Kinetic and fluid descriptions of charged particle swarms and its applications in modeling of particle detectors

Saša Dujko and Danko Bošnjaković

Gaseous Electronics Laboratory
Institute of Physics University of Belgrade
Serbia

In cooperation with: I. Simonović. J. Mirić, Z.Lj. Petrović, O. Šašić, R.D. White,
A. Markosyan and U. Ebert

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CERN

Outline

Introduction

- What is a swarm of charged particles?
- Swarm method of deriving cross sections (Example: $C_2H_2F_4$)

How do we solve the Boltzmann equation?

- Two-term approximation vs. Multi term theory
- Legendre polynomial expansion: yes or no?

What can swarms bring to particle detectors?

- Transport coefficient duality.
- What kind of transport properties should be used in modeling of particle detectors?
- Why do we need the high-order transport coefficients?
- Electron transport in electric and magnetic fields.
- Electron transport in strongly attaching gases.
- Electron transport in liquid Ar and Xe and transition of an avalanche into a streamer

Kinetic and fluid models – Big picture

- How to derive, truncate and close the system of fluid equations?
- Correct implementation of data in fluid modeling.

Concluding Remarks

SERBIA and CERN

September, 1954: The Former Yugoslavia was one of twelve European founding states of CERN

January, 1961: Yugoslavia pulls out from CERN and receives an observer status

June, 1995: CERN Council abolishes an observer status of Federal Republic of Yugoslavia and Serbia establishes formal relations with CERN as an independent state

June 9, 2001: Serbia signs with CERN the General Agreement on Scientific and Technical Cooperation

SERBIA and CERN

August 12, 2005: Serbia signs Memorandum of Understanding for M&O for ATLAS and CMS Experiment

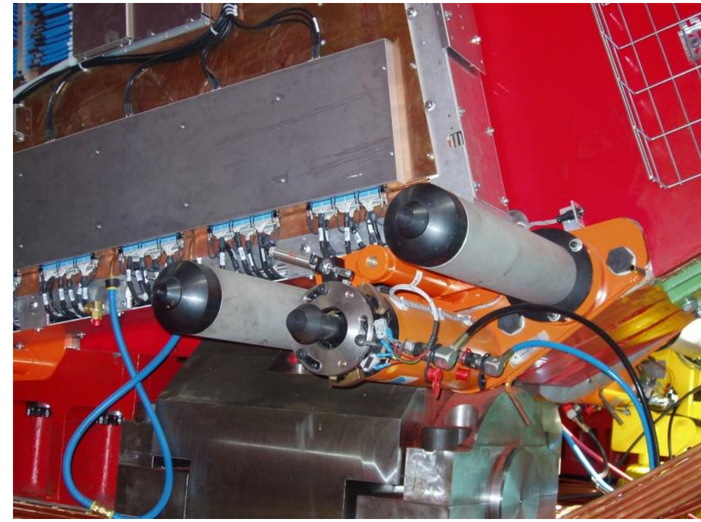
November, 2008: Serbia sends a letter of intent for admission to the CERN membership

March, 2009: Serbia applies for a candidate for the CERN Membership

January 10, 2012: Serbia signs the Agreement on an associate CERN membership as pre-stage to the full membership

March, 2012: Serbia's parliament ratifies this Agreement and Serbia becomes an associate member of CERN

In-kind contribution to the **CMS** experiment



75 hydraulic jacks

for the CMS magnet

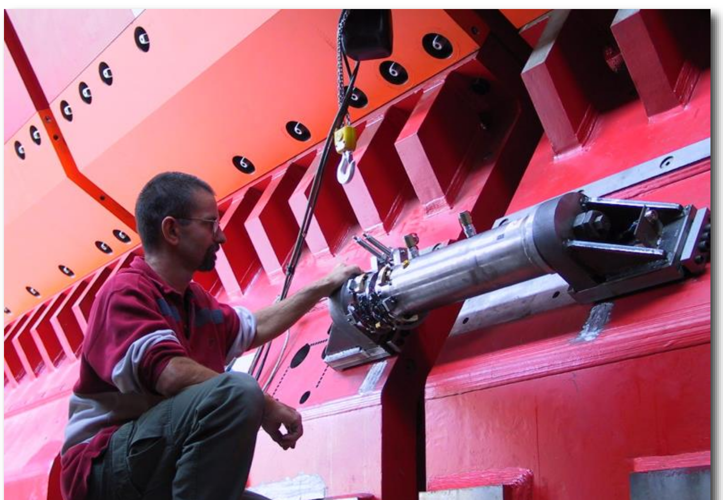
were made in 2002

by “ZASTAVA Alati”

in Kragujevac and

delivered to CMS

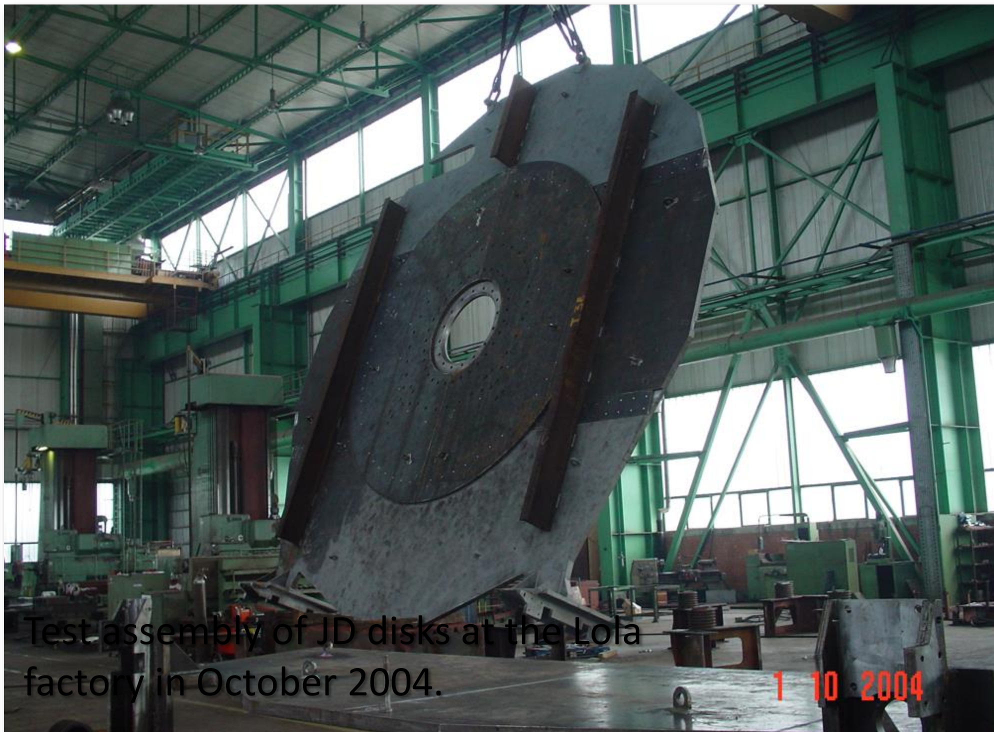
in July 2003.



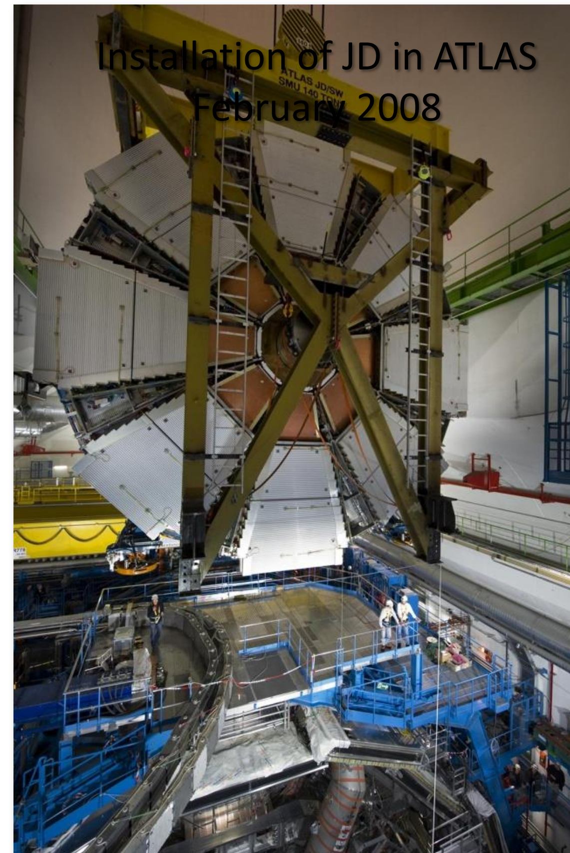
Contributions to the **ATLAS** experiment

In-kind contribution to the forward shielding system:

Disk Shielding (JD) and A-frame supports for the forward shielding (JF), produced by Lola Korporacija (Zeleznik) and Kryooprema (Belgrade), and transported to CERN in 2004.



Test assembly of JD disks at the Lola factory in October 2004.

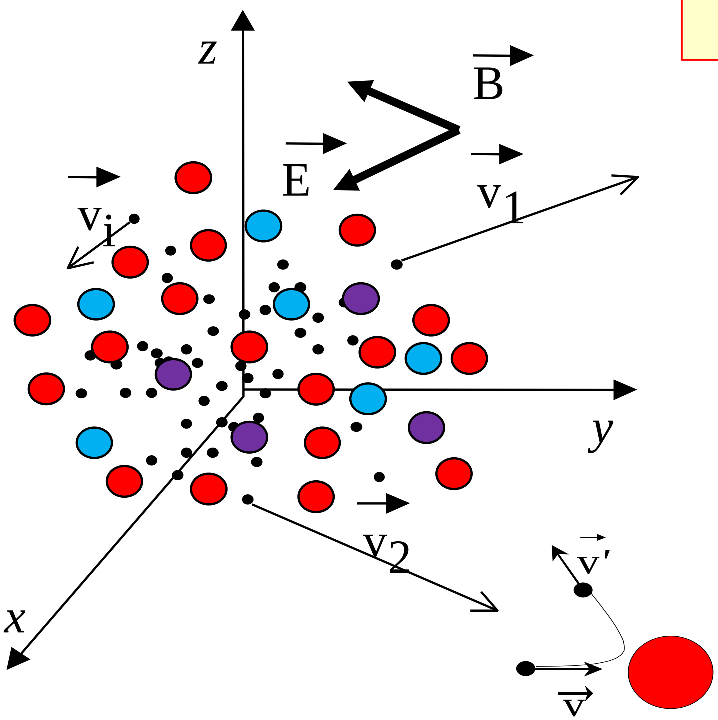


Installation of JD in ATLAS February 2008

Physics studies since 2003:

- until 2010: preparation of the experiment
- since 2010: physics analysis of experimental data

What is a swarm of charged particles?



Swarm conditions $\equiv$ Free diffusion plasma limit

Ludwig Boltzmann (1844-1906)

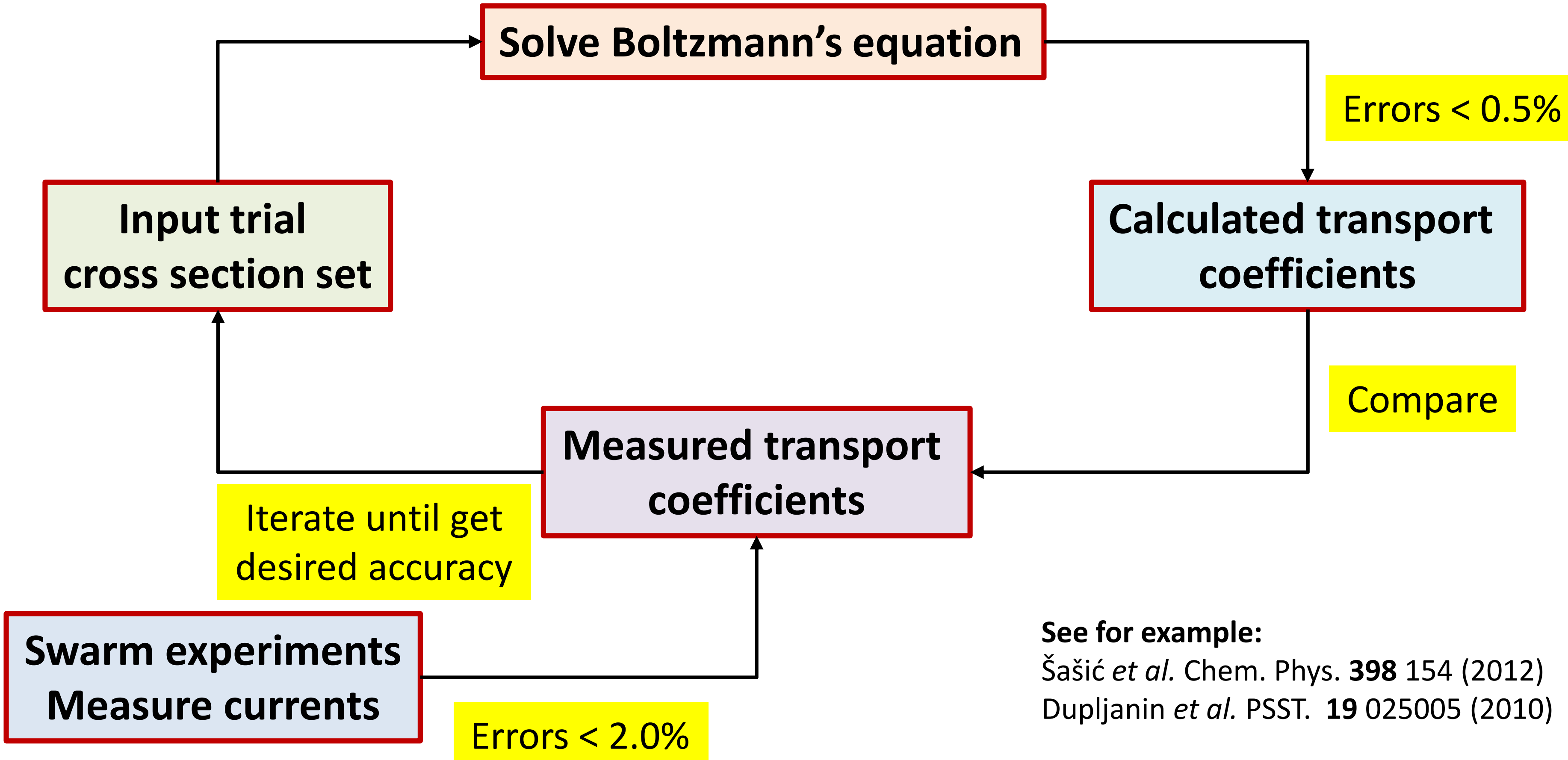
Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{q}{m}(\mathbf{E} + \mathbf{c} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{c}} = -J(f, F_0)$$

$f(\boldsymbol{r},\boldsymbol{c},t)$ - phase space distribution function;
r - space co-ordinate; c - velocity co-ordinate;
E, B - electric and magnetic field strengths;
$J(f,F_0)$ - collision operator.

- Low density of charged particle in gases:
  - Neglect charged particle – charged particle interaction.
  - Neglect space charge effects.
- **E** and **B** fields are spatially homogeneous and externally prescribed.
- Small spatial gradients in number density.
- Minimal boundary effects.

