical reactors a DC self bias builds up, if the discharge is driven by a waveform which contains an even harmonic of the fundamental frequency.

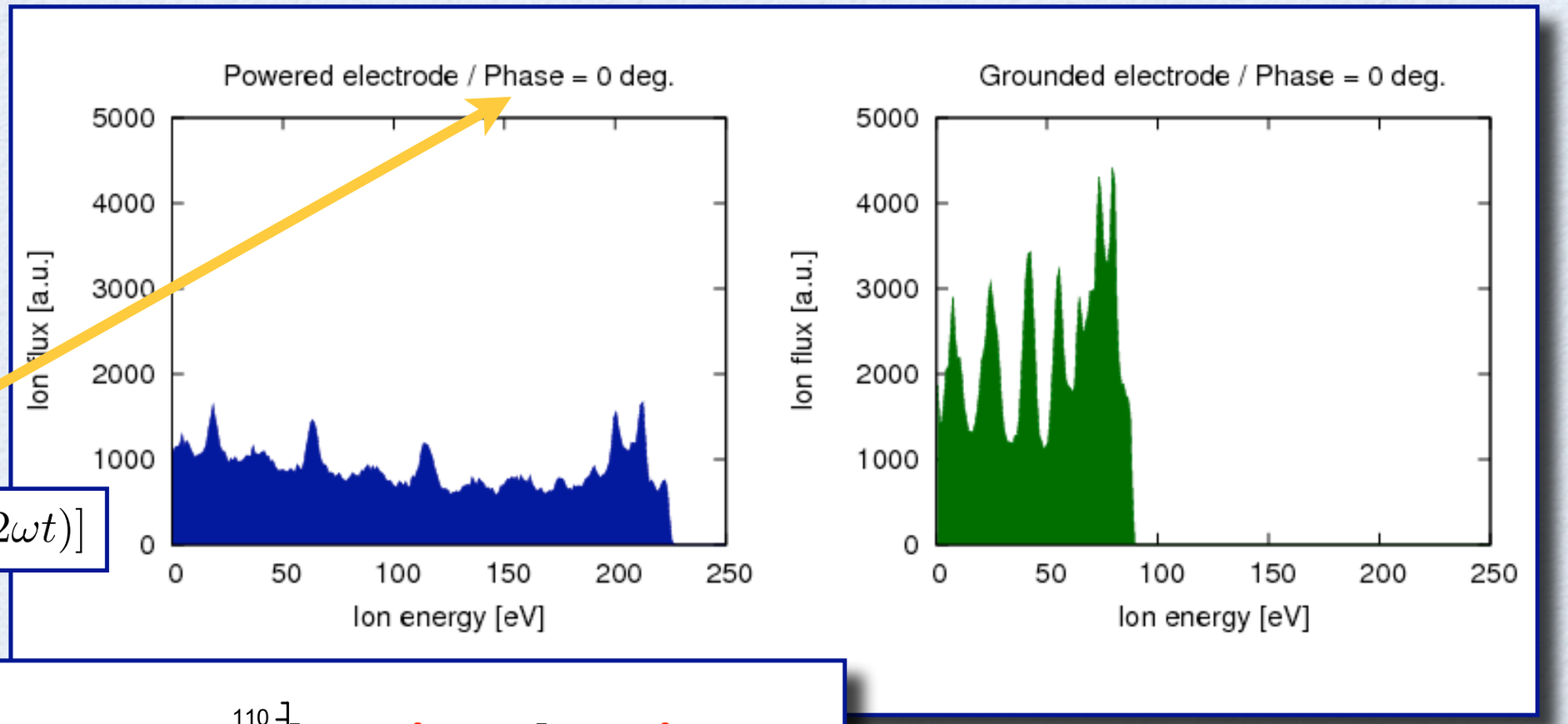
See much more: Uwe Czaretzki: “The Electrical Asymmetry Effect in Capacitive RF Discharges” [ESCAMPIG 2010]

