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

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" Back to Basics "

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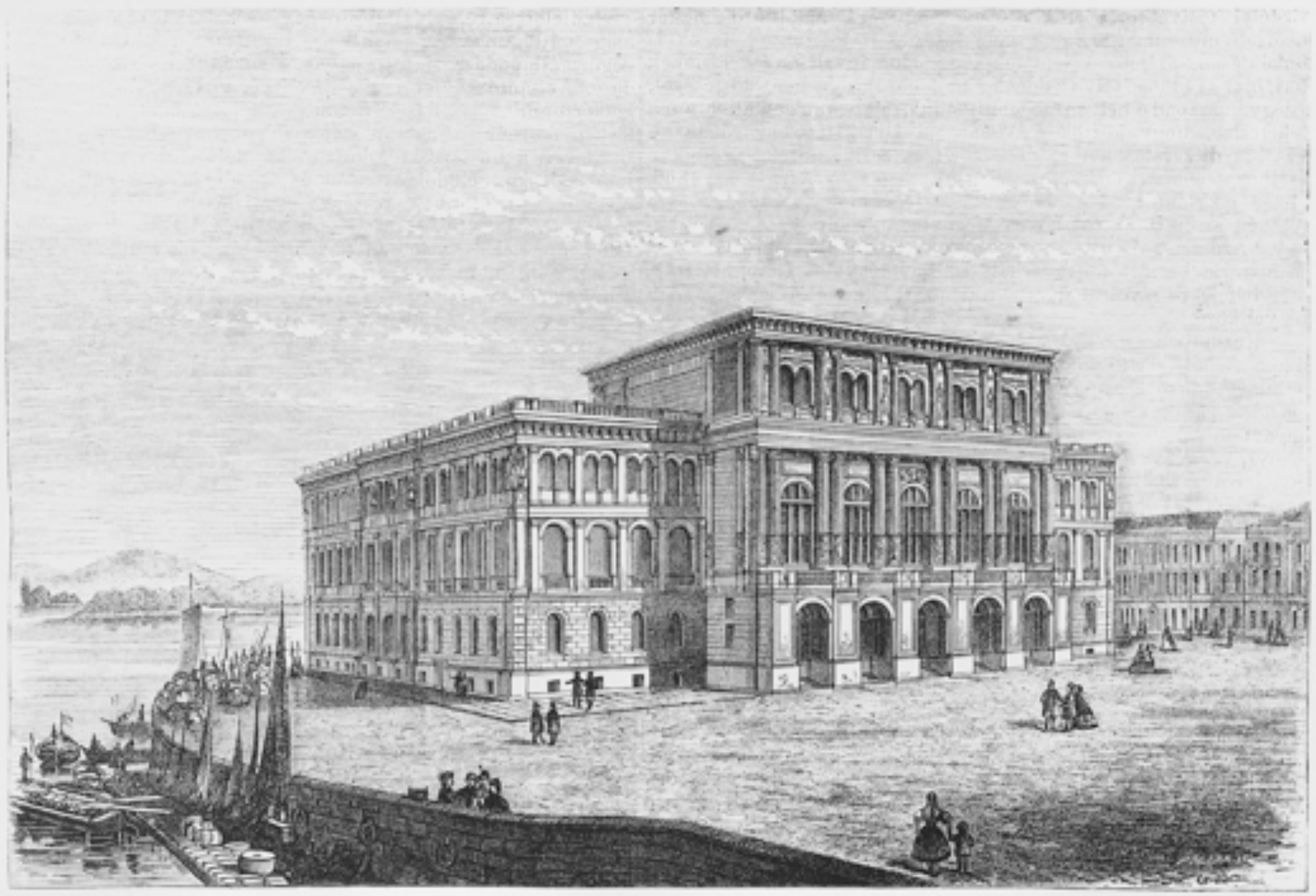

Az akademiai palota terve, a végleges megállapodás szerint

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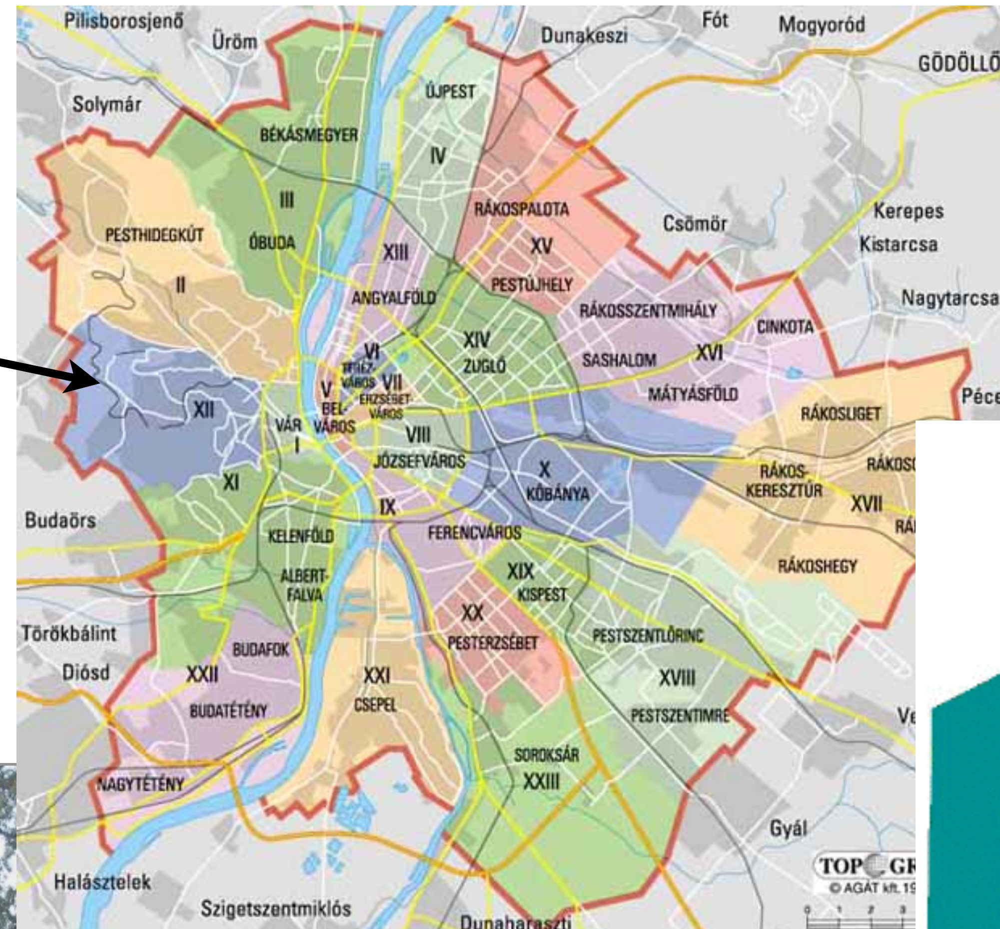

Acknowledgments

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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

1) The Monte Carlo technique, description of collisions

2) Simulation of particle swarms and Townsend discharges

3) Modeling of DC glow discharges

4) Heavy-particle processes in DC discharges

4) Particle-in-Cell + Monte Carlo collision: method

5) PIC/MCC simulation: results for CCRF discharges

(Few words about) Computational resources

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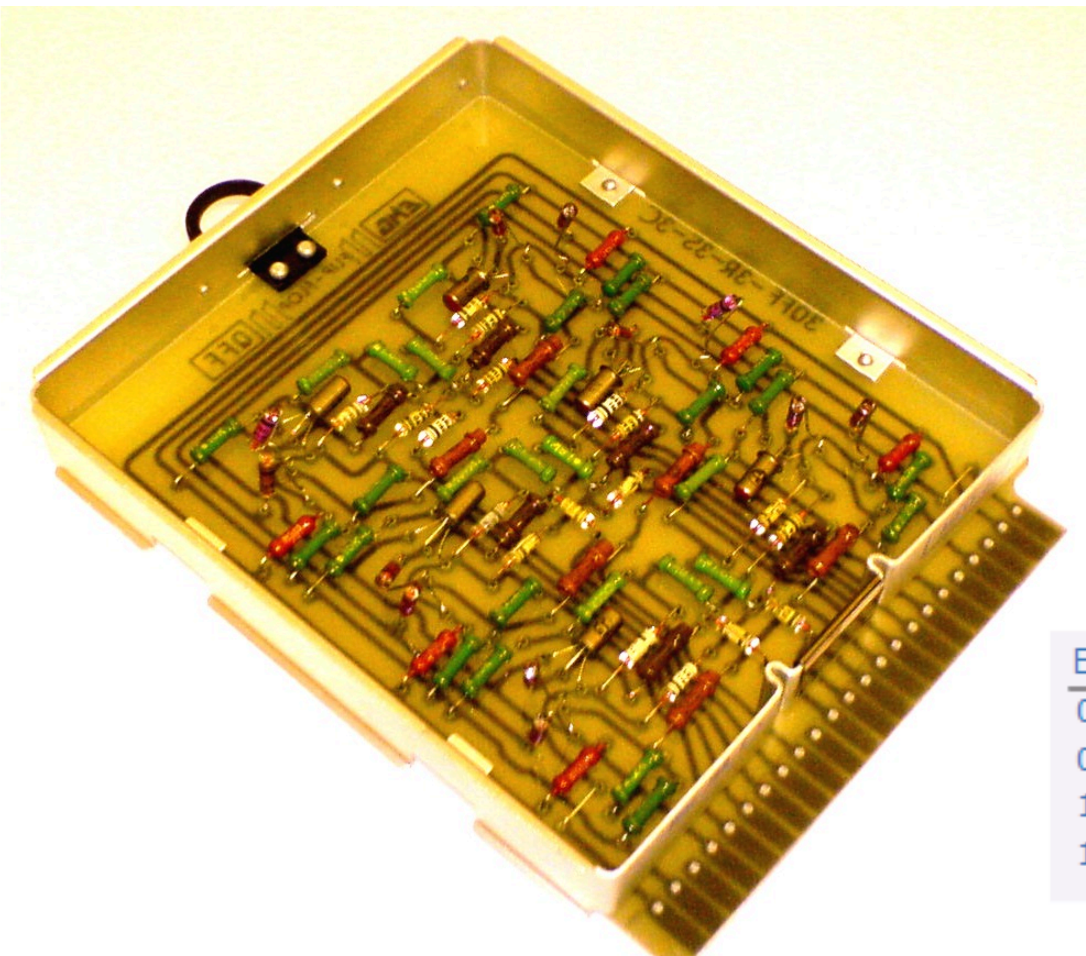
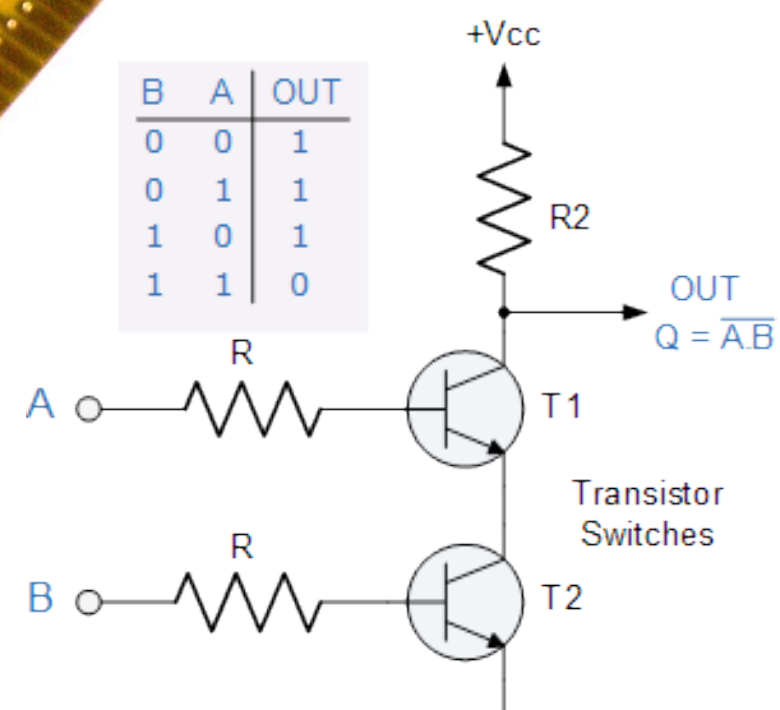
3 bits (transistor flip-flop)
storage card (1960s)



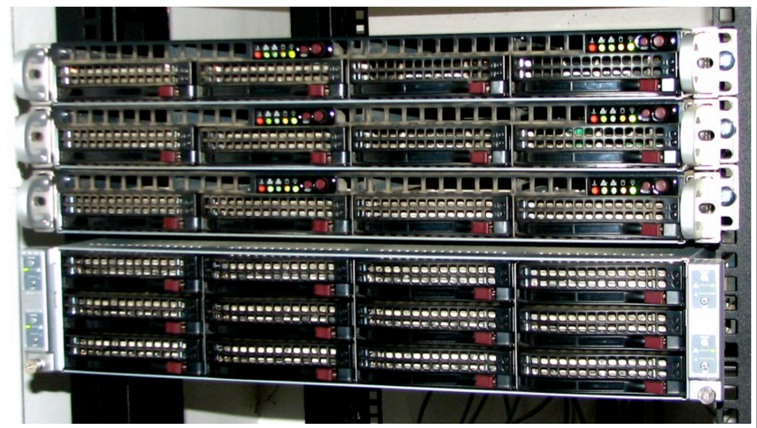
32 GB memory card



NAND gate

One of the most popular
processors

(Few words about) Computational resources



- Amazing progress of resources
- Strong feedback of plasma science and technology on the development of devices

(???)

GPU

Clusters

PCs

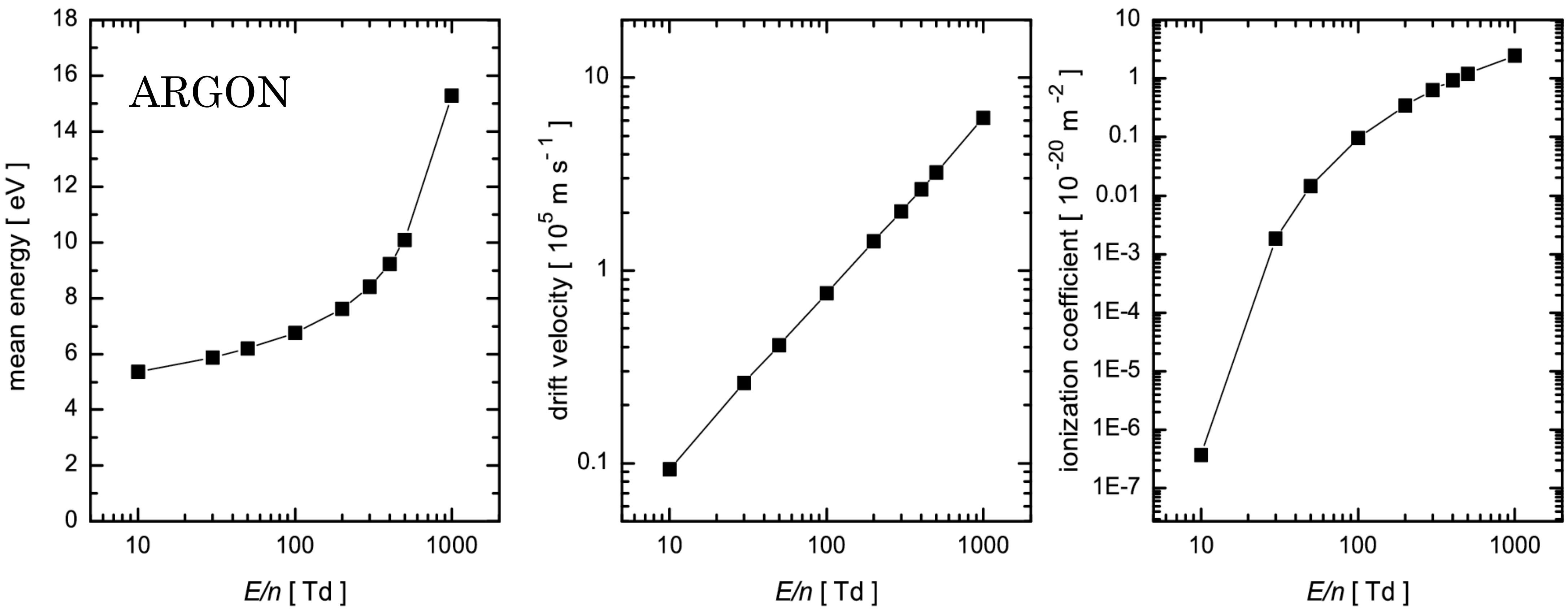
PC

I. Charged particle kinetics

- Fluid vs. kinetic description of transport
- Basics of Monte Carlo simulation
- Velocity distribution functions and transport parameters in homogeneous field
- Spatio-temporal relaxation of the electron gas

Passage of electrons through a gas: electron transport coefficients

- Transport = free flights + collisions
- Look from a distance at the ensemble of particles: transport coefficients
- Transport coefficients can be measured or can be derived from cross section data
- Such calculations are zero-dimensional (homogeneous electric field, infinite space)



Are these data applicable to describe electron behavior in discharges??

Fluid vs. kinetic description of transport

- Fluid models : hydrodynamic transport
- Transport coefficients are functions of local E/n (or on local mean electron energy)
- (Typical) Fluid equations:

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

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

$$S_\mathrm{e} = \alpha\ \phi_\mathrm{e}$$

where

$$\mu_\mathrm{e} n = f_1(E/n)$$

$$D_\mathrm{e} n = f_2(E/n)$$

$$\alpha/n = f_3(E/n)$$

Need: $\frac{\mathrm{d}E}{\mathrm{d}x}\lambda \ll E \qquad \frac{\mathrm{d}E}{\mathrm{d}t}\nu^{-1} \ll E$

- Such a description becomes invalid when the electric field changes rapidly in space/time ⇒ kinetic theory (to describe non-hydrodynamic / non-equilibrium / non-local transport)

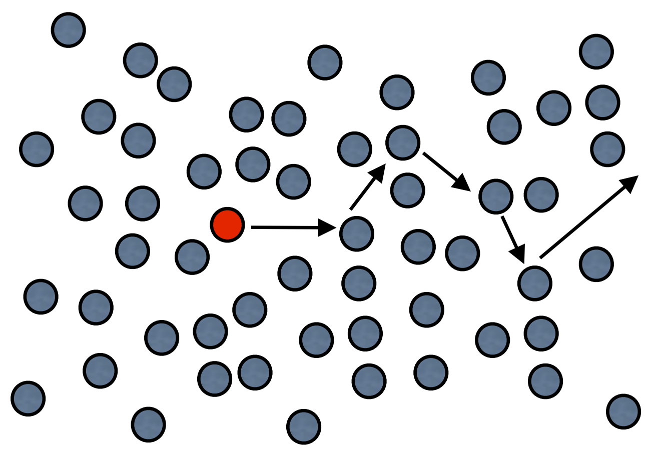
Boltzmann equation

$$\left[\frac{\partial}{\partial t} + \mathbf{a}\cdot\nabla_\mathrm{v} + \mathbf{v}\cdot\nabla_\mathrm{r}\right] f = \left(\frac{\partial f}{\partial t}\right)_\mathrm{coll}$$

$$f = f(\mathbf{r}, \mathbf{v}, t)$$

velocity distribution function

Particle simulation



How good are the transport coefficients ?
Equilibrium vs. non-equilibrium transport

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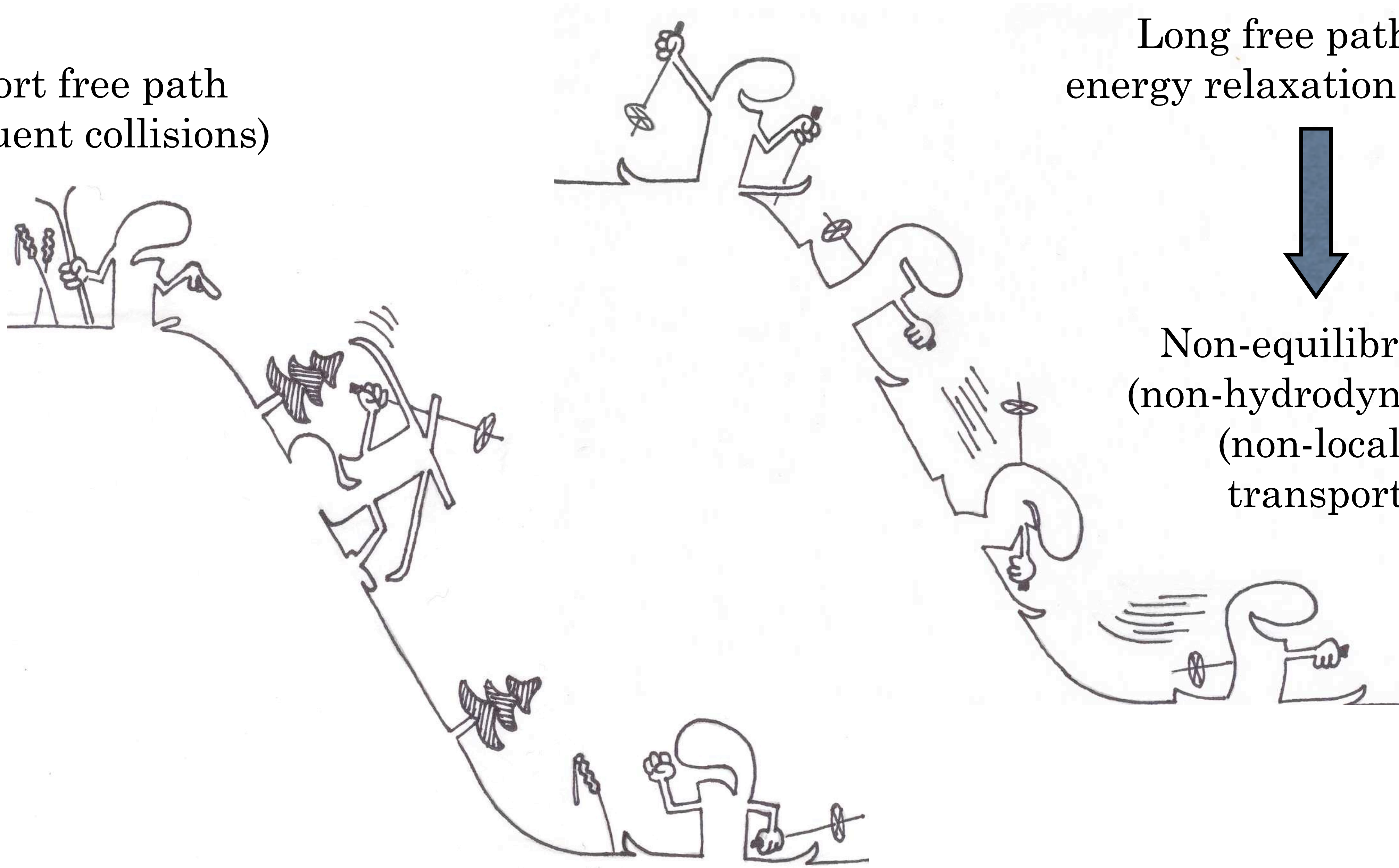
Short free path
(frequent collisions)



Long free path &
energy relaxation length

Non-equilibrium
(non-hydrodynamic)
(non-local)
transport

v

Thanks G. Bánó

Monte Carlo methods

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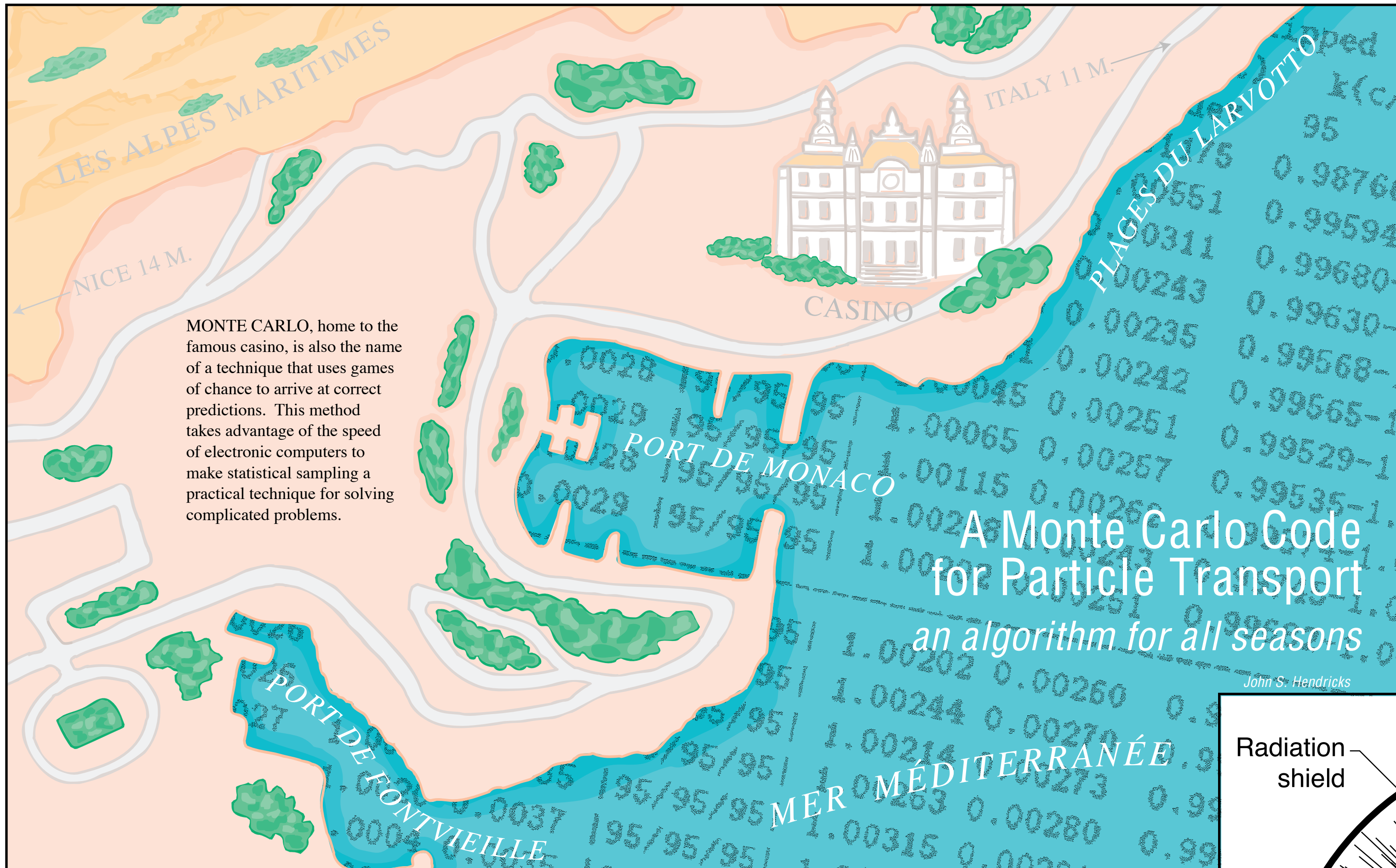
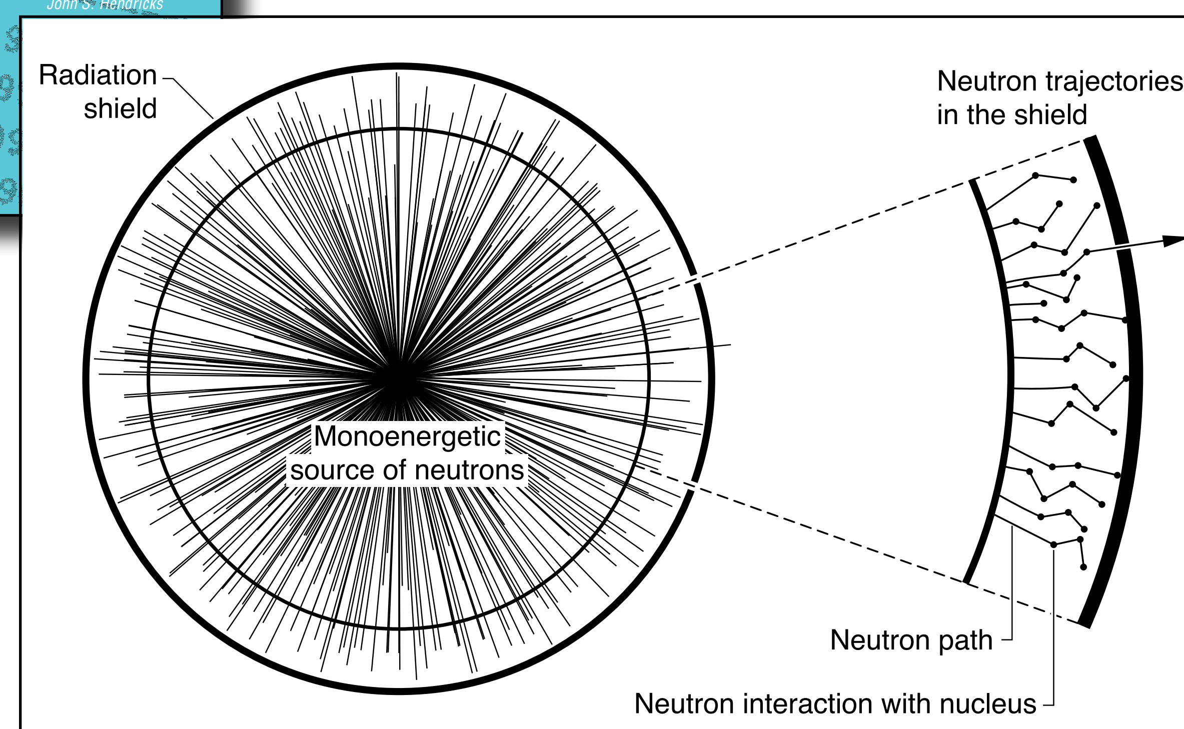