Swarm analysis: block schema



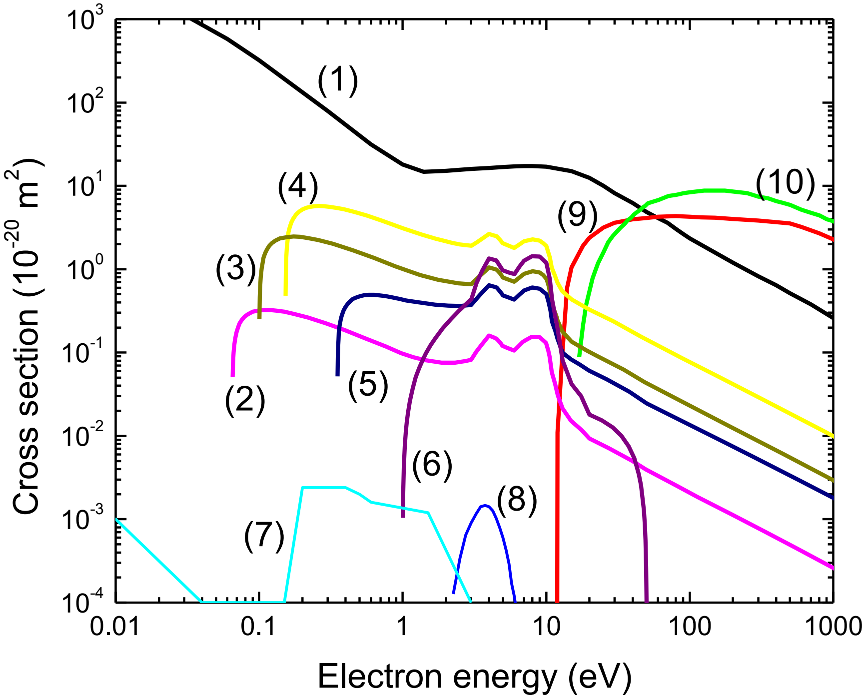
See for example:
Šašić *et al.* Chem. Phys. **398** 154 (2012)
Dupljanin *et al.* PSST. **19** 025005 (2010)

- **Advantages:** completeness, absolute cross sections, and direct applicability to model plasmas and particle detectors.

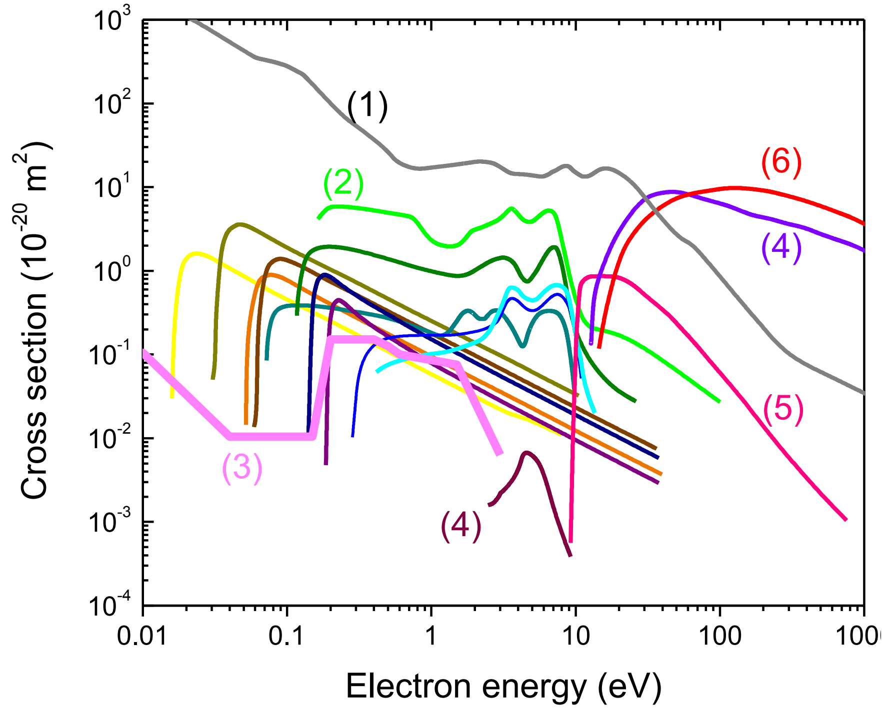
- **Disadvantages:** non-uniqueness, limited resolution, averaging over angular distribution, complexity, indirect nature of the procedure
- This procedure was used to normalize (and develop) cross sections for a range of molecules, including NO, N_2O, CH_4, CF_4, HBr, BF_3, $C_2H_2F_4$, …

Cross sections for electron scattering in $C_2H_2F_4$

S. Biagi – MAGBOLTZ 8.9.1



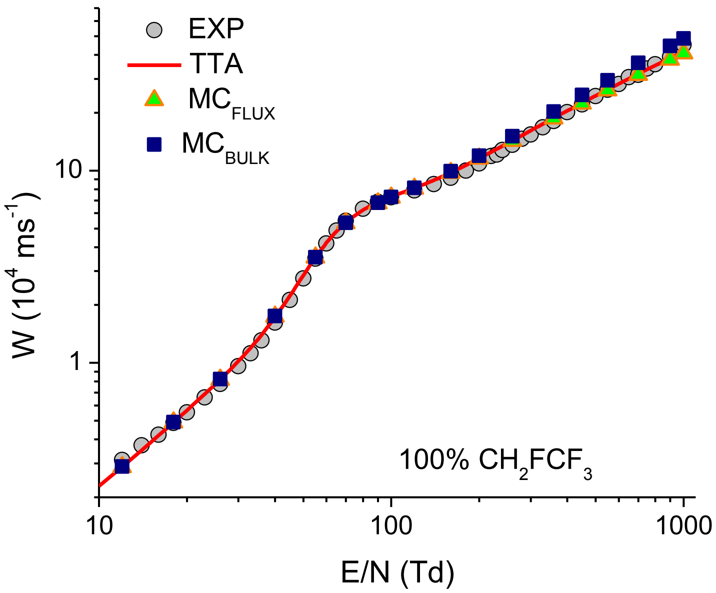
Our laboratory - unpublished



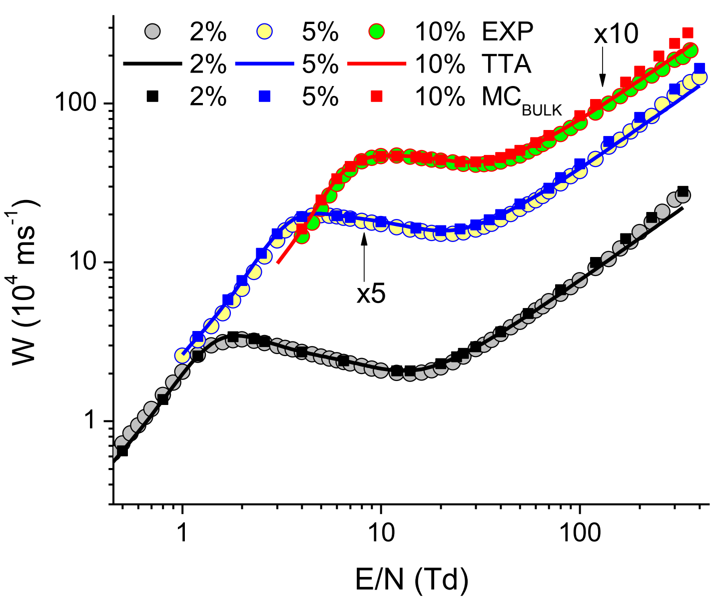
- Used scaled C_2F_6 x-sections.
- Fit to Pulsed-Townsend data of Urquijo et al.
- Included 3-body attachment to fit pressure dependent data of Basile et al.
- Extensively used in modeling of RPC detectors.

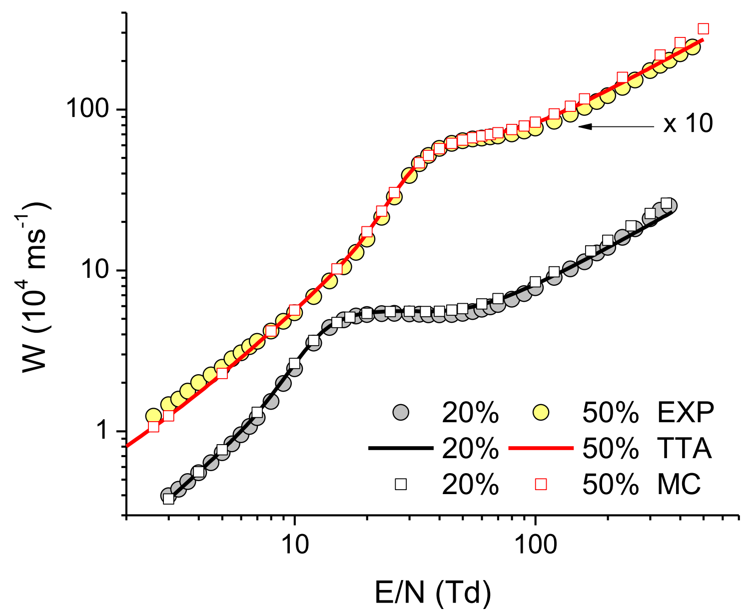
- Better representation of low-energy inelastic processes.
- X-sections for diss. electron attachment, electronic excitations and ionization are calculated by QUANTEMOL.
- Fit to PT data of Urquijo et al. and pressure dependent data of Basile et al.

Drift velocity for electrons in pure $C_2H_2F_4$ and its mixtures with Ar



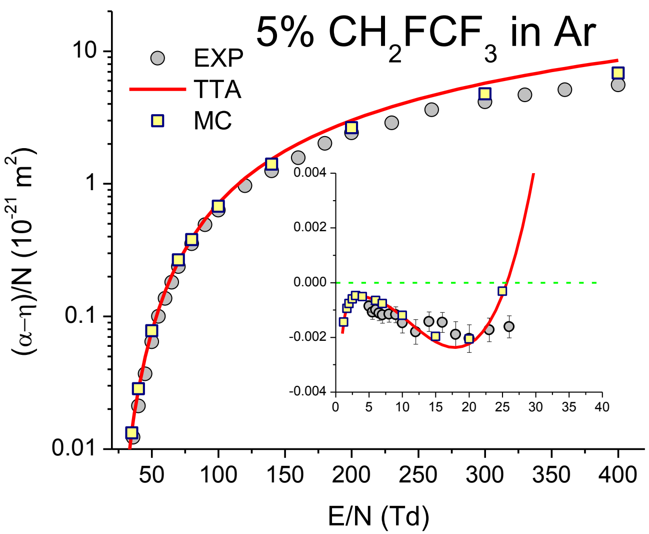
- Cross sections for total momentum transfer was modified to fit the drift velocity.
- Agreement between our and experimental data is very good.
- It is interesting to note that for higher abundances of $C_2H_2F_4$ in the mixture the NDC is firstly suppressed and then for even higher abundances of $C_2H_2F_4$ NDC is removed from the profile of drift velocity.

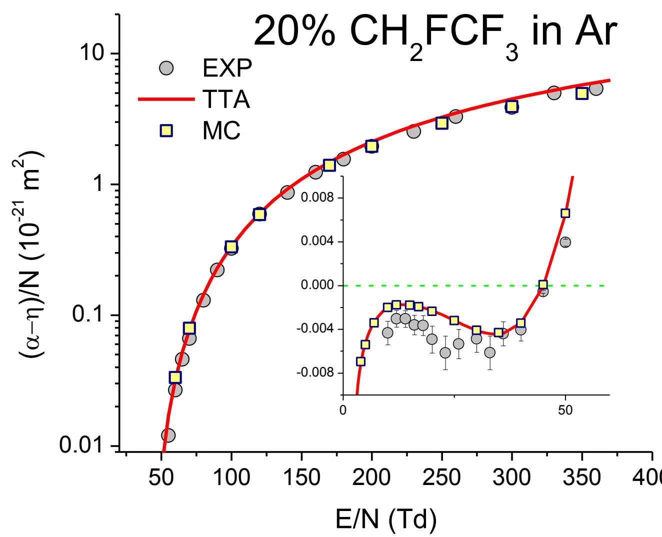


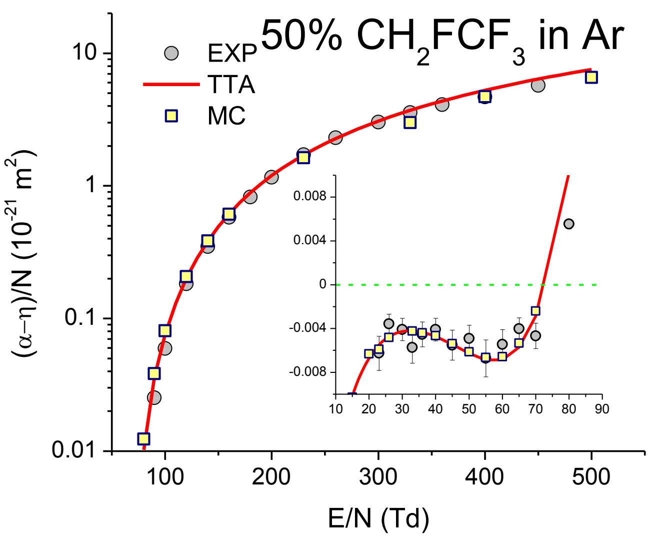


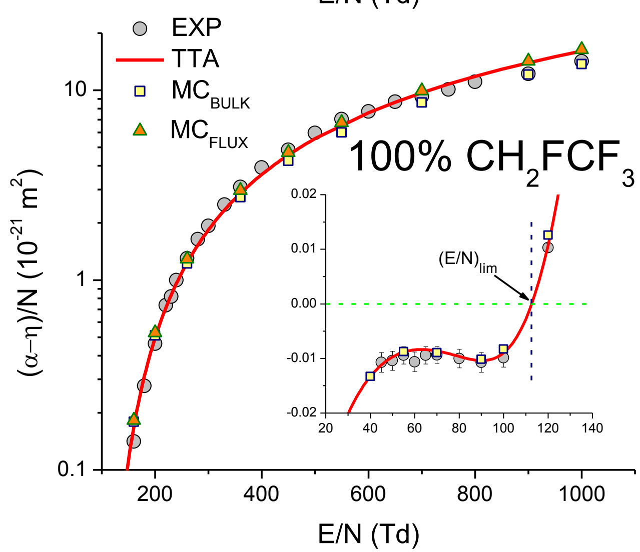
Effective ionization coefficient for electrons in pure $C_2H_2F_4$ and its mixtures with Ar

- In most cases differences are about 10% indicating that the inelastic losses are determined with sufficient accuracy over the wide range of the applied E/N.
- Critical electric field of 112.5 Td for pure $C_2H_2F_4$ agrees very well with the value determined by Basile et al.









How do we solve the Boltzmann equation?