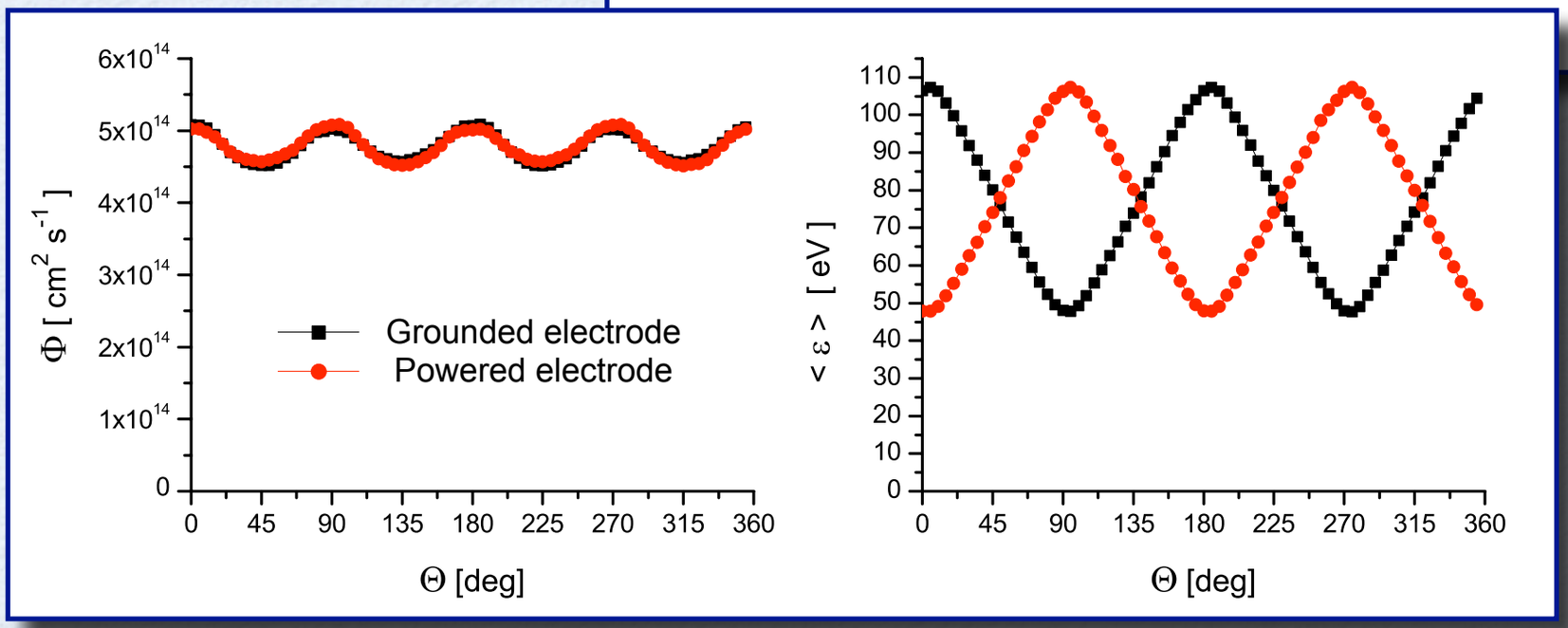
# Electrical asymmetry effect: flux-energy distributions of ions