Los Alamos Science. No. 22 (1994)

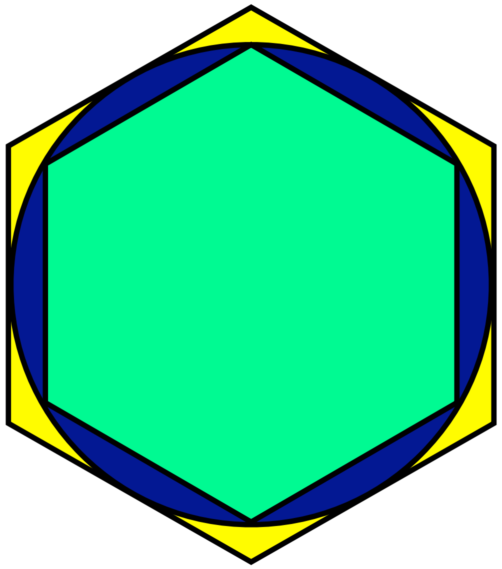
"The Monte Carlo method was first applied on the MANIAC computer at the Laboratory to predict the rate of neutron chain reactions in fission devices..... "

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



Monte Carlo methods: example 1

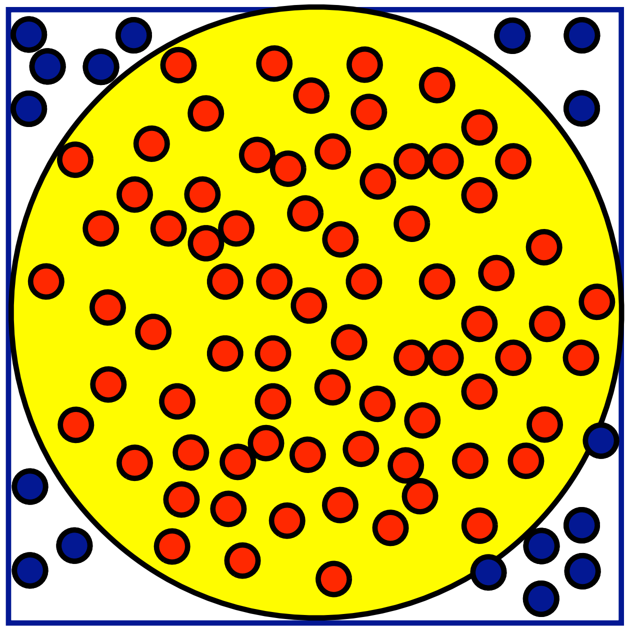
How to approximate π ?



.... 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



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

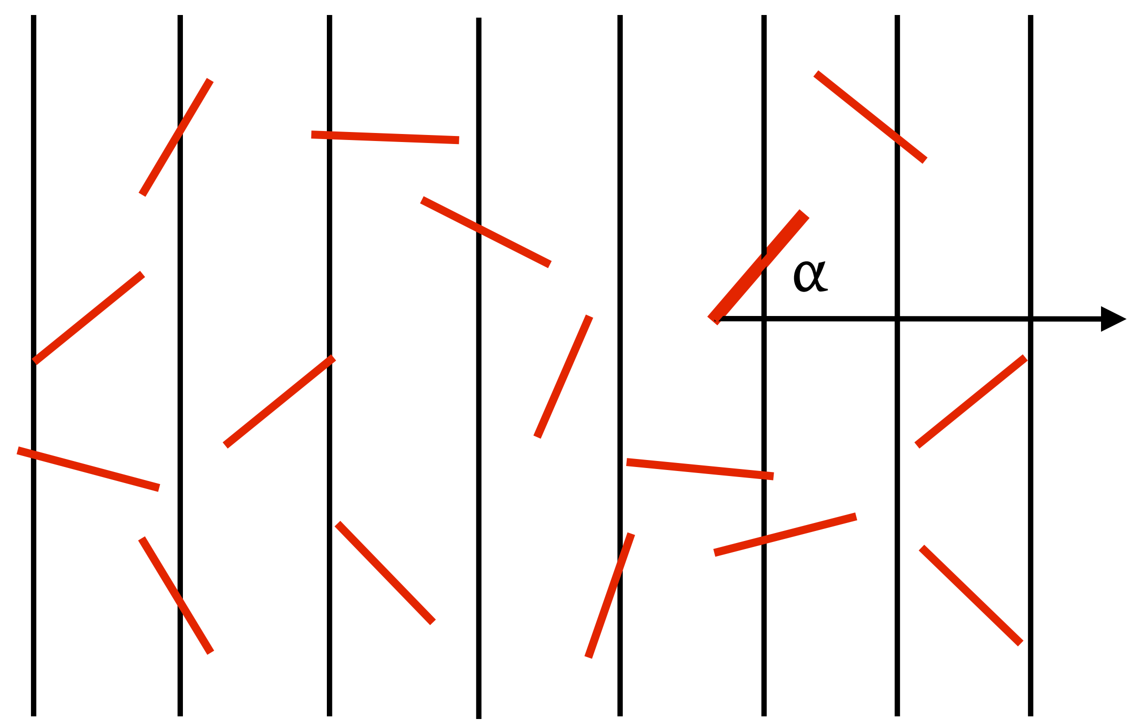
Efficiency / computing speed

A different way of thinking...

Monte Carlo methods: example 2

"Buffon's Needle problem"

Throw needles with length L on a paper, which has parallel lines with distance D



George Louis le Clerq, *Comte de Buffon*

P (needle crosses a line) : $\quad P(\alpha) = \dfrac{L|\cos\alpha|}{D}$

$$P = \frac{1}{2\pi}\int_0^{2\pi} P(\alpha)\mathrm{d}\alpha = \frac{L}{2\pi D}\int_0^{2\pi} |\cos\alpha|\mathrm{d}\alpha = \frac{2L}{\pi D}$$

If $L = D$: $\quad \dfrac{N}{N_\mathrm{C}} \to \dfrac{\pi}{2}$

Monte Carlo method: particle transport

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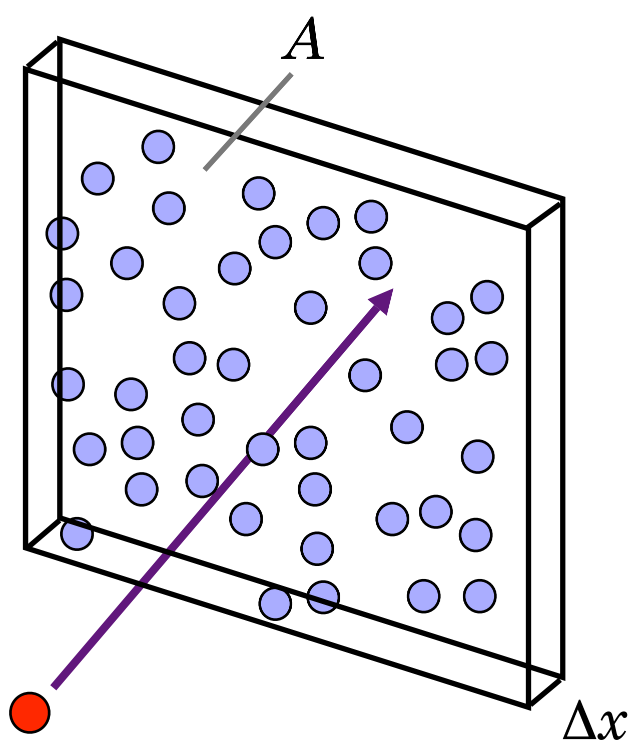
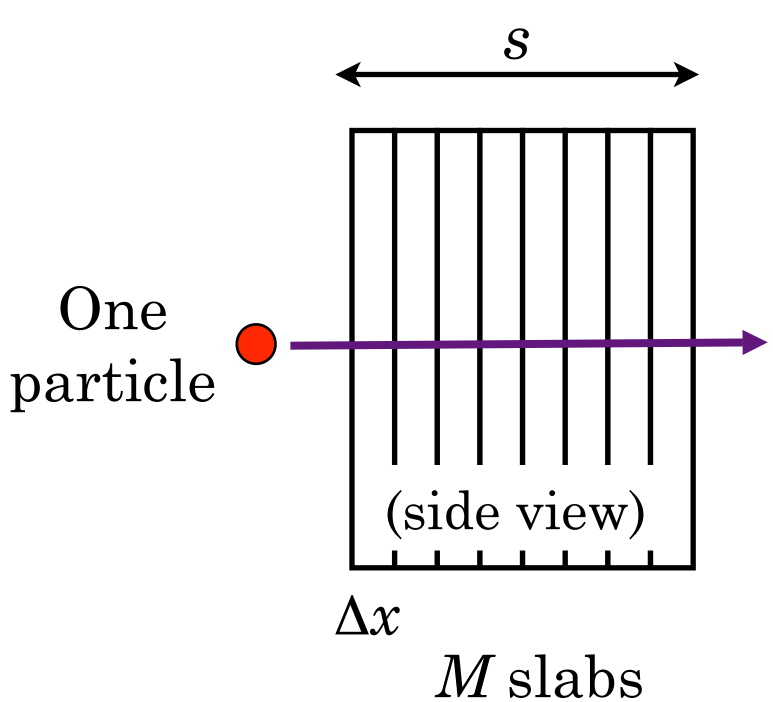


Transit of a particle through a narrow slab of background gas

N background gas particles with same cross section

$$P_{\text{coll}} = \frac{A'}{A} = \frac{N\sigma}{A} = \frac{(nA\Delta x)\sigma}{A} = n\sigma\Delta x$$

valid in the $\Delta x \rightarrow 0$ limit

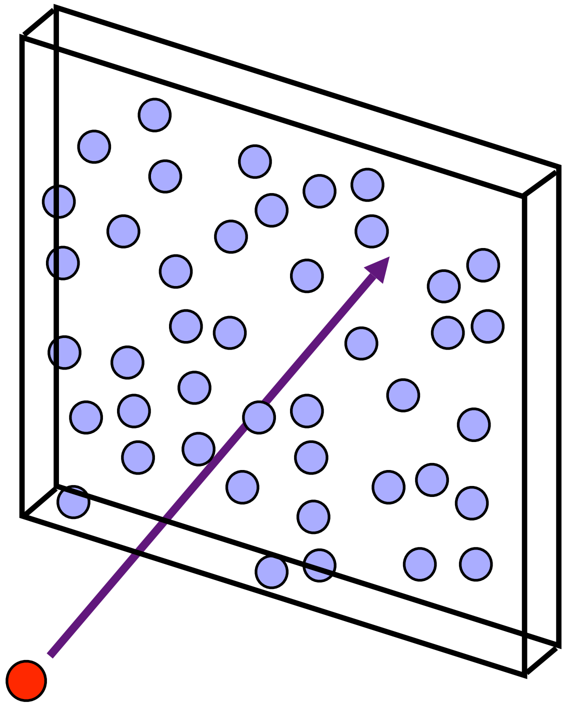


Transit of a particle through a stack of slabs (macroscopic width)

$$P_{\text{transfer}} = (1 - P_{\text{coll}})^M$$
$$= (1 - n\sigma\Delta x)^M = (1 - n\sigma\Delta x)^{\frac{s}{\Delta x}}$$
$$= (1 - n\sigma\Delta x)^{-\frac{1}{n\sigma\Delta x}(-sn\sigma)} \rightarrow \mathrm{e}^{-n\sigma s} \quad \text{if} \quad \Delta x \rightarrow 0$$

$$\boxed{P_{\text{coll}} = 1 - \mathrm{e}^{-n\sigma s} = 1 - \mathrm{e}^{-n\sigma v \Delta t}}$$

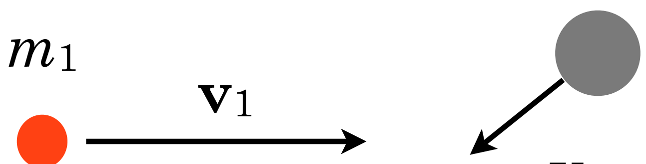
Monte Carlo method: particle transport



Collisions with background gas atoms with thermal distribution

$$P(\Delta t) = 1 - \exp[-n\overline{\sigma_\mathrm{T}(v_r)v_r}\Delta t]$$

$$\mathbf{v}_r = \mathbf{v}_1 - \mathbf{v}_2$$



$$\overline{\sigma_\mathrm{T} v_r} = \int\int\int \sigma_\mathrm{T}(|\mathbf{v}_1 - \mathbf{v}_2|)|\mathbf{v}_1 - \mathbf{v}_2|\left(\frac{m_2}{2\pi k T_2}\right)^{3/2}\exp\left(-\frac{m_2 v_2^2}{2kT_2}\right)\mathrm{d}v_{2x}\mathrm{d}v_{2y}\mathrm{d}v_{2z}$$

Cold gas approximation

$$T_2 = 0$$

$$P_\mathrm{coll}(\Delta t) = 1 - \exp[-n\sigma_\mathrm{T} v_1 \Delta t]$$

- valid for electrons as long as $\overline{\varepsilon} \gg kT_2$
- normally not valid for ions

Monte Carlo method: particle transport

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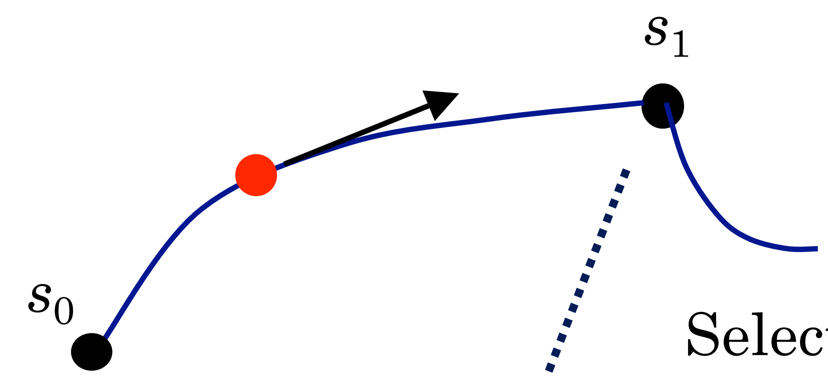
Tracing of individual particles
(cold gas approx.)

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

$t \rightarrow t + \Delta t$

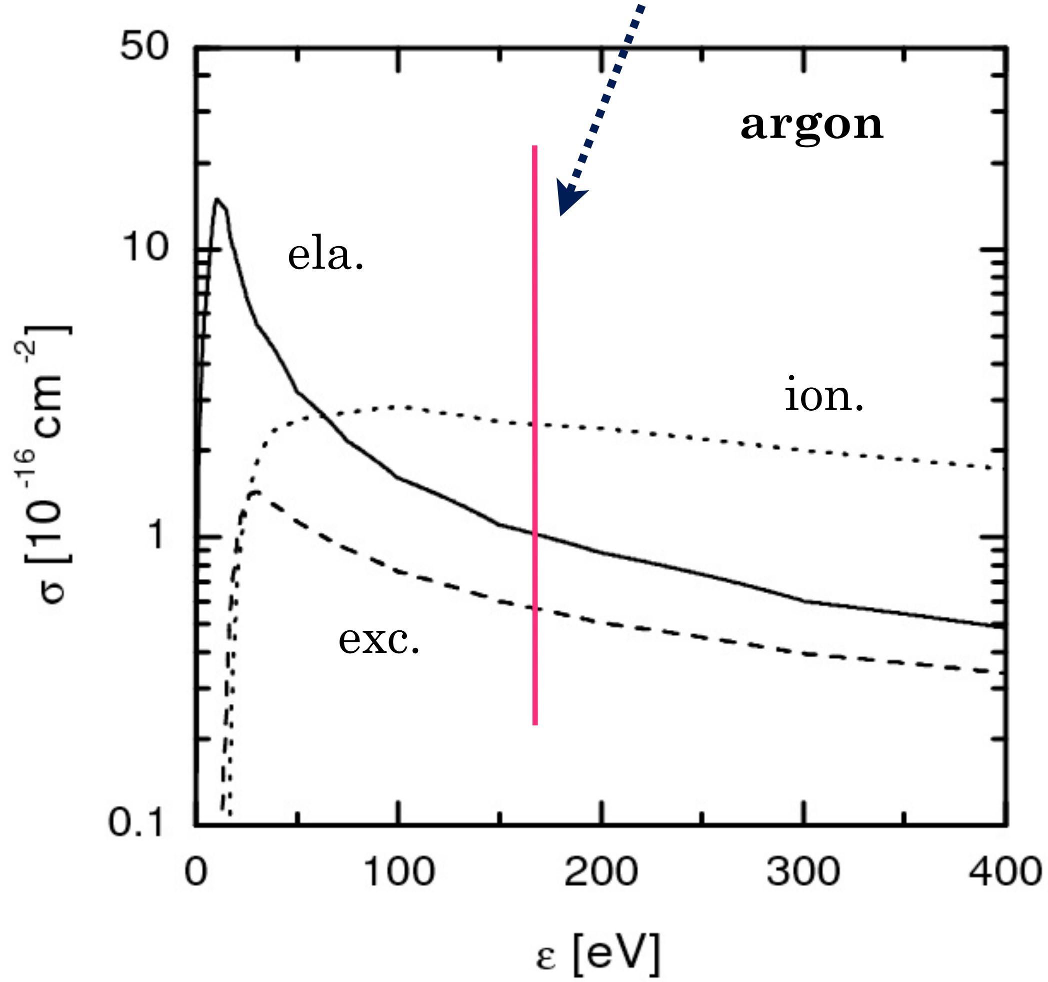
Probability of collision: $P_{\mathrm{coll}} = 1 - \mathrm{e}^{-n\sigma v \Delta t}$

total cross section



Select type:

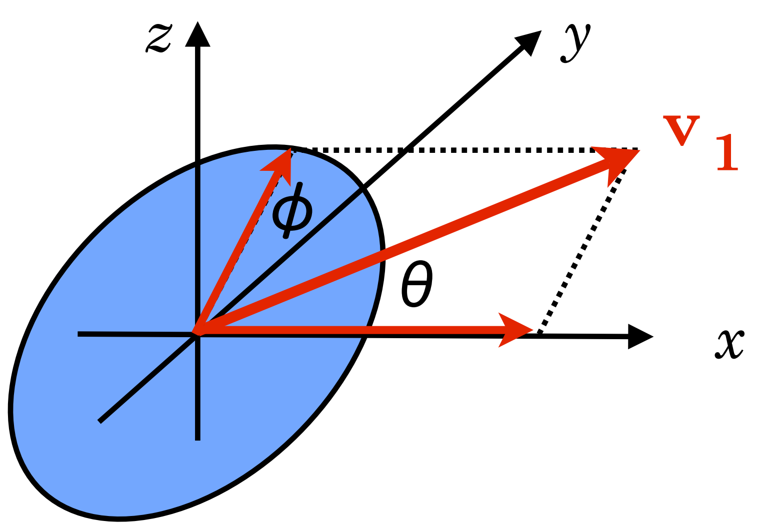
$$P_k = \frac{\sigma_k(\varepsilon)}{\sigma_{\mathrm{T}}(\varepsilon)}$$



- Processes
  - elastic scattering,
  - electronic excitation,
  - ionization

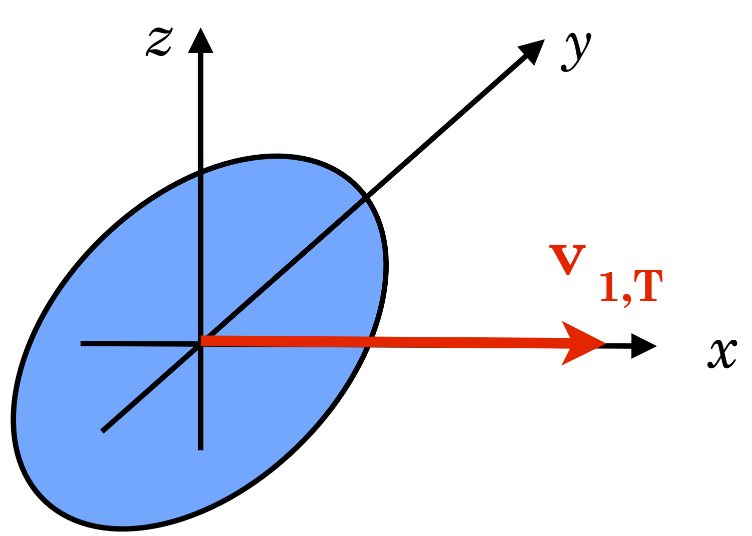
- Chosen in a probabilistic manner:
  - free path,
  - type of collision,
  - new direction

Electron collisions: steps



1. Find velocity components (Euler angles)

$$\mathbf{v}_1 = \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = v_1 \begin{bmatrix} \cos\theta \\ \sin\theta\cos\phi \\ \sin\theta\sin\phi \end{bmatrix}$$



2. Transform velocity vector into z direction

$$\mathbf{v}_{1,\mathrm{T}} = \mathbf{T}_z(-\theta)\mathbf{T}_x(-\phi)\mathbf{v}_1 = v_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

(this calculation doesn't need to be carried out)

Electron collisions: steps

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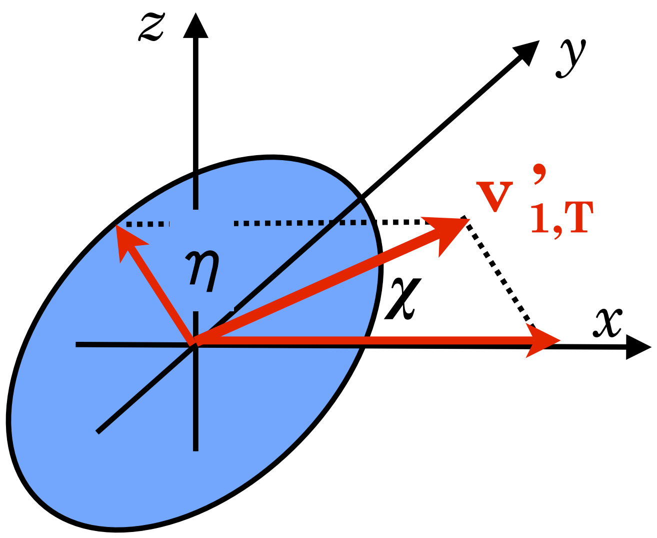
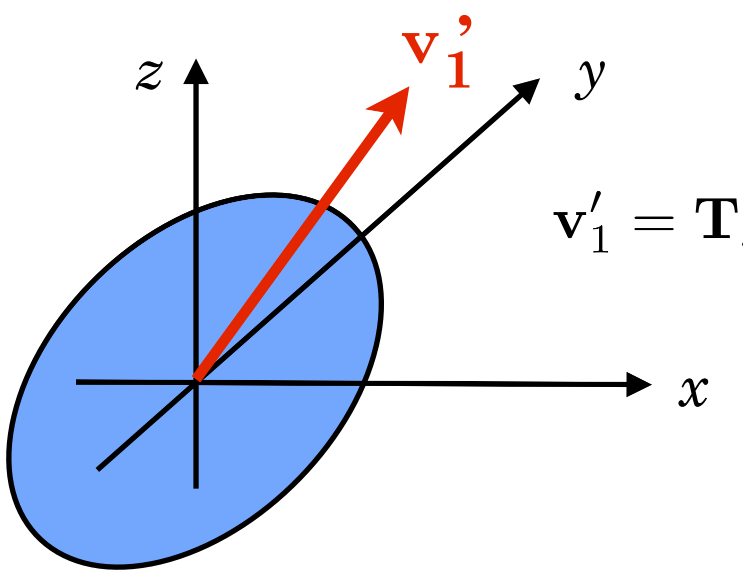


3. Deflect velocity vector (collision)

$$\mathbf{v}'_{1,\mathrm{T}} = v'_1 \begin{bmatrix} \cos\chi \\ \sin\chi\cos\eta \\ \sin\chi\sin\eta \end{bmatrix}$$

(details discussed later on)



4. Transform "back"

$$\mathbf{v}'_1 = \mathbf{T}_x(\phi)\mathbf{T}_z(\theta)\mathbf{v}'_{1,\mathrm{T}} = v'_1 \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \end{bmatrix} \begin{bmatrix} \cos\chi \\ \sin\chi\cos\eta \\ \sin\chi\sin\eta \end{bmatrix}$$

$$\mathbf{v}'_1 = v'_1 \begin{bmatrix} \cos\theta\cos\chi - \sin\theta\sin\chi\cos\eta \\ \sin\theta\cos\phi\cos\chi + \cos\theta\cos\phi\sin\chi\cos\eta - \sin\phi\sin\chi\sin\eta \\ \sin\theta\sin\phi\cos\chi + \cos\theta\sin\phi\sin\chi\cos\eta + \cos\phi\sin\chi\sin\eta \end{bmatrix}$$

Electron collisions: velocity change during collision

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Choosing the angles:

Scattering angle

based on differential cross sec.:

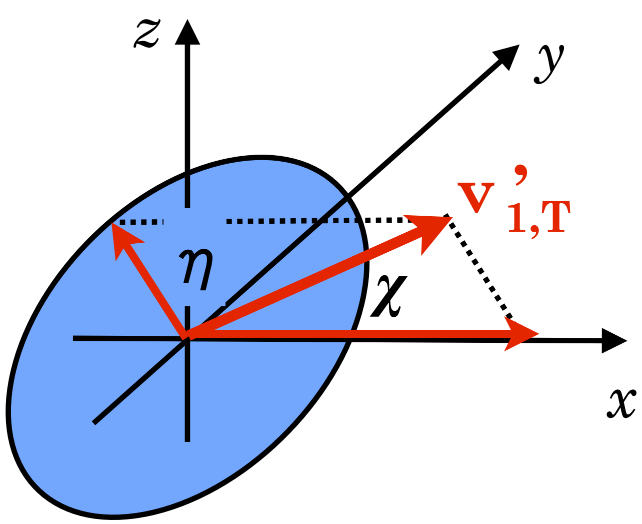
$$\frac{\int_0^{\chi} \sigma(\varepsilon, \chi') \sin \chi' \mathrm{d}\chi'}{\int_0^{\pi} \sigma(\varepsilon, \chi') \sin \chi' \mathrm{d}\chi'} = R_{01}$$

or, assuming isotropic scattering:

$$\chi = \arccos(1 - 2R_{01})$$

Azimuth angle

$$\eta = 2\pi R_{01}$$



Energy change:

Elastic scattering

$$\frac{\Delta\varepsilon}{\varepsilon} = -\frac{2m_1 m_2}{(m_1 + m_2)^2}(1 - \cos\chi)$$

$$\frac{\Delta\varepsilon}{\varepsilon} = -2\,\frac{m_1}{m_2}(1 - \cos\chi) \quad \text{if} \quad m_1 \ll m_2$$

Excitation

$$\Delta\varepsilon = -\varepsilon_j$$

Ionization

$$\varepsilon_{\mathrm{scatt}} + \varepsilon_{\mathrm{eject}} = \varepsilon - \varepsilon_{\mathrm{ion}}$$

$$\varepsilon_{\mathrm{eject}} = \bar{E} \tan\left[R_{01} \arctan\left(\frac{\varepsilon - \varepsilon_{\mathrm{ion}}}{2\bar{E}}\right)\right]$$

For electrons we did not use here transformation to Center of Mass system for the scattering ...