Expansion; Truncation → **Boltzmann equation**

↓

Orthogonality relations;
Symmetry and reality considerations

↓

System of equations for the moments of the dist. function

↓

Transport coefficients and transport properties

↓

Convergence checking
incremented (independently) parameters which are truncated until the convergence criterion is met.

$$\frac{\partial f}{\partial t}+\mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{q}{m}\left(\mathbf{E}+\mathbf{c}\times\mathbf{B}\right)\cdot\frac{\partial f}{\partial \mathbf{c}}=-J\left(f,F_0\right)$$

- Resolving the angular dependence in velocity space:

$$f(\mathbf{r},\mathbf{c},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_m^{(l)}(\mathbf{r},c,t)Y_m^{[l]}(\hat{\mathbf{c}})$$

- Projecting out the space dependence:
  - Hydrodynamic regime:

$$f_m^{(l)}(\mathbf{r},c,t)=\sum_{s=0}^{\infty}\sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda} f(lm\,|\,s\lambda\mu;c,t)G_{\mu}^{(s\lambda)}n(\mathbf{r},t)$$

  - Non-hydrodynamic regime:
    - finite difference
    - pseudo-spectral
- Resolving the speed dependence:

$$f(lm\,|\,s\lambda\mu;c,t)=\omega(\alpha,c)\sum_{\nu=0}^{\infty}F(\nu lm\,|\,s\lambda\mu;\alpha,t)R_{\nu l}(\alpha c)$$

Dujko *et al.* Phys. Rev. E **81** (2010) 046403

Transport coefficient duality

$$\frac{\partial n(\mathbf{r},t)}{\partial t} + \nabla\cdot\boldsymbol{\Gamma}(\mathbf{r},t) = S(\mathbf{r},t)$$

Eq. of continuity

Hydrodynamic approximation:

$$f(\mathbf{r},\mathbf{c},t) = \sum_{k=0}^{\infty} f^{(k)}(\mathbf{c},t)\otimes(-\nabla)^k n(\mathbf{r},t)$$

Flux-gradient relation:

$$\boldsymbol{\Gamma}(\mathbf{r},t) = \mathbf{W}^{(*)}(t)n(\mathbf{r},t) - \mathbf{D}^{(*)}(t)\cdot\nabla n(\mathbf{r},t)$$

$\mathbf{W}^*$ Flux drift velocity

$\mathbf{D}^*$ Flux diffusion tensor

Diffusion equation:

$$\frac{\partial n}{\partial t} + \mathbf{W}(t)\cdot\nabla n - \mathbf{D}(t):\nabla\nabla n = -R_a(t)n$$

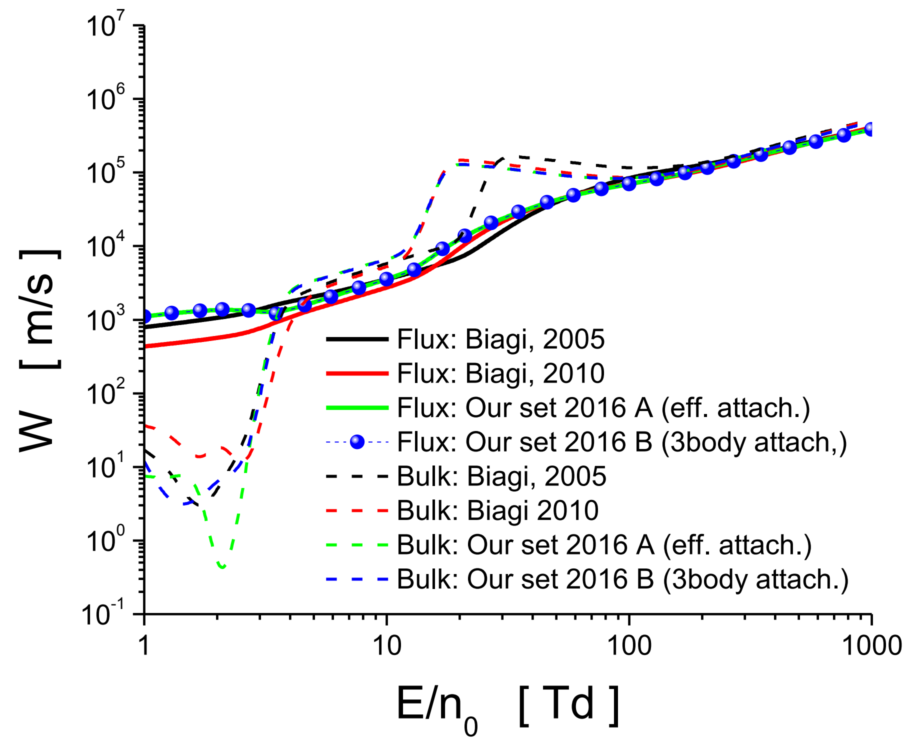
R_a Reaction rate

$\mathbf{W}$ Bulk drift velocity

$\mathbf{D}$ Bulk diffusion tensor

Bulk transport coefficients:
- Measured in swarm experiments.
- Determined according to the diffusion eq.
- Required for cross section renormalization.

Flux transport coefficients:
- Not measurable.
- Determined via the flux gradient eq.
- Required in fluid plasma models as input data.



Drift velocity for electrons in an ALICE TOF RPC system.
Gas mixture used: $C_2H_2F_4$:iso-C_4H_{10}:SF_6=90:5:5

Why do we need high order transport coefficients?

- Required in swarm analysis for converting transport data measured in various experiments into hydrodynamic transport coefficients.
- Necessary for describing deviations of spatial density profile from an ideal Gaussian.
- Since they are very sensitive with respect to the energy dependence of cross sections - their measurement and calculation would improve the accuracy of cross section fitting procedure.
- Required for analysis of systems which shows the signs of non-hydrodynamic behavior.

They appear in the flux-gradient and diffusion equations:

$$\Gamma_a = n(\vec{r},t)W_a - \sum_{b=1}^{3} D_{ab}\frac{\partial n(\vec{r},t)}{\partial r_b} + \sum_{b,c=1}^{3} Q_{abc}\frac{\partial^2 n(\vec{r},t)}{\partial r_b \partial r_c} + \dots$$

$$\left(\frac{\partial}{\partial t} + W^{(B)}\cdot\nabla - \hat{D}^{(B)} : \nabla\nabla + \hat{Q}^{(B)} \vdots \nabla\nabla\nabla + \dots\right) n(\vec{r},t) = -R_a n(\vec{r},t)$$

How to sample them in Monte Carlo codes?

$$n_0{}^2 Q_L = n_0{}^2 Q_{zzz}$$

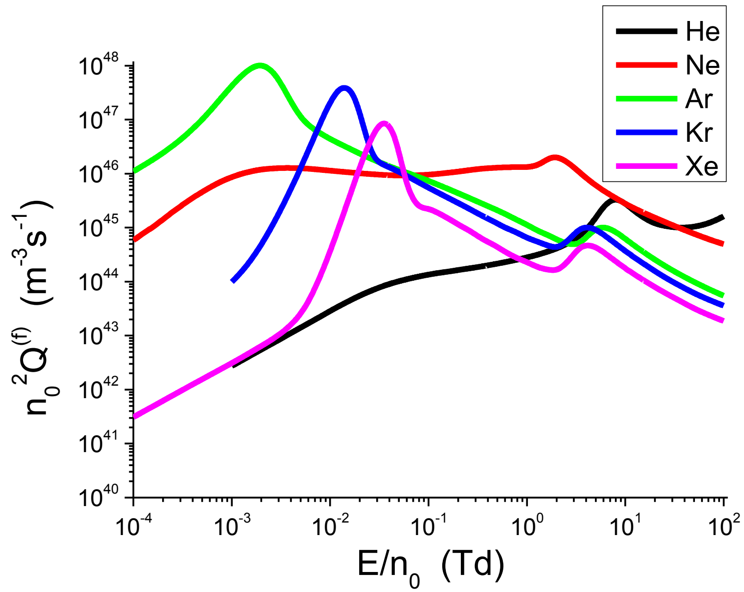
$$n_0{}^2 Q_T = n_0{}^2 (Q_{xxz} + Q_{xzx} + Q_{zxx})$$

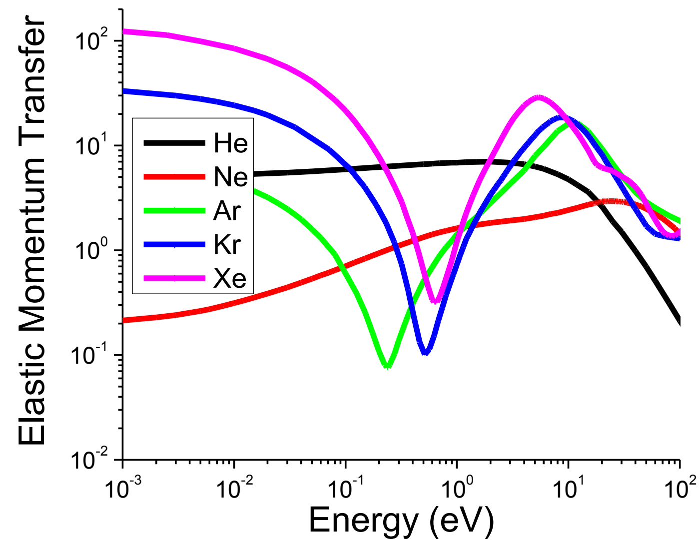
Structure of the skewness tensor: **E** = E**e**$_z$

$$Q_{xab} = \begin{pmatrix} 0 & 0 & Q_{xxz} \\ 0 & 0 & 0 \\ Q_{xxz} & 0 & 0 \end{pmatrix} \qquad Q_{yab} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & Q_{xxz} \\ 0 & Q_{xxz} & 0 \end{pmatrix} \qquad Q_{zab} = \begin{pmatrix} Q_{zxx} & 0 & 0 \\ 0 & Q_{zxx} & 0 \\ 0 & 0 & Q_{zzz} \end{pmatrix}$$

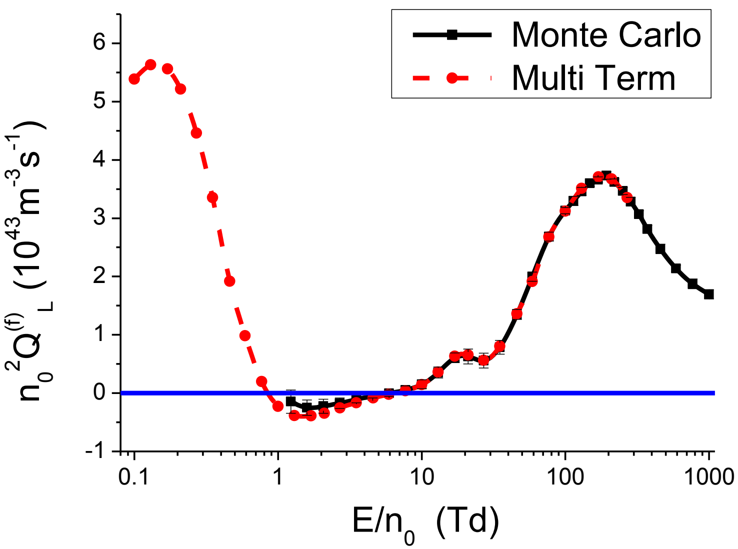
Examples of high order transport coefficients in atomic and molecular gases

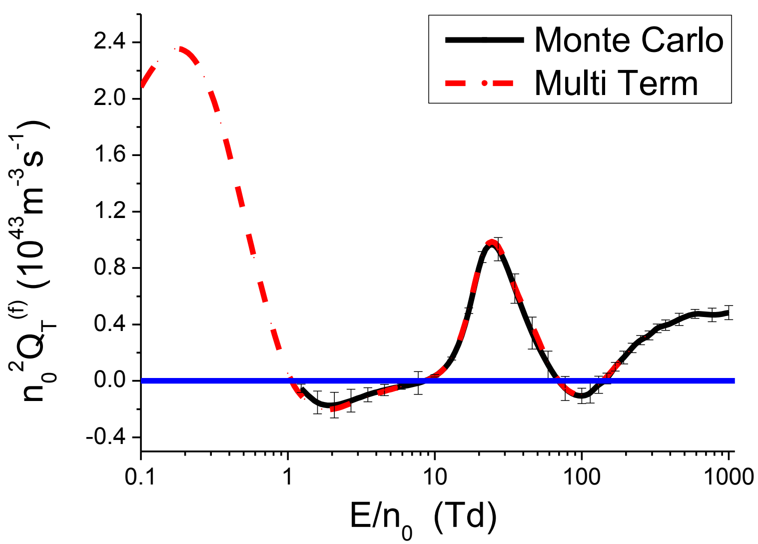
- How to determine the depth and position of Ramsauer Townsend minimum?





- First observation of negative steady-state transport coefficients! Electrons in CF_4

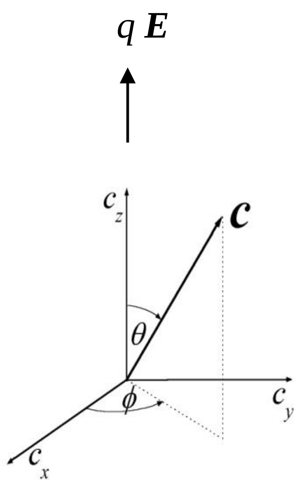




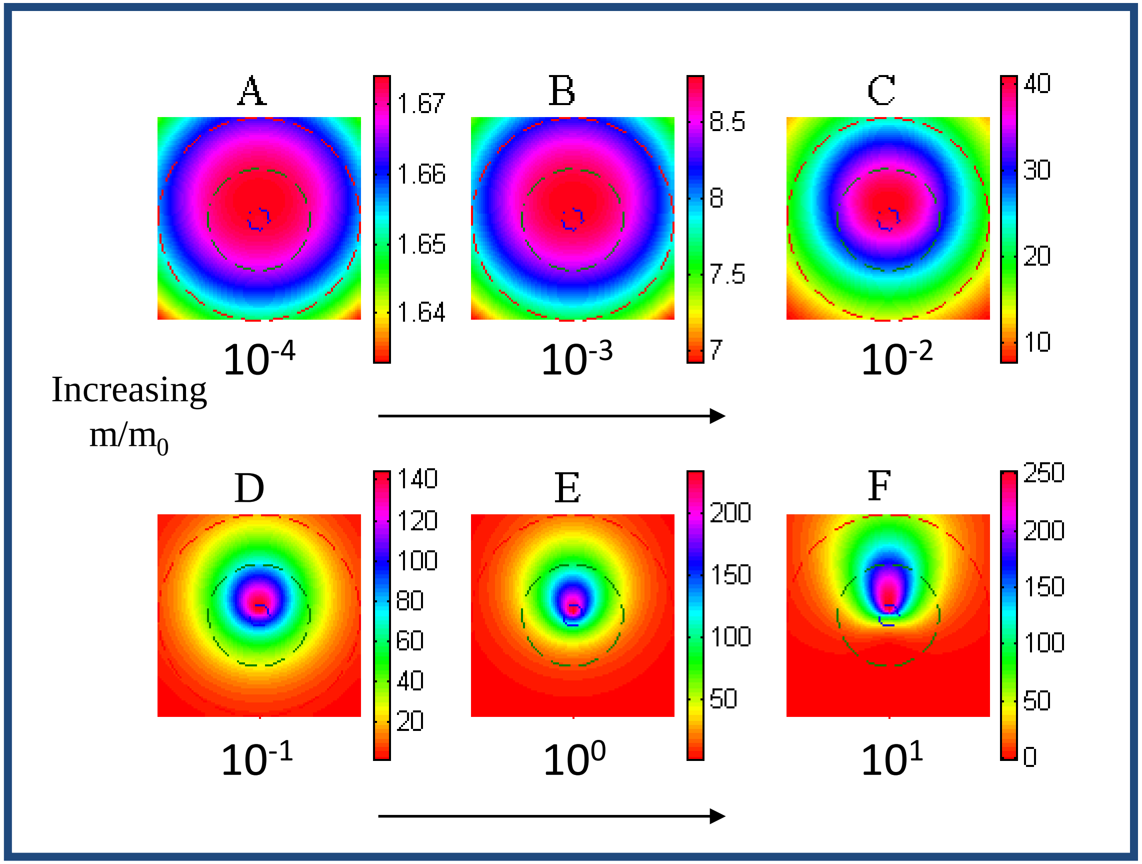
Spherical harmonic representation of the velocity distribution function

$$f^{(s)}(\boldsymbol{r},\boldsymbol{c},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}f_m^{(s,l)}(\boldsymbol{r},c,t)Y_m^{[l]}(\hat{\boldsymbol{c}})$$

- For light particles m/m_0 *<<1,* truncation at l_{max} *=1 ('two-term approximation')* is *generally* satisfactory if collisions are *elastic.*
- **For ions $m \approx m_0$ and two-term approximation is never valid!**



- **Both** angles θ, ϕ are generally needed!
- Legendre polynomial representation is generally inadequate!