Ar @ 5 Pa,
L = 2.5 cm,
f = 13.56 MHz,
$V_0$ = 200 V

$$\tilde{\phi} = V_0[\cos(\omega t + \theta) + \cos(2\omega t)]$$

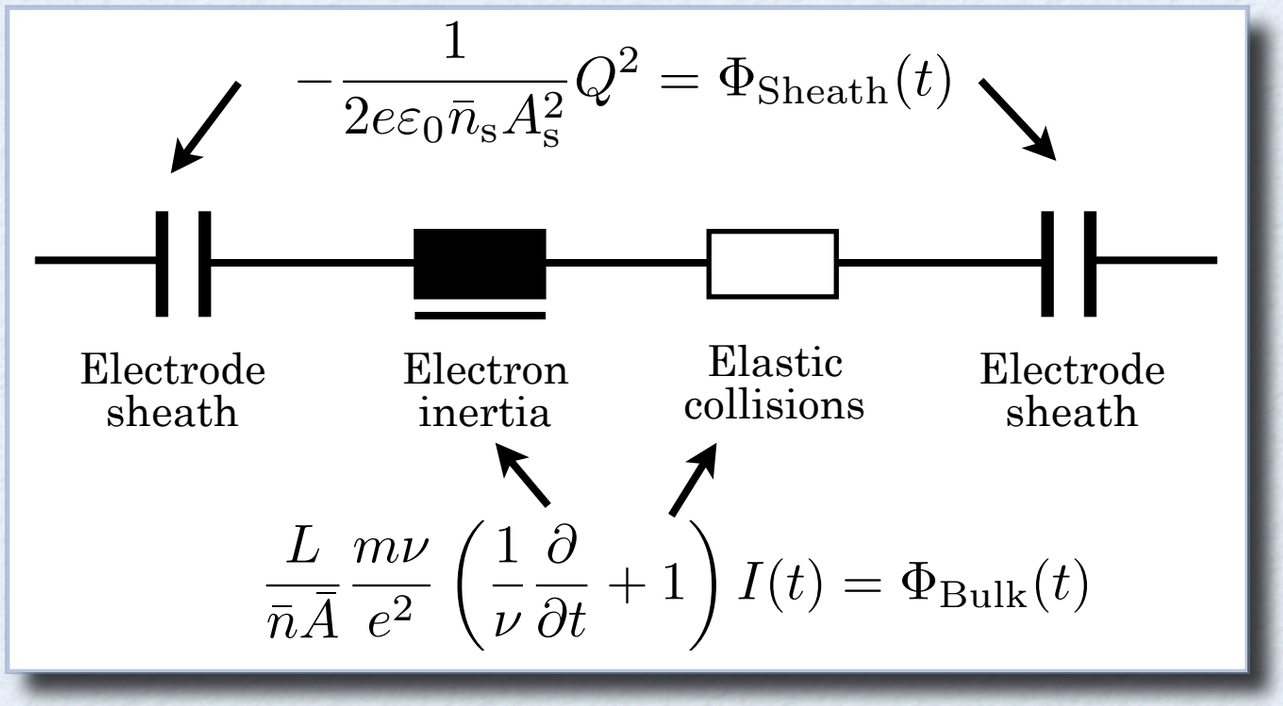



The mean energy of ions can be tuned over a wide range by changing the phase angle between the driving frequencies.

# Plasma Series Resonance

Equivalent circuit of the discharge:



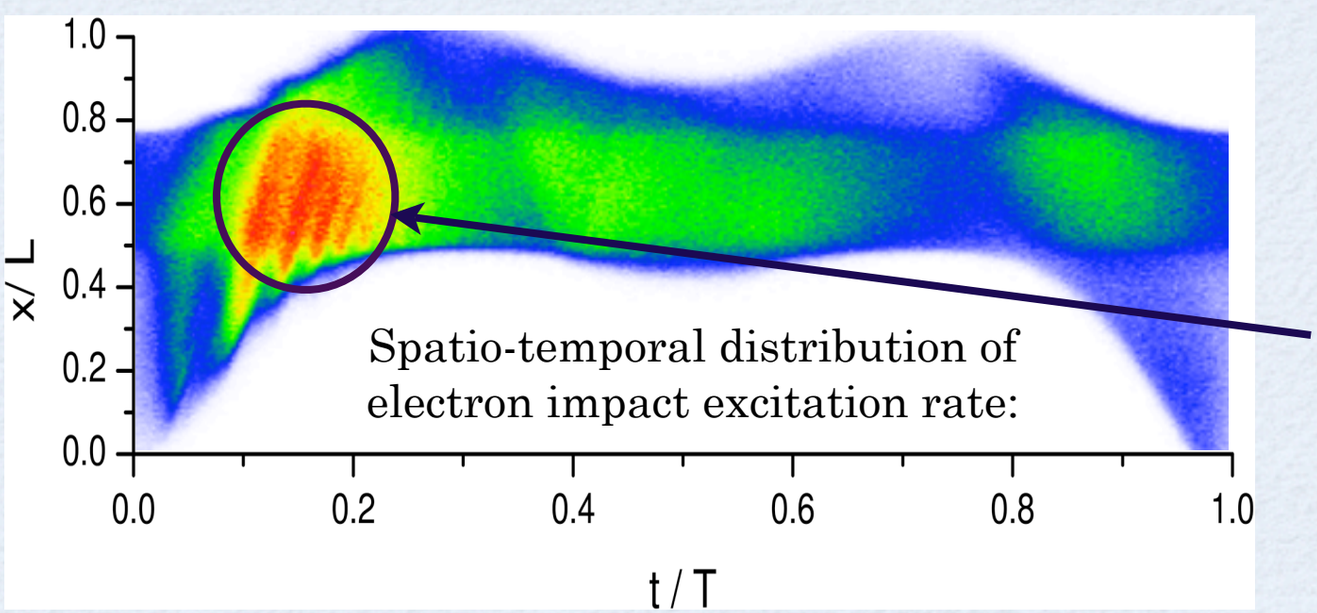

e.g.
U. Czarnetzki, T. Mussenbrock and R. P. Brinkmann, Phys. Plasmas **13**, 123503 (2006).

T. Mussenbrock, R. P. Brinkmann, M. A. Lieberman, A. J. Lichtenberg, and E. Kawamura, Phys. Rev. Lett. **101** 085004 (2008).

PSR equation:

$$\Phi(t) = \Phi_{\mathrm{sheath},1}(t) + \Phi_{\mathrm{sheath},2}(t) + \Phi_{\mathrm{Bulk}}(t)$$

special cases: (1) strongly asymmetric,
(2) symmetrical: sheaths cancel




Observation of PSR in a geometrically symmetric, electrically asymmetric discharge

$$\tilde{\phi} = V_0[\cos(\omega t + \theta) + \cos(2\omega t)]$$

$V_0$ = 1000 V, $\Theta$ = 7.5°, L = 2.5 cm, p = 3 Pa

Electron beams with a speed of $\approx 3 \times 10^6$ m/s.

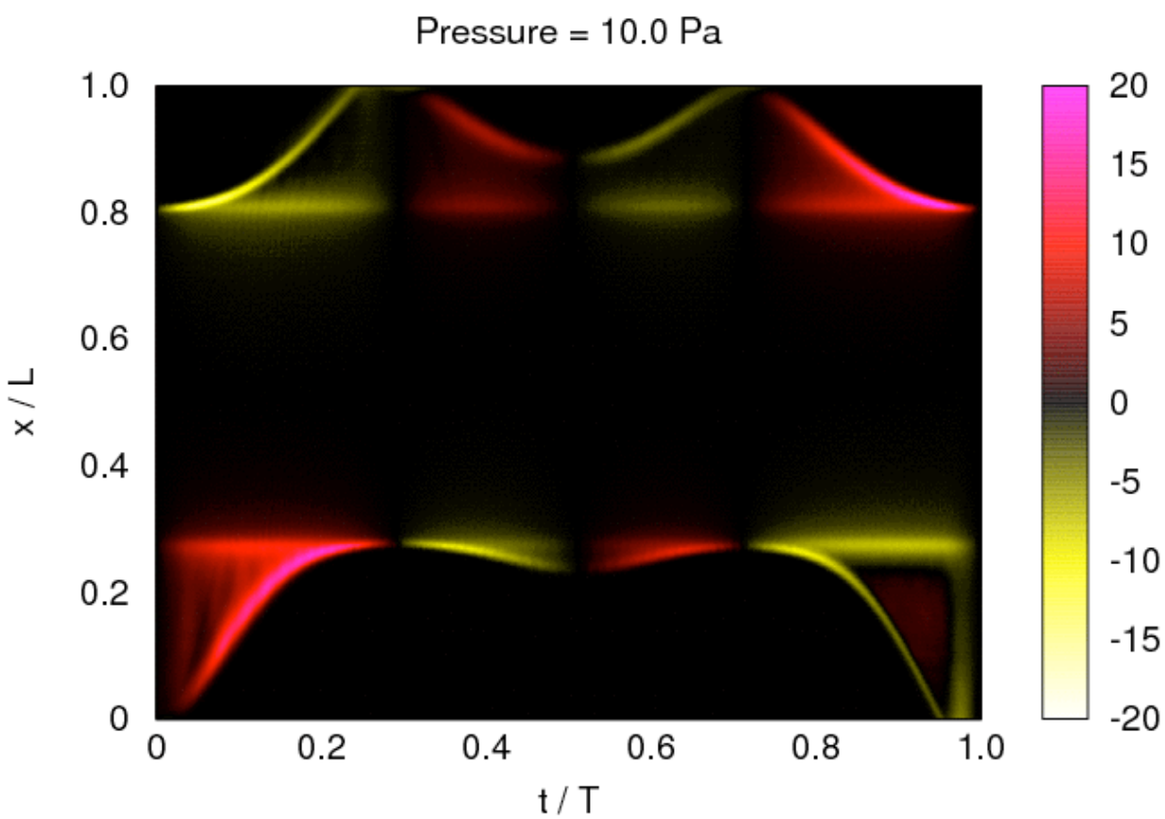
Z. Donkó, J. Schulze, B. G. Heil and U. Czarnetzki, J. Phys. D: Appl. Phys. **42**, 025205 (2009);