Ion collisions

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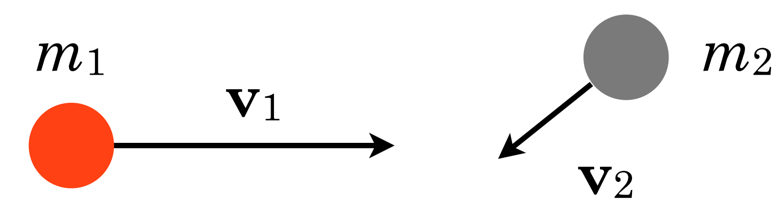
Unlike for electrons, here the mass of the projectile and the target are comparable
→ one has to work in the *Center of Mass* system



$\mathbf{v}_2$ has to be sampled from a Maxwellian distribution of the background gas atoms

Velocity of center of mass: $\mathbf{w} = \dfrac{m_1\mathbf{v}_1 + m_2\mathbf{v}_2}{m_1 + m_2}$

Relative velocity: $\mathbf{v}_\mathrm{r} = \mathbf{v}_1 - \mathbf{v}_2$

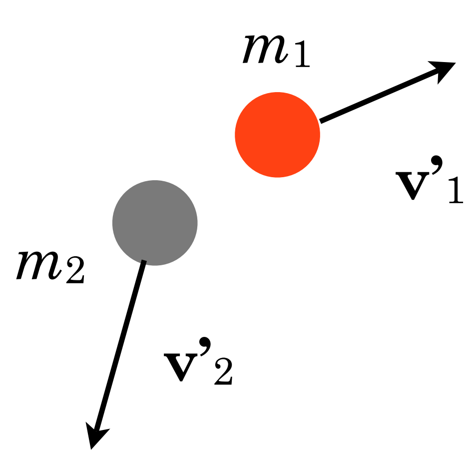
Velocities in the COM frame: $\begin{cases} \mathbf{V}_1 = \mathbf{v}_1 - \mathbf{w} \\ \mathbf{V}_2 = \mathbf{v}_2 - \mathbf{w} \end{cases}$

An elastic collision changes the direction of the relative velocity but keeps the magnitude unchanged

$\mathbf{v}_\mathrm{r} \rightarrow \mathbf{v}_\mathrm{r}'$

Postcollision velocities in the LAB frame:

$$\begin{cases} \mathbf{v}_1' = \dfrac{m_2}{m_1+m_2}\mathbf{v}_\mathrm{r}' + \dfrac{m_1\mathbf{v}_1 + m_2\mathbf{v}_2}{m_1+m_2} \\[2ex] \mathbf{v}_2' = -\dfrac{m_1}{m_1+m_2}\mathbf{v}_\mathrm{r}' + \dfrac{m_1\mathbf{v}_1 + m_2\mathbf{v}_2}{m_1+m_2} \end{cases}$$



For noble gases the ion-atom collisions can in most cases be restricted to elastic scattering. Using the model of Phelps [J. Appl. Phys. **76**, 747 (1994)] this process is assumed to have two parts: (i) isotropic part + (ii) backward scattering part.

MC simulation: electron avalanches

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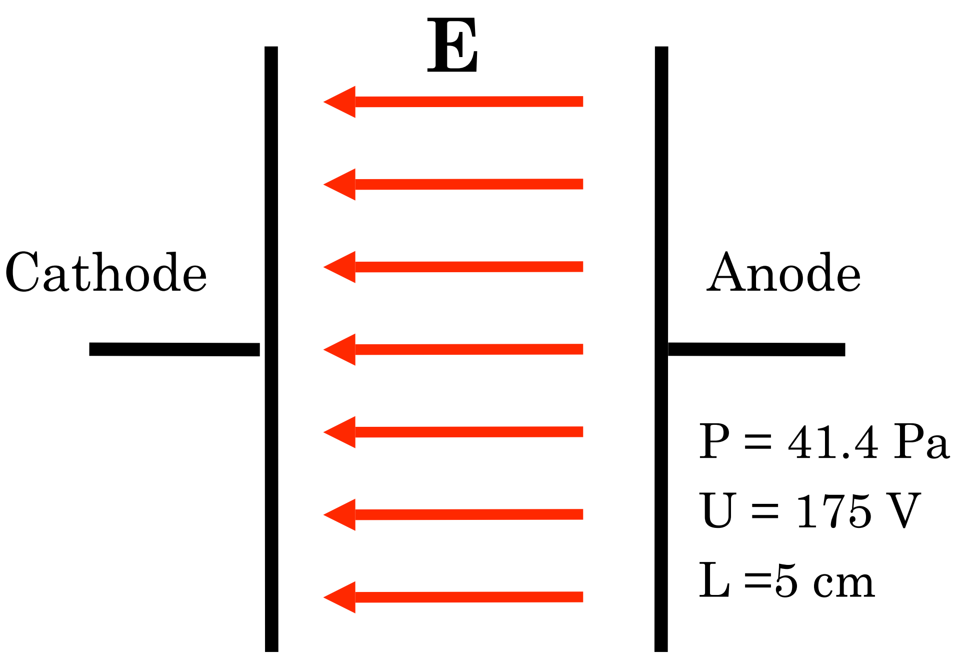
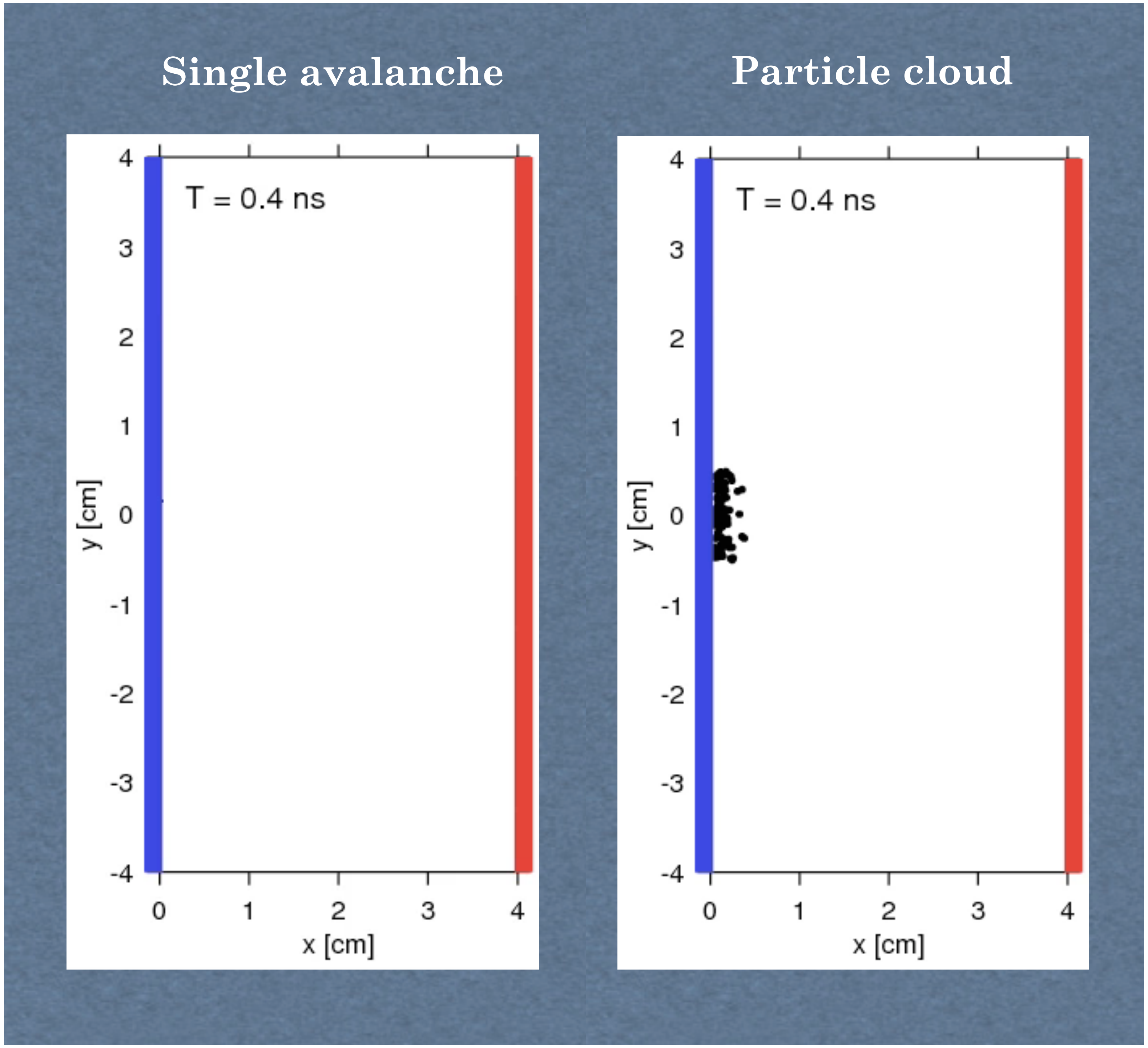
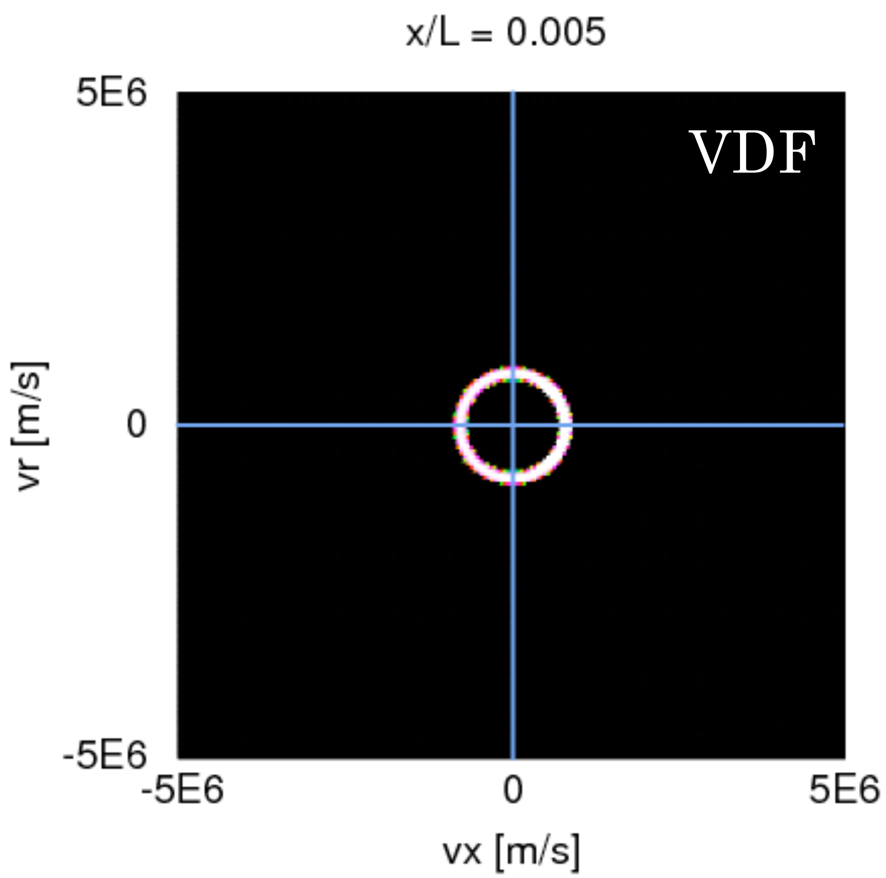


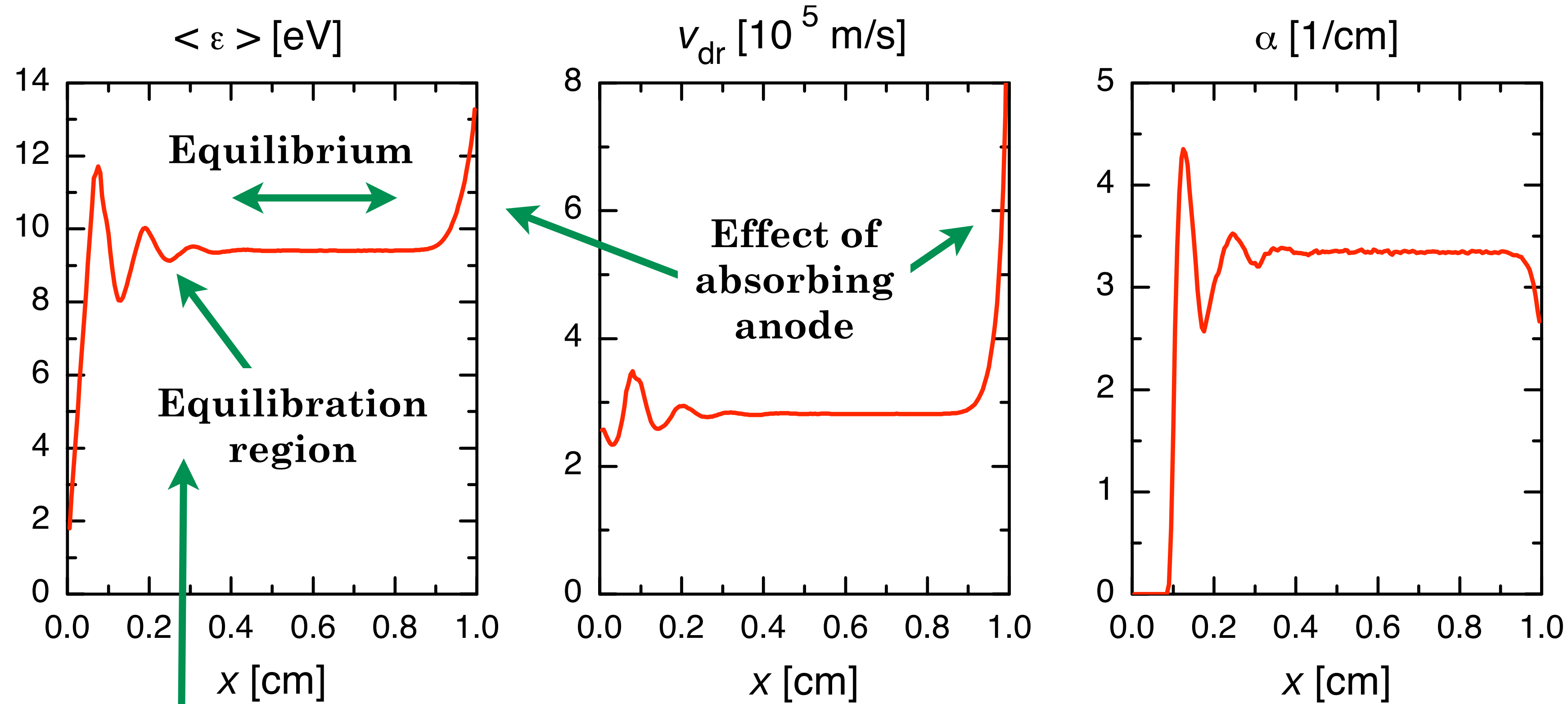
- 1D - simplest geometry
- infinite, plane, parallel electrodes
- homogeneous field
- already requires kinetic treatment (see more later)



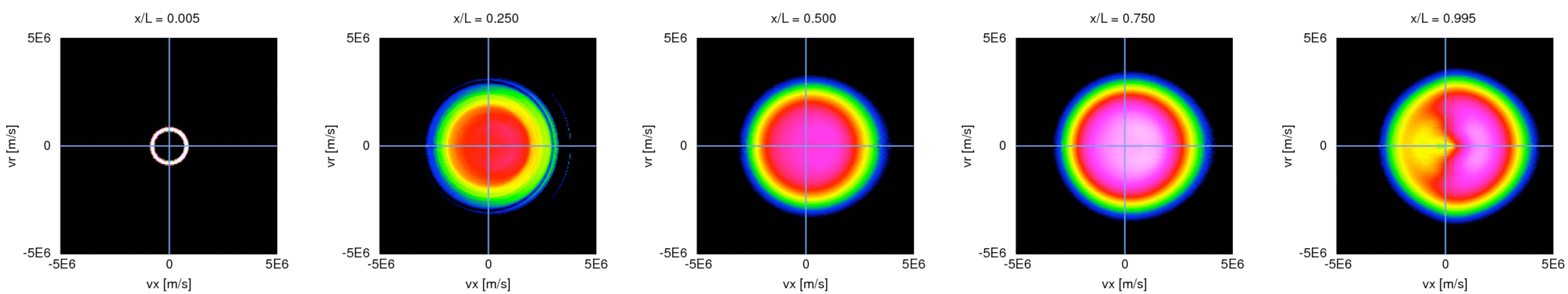
Electron swarms in homogeneous electric field

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).



Z. Donkó, PSST (2010).

Electron swarms in homogeneous electric field

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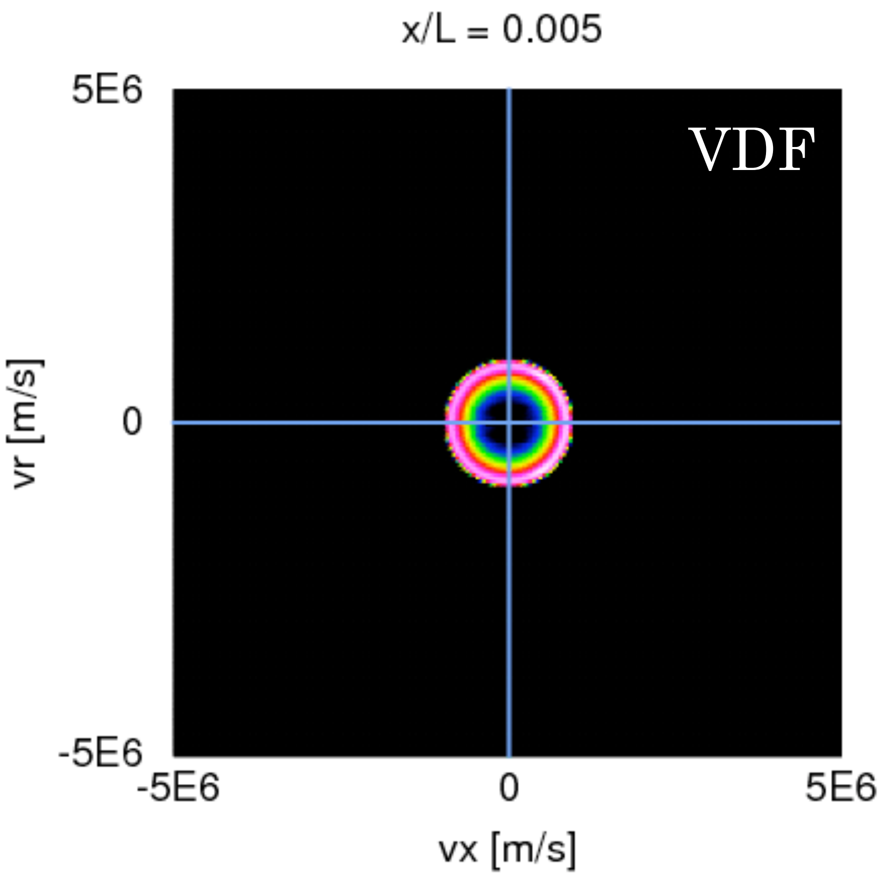
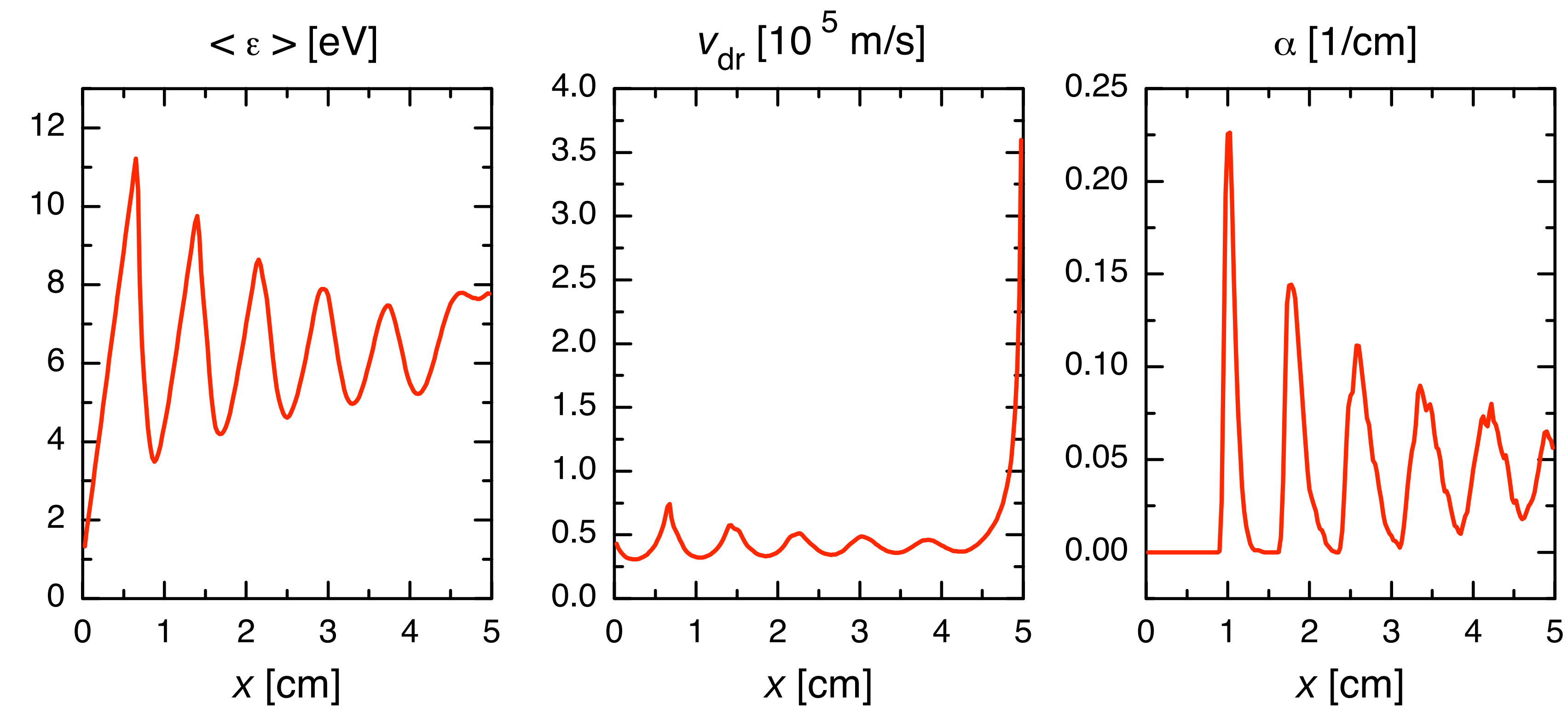
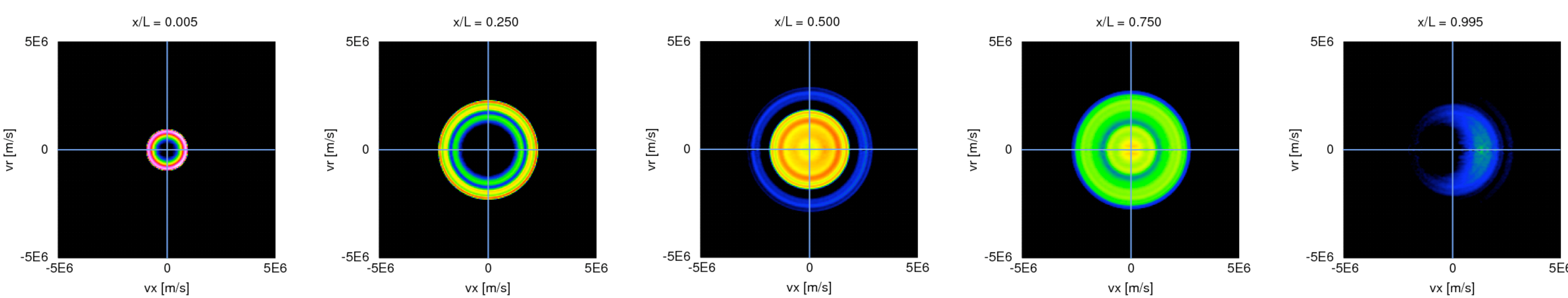


E/n = 50 Td, L = 5 cm, p = 1 Torr



Complete lack of equilibrium region



Spatio-temporal relaxation of an electron swarm

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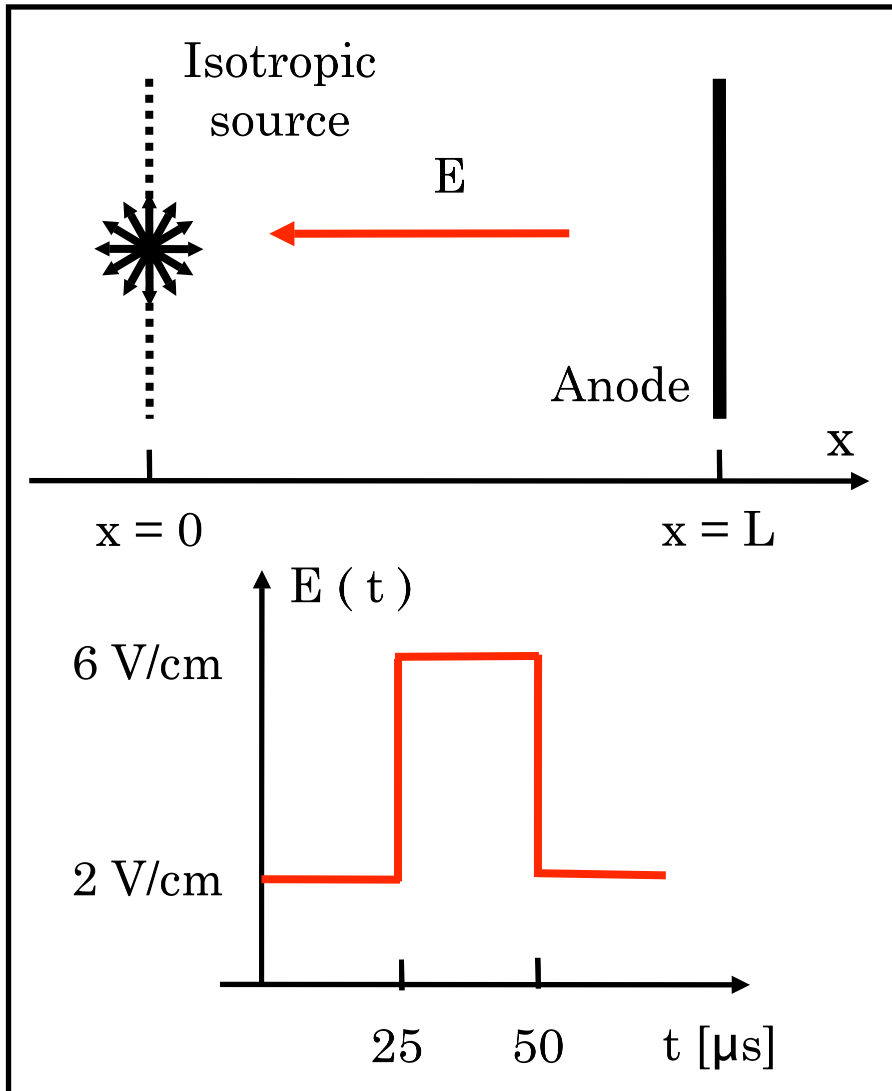