Legendre polynomial expansion procedure: yes or no?

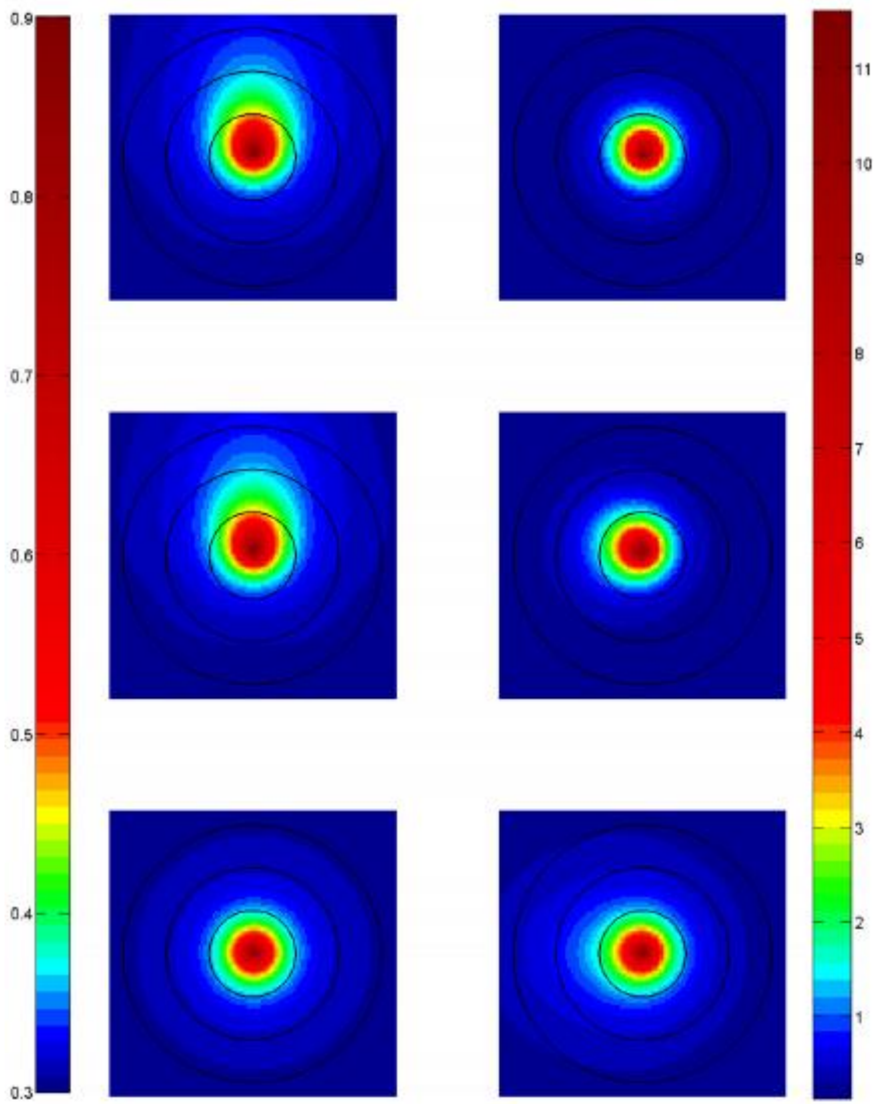
B/n_0 = 0 Hx

B/n_0 = 200 Hx

Plane: $\phi=0,\pi$
(x-z plane)

Plane:
$\phi=\pi/2,3\pi/2$
(y-z plane)

Plane: $\theta=\pi/2$
(x-y plane)



Observed phenomena:
- Magnetic cooling effect;
- Directional effects;
- Distraction of symmetry.

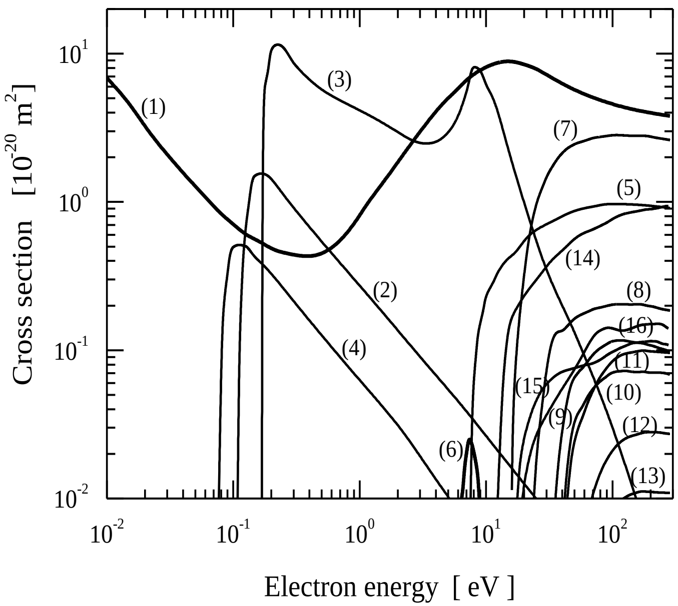
No axis of rotational symmetry: Legendre expansion is flawed

Rotational symmetry destroyed by application of perpendicular component of B field!

CO_2: E/n_0 = 5 Td, B/n_0 = 200 Hx

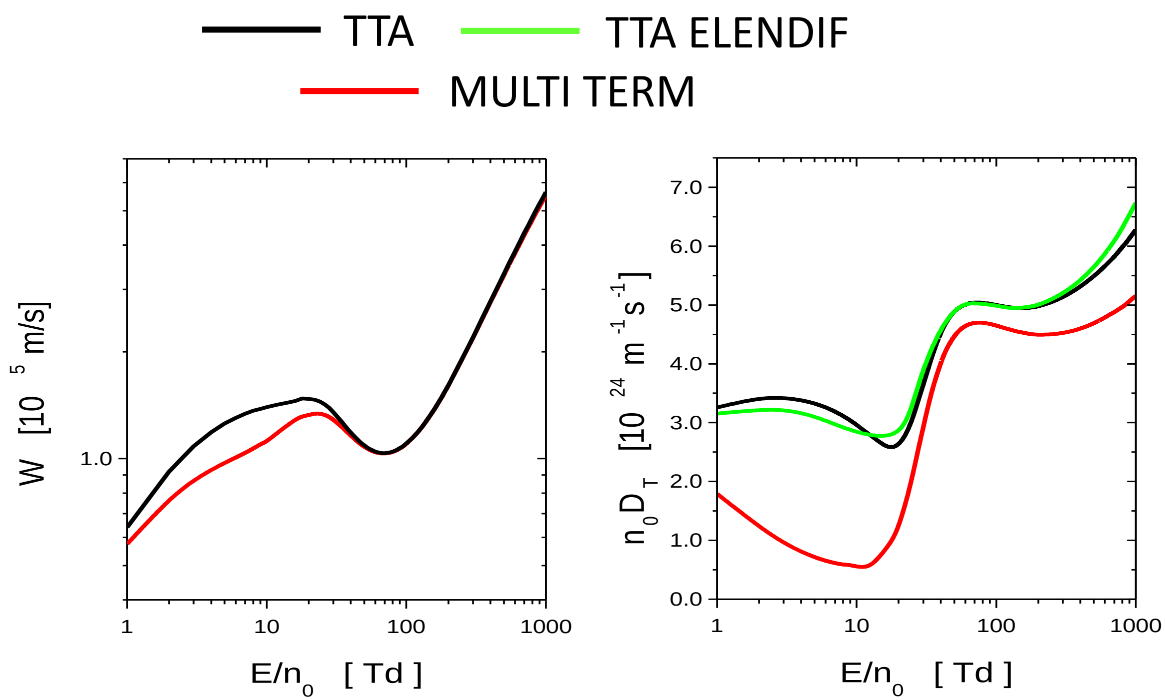
White et al. 2009 J. Phys. D: Appl. Phys. **42** 194001

CF_4: TTA vs. Multi Term Boltzmann Equation Analysis



Electron impact cross section for CF_4

(Kurihara *et al.* J.Phys.D:Appl. Phys. 33 (2000) 2146)
momentum transfer cross section (1), vibrational excitation (2–4)
electronic excitation (5), attachment cross section (6),
dissociative ionization cross sections (7–13) and
cross sections for neutral dissociation (14–16).



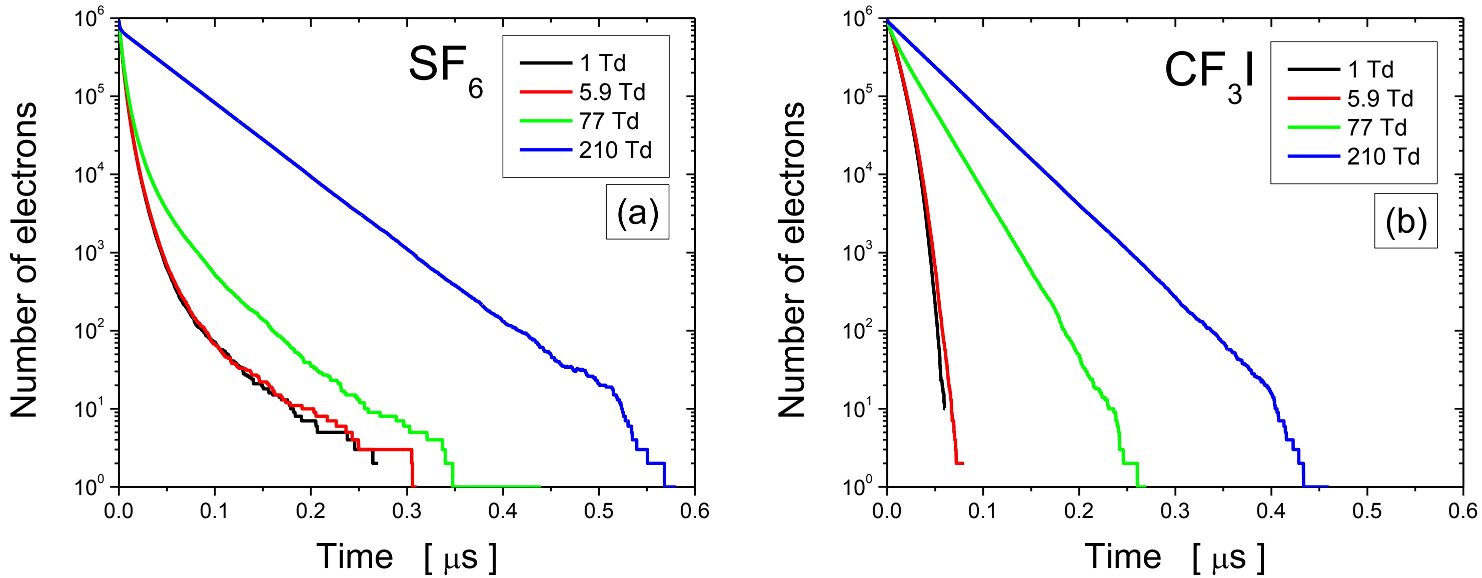
- Need 7-terms in the spherical harmonic expansion to achieve error <1%;

- Two-term approximation can produce the wrong results for both the drift and diffusion.

- The errors associated with W: ~ 30%;
- The errors associated with n_0D_T: ~ 400% !

S. Dujko, R.D. White and Z.Lj. Petrović
Facta Univ. 6 (2008) 57

How to simulate electron transport in very strong attaching gases?



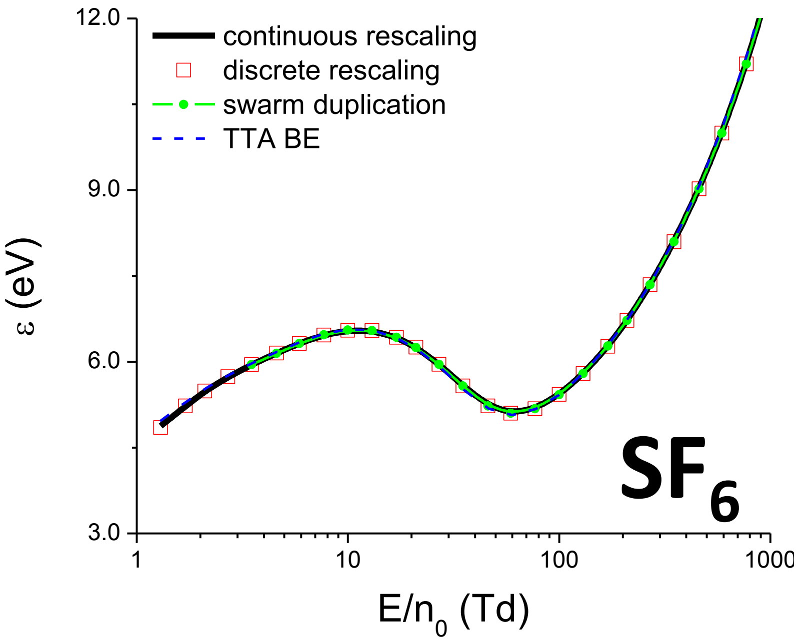
• Electron number density drops down by six orders of magnitude over the course of several hundred nanoseconds in both gases.
• To facilitate the numerical simulation, it is clear that some kind of rescaling of the number density is necessary to compensate for the electrons consumed by electron attachment.

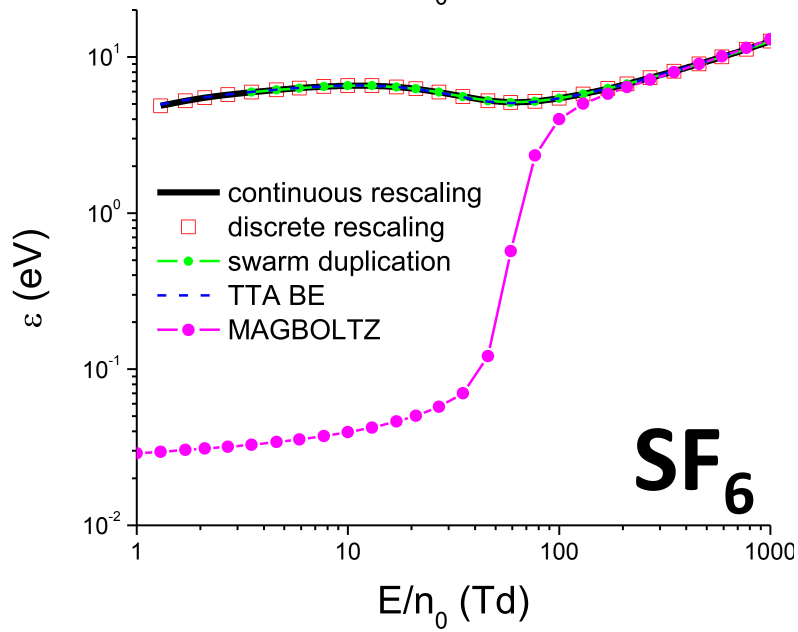
❖ **DISCRETE RESCALING:** Uniform generation of new electrons with initial properties taken from the remaining electrons.

❖ **SWARM DUPLICATION:** Uniform scaling of an electron swarm by a factor of 2 or 3 at certain instants of time or distance depending on the simulation conditions where the probability of scaling for each electron is set to unity.