Z. Donkó, J. Schulze, U. Czarnetzki, D. Luggenhölscher, Appl. Phys. Lett. **94**, 131501 (2009).

# Plasma Series Resonance

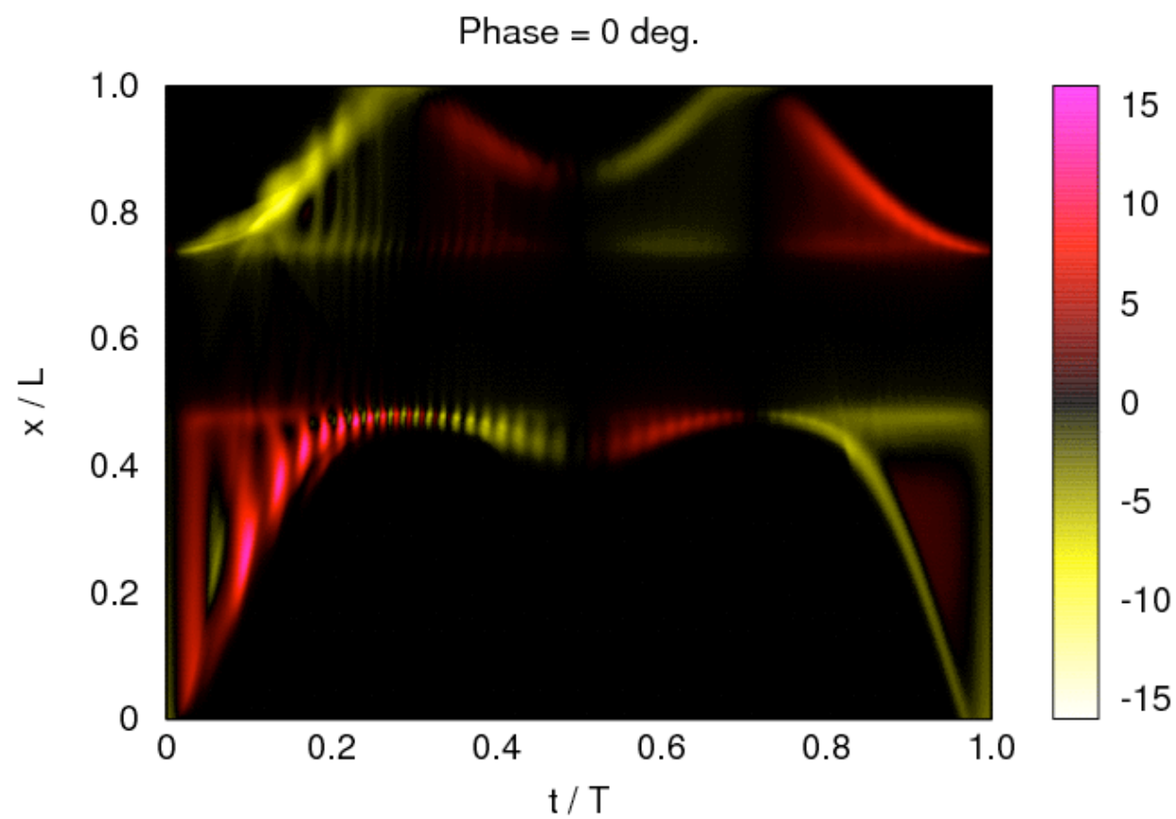
Observation of PSR oscillations in **electrically asymmetric** discharges

Electron heating rate:




$V_0$ = 1000 V, Θ = 7.5°, L = 2.5 cm

Electron heating rate:

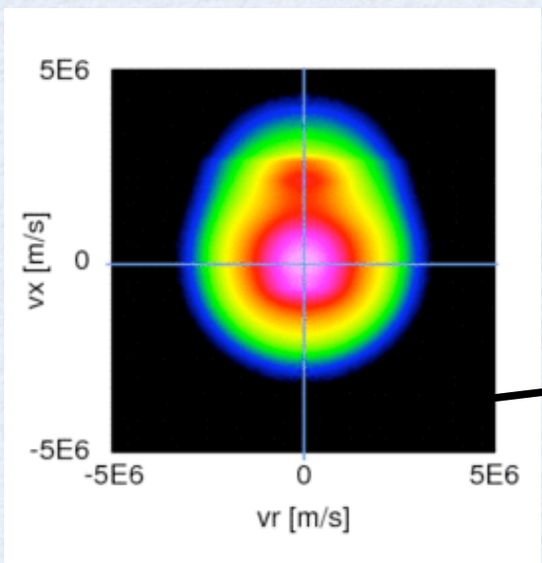



$V_0$ = 1000 V, p = 3 Pa, L = 2.5 cm

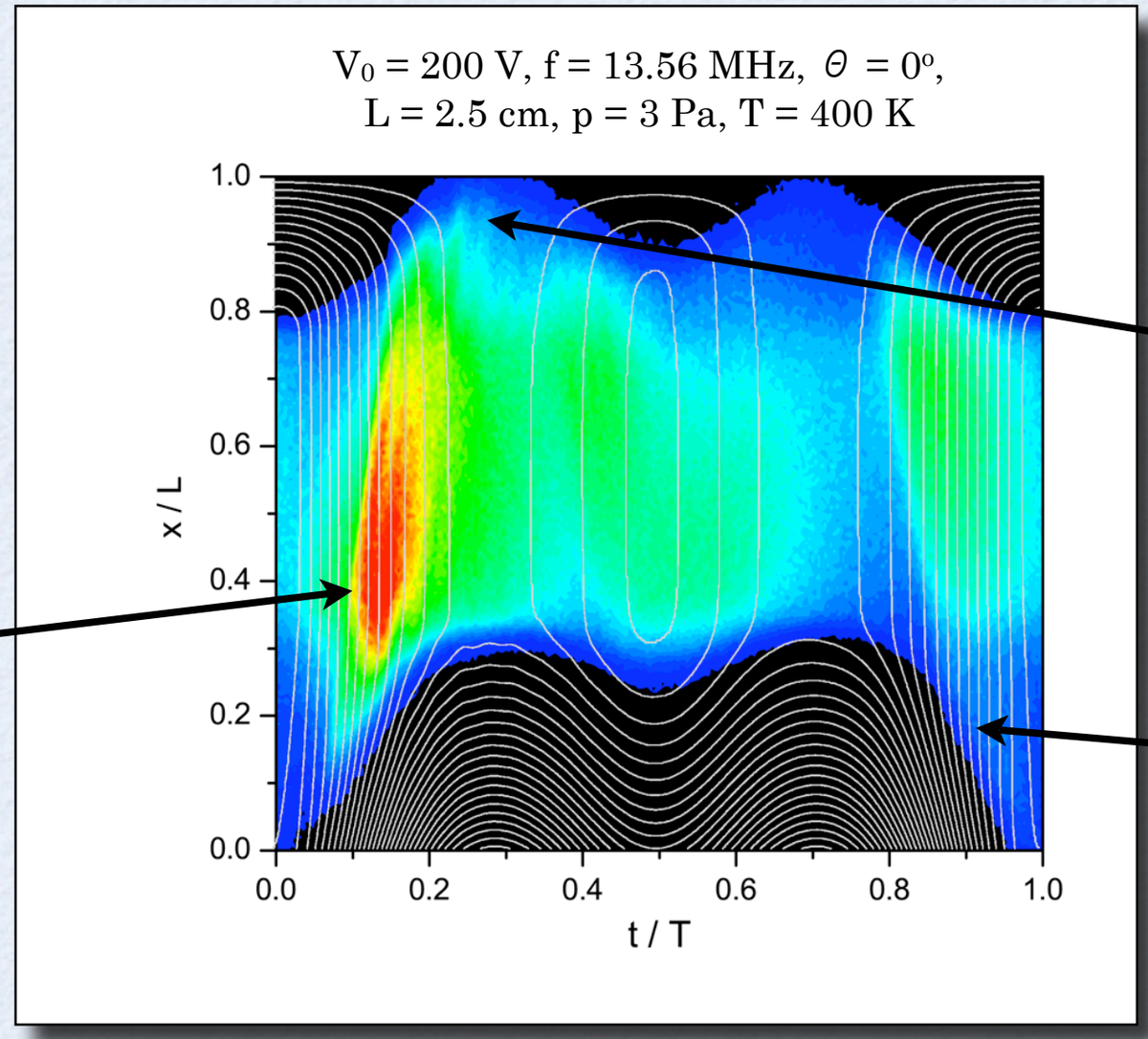
Z. Donkó, J. Schulze, B. G. Heil and U. Czarnetzki, J. Phys. D: Appl. Phys. 42, 025205 (2009);
Z. Donkó, J. Schulze, U. Czarnetzki, D. Luggenhölscher, Appl. Phys. Lett. 94, 131501 (2009).