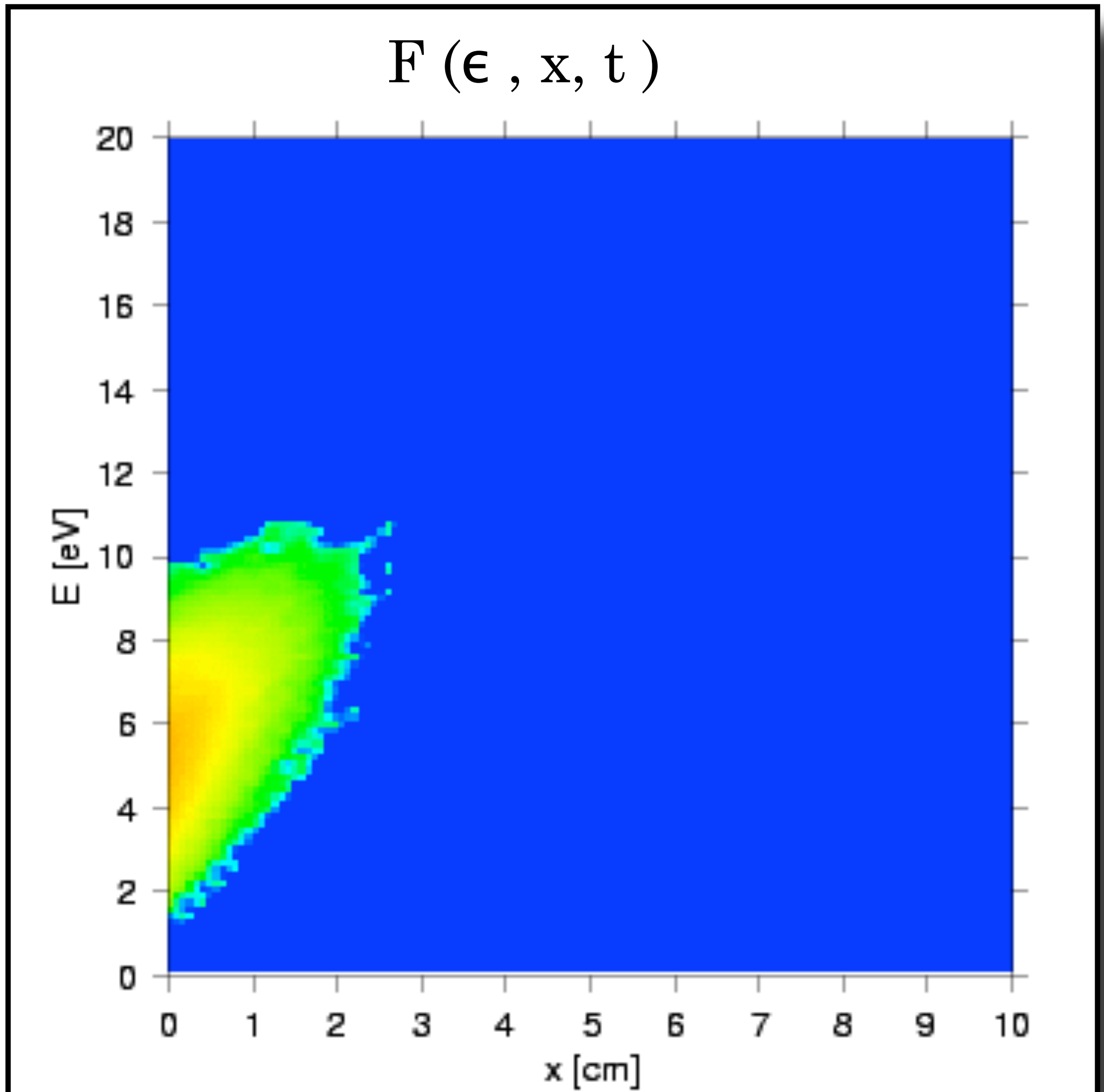

D. Loffhagen, R. Winkler, Z. Donkó, Eur. Phys. J. Appl. Phys. 18, 189 (2002).

(calculated with both MC simulation and Boltzmann equation)

Monte Carlo method: particle transport

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- *Monte Carlo simulation of charged species kinetics in weakly ionized gases* [S. Longo, Plasma Sources Sci. Technol. **15**, S181 (2006)]
- *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, Greifswald & Belgrade groups, ...)
- *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.]

The "null-collision" technique

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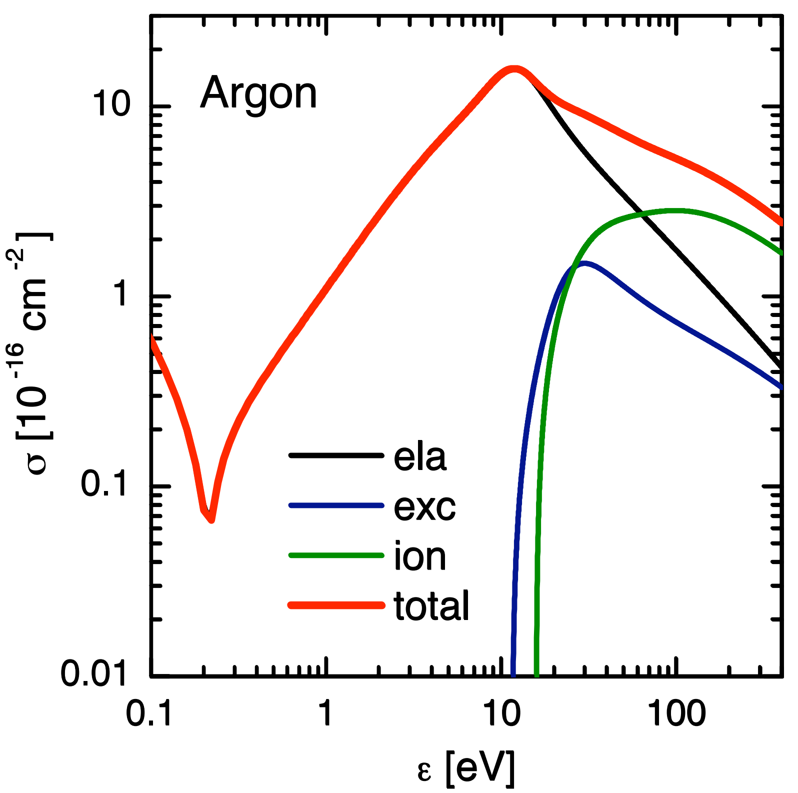
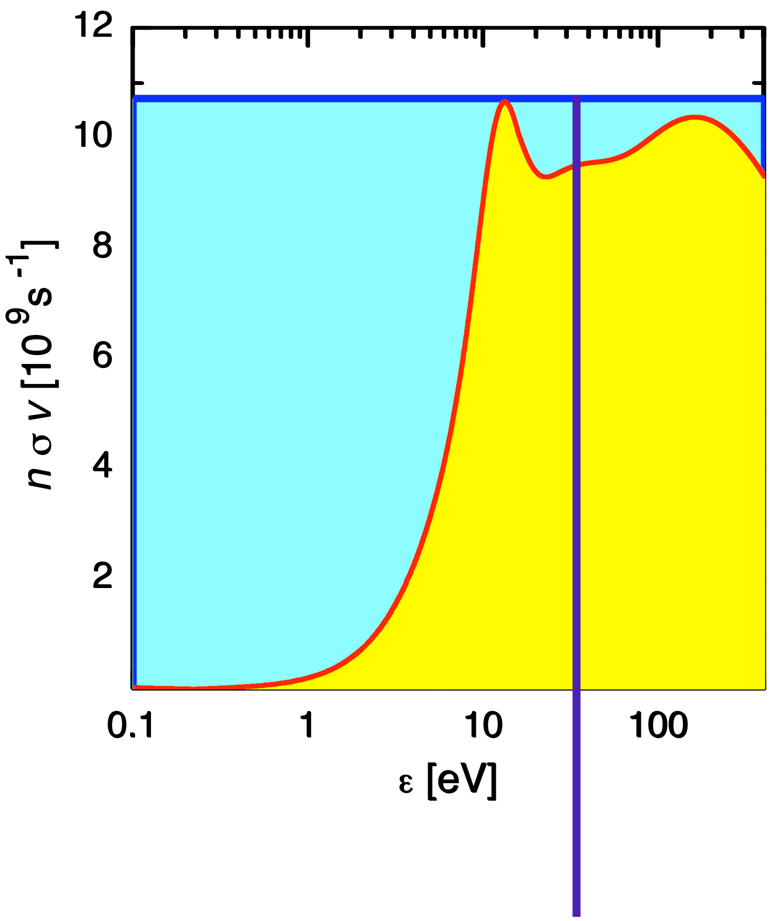
$$P_{\mathrm{coll}}(\Delta t) = 1 - \exp[-n\sigma_{\mathrm{T}} v_1 \Delta t] = 1 - \exp[-\nu \Delta t]$$

ν : collision frequency





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

$$\nu^* = \max\{n\sigma_{\mathrm{T}}(v_1)v_1\}$$

$$\nu^*(v_1) = \nu(v_1) + \nu_{\mathrm{null}}(v_1)$$

Flight time:

$$\tau = -\frac{1}{\nu^*}\ln(1 - R_{01})$$

No need to check for collision after each small Δt, after a free flight τ the occurrence of a real/null collision is checked

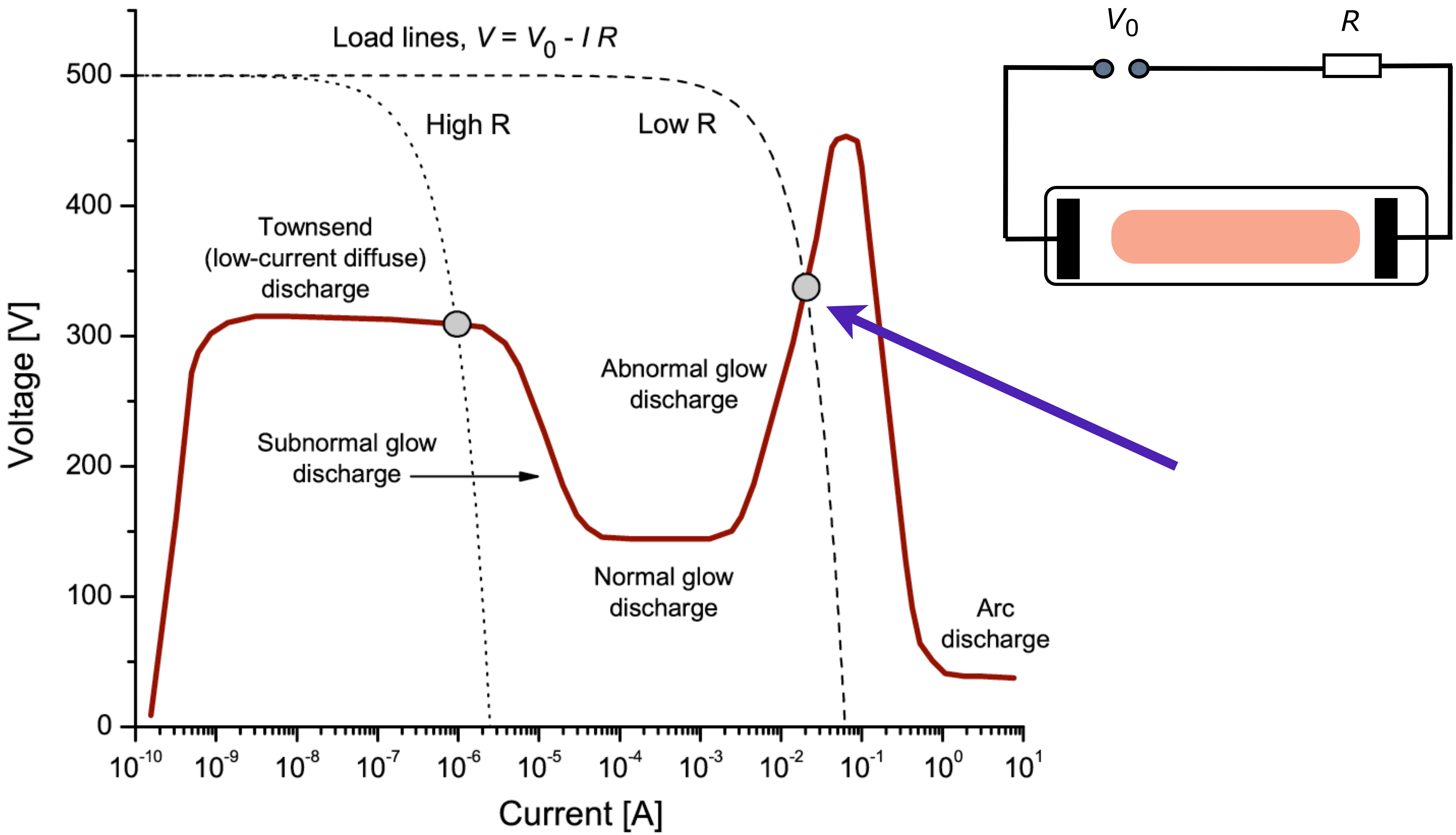
$$P_{\mathrm{real}} = \frac{\nu_{\mathrm{real}}}{\nu^*} = \frac{n\sigma_{\mathrm{T}}(v_1)v_1}{\nu^*}$$

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"

II. Modeling of cold-cathode DC glow discharges

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

DC discharges



DC discharges

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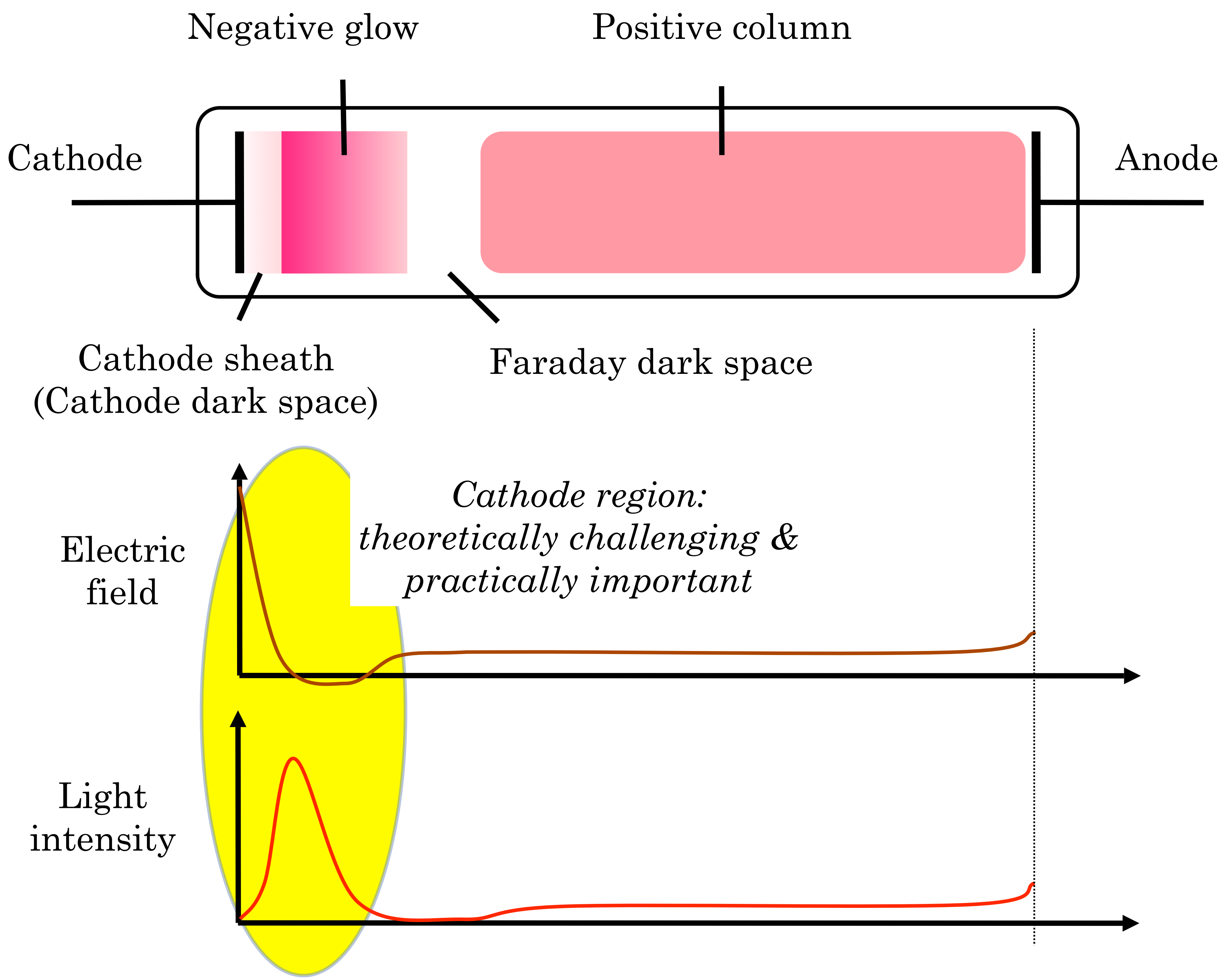

- CDS: strong electric field, electrons (emitted from the cathode + secondaries) are accelerated
- NG: deposition of electron energy, intensive ionization & excitation
- FDS: low electron energy, no excitation and ionization
- PC: quasi-neutral plasma, ionization (in weak electric field) and wall losses balance each other.

Self-consistent gas discharge models: a simple fluid model

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

Continuity equations:

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

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

Source functions:

$$S_\mathrm{i} = S_\mathrm{e} = \alpha \Phi_\mathrm{e}$$

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

local field approximation

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:

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

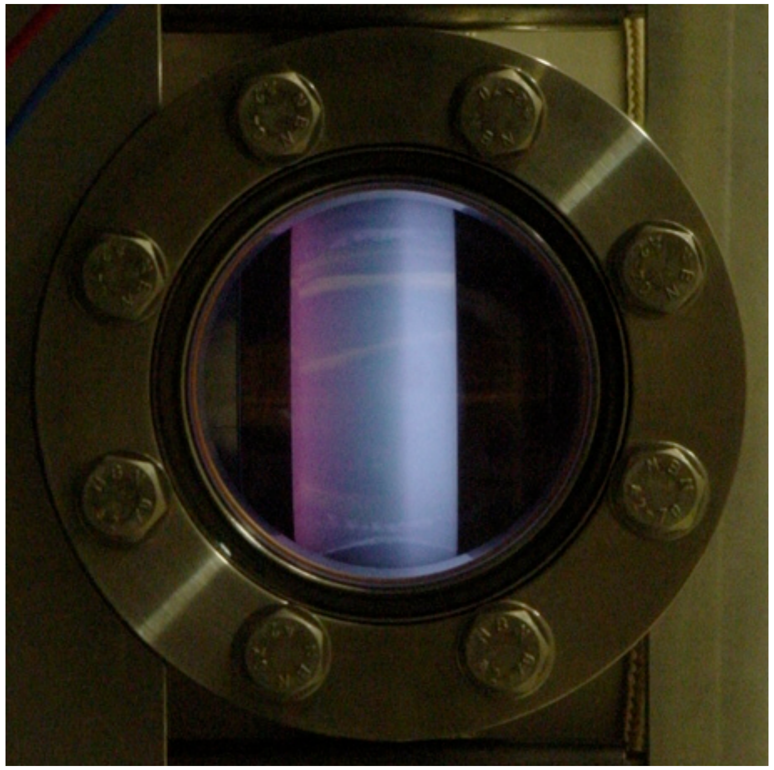
Boundary conditions:

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

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

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

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



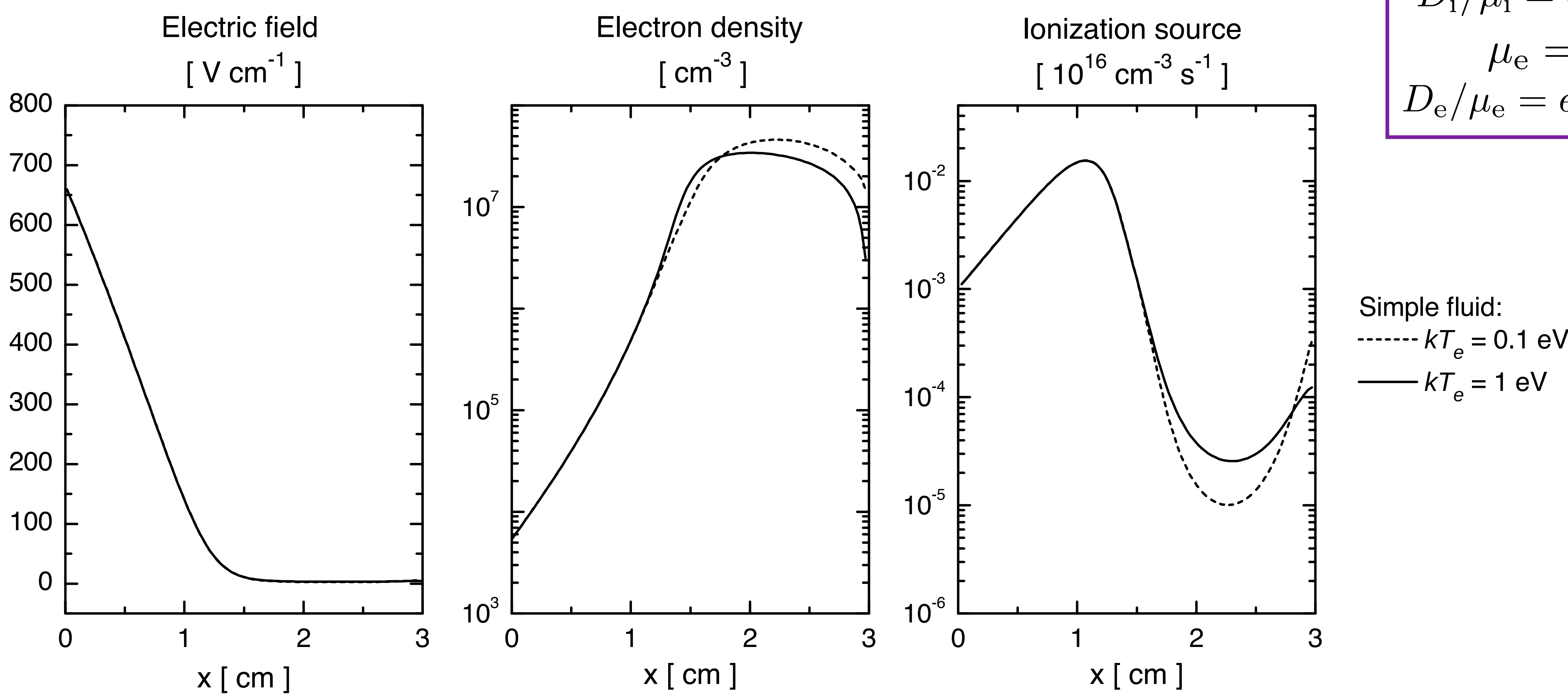
- **Cold-cathode abnormal glow**
- 1 dimension
- “short discharge”: D >> L
- Radial losses can be neglected
- 1-dimensional model
- Processes:
  - Drift
  - Diffusion
  - Ionization

Results: simple fluid model

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

transport coefficients

$$\mu_i = f(E/n)$$
$$D_i/\mu_i = ekT_i = ekT_g$$
$$\mu_e = \text{const.}$$
$$D_e/\mu_e = ekT_e \leftarrow \text{input}$$



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

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

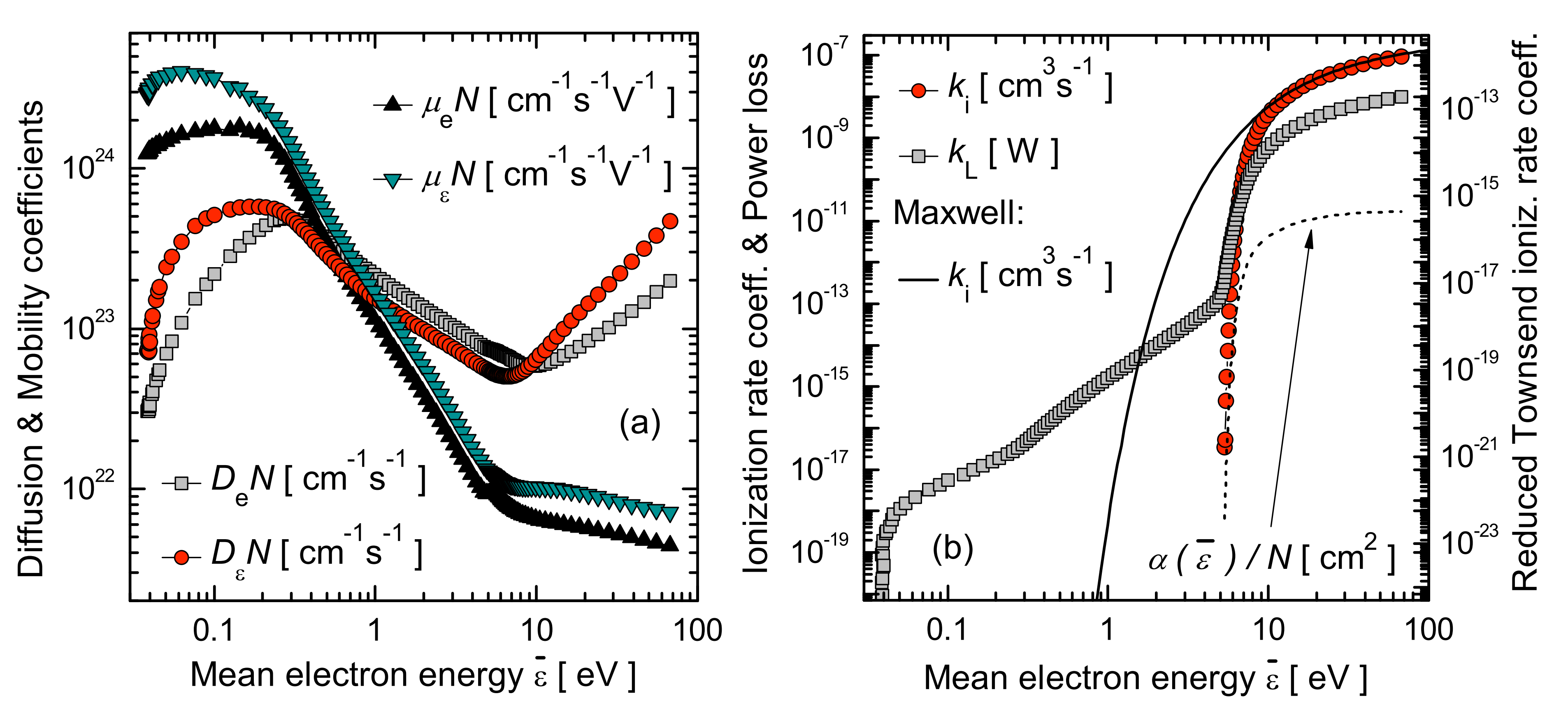
Rate coefficient - based: $$S(x) = k_\mathrm{i}[\bar{\varepsilon}(x)]n_\mathrm{e}(x)N \qquad k_\mathrm{i}(\bar{\varepsilon}) = \sqrt{\frac{2e}{m}}\int_0^\infty \varepsilon\sigma_\mathrm{i}(\varepsilon)F_0(\varepsilon)\mathrm{d}\varepsilon$$