❖ **CONTINOUS RESCALING:** Introduction of an additional fictitious ionization process with a constant ionization frequency (that is close to the rate for attachment), which artificially increases the number of simulated electrons.

Electron transport in strongly attaching gases





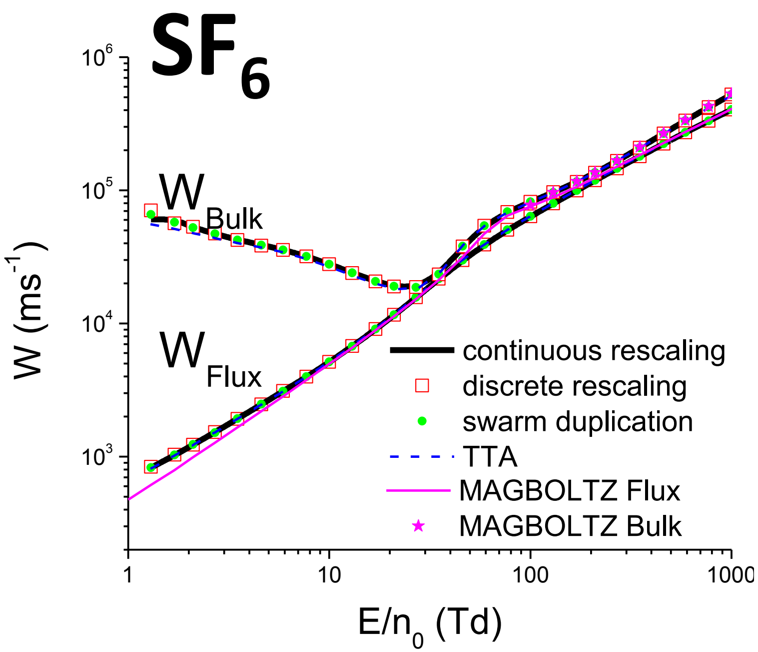
Simulation conditions: SF_6 T=293K p = 1atm.
Cross sections for electron scattering in SF_6:
Itoh et al. J. Phys. D **26** (1993) 1975

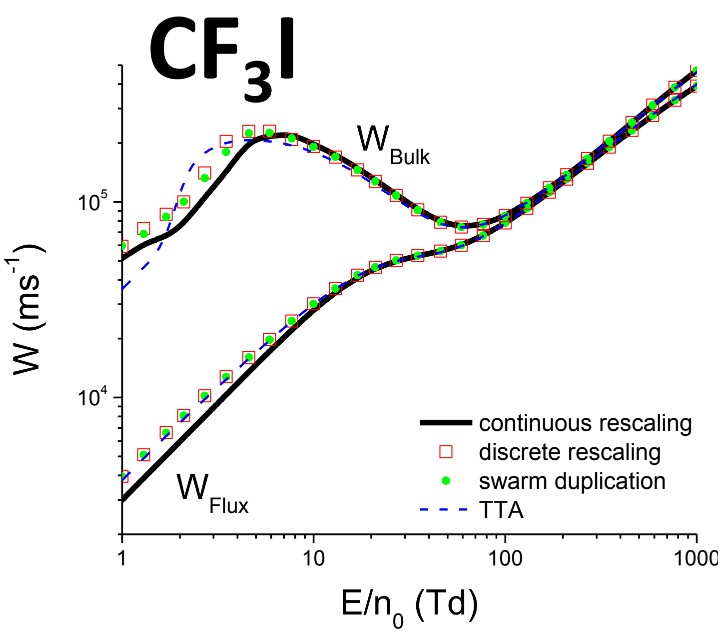
We observe the following interesting points:

- All rescaling procedures and our TTA for solving the Boltzmann equation agree very well.
- Mean energy initially increases with E/n_0, reaching a peak around 10 Td, and then surprisingly it starts to decrease with E/n_0!
    - attachment heating.
    - inelastic cooling.
- Deviations between our and MAGBOLTZ results are huge: MAGBOLTZ has some issues with the explicit influence of electron attachment!

Mirić et al. Submitted to PSST

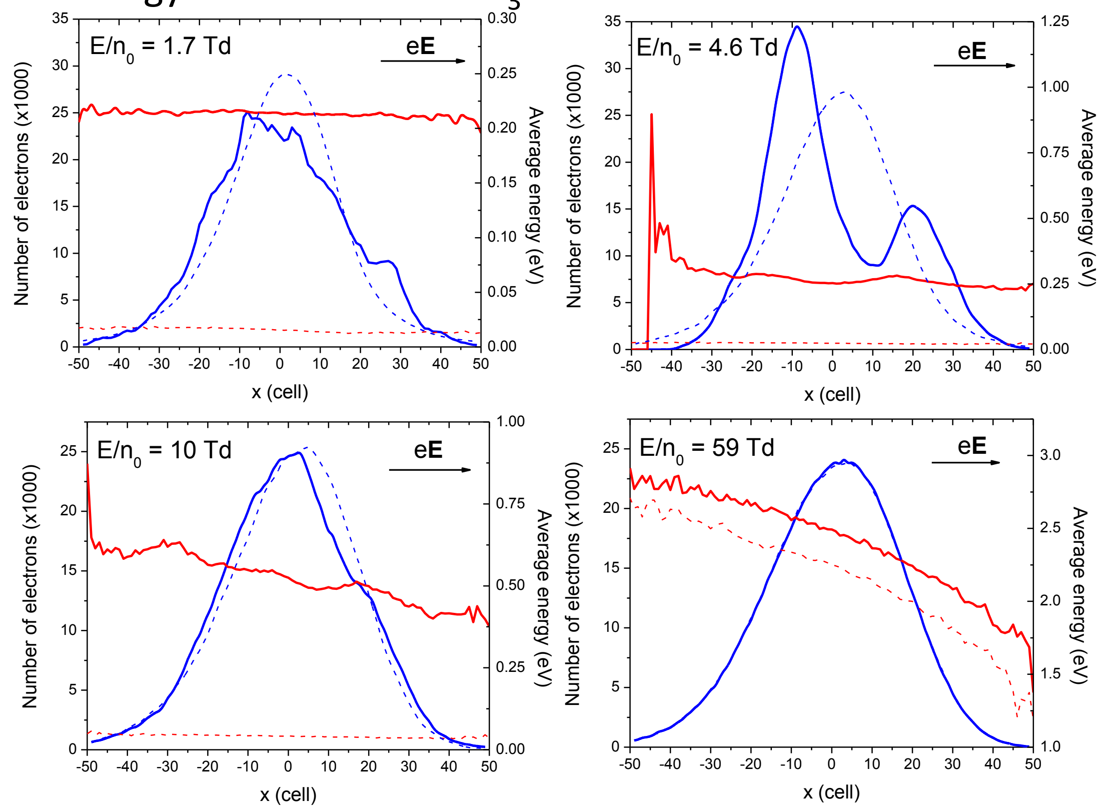
Electron transport in strongly attaching gases





- For both SF_6 and CF_3I, the bulk dominates the flux drift velocity over the entire E/n_0 .
    - Lower E/n_0: attachment heating.
    - Higher E/n_0: explicit effects of ionization .
- **New phenomenon:** A very strong NDC effect is present only in the bulk component!

Spatial profiles of electrons and spatially resolved average energy for electrons in CF_3I.



Spatiotemporal development of electron swarms

Dujko et al. Eur. Phys. J. D **68** (2014), 166

The Lucas and Saelee ionization model:

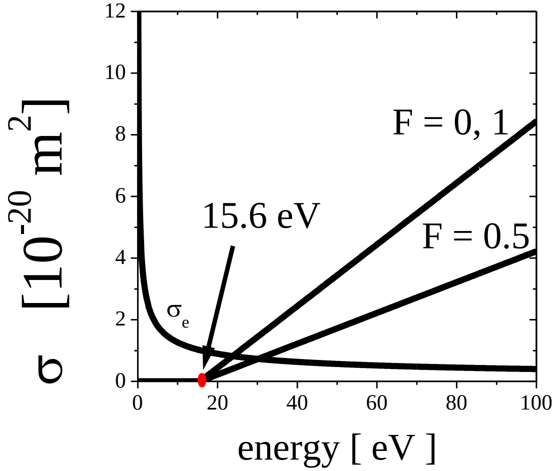
$$\sigma_e = \frac{4}{\sqrt{\varepsilon}} 10^{-20}\ \mathrm{m}^2$$

$$\sigma_{ex} = \begin{cases} 0.1(1-F)(\varepsilon-\varepsilon_i)10^{-20}\ \mathrm{m}^2,\ \varepsilon \geq \varepsilon_i \\ 0,\ \varepsilon \leq \varepsilon_i \end{cases}$$

$$\sigma_i = \begin{cases} 0.1F(\varepsilon-\varepsilon_i)10^{-20}\ \mathrm{m}^2,\ \varepsilon \geq \varepsilon_i \\ 0,\ \varepsilon \geq \varepsilon_i \end{cases}$$

$$\frac{m}{m_0} = 0.001,\ n = 1\times 10^{-20}\ \mathrm{m}^{-3},\ T_0 = 0\ K$$

E/n_0 = 27 Td



F = 0 conservative case

F = 1 non-conservative case

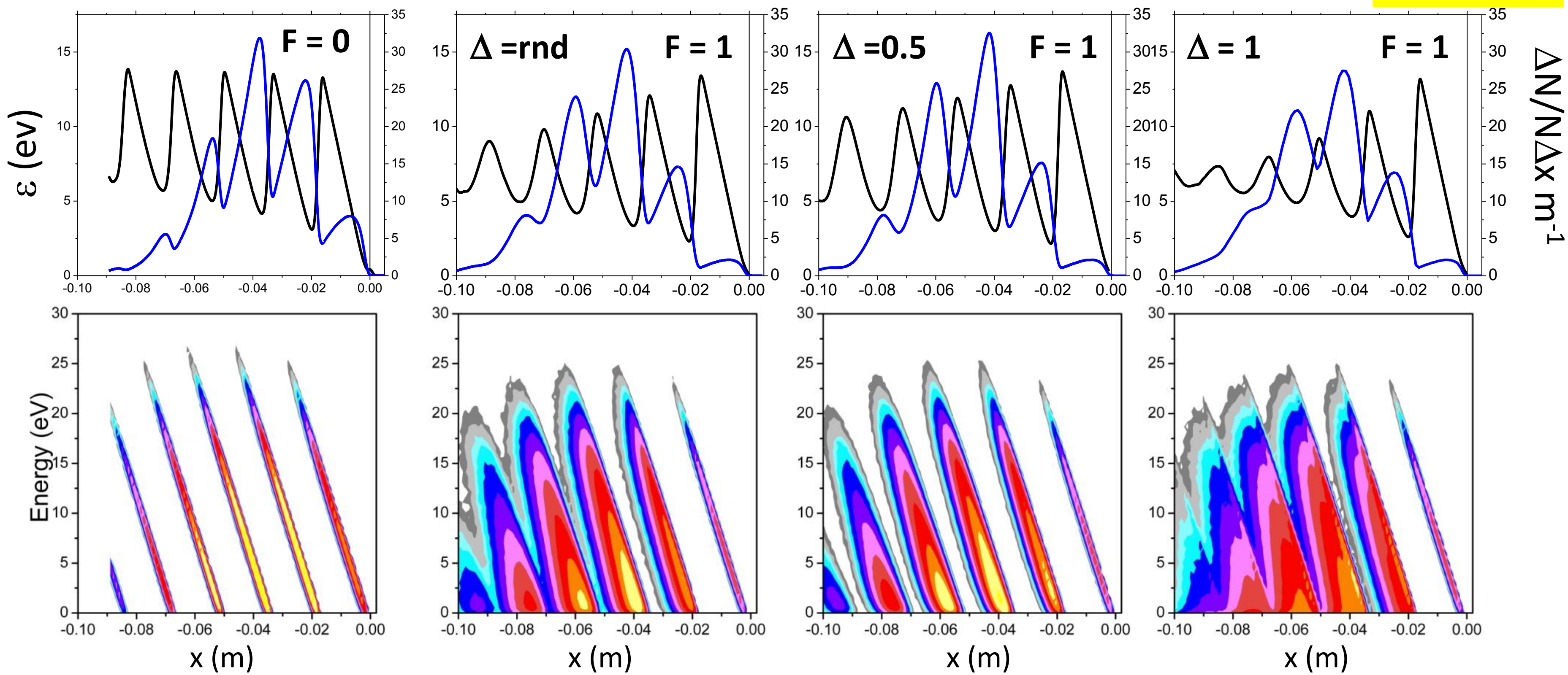
Energy partitioning:

Δ = rnd random

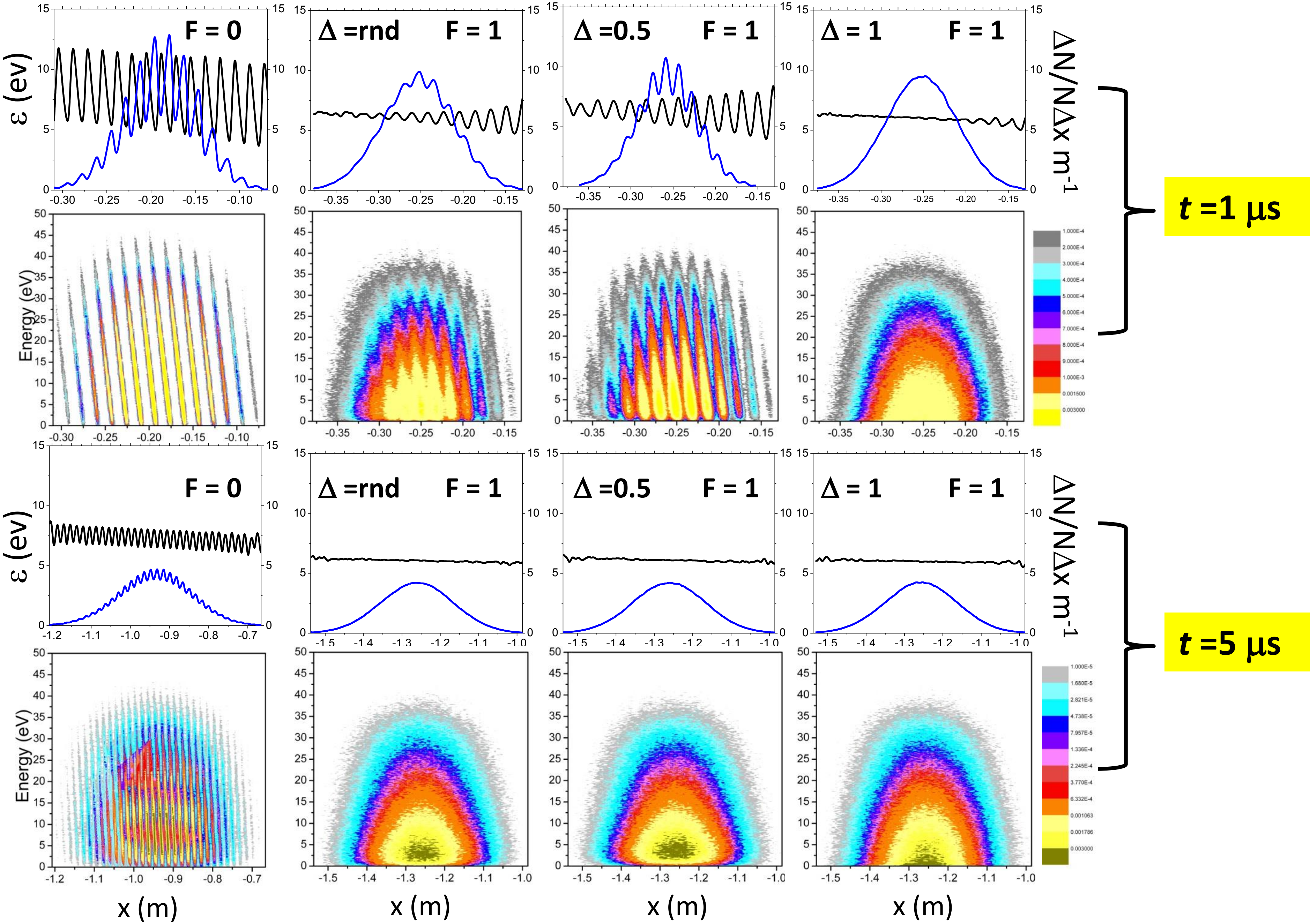
Δ= 0.5 equal

Δ = 1 zero energy progeny

t =0.2 μs



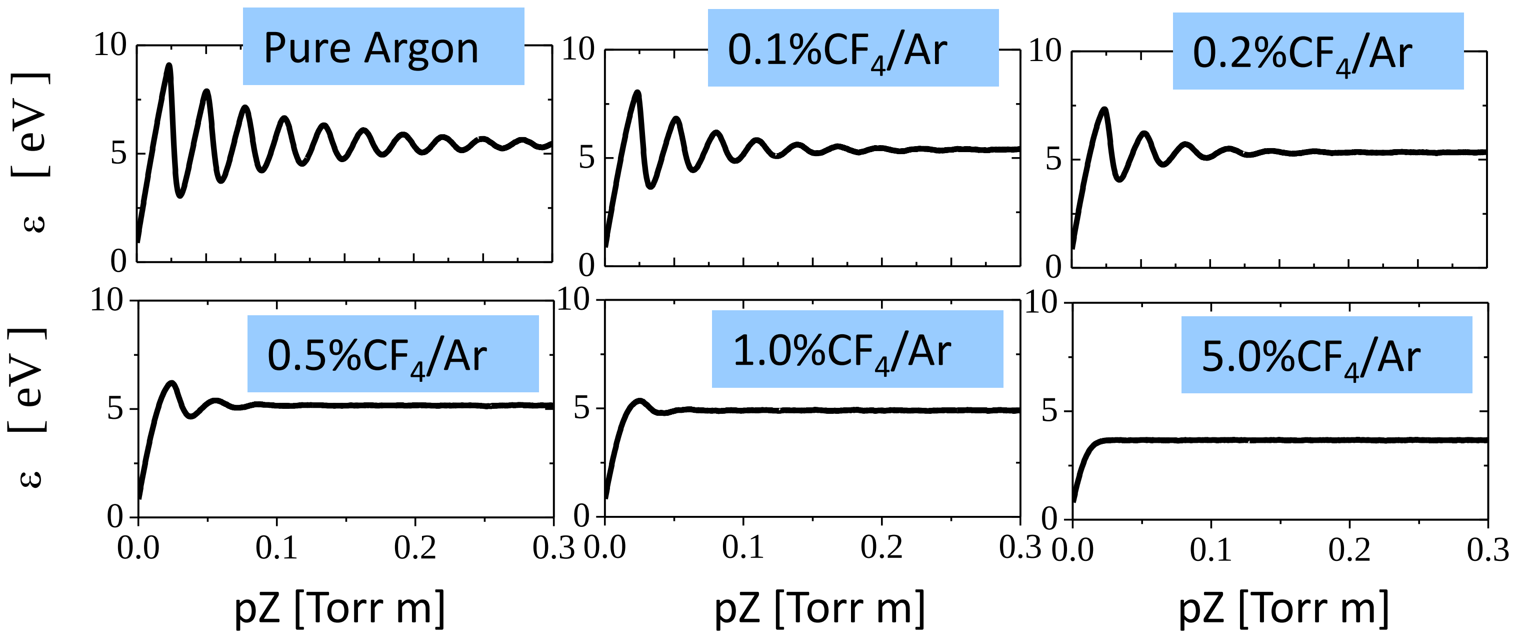
Spatiotemporal development of electron swarms



Non-hydrodynamic conditions: Spatial relaxation of electrons in real gases

- by introducing a small amount of molecular gas admixture, the oscillations are quenched;

- by adding a molecular admixture, the new collisional processes (preferentially vibrational excitation processes in case of CF_4 for E/n_0 of 15 Td) are introduced, and these new inelastic processes are more efficient in damping than elastic collisions;



Dujko et al. **20** (2011) 024013

Boltzmann equation analysis of electron transport in RPCs

Primary motivation:

- Modeling of RPC detectors.

Application:

- Used in high-energy physics experiments for timing and triggering purposes.
- Medical physics and geophysics.

Modeling input requirements:

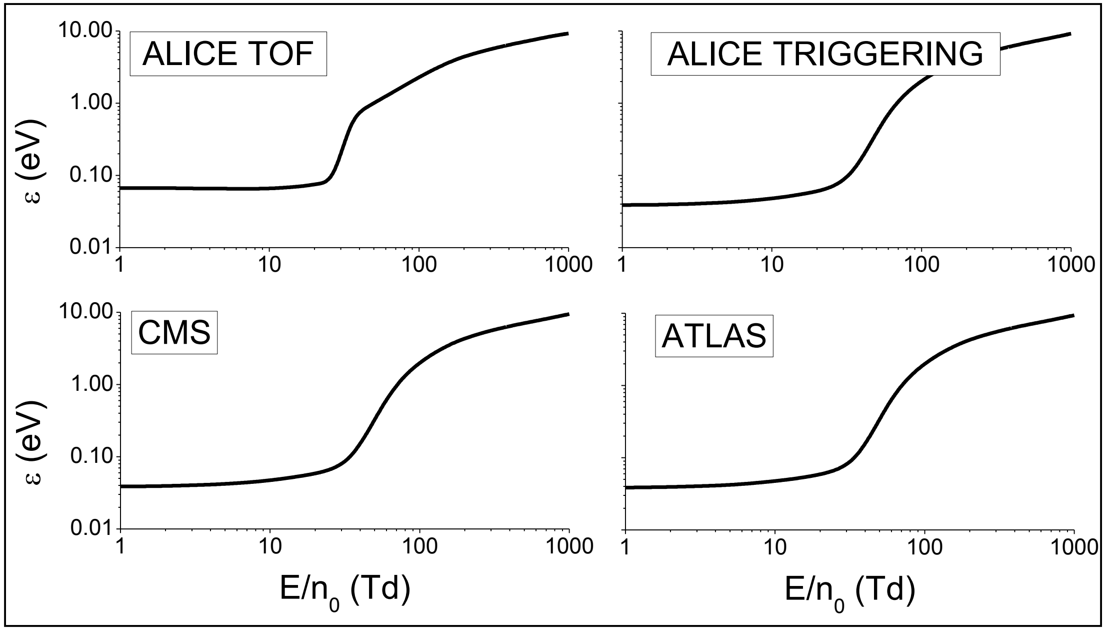
- Rate coefficients, drift velocity and diffusion coefficients as a function of E/n_0.

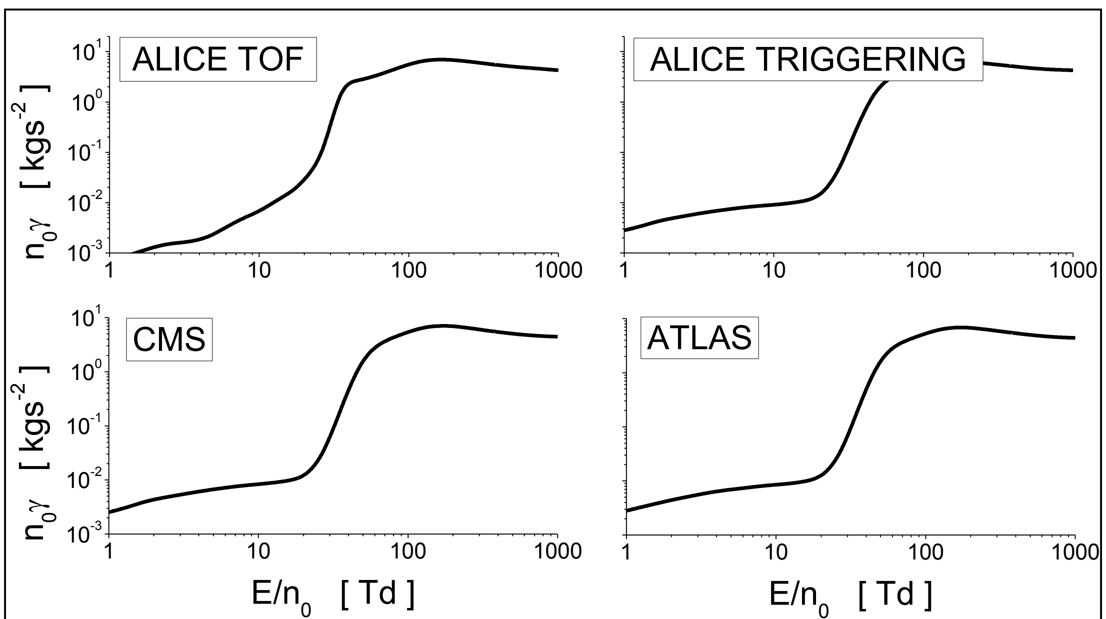
Aims:

- To understand the explicit influence of non-conservative collisions and induced phenomena including transport modification and duality of transport coefficients.
- Correct implementation of data in fluid models.

- **Gas mixtures:**
  $C_2H_2F_4$: iso-C_4H_{10} : SF_6 =
  90 : 5 : 5 (ALICE timing)
  89.7 : 10 : 0.3 (ALICE triggering)
  94.7 : 5 : 0.3 (ATLAS)
  96.2 : 3.5 : 0.3 (CMS)
- Calculations are performed using Boltzmann equation and Monte Carlo technique.

Boltzmann equation analysis of electron transport in RPCs





- Cross sections are reflected in the profiles of the mean energy.
- Variation of the mean energy with E/n_0 for Alice Triggering, CMS and ATLAS RPC systems is almost identical.
- For Alice TOF system the mean energy is higher than thermal energy due to the combined effects of attachment heating and inelastic cooling.
- The gradient expansion of the average energy is given by:

$$\varepsilon(\mathbf{r},t)=\sum_{s=0}^{\infty}\varepsilon_s(-\nabla)^s n(\mathbf{r},t)=\tilde{\varepsilon}+\boldsymbol{\gamma}\cdot\frac{\nabla n}{n}+\ldots$$

Spatially homogenous mean energy

Gradient energy vector

- This quantity illustrates the slope of the average energy along the swarm.

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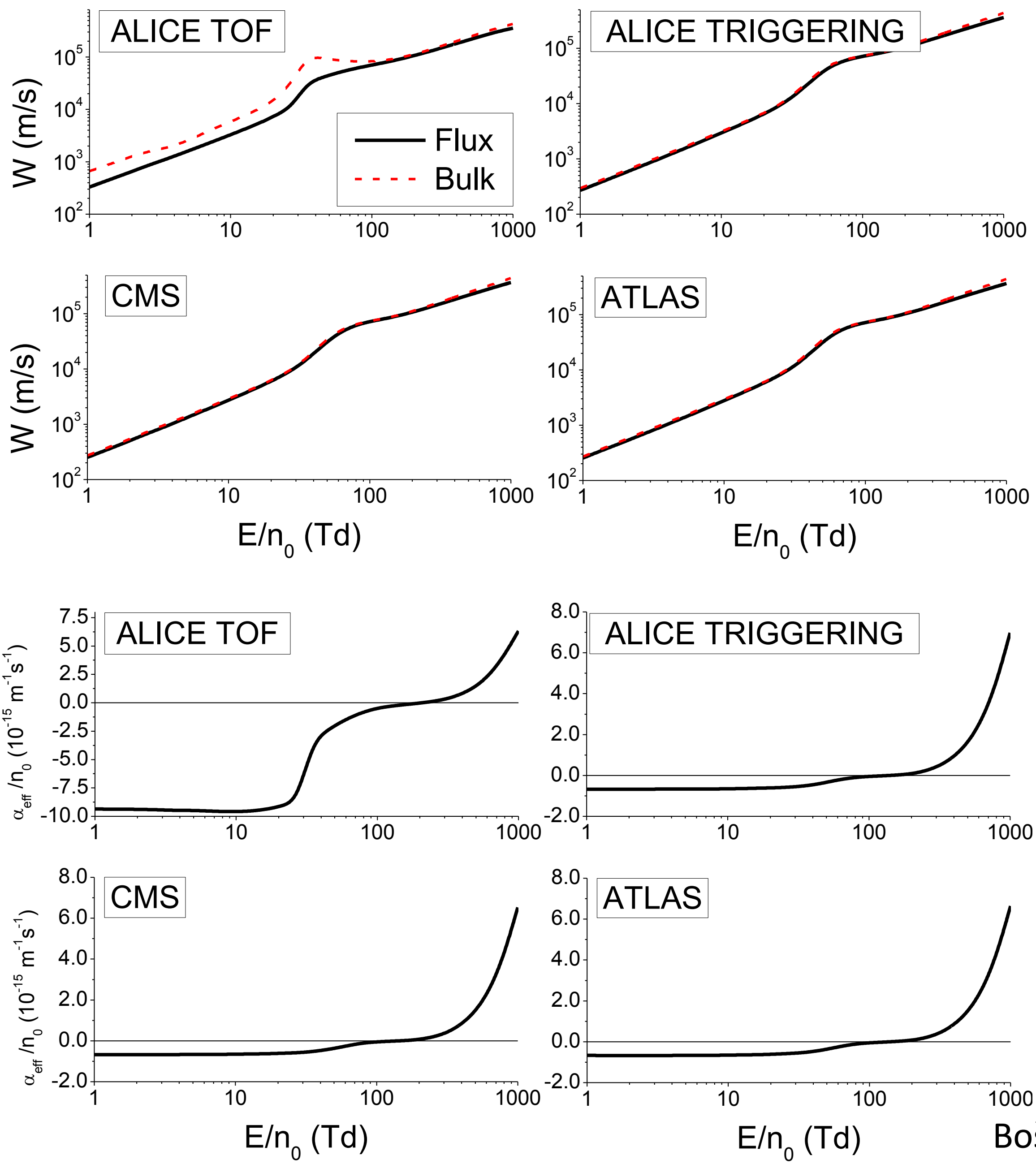
Boltzmann equation analysis of electron transport in RPCs



• In all experiments the bulk component dominates the flux component over the entire E/n_0 range. For lower E/n_0 this follows from the attachment heating while for higher E/n_0 this is a consequence of the explicit effects of ionization on the drift velocity.

• The most striking phenomenon is the existence of negative differential conductivity (NDC) in the bulk drift velocity component with no indication of any NDC for the flux component in the ALICE timing RPC system.

• Variation of the effective ionization coefficients with E/n_0 is almost identical for ALICE triggering, CMS and ATLAS RPC systems due to small variations in the abundances of $C_2H_2F_4$ and iso-C_4H_{10} in the gas mixtures. The critical electric field for these systems is around 140 Td. For Alice TOF the critical electric field is around 215 Td.