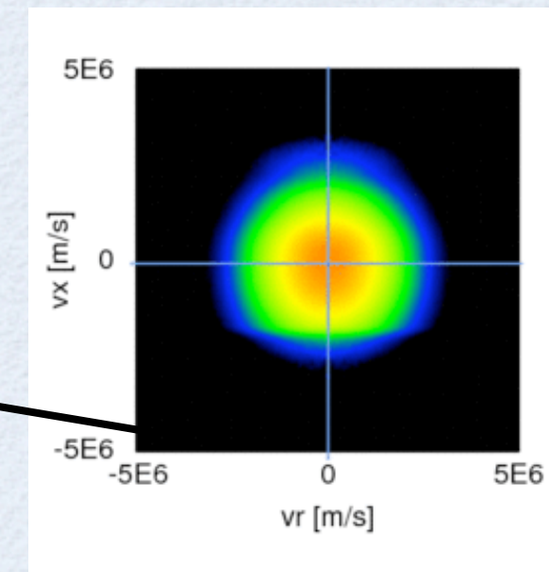
# Velocity distribution functions in RF discharges

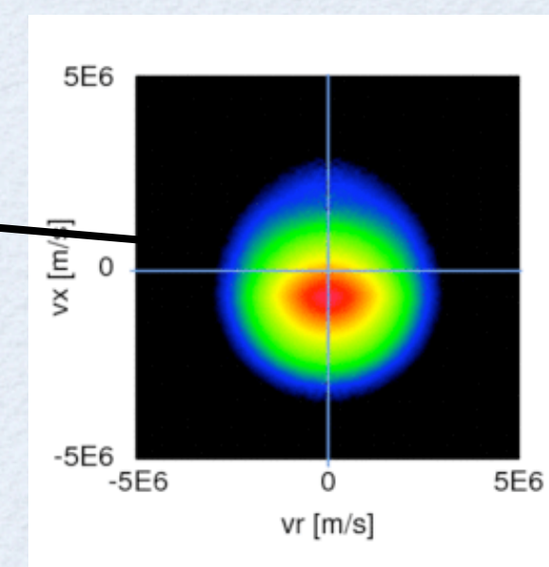
$$\tilde{\phi} = V_0[\cos(\omega t + \theta) + \cos(2\omega t)]$$




distance between contour lines: 20 V




http://plasma.szfki.kfki.hu/~zoli/research/rf1/

# Summary

- This talk intended to illustrate the usefulness and applications of particle simulation methods in specific fields of gas discharge physics - from simple examples to more complicated systems:
  - Charged particle kinetics in homogeneous field
  - Modeling of glow discharges
  - Particle in Cell simulation of radiofrequency discharges
- Important: (i) connection with experiments, (ii) benchmarking, cross-checking

# Thanks

COLLABORATORS, COLLEAGUES, FRIENDS, ....


TO HOST AND
FUNDING
INSTITUTIONS

Hungarian Academy
of Sciences

OTKA
HUNGARIAN SCIENTIFIC RESEARCH FUND

Research Institute for
Solid State Physics and Optics

..... TO ALL OF YOU FOR YOU ATTENTION