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



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

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

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

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

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

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

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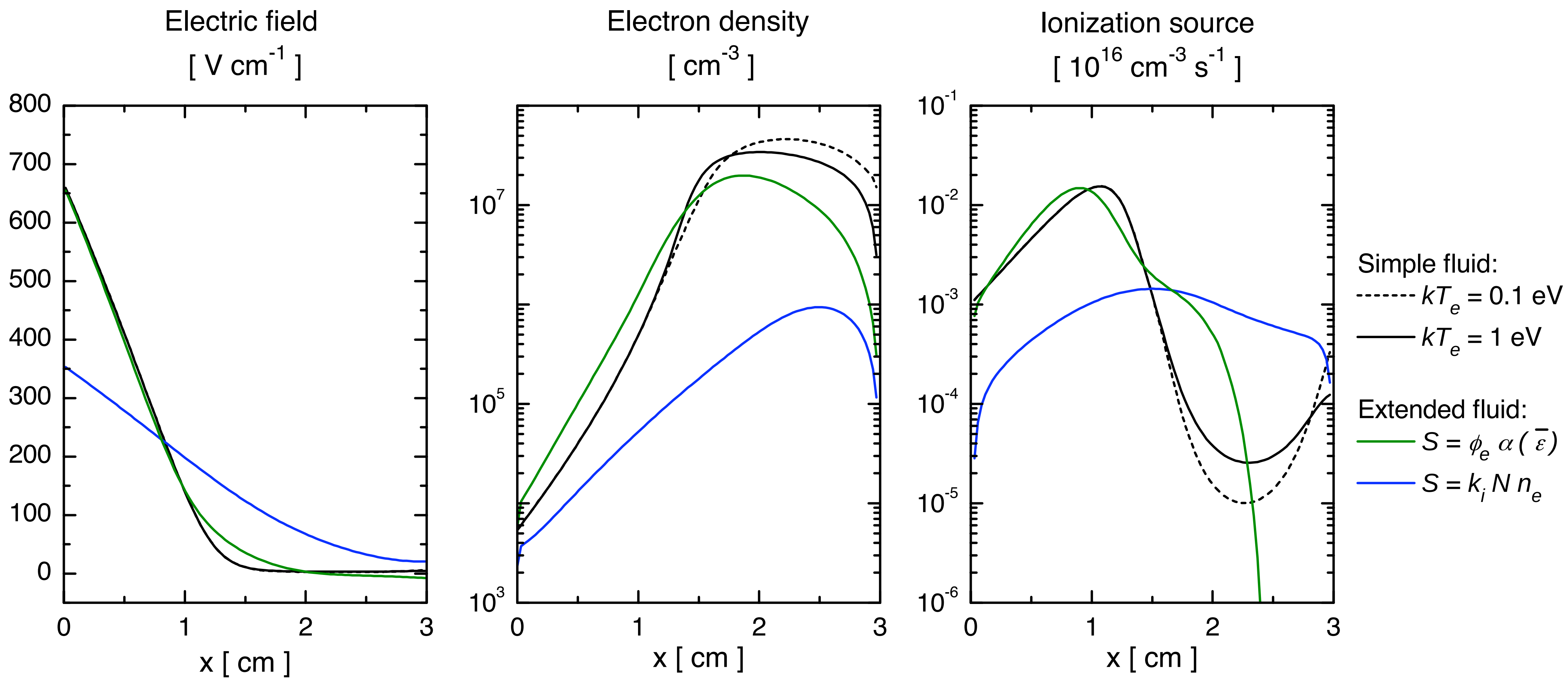
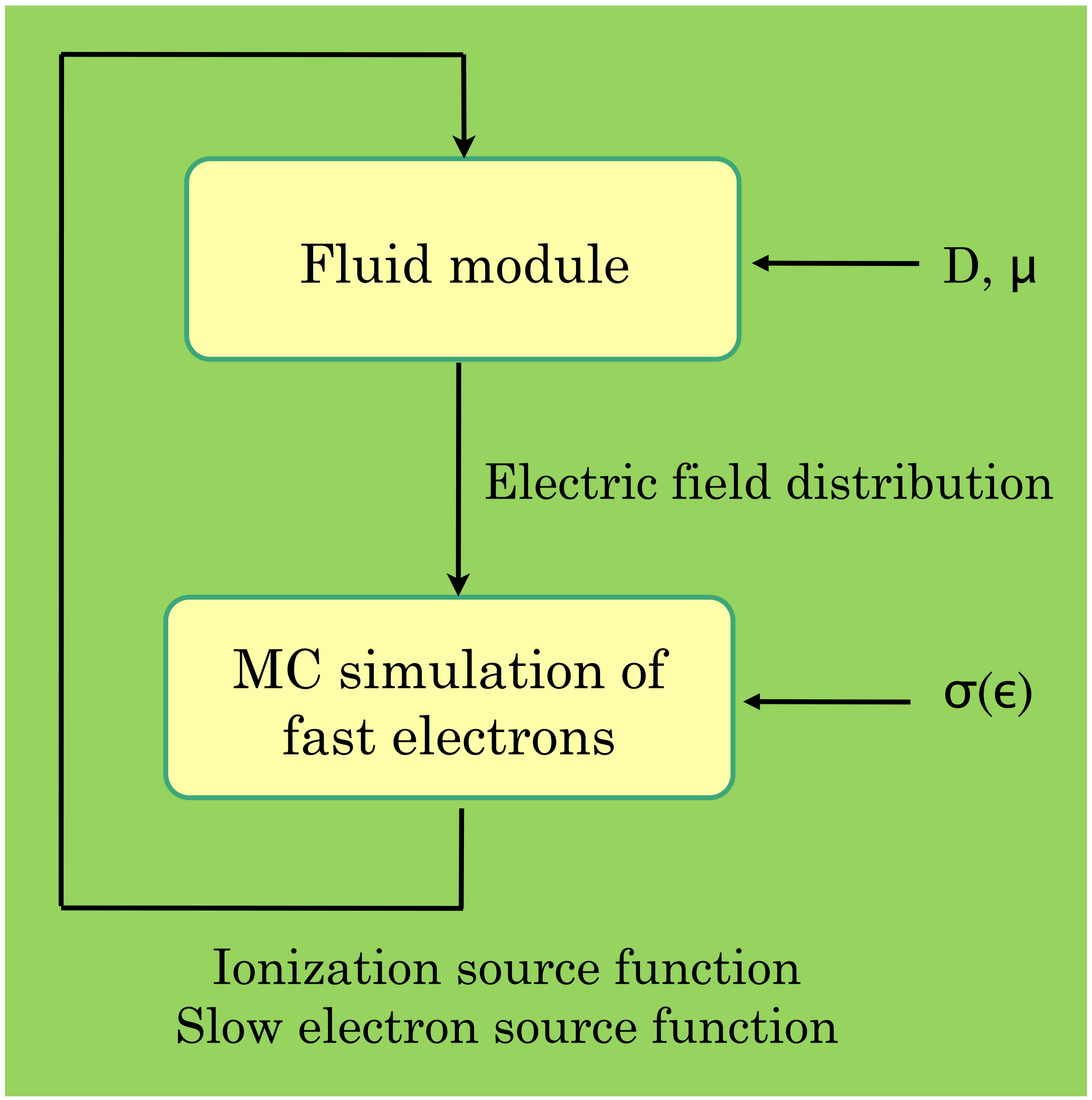
p = 40 Pa (Ar), V = 441 V, T_g = 300 K, L = 3 cm, γ = 0.033



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

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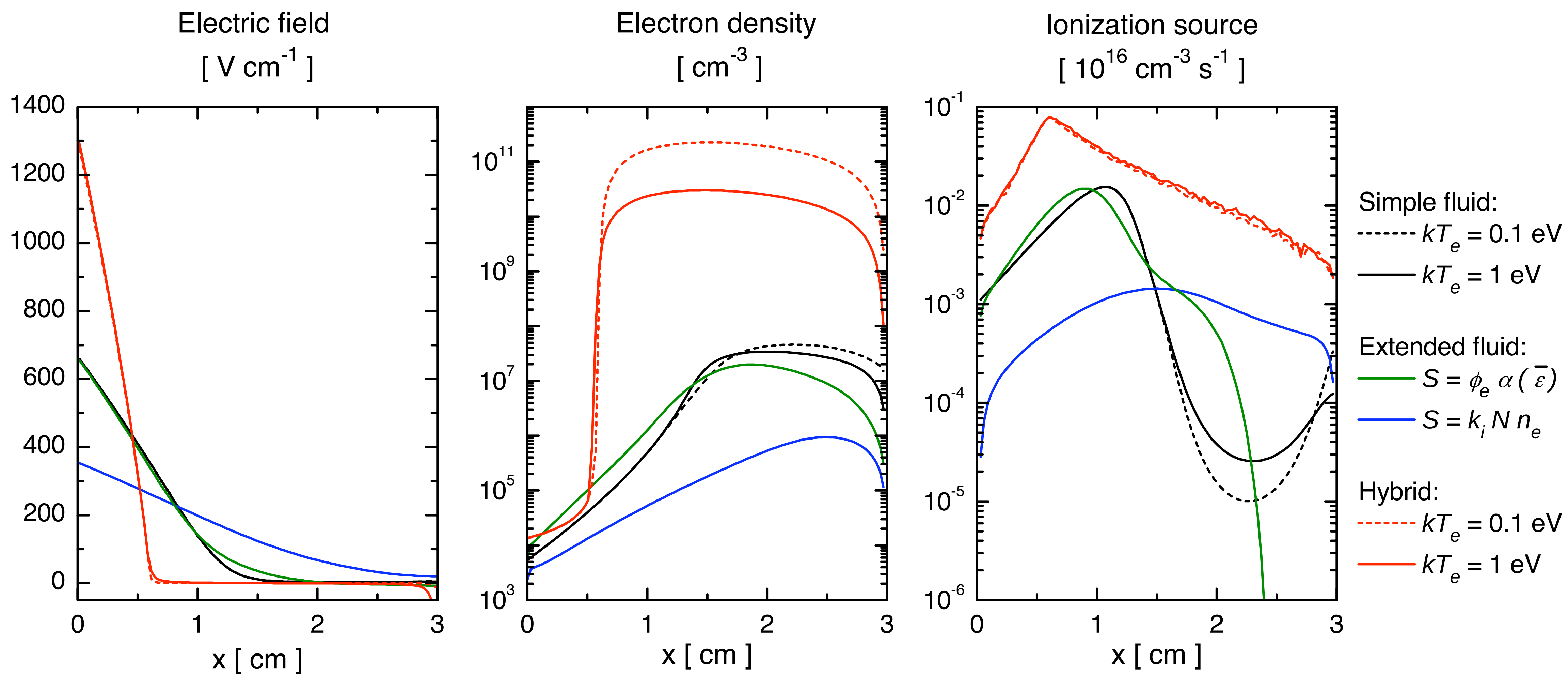
p = 40 Pa (Ar), V = 441 V, T_g = 300 K, L = 3 cm, γ = 0.033



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 (I)

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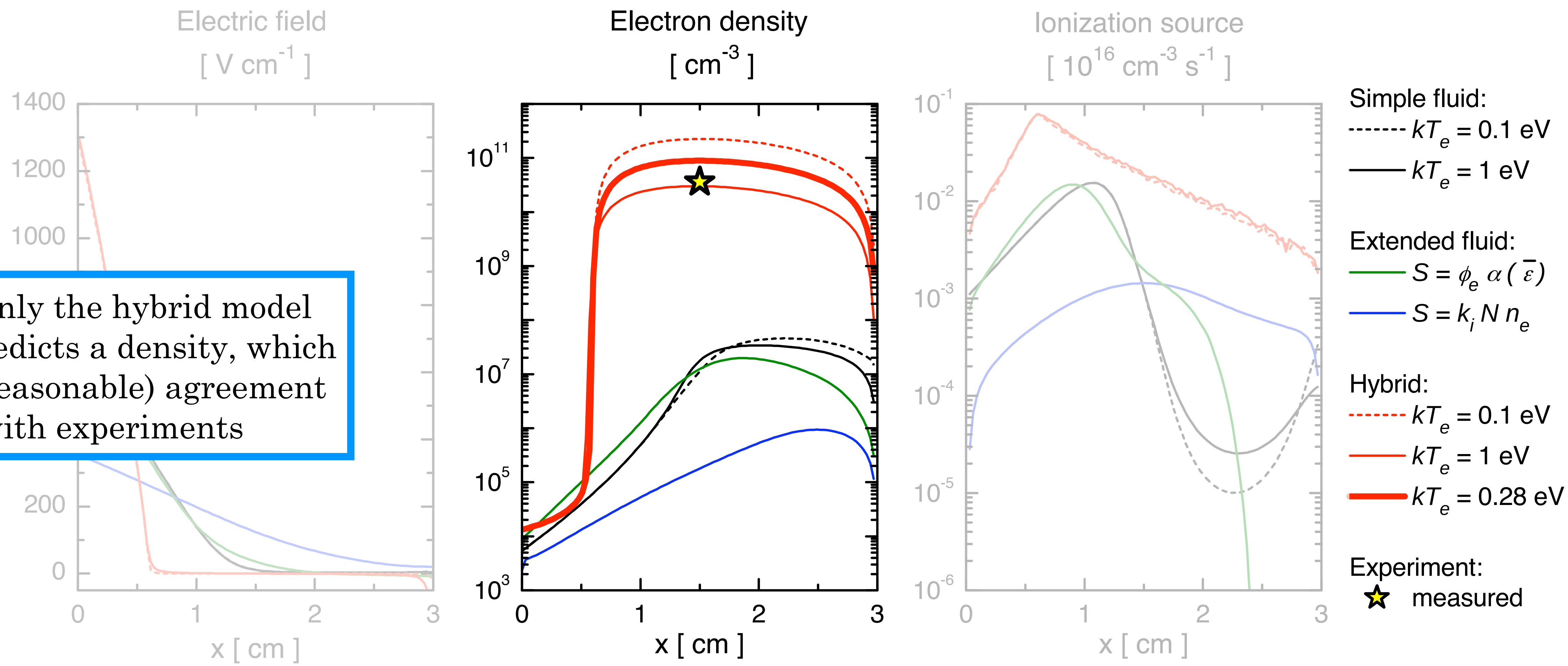
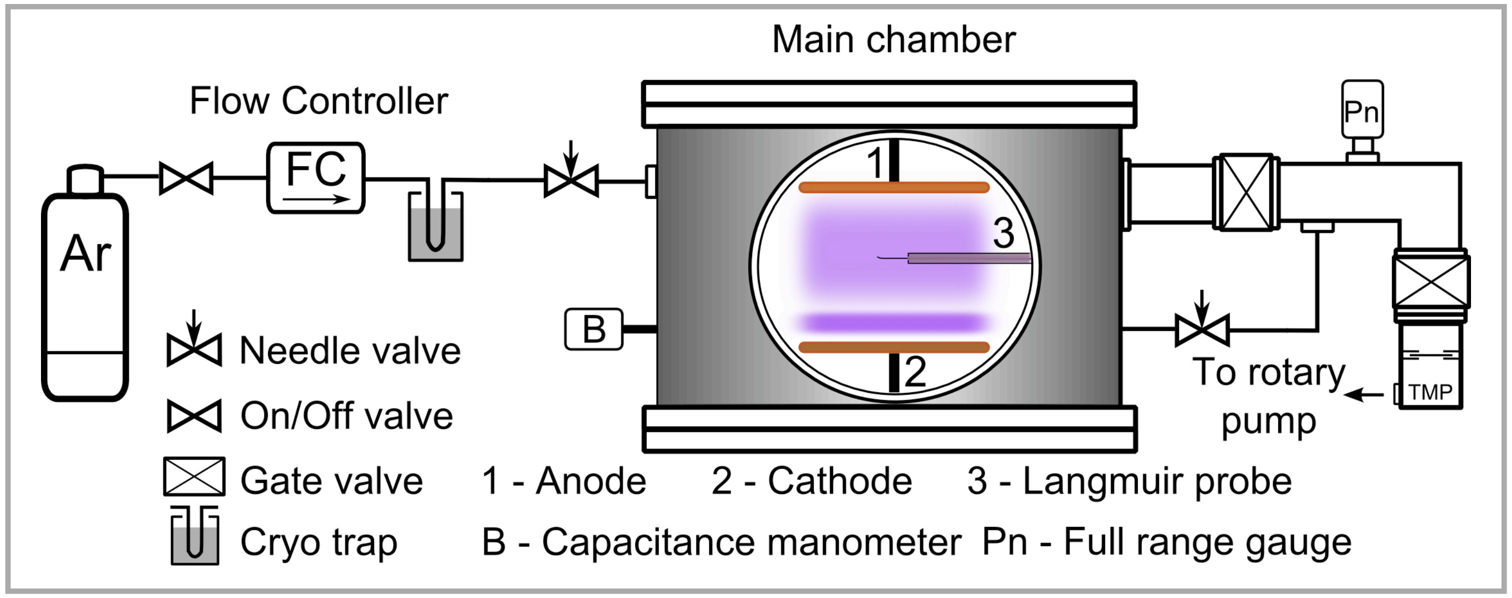


It is only the hybrid model that predicts a density, which is in (reasonable) agreement with experiments

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

Measurements with Langmuir probe



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)

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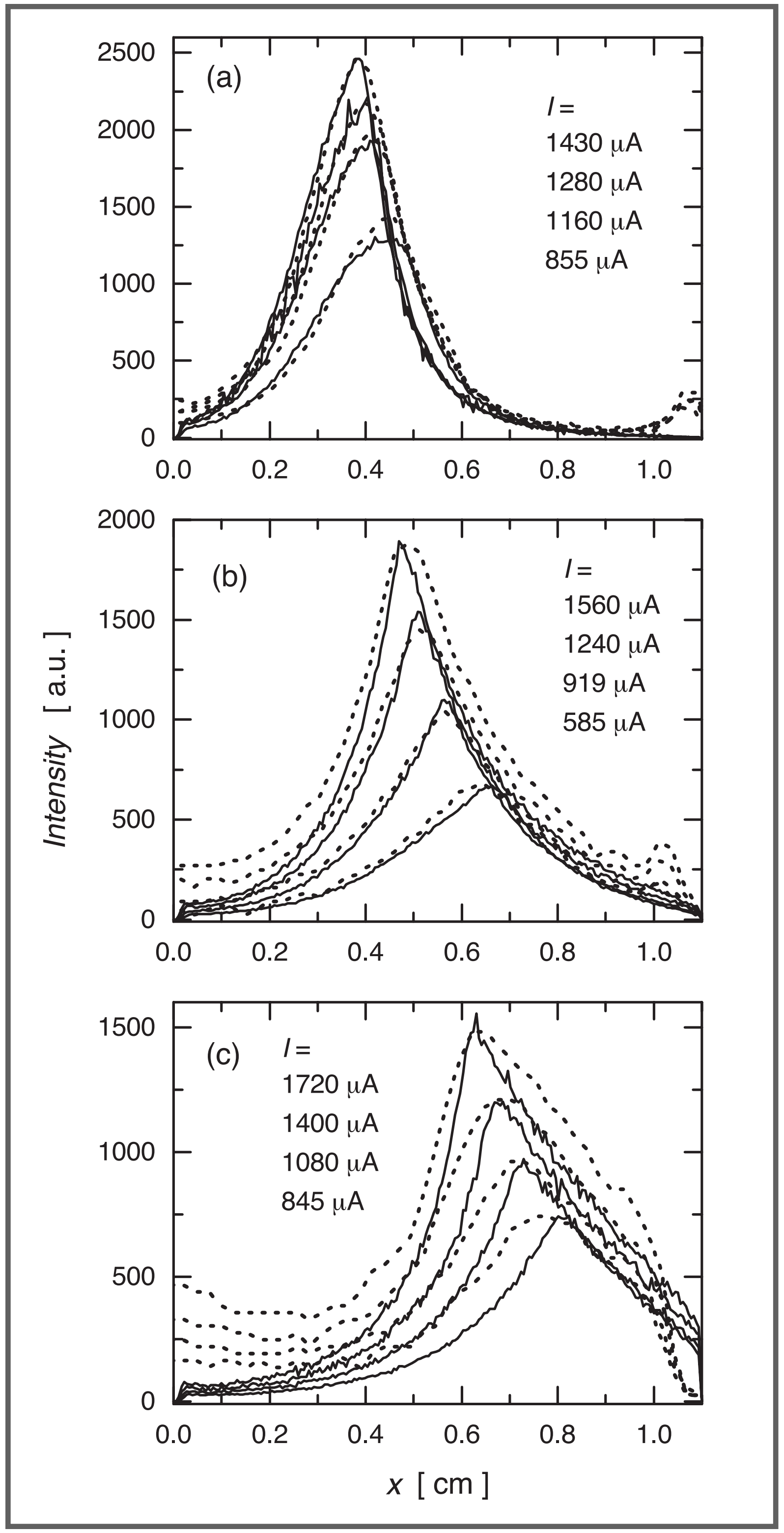
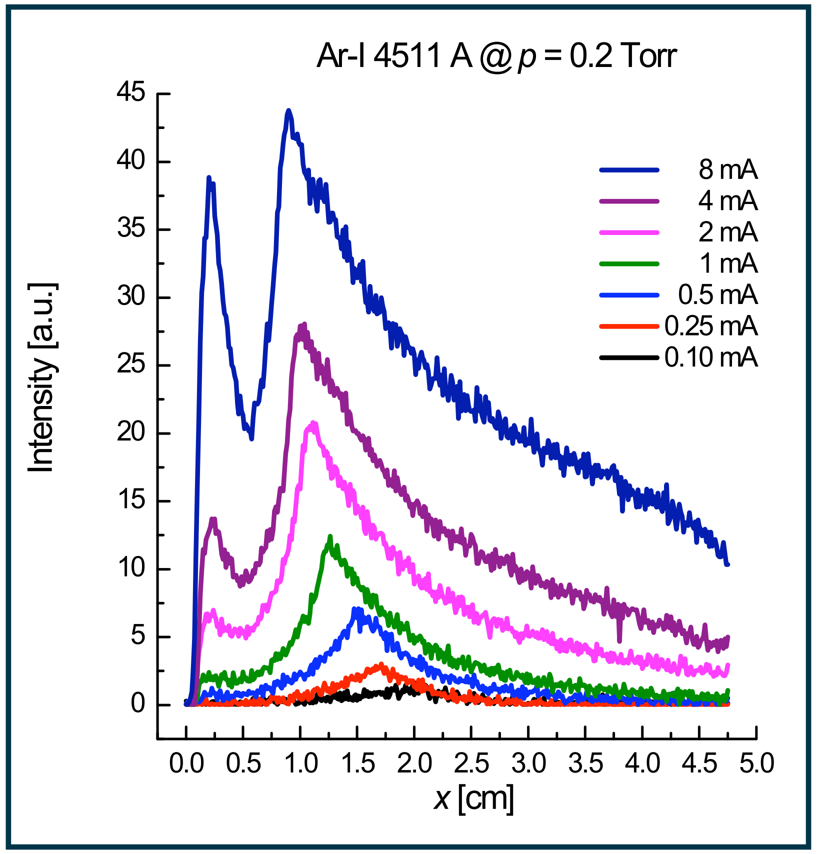
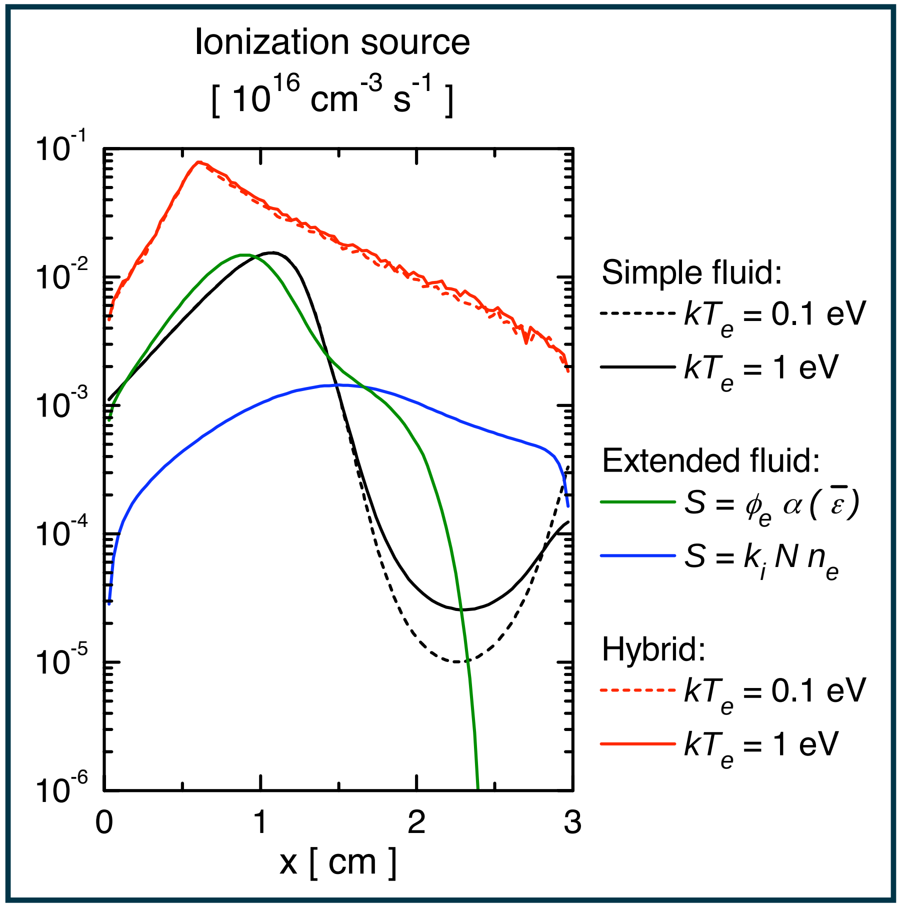
EXPERIMENT & MODELS