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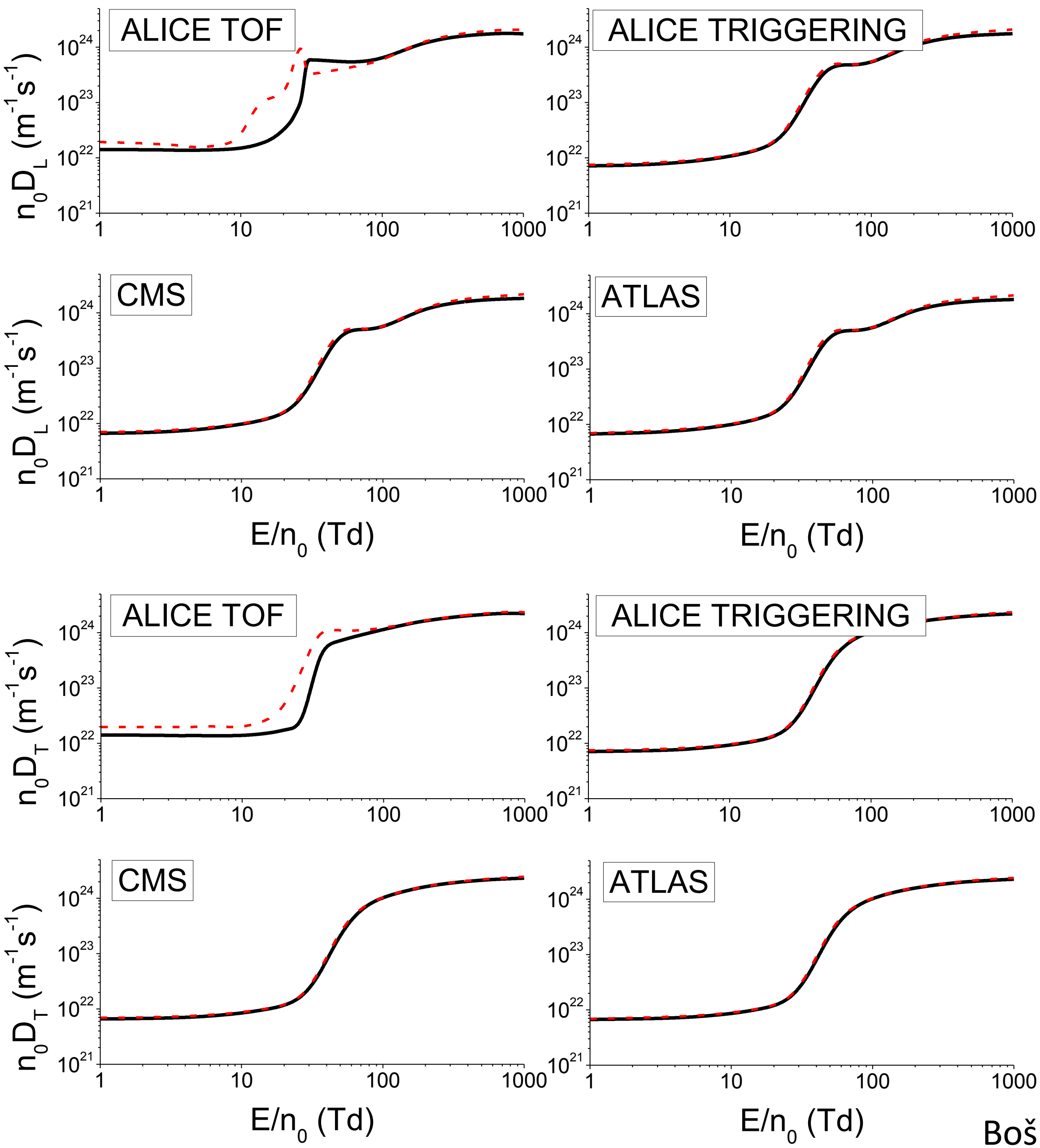
Boltzmann equation analysis of electron transport in RPCs



- For ALICE triggering, CMS and ATLAS RPC systems, the variations of bulk and flux components of ND_L and ND_T with E/N are almost identical. The differences between the bulk and flux are within 20%.

- For ALICE time-of-flight e the bulk and flux components of the diffusion coefficients exhibit qualitatively different behavior.

- To understand diffusion one must consider:
  - thermal anisotropy effect.
  - anisotropy at elevated reduced electric fields.
  - the contribution of non-conservative collisions and the complex energy dependence of electron attachment and ionization.

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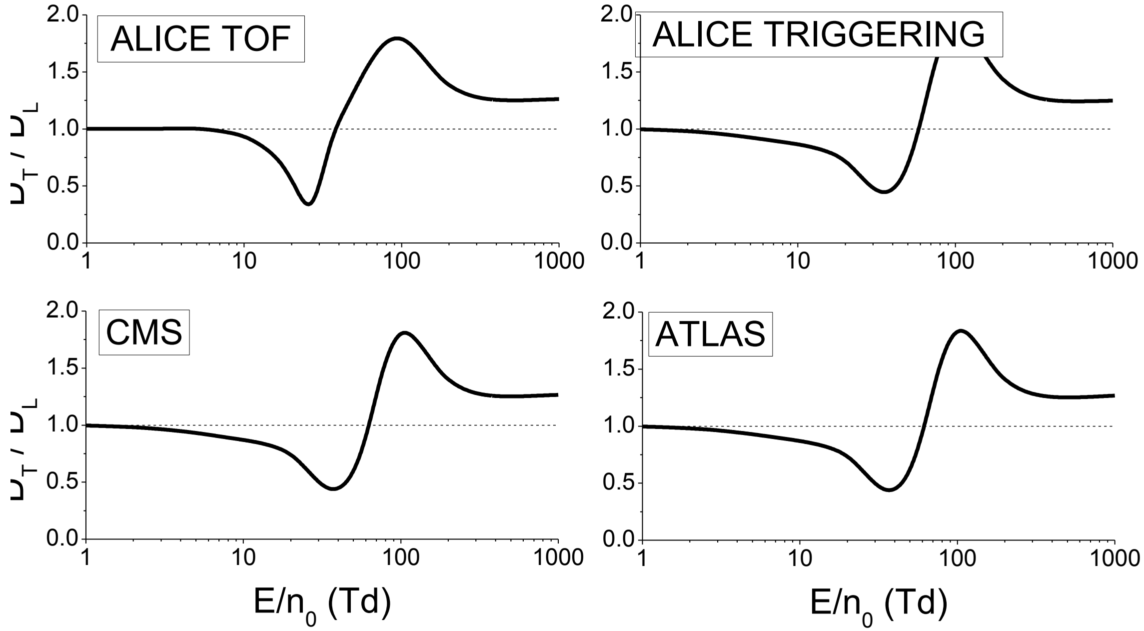
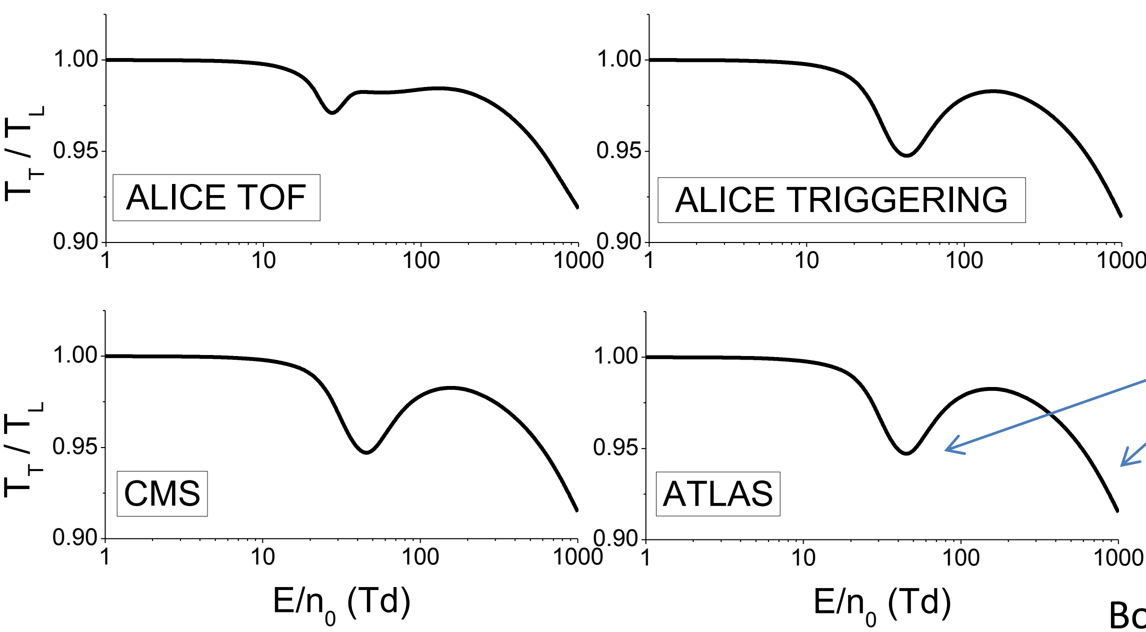
Boltzmann equation analysis of electron transport in RPCs





Anisotropy of the diffusion tensor

- For all RPC systems in the limit of the lowest E/n_0 the diffusion is isotropic.
- For increasing E/n_0 D_T<D_L and then for higher E/n_0 the opposite situation holds: D_T>D_L.
- Comparing to other gases the degree of anisotropy is not high: there is a factor of 2 between the two components.

Anisotropy of the temperature tensor

- The anisotropy in the temperature tensor reflects the anisotropy of the distribution function in velocity space.

E/n_0 regions where the TTA (two-term approximation) for solving the Boltzmann eq. will generally fail.

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Transport of electrons in electric and magnetic fields

- **Primary motivation:**
  - Time-projection chambers

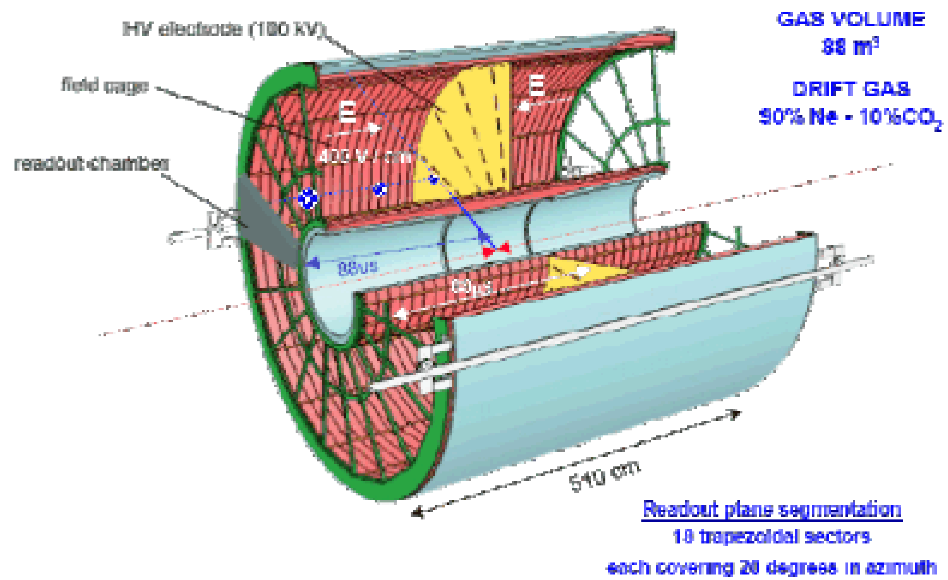
Application:
  - A 3D reconstruction of a particle trajectory.

- **Modeling input requirements:**
  - Transport coefficients
    - Mean energy
    - Drift velocity
    - Diffusion tensor

  - **As a function of:**
    - Reduced electric field
    - Reduced magnetic field
    - Angle between the fields

- **Previous modeling:**
  - Langevin elementary theory
  - Scaled transport coeffciients

ALICE TPC LAYOUT

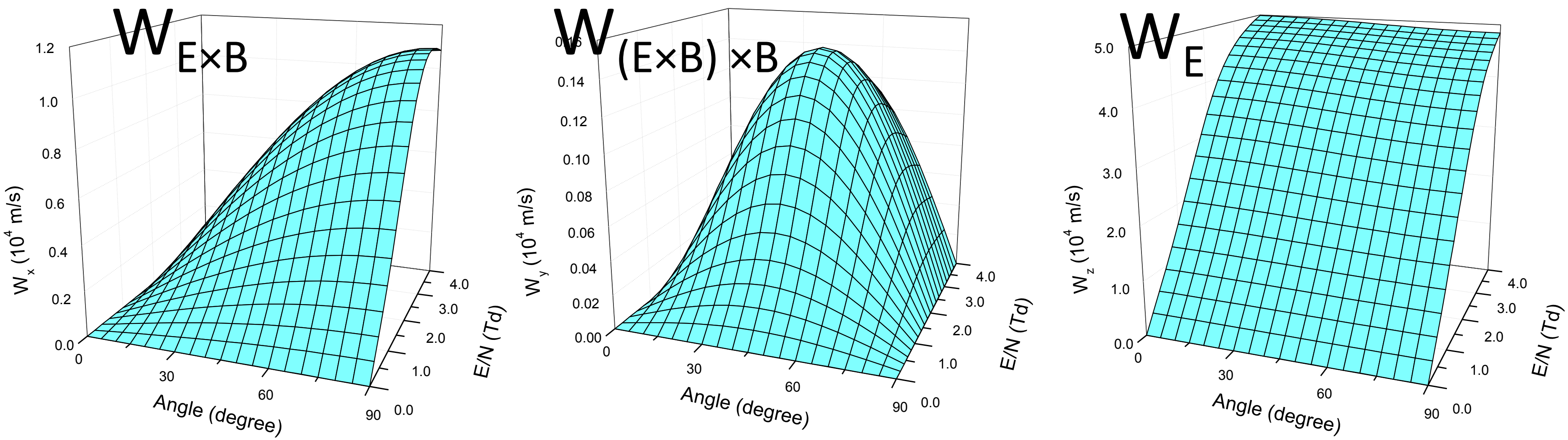


Simulation conditions:
- Gas mixture: 90% Ne +10% CO_2
- T = 293 K and p = 1 atm.
- E/N 0 – 4 Td (0 – 1200 kV/cm).
- B/N 16 – 160 Hx (0.5 – 5 T at p=1 atm).

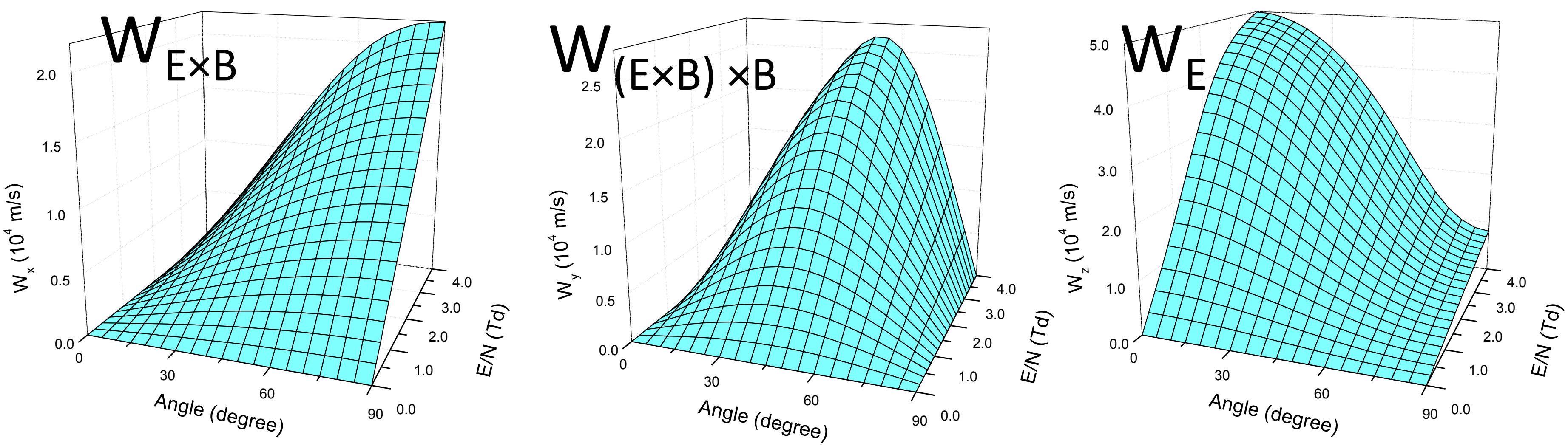
- **Important to consider:**
  - Sensitivity to the ambient temperature.
  - Variations induced by changes of CO_2 amount .
  - influence of magnetic field inhomogeneity.