EXPERIMENT



MODELS



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

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

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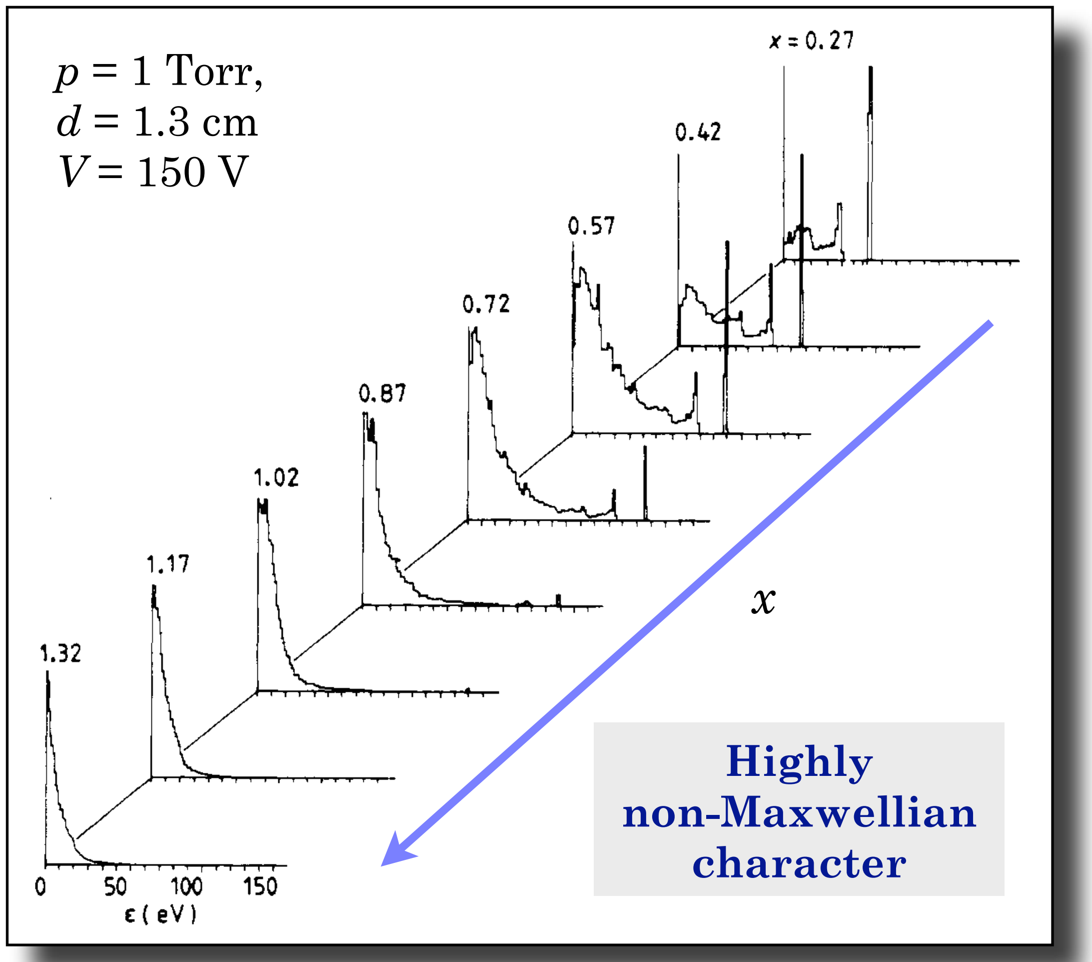
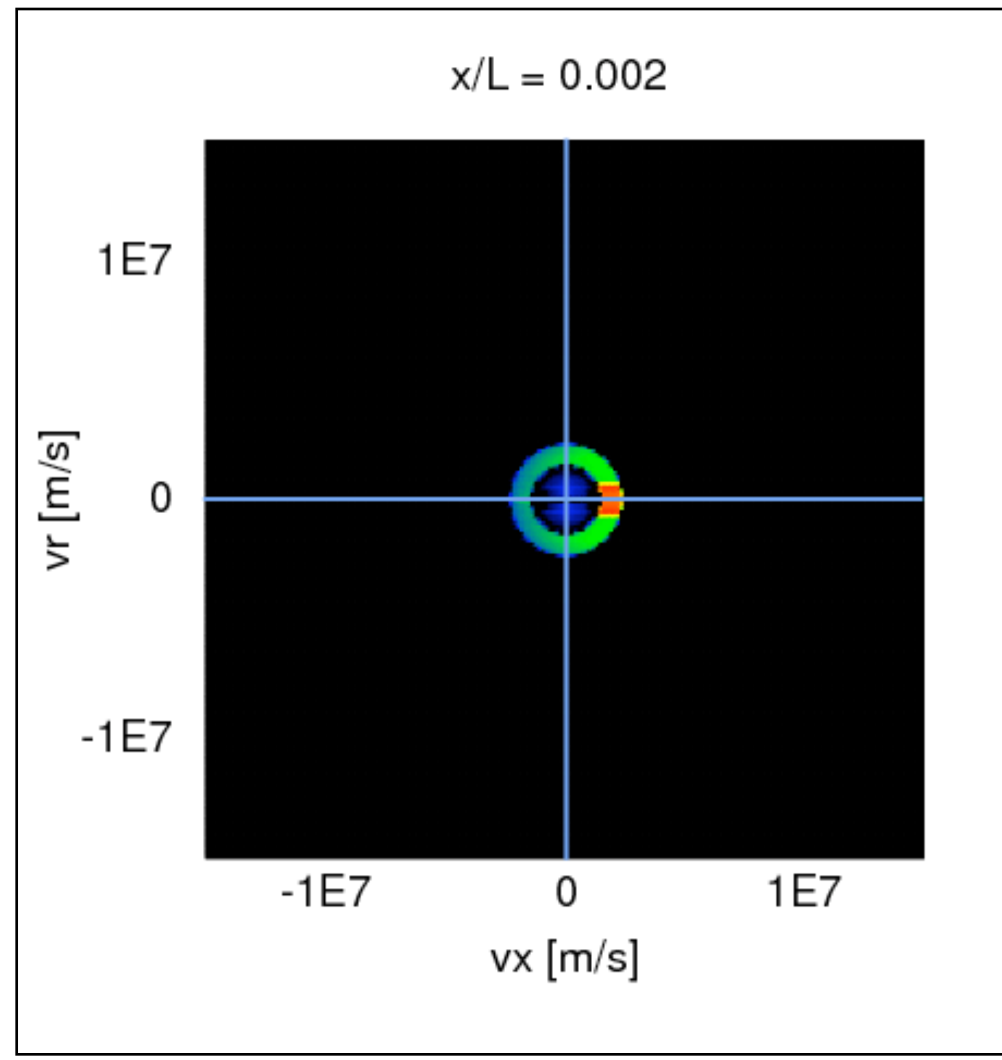
The spatial variation of the distribution function in the cathode sheath



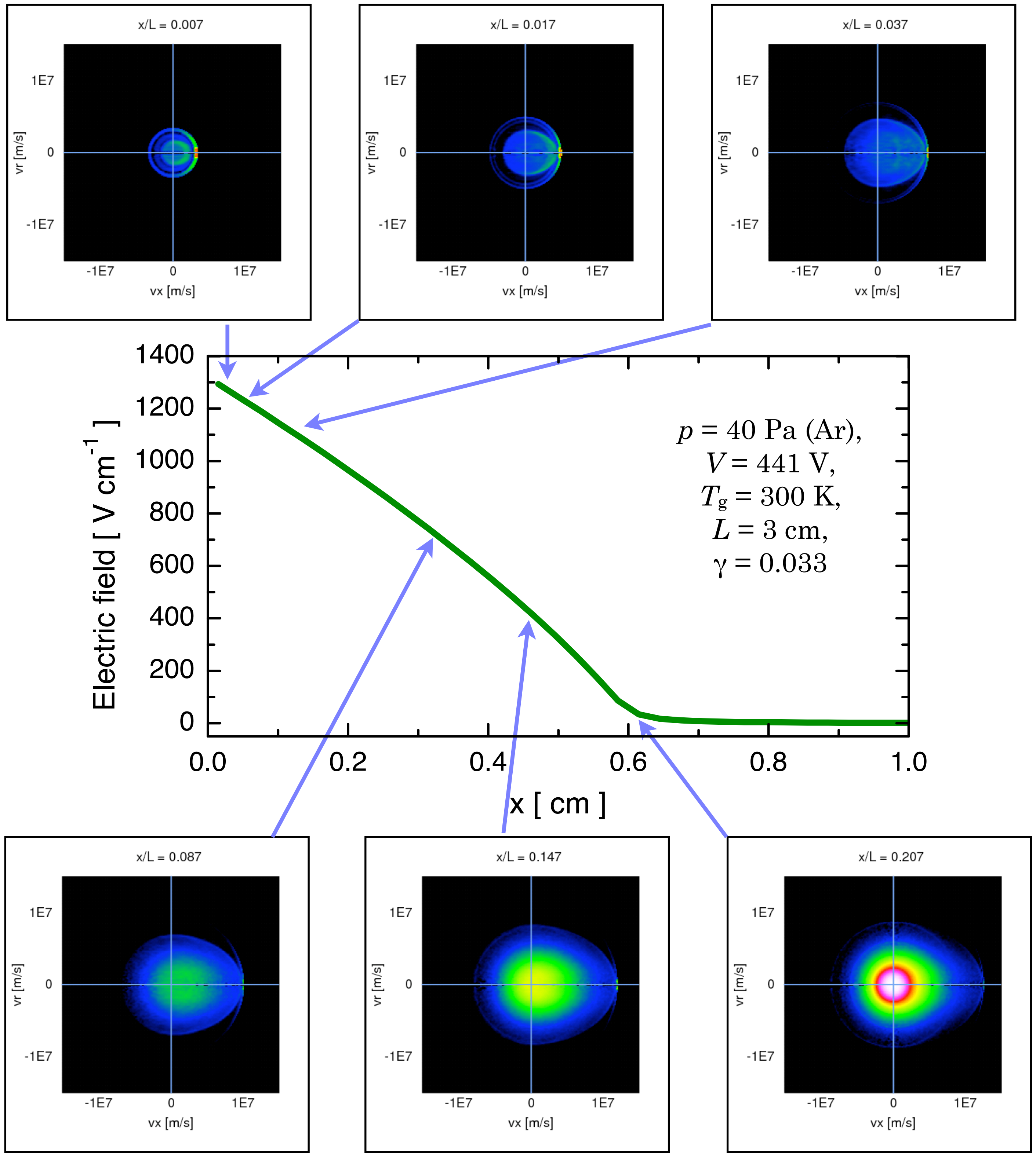
J. P. Boeuf and E. Marode J. Phys. D **15** 2169 (1982)
"A Monte Carlo analysis of an electron swarm in nonuniform field: the cathode region of a glow discharge in helium"

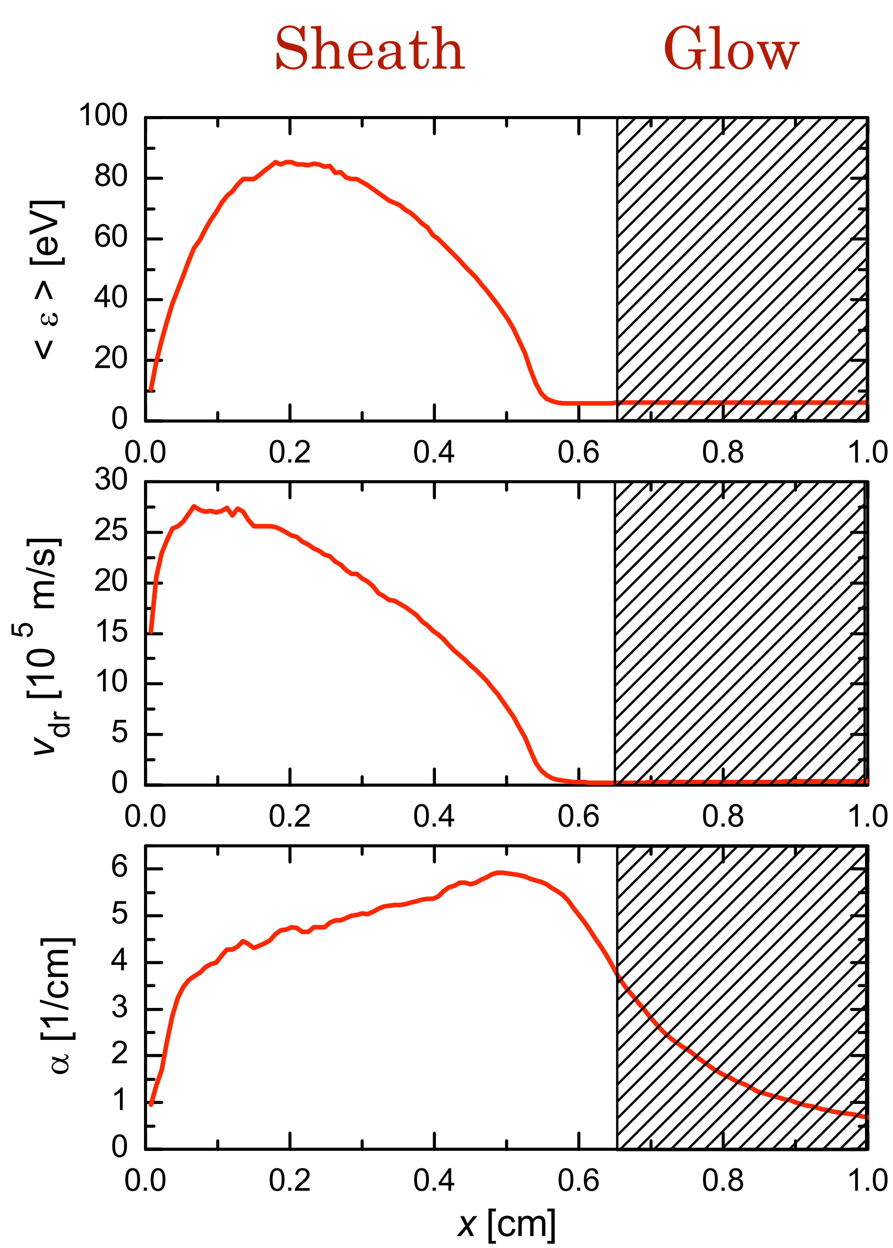
The VDF:

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



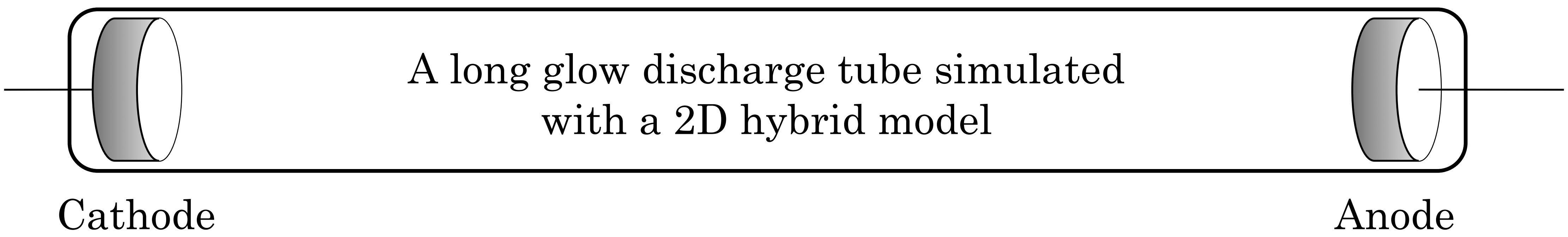
Analysis of the VDF in the DC glow sheath

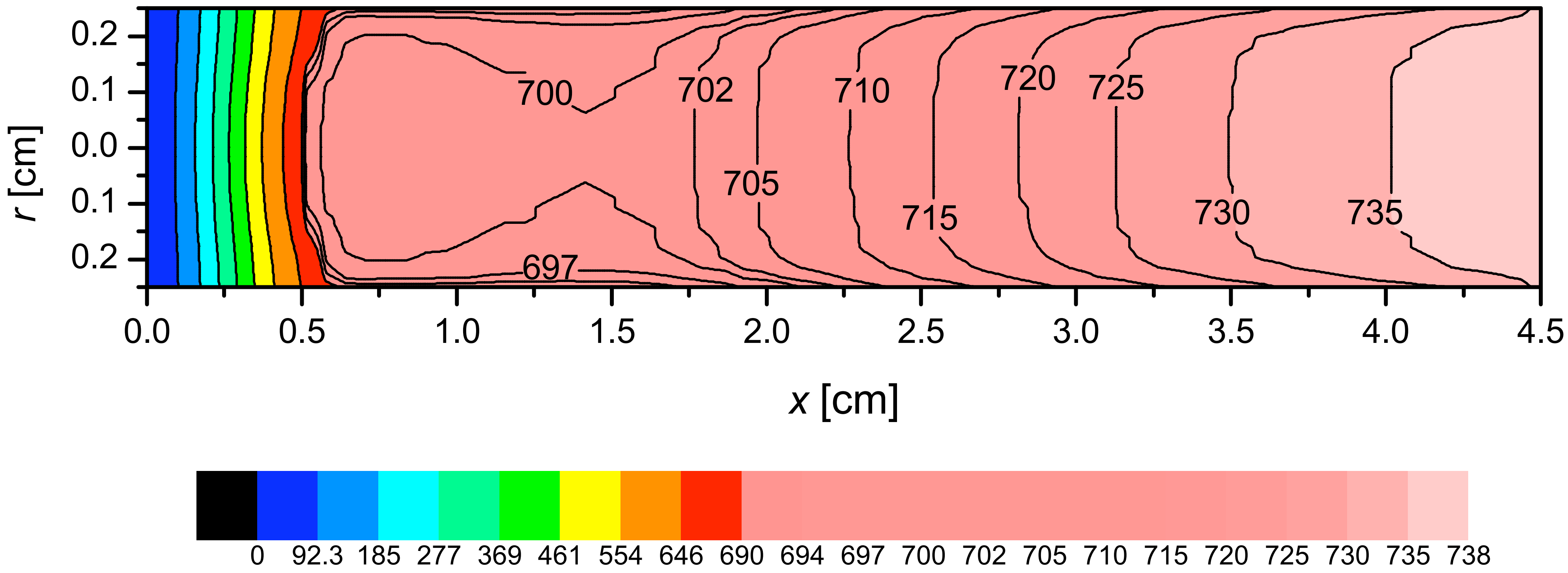




Conclusion: characteristic features captured by kinetic description only

Applications of hybrid models: Simulation of a "long" glow discharge





Potential distribution

All characteristic regions reproduced

DC discharges: dynamics

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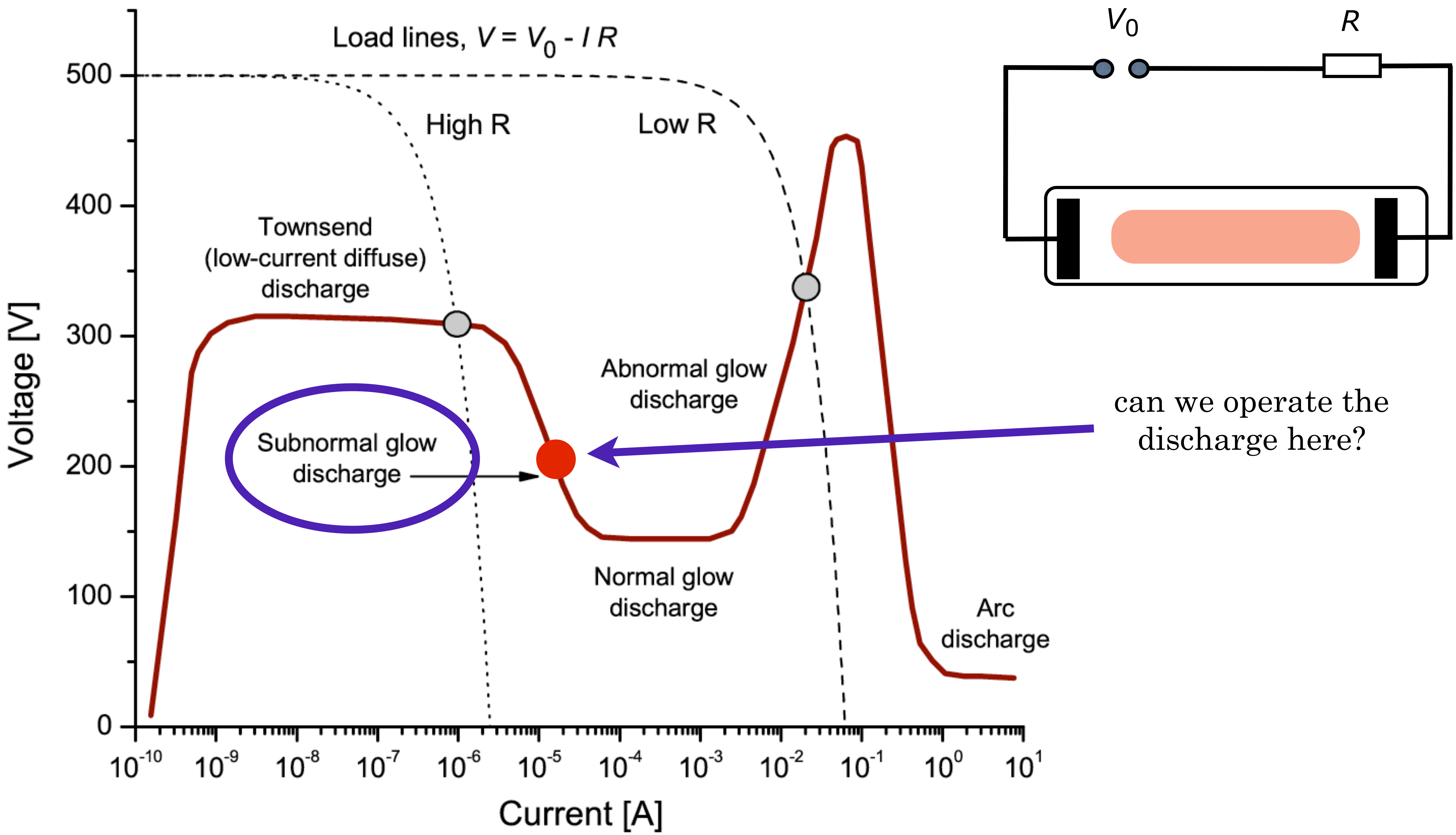
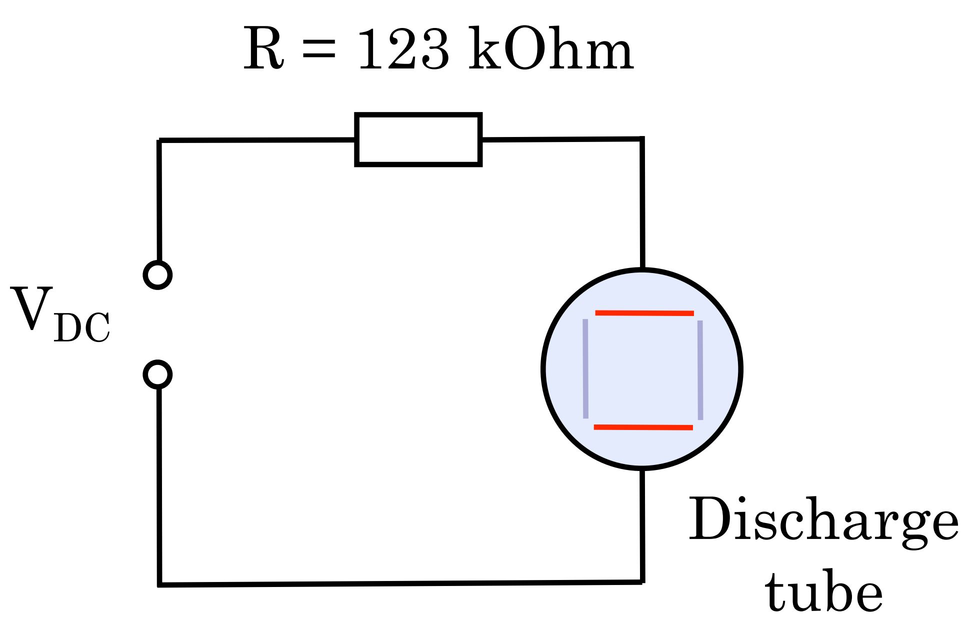
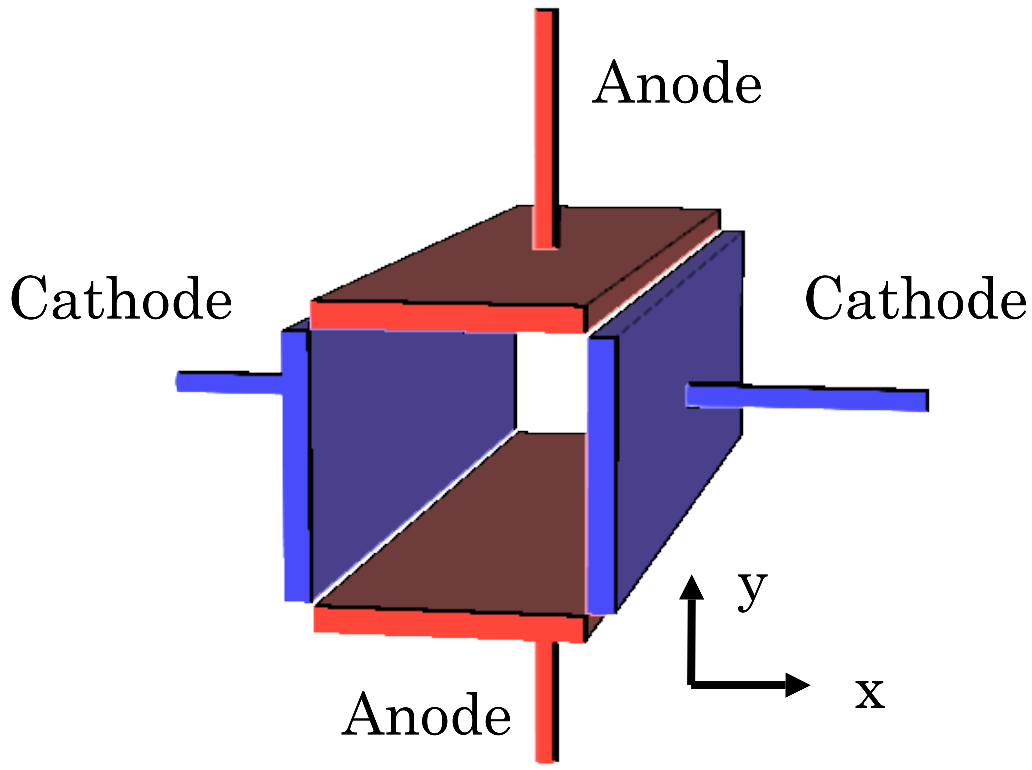


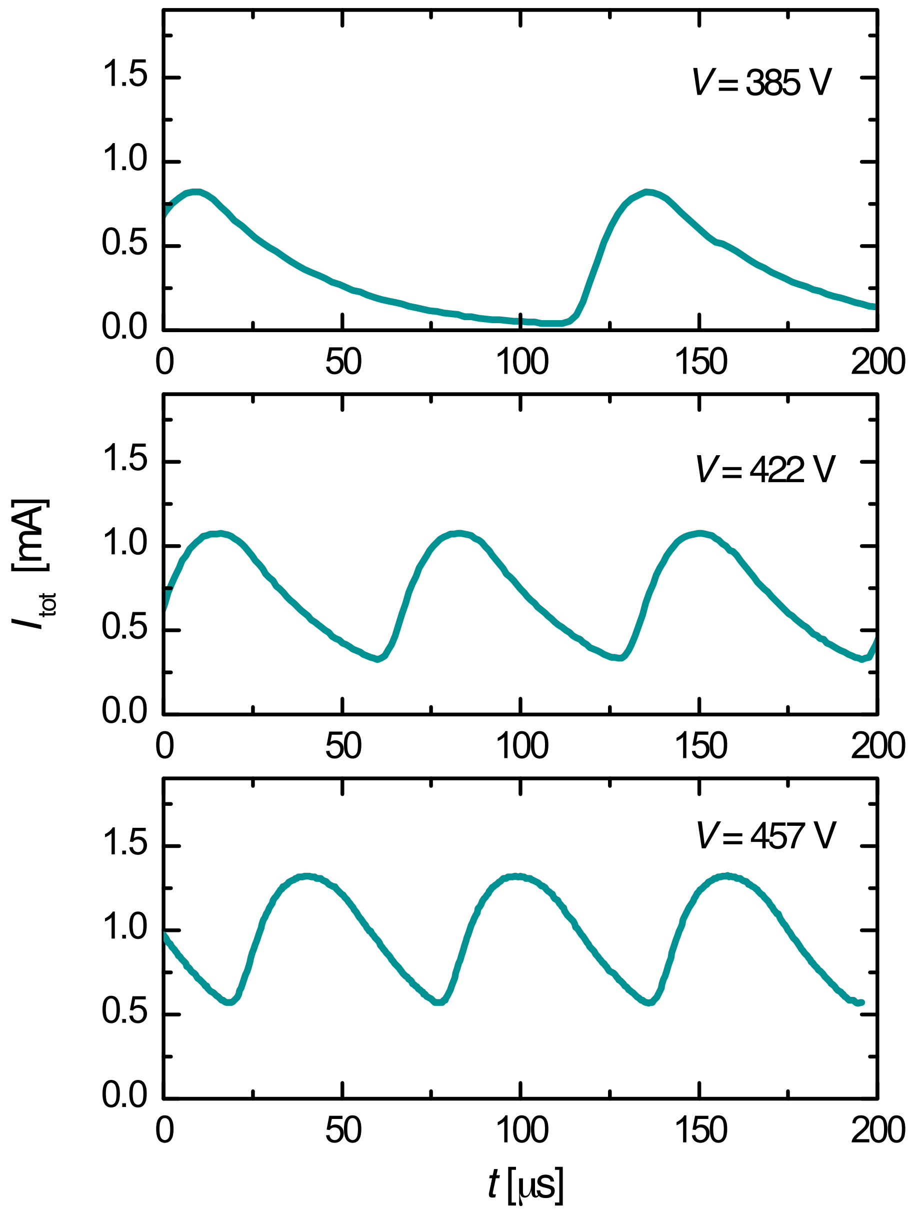
can we operate the discharge here?

Applications of hybrid models: Self-generated oscillations in a hollow cathode discharge

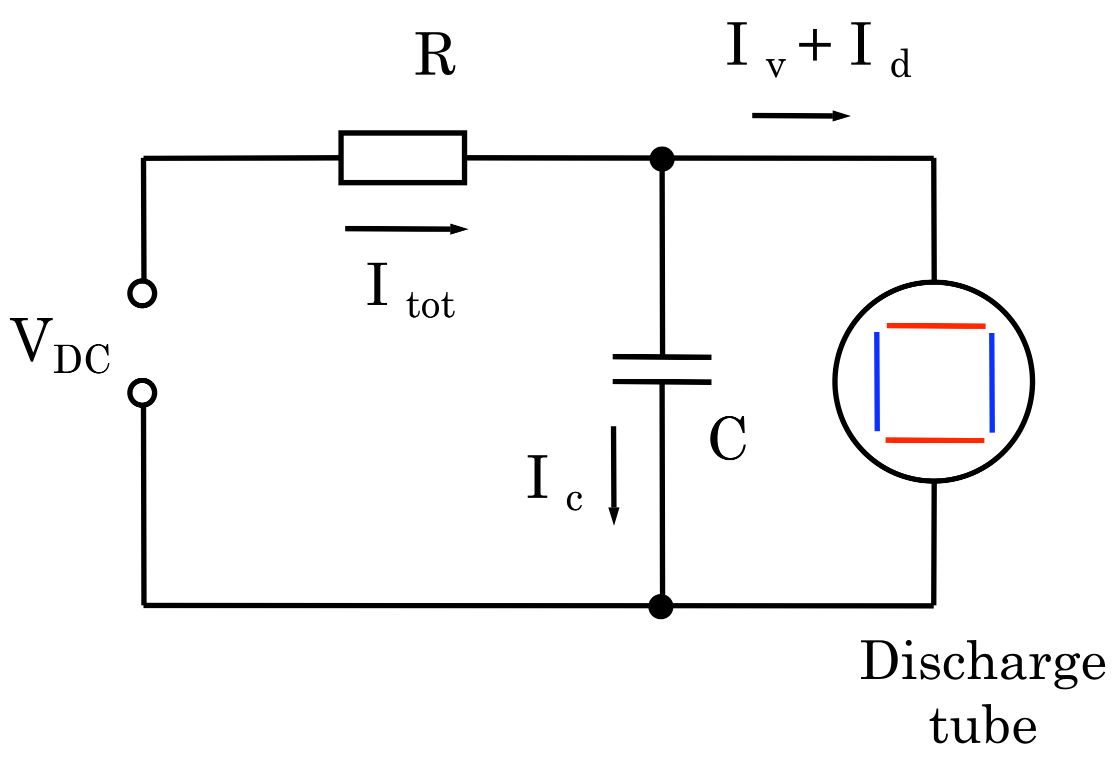


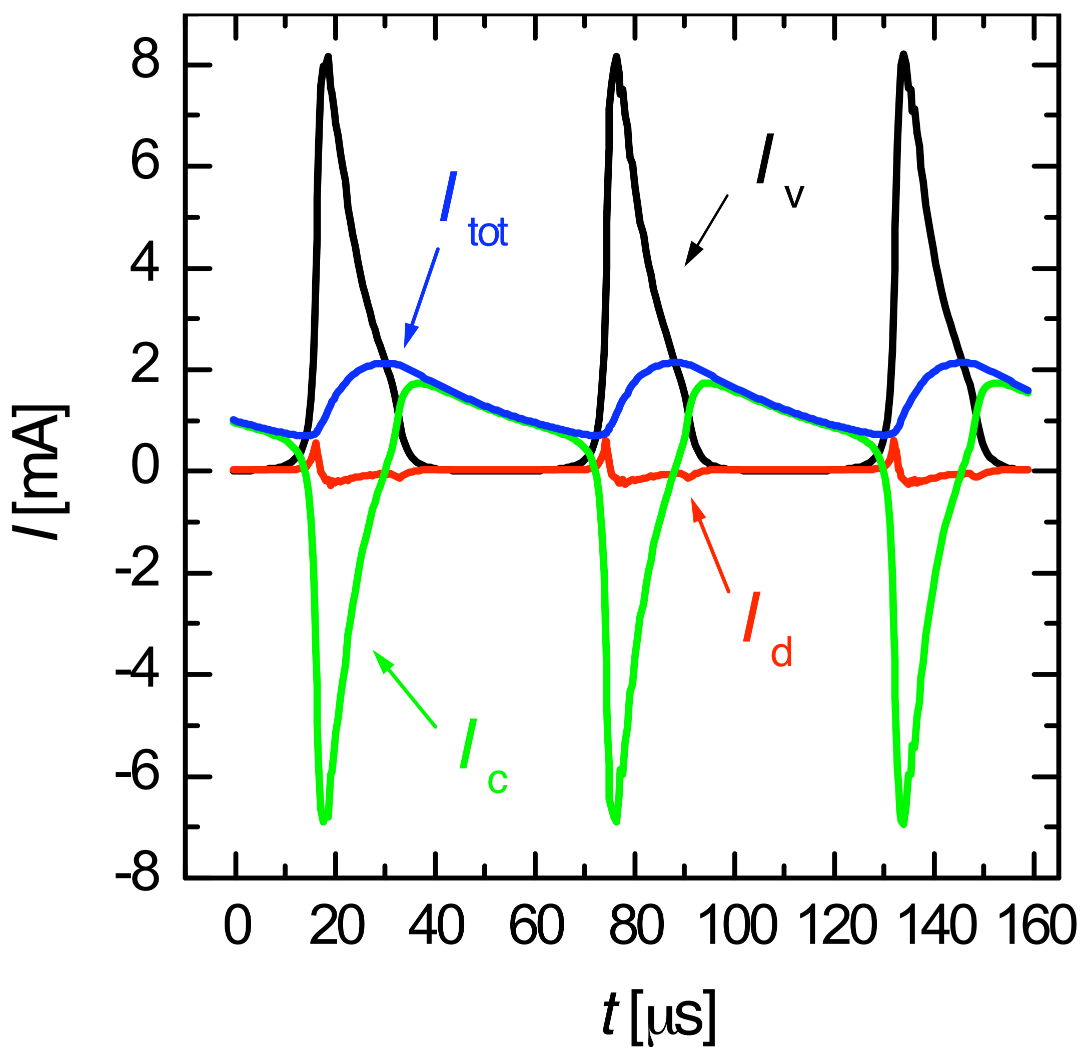


Experimentally observed oscillations:



Applications of hybrid models: Self-generated oscillations in a hollow cathode discharge



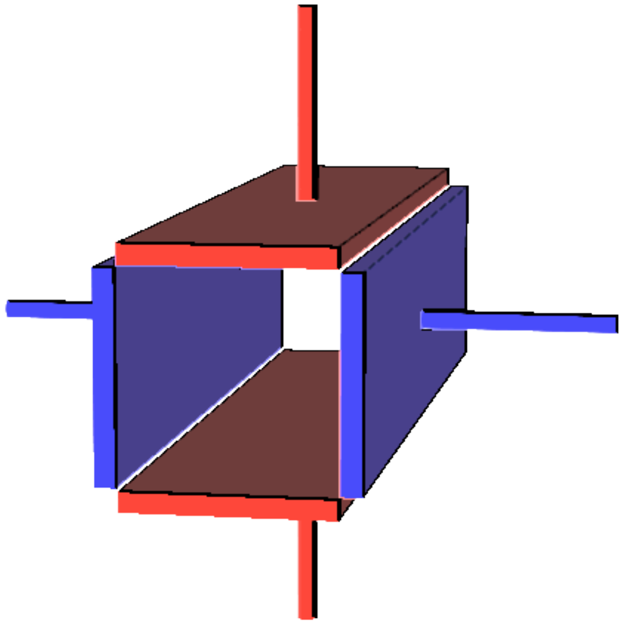


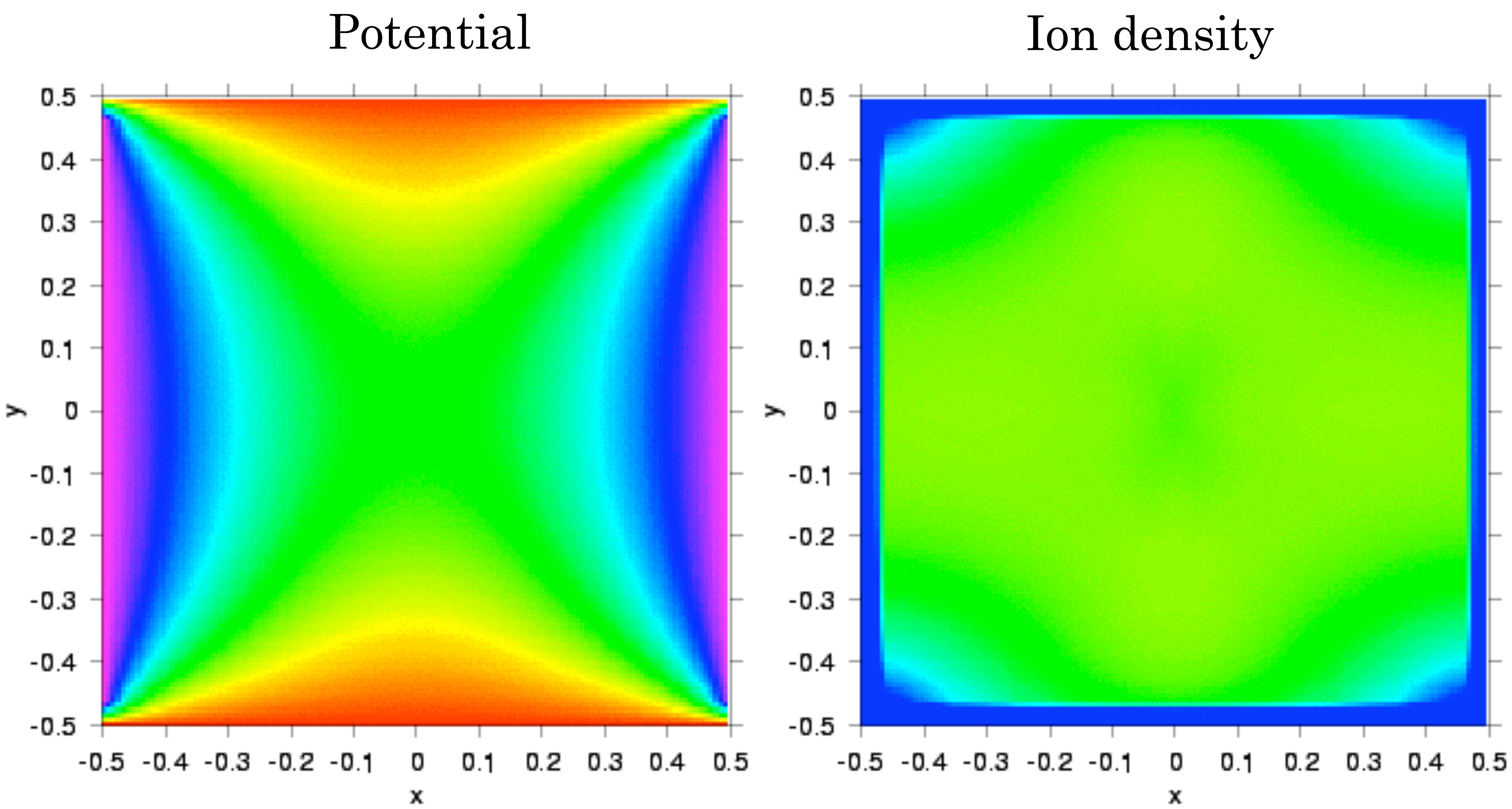
2D hybrid model +

$$I_{\rm tot} = I_{\rm v} + I_{\rm d} + I_{\rm C} \qquad V_{\rm DC} = V - RI_{\rm tot}$$

$$I_{\rm d} = \varepsilon_0 \int_{\rm (Cath.)} \frac{{\rm d}E_{\rm n}}{{\rm d}t} {\rm d}A \qquad I_{\rm C} \cong C\frac{\Delta V}{\Delta t}$$

Applications of hybrid models: Self-generated oscillations in a hollow cathode discharge



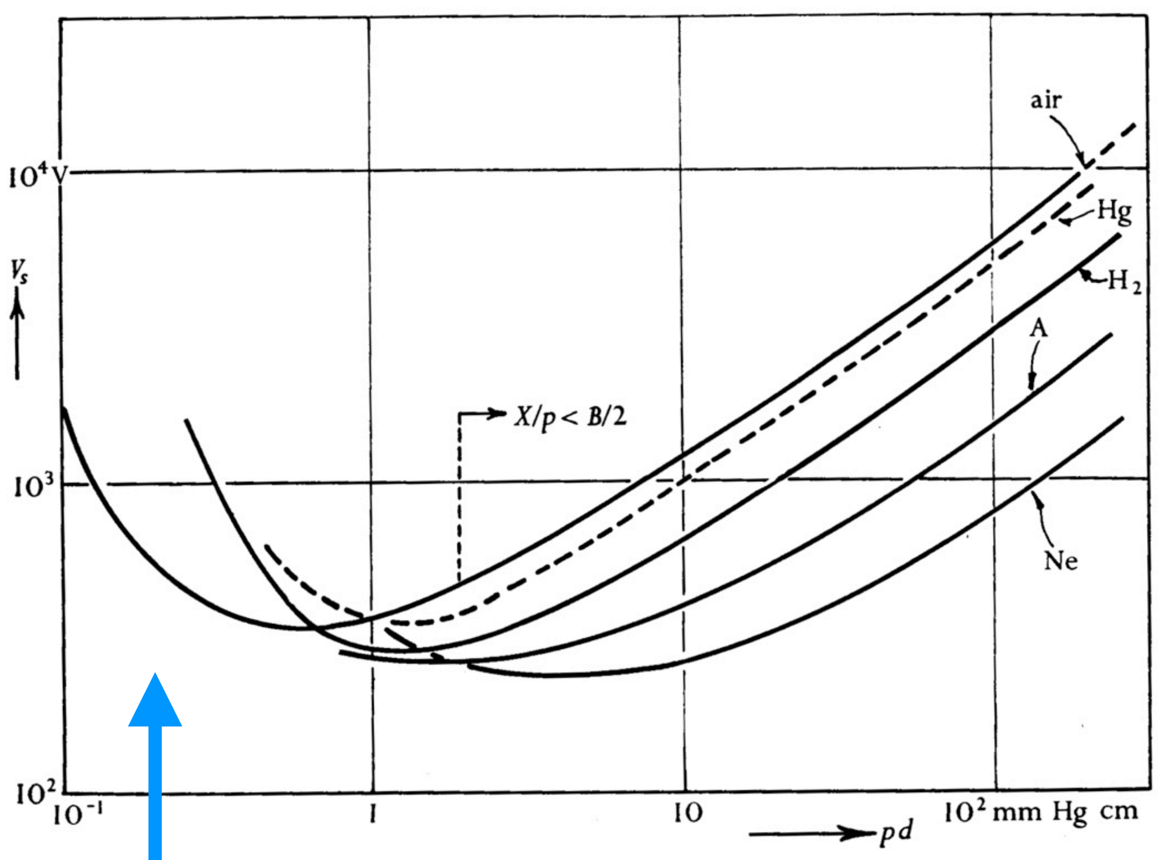


Z. Donkó, J. Phys. D. 32, 1657 (1999)

Heavy particle processes in low-pressure discharges

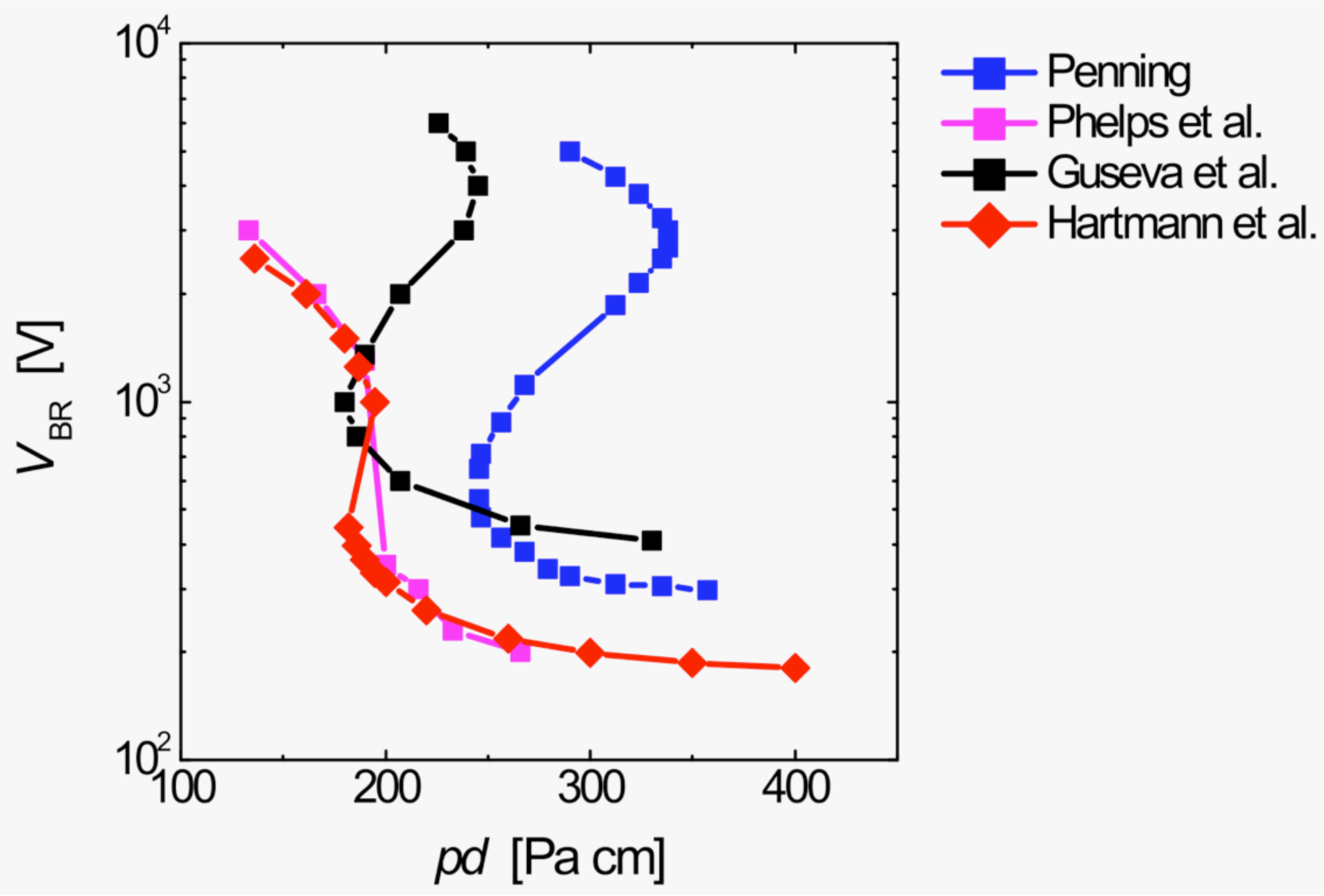
Gas breakdown

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



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

Measured breakdown curves for helium gas:



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

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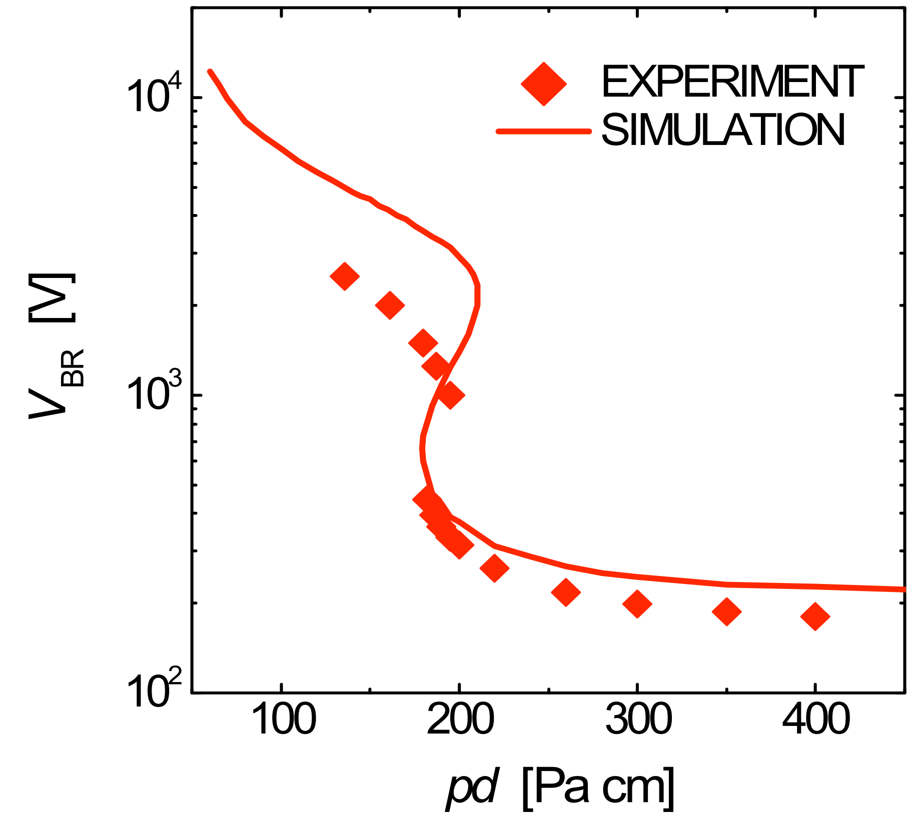
Simulation including the Monte Carlo treatment of electrons, ions, as well as fast atoms

$e^- + X \rightarrow e^- + X$	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

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

+ reasonable data for secondary yields for all these species

Townsend discharge – abnormal glow transition

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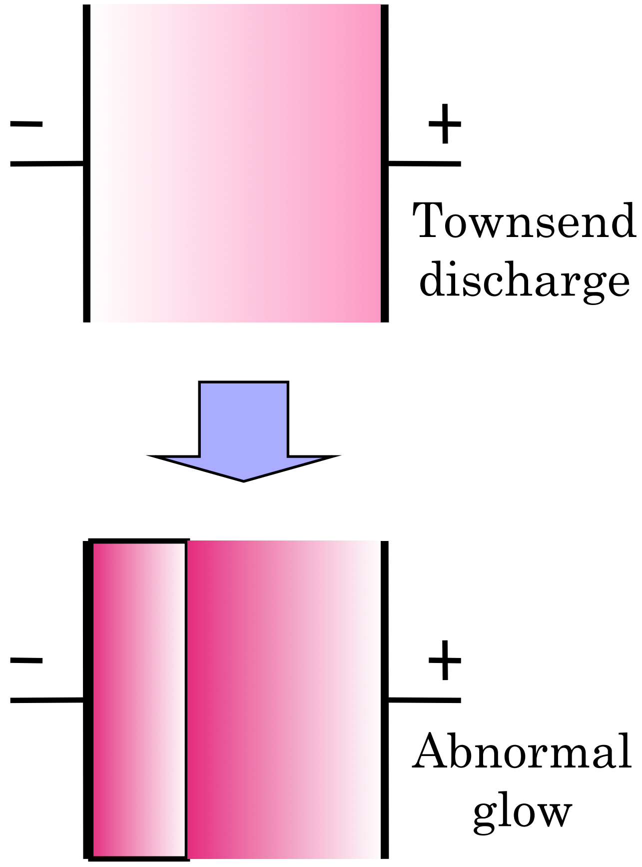
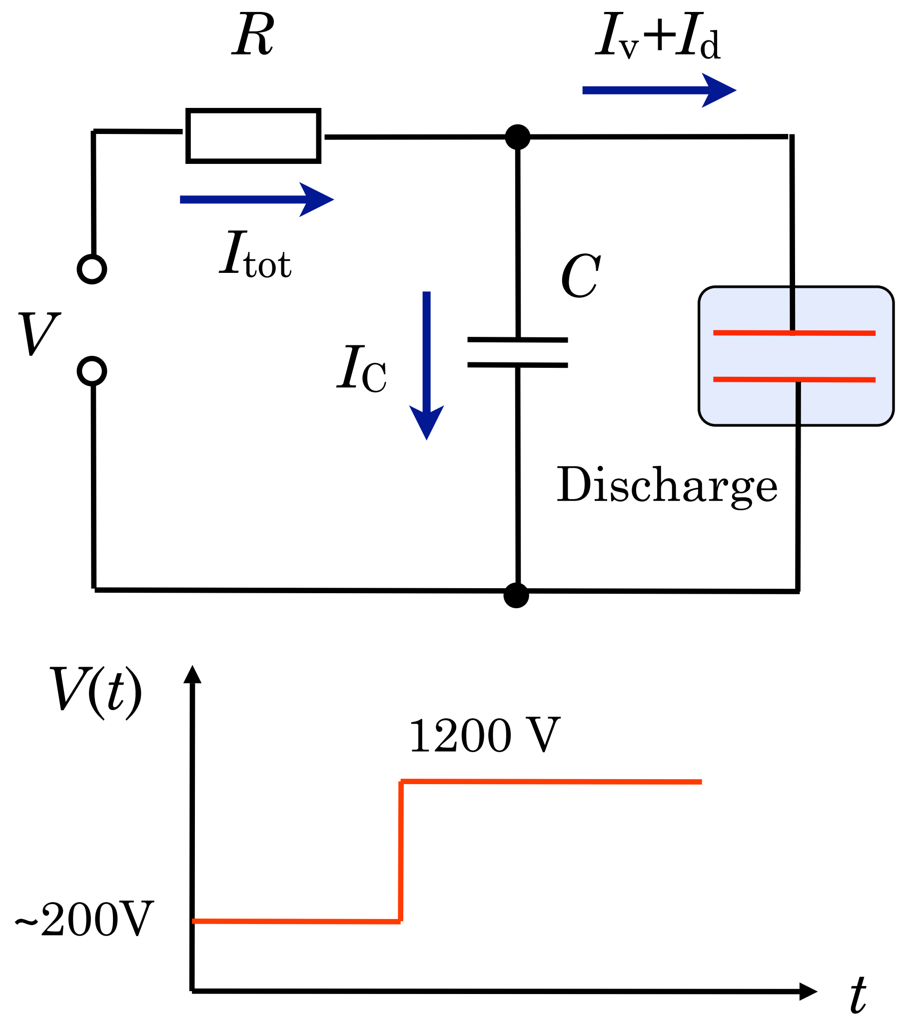
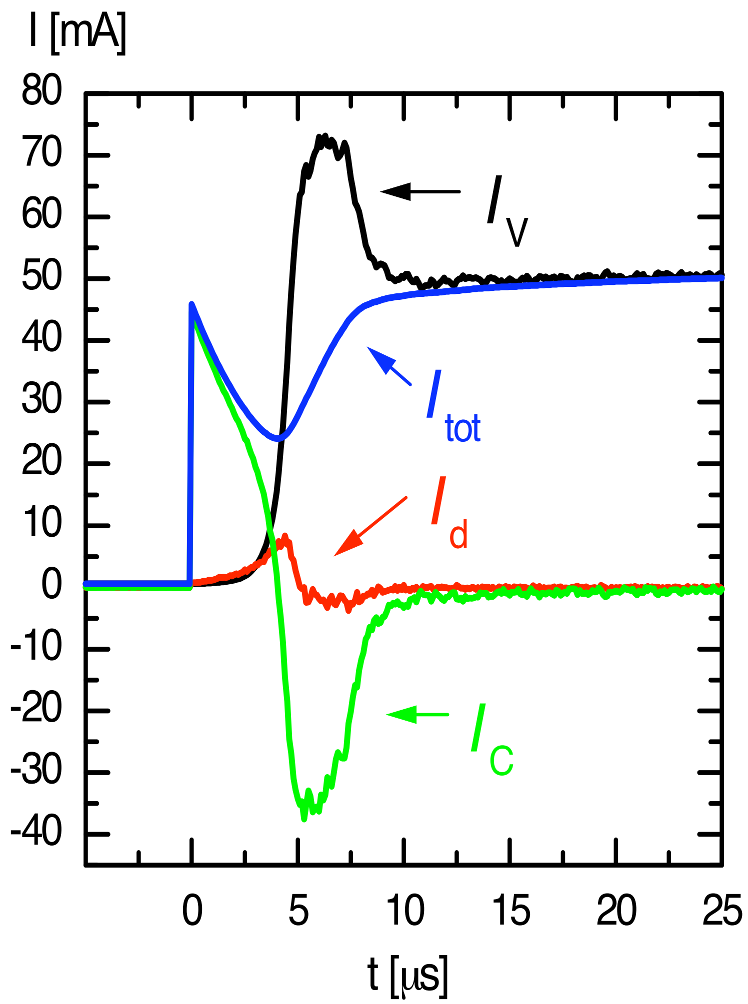
Heavy particle hybrid model:
Monte Carlo simulation of
fast electrons,
fast positive ions and
fast neutrals



$$I_{\mathrm{tot}} = I_{\mathrm{v}} + I_{\mathrm{d}} + I_{\mathrm{C}} \qquad V_{\mathrm{DC}} = V - RI_{\mathrm{tot}}$$

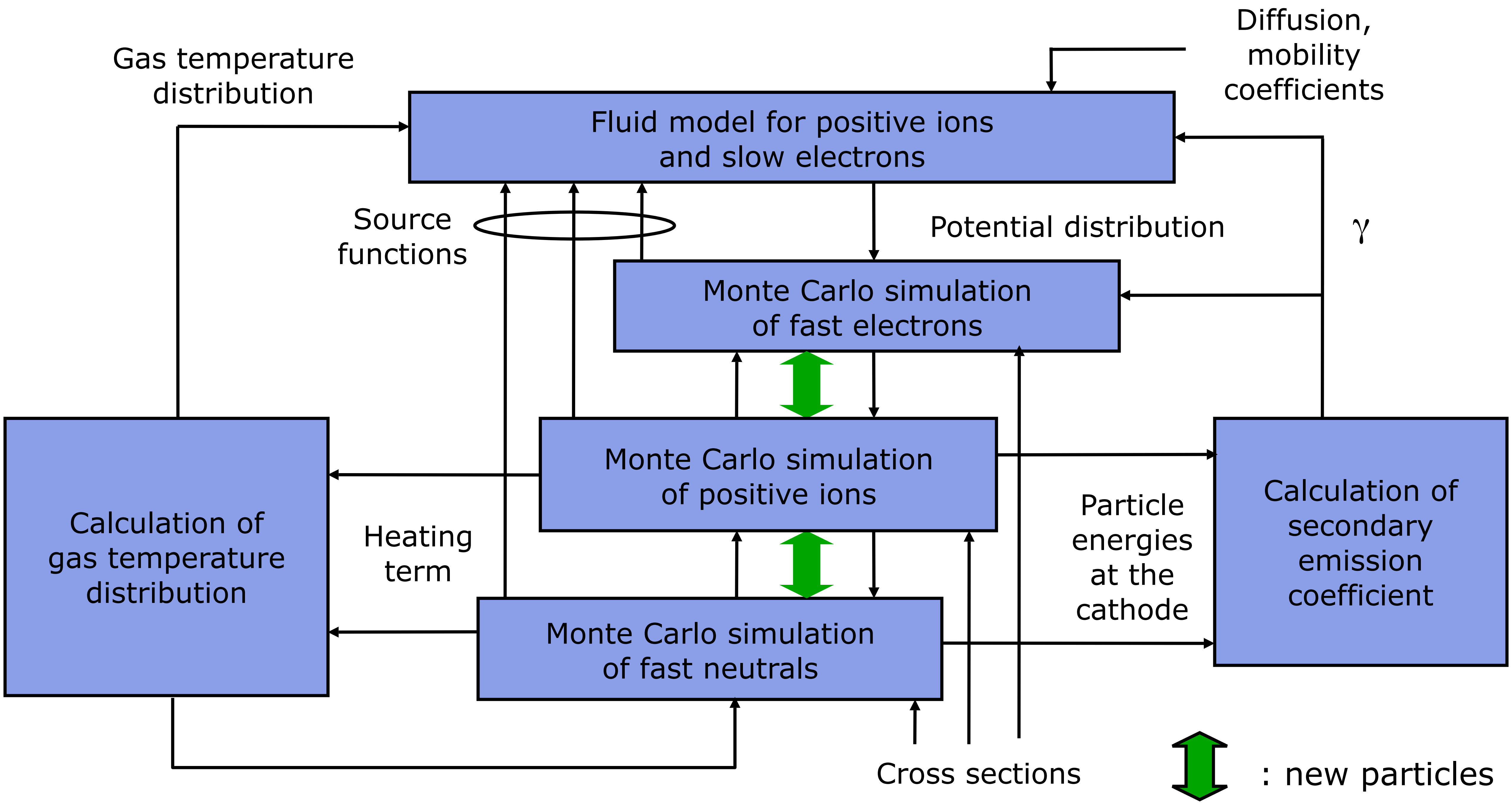
$$I_{\mathrm{d}} = \varepsilon_0 \int_{(\mathrm{Cath.})} \frac{\mathrm{d}E_{\mathrm{n}}}{\mathrm{d}t} \mathrm{d}A \qquad I_{\mathrm{C}} \cong C \frac{\Delta V}{\Delta t}$$





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

Heavy-particle hybrid model



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

Discharge transient: temporal changes of light intensity

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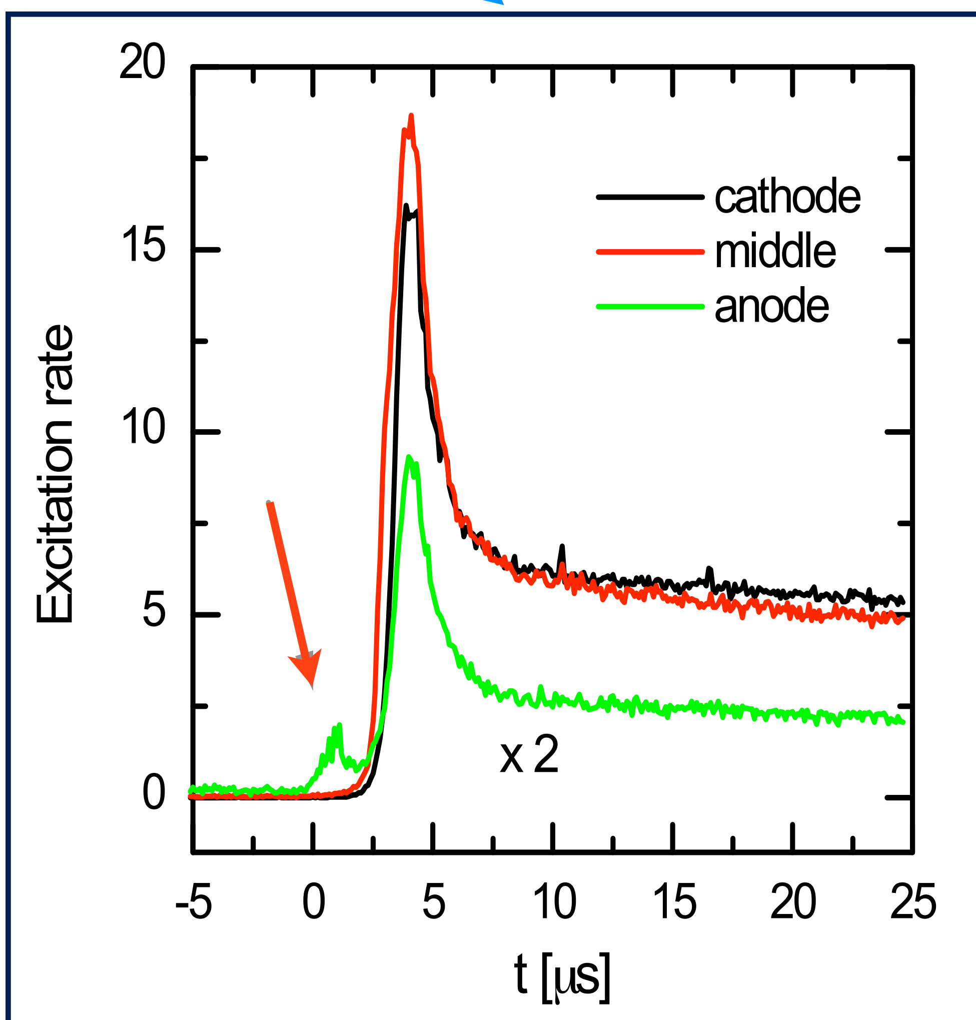
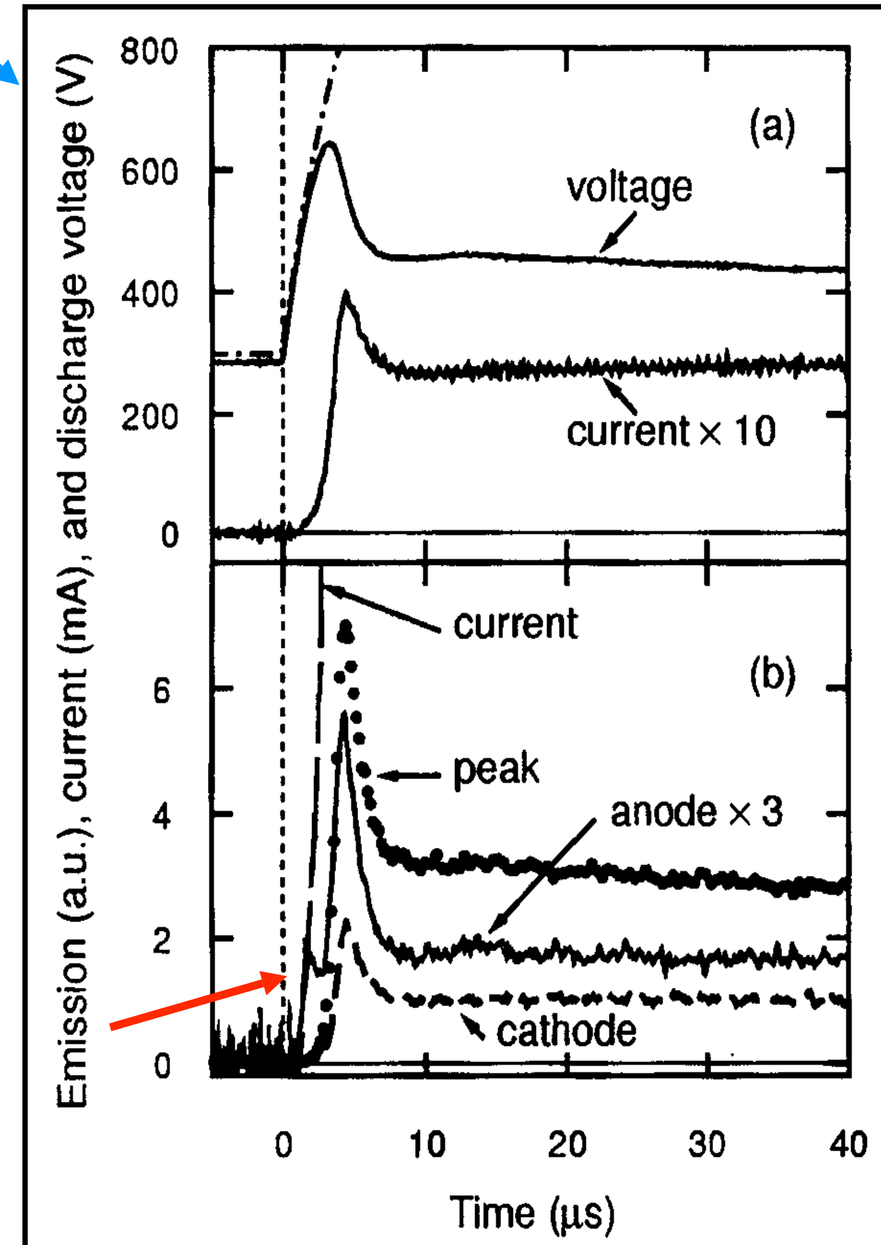
Simulations

Measurement





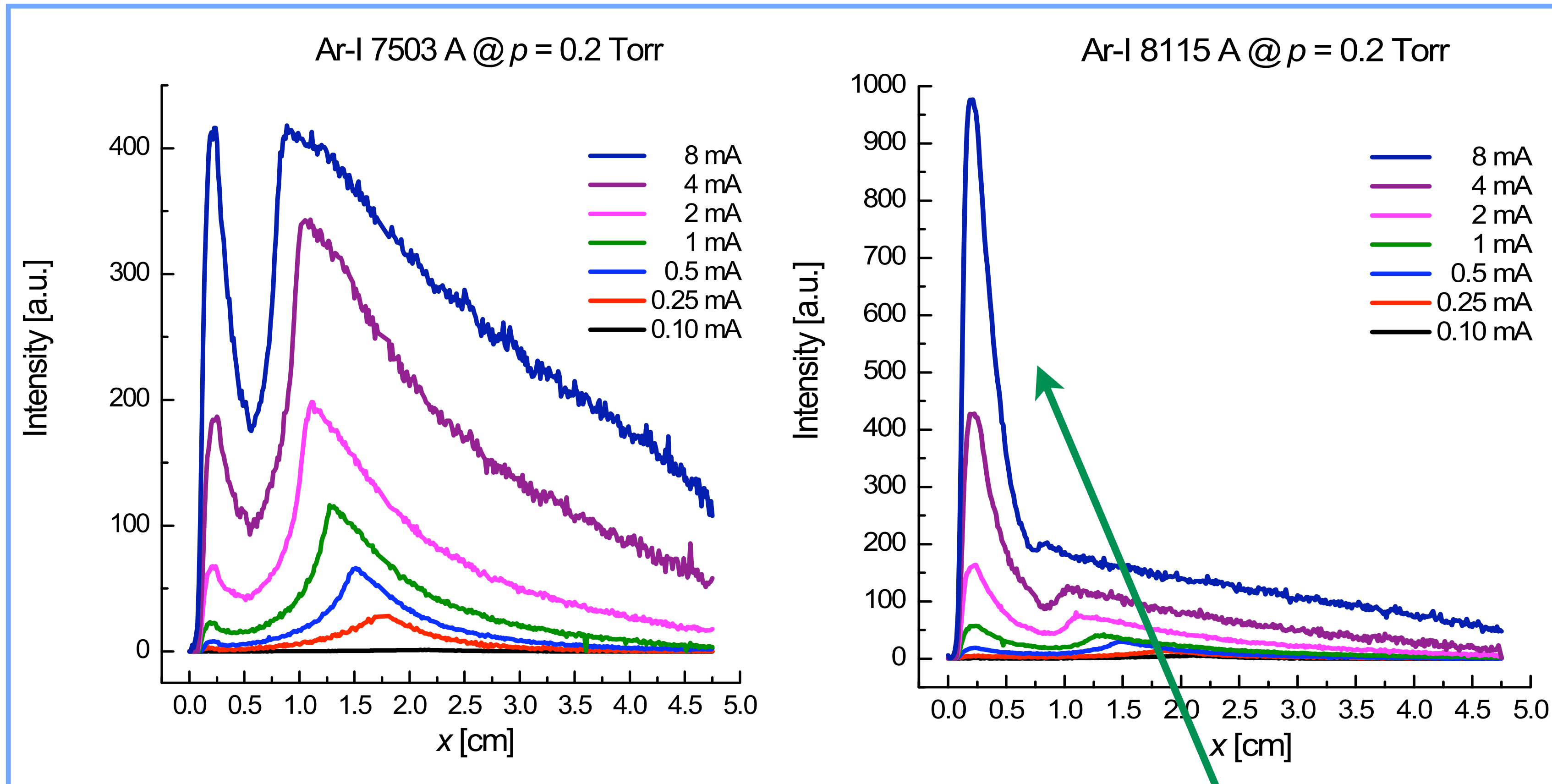
Z. Donkó, J. Appl. Phys. 88, 2226 (2000)

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

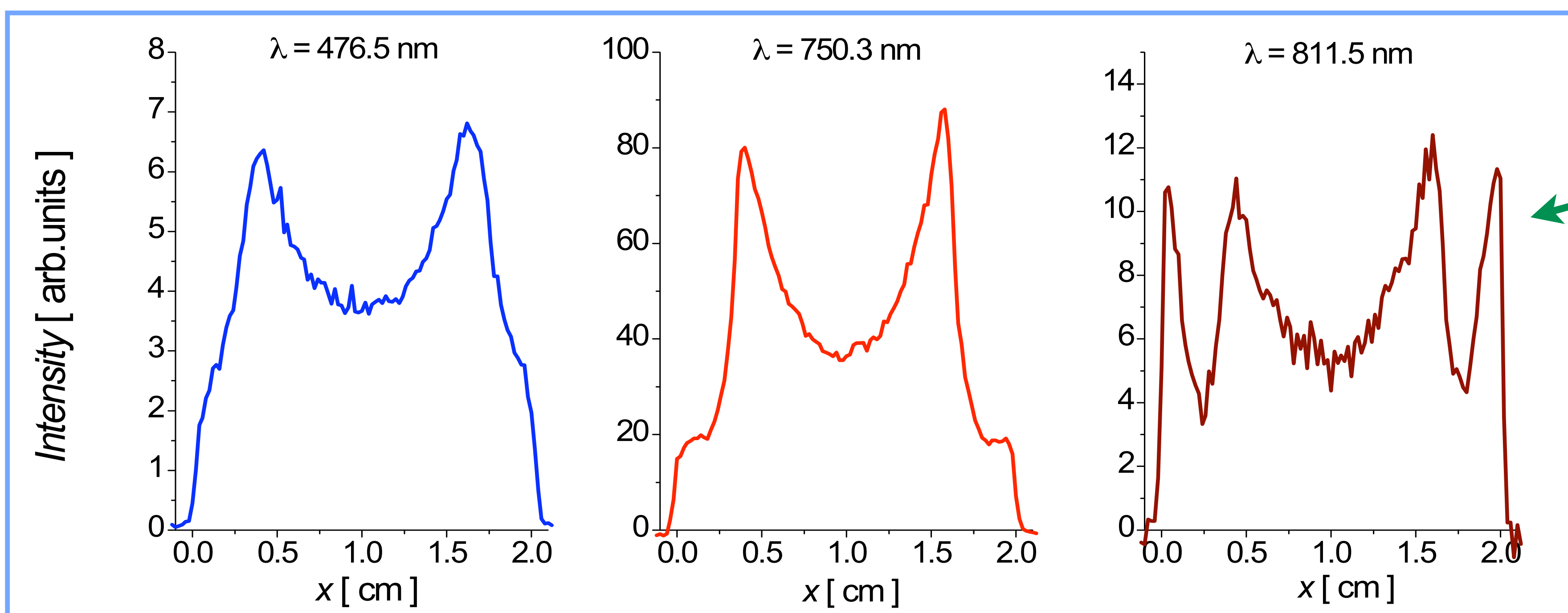
Heavy-particle excitation in the cathode region

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



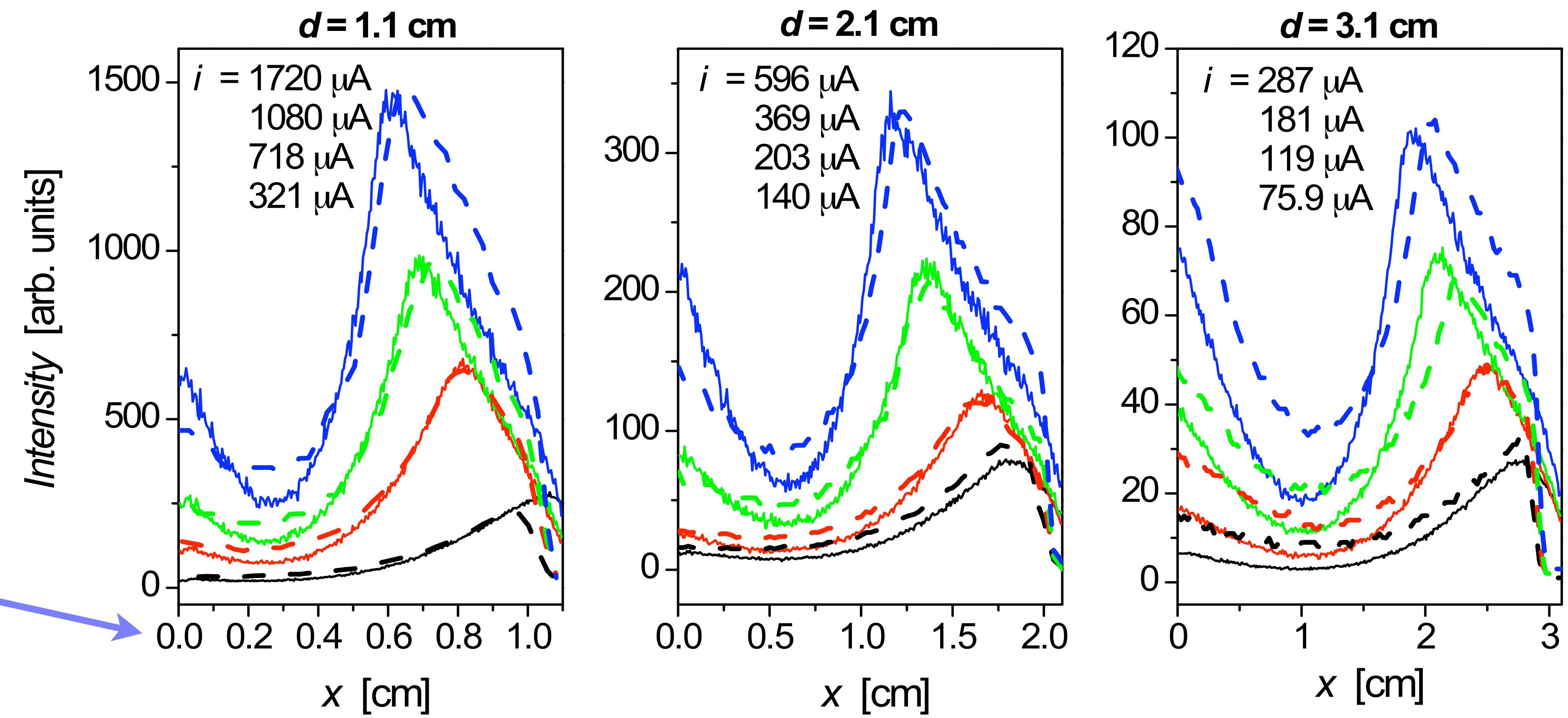
Line intensities in a hollow cathode discharge with plane & parallel cathodes

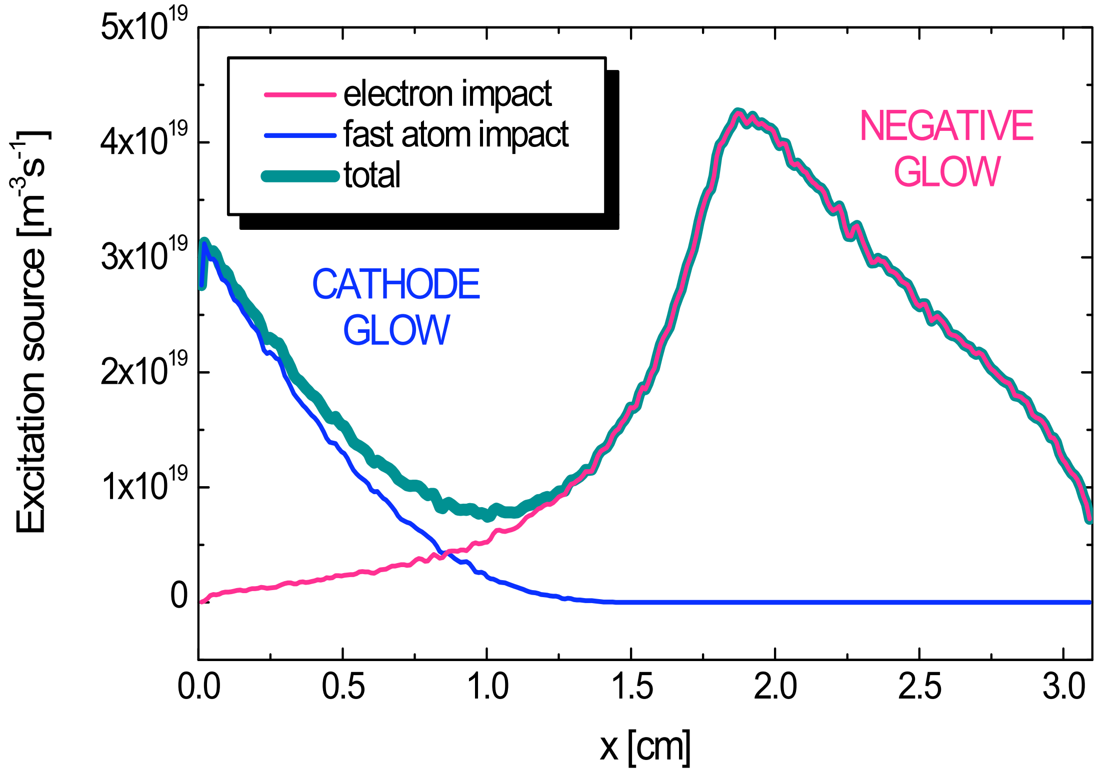
K. Kutasi and Z. Donkó, J. Phys. D. **33**, 1081 (2000).

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).

Summary

- **Charged particle kinetics**
  - Fluid vs. kinetic description of transport
  - Basics of Monte Carlo simulation
  - Velocity distribution functions and transport parameters in homogeneous field
  - Spatio-temporal relaxation of the electron gas
- **Modeling of cold-cathode DC glow discharges**
  - Fluid models - how far can we go without kinetic simulations?
  - Hybrid models - ionization source calculated at kinetic level
- **Heavy particle processes in low-pressure discharges**
  - Breakdown, transients, light emission