Transport of electrons in electric and magnetic fields

B/n_0 = 16 Hx (B = 0.5 T and p =1 atm)

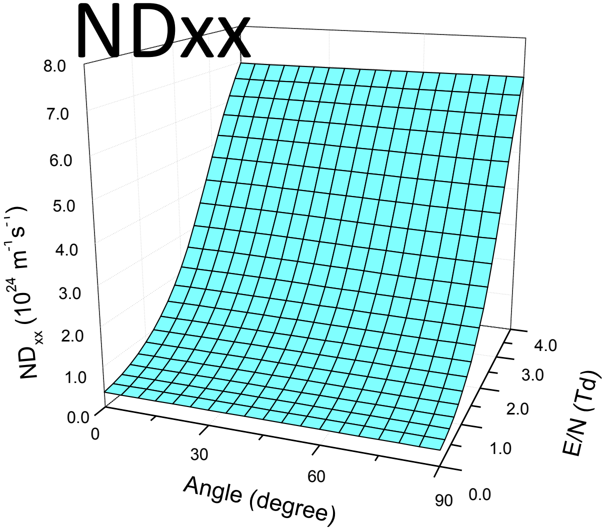


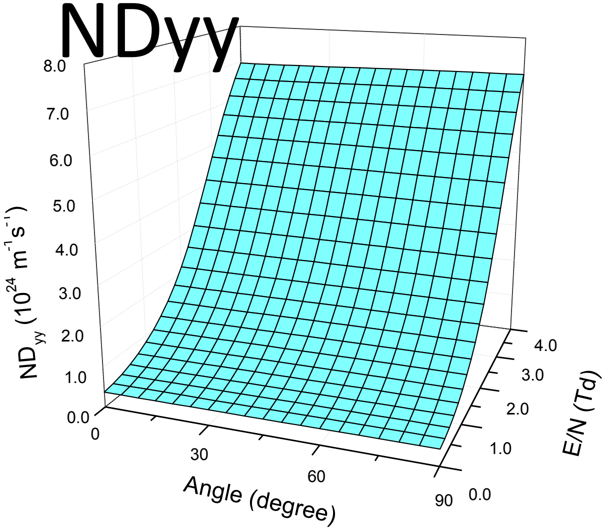
B/n_0 = 160 Hx (B = 5.0 T and p =1 atm)

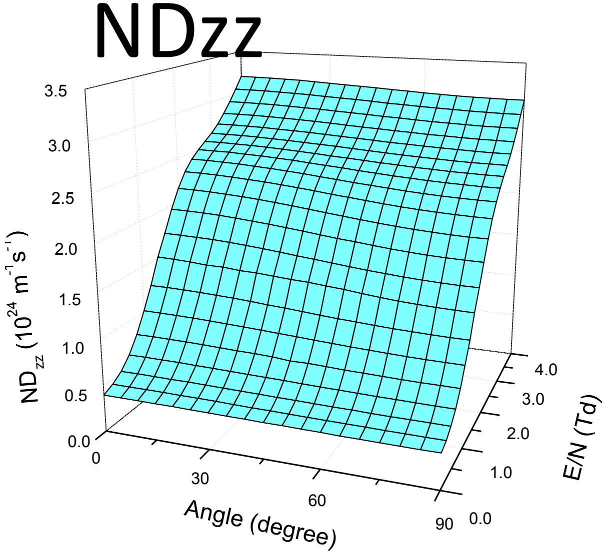


Transport of electrons in electric and magnetic fields

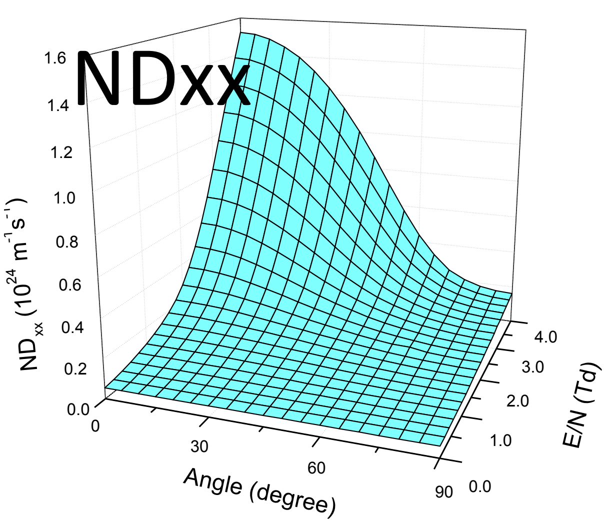
B/n_0 = 16 Hx (B = 0.5 T and p =1 atm)

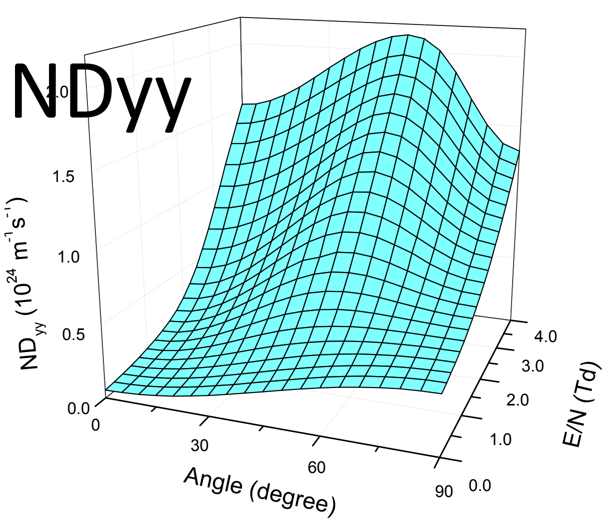


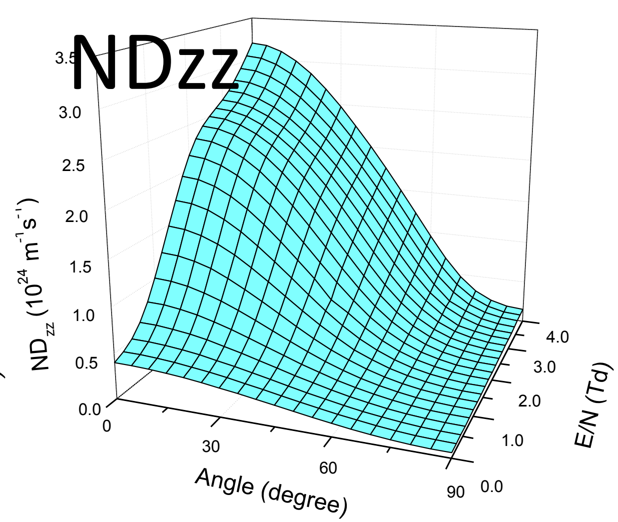




B/n_0 = 160 Hx (B = 5.0 T and p =1 atm)

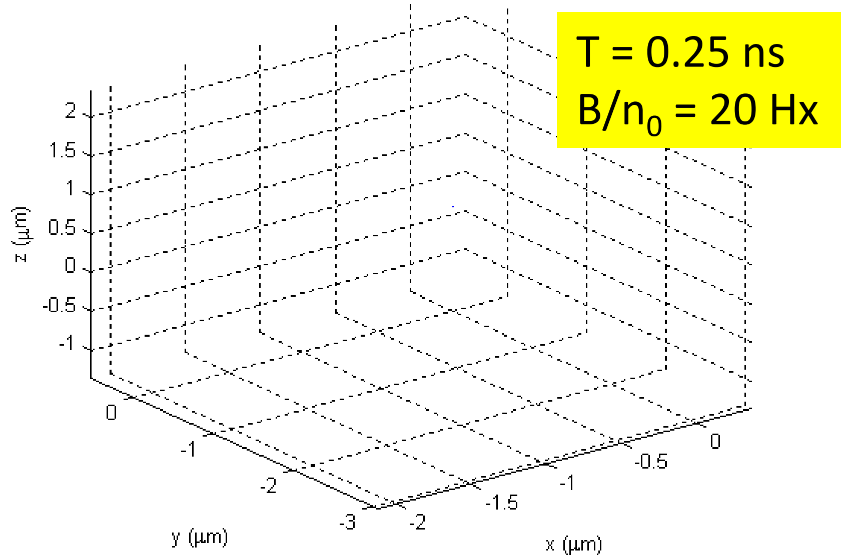






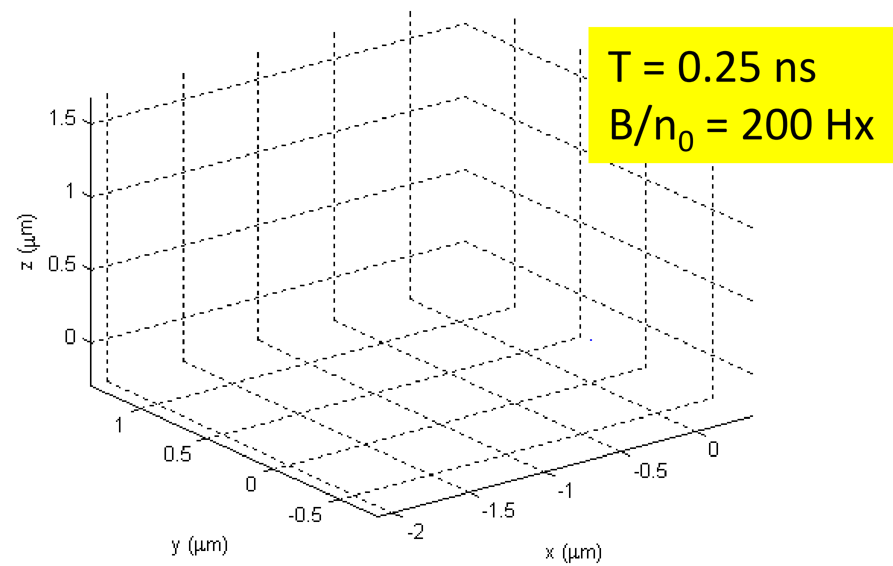
Simulation of an electron path in time projection chambers (TPC)

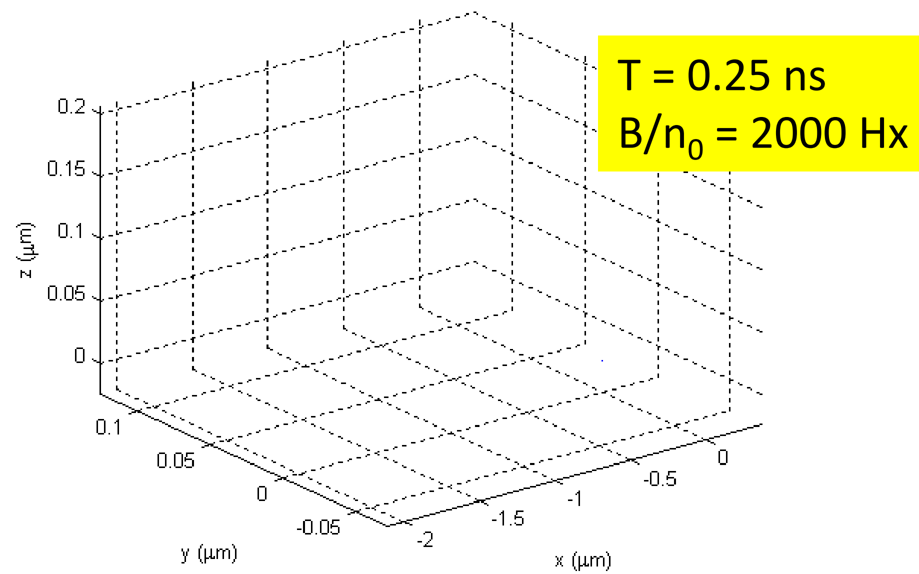
- E/n_0 = 1.6 Td; Ne/CO_2 = 90:10, Parallel field orientation.



- We observe that as the magnetic field strength is increased the fraction of the orbit completed before collision is increased.

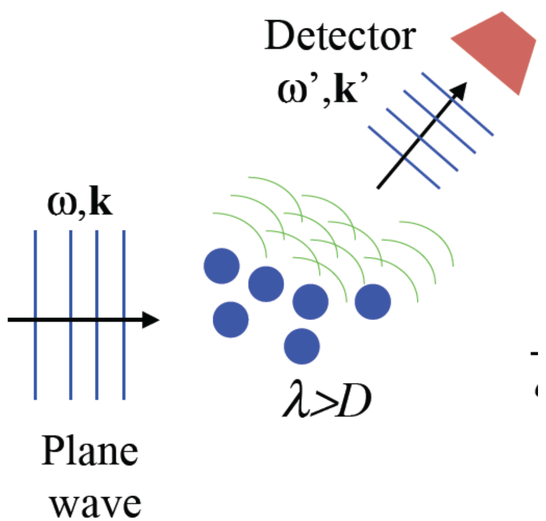
- In the limit of very high magnetic fields the electrons may complete many orbits before collision takes place.





How do we simulate electron transport in liquids?

- **Aim:** Exact transport theory for electrons in liquid noble gases.
- **Applications:** Modeling of Liquid Argon and Liquid Xe TPC for dark matter searches and neutrino detection.



Electrons are coherently scattered by atoms that are correlated to each other.

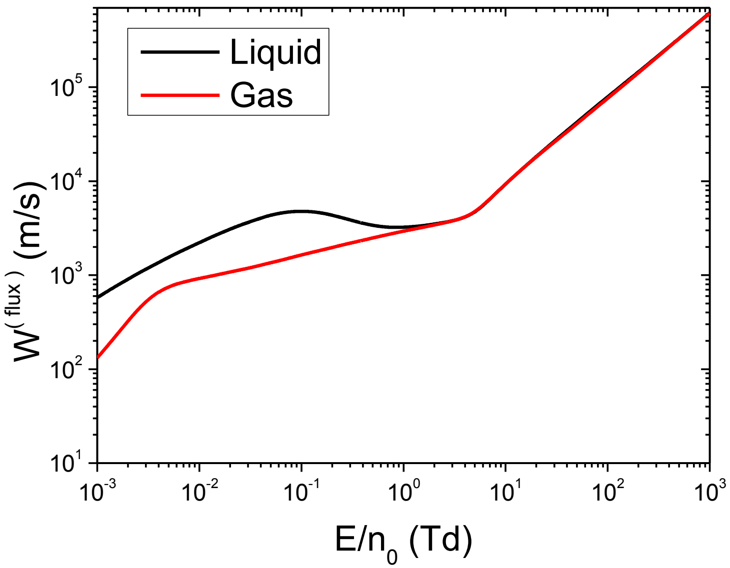
$$\frac{d^2\sigma}{d\Omega_k d\omega'} = S(\Delta\mathbf{k}, \Delta\omega)\left(\frac{d\sigma}{d\mathbf{k}'}\right)$$

Dynamic structure factor (properties of the medium)

Single scattering DCS (properties of interaction)

- **Boltzmann equation** that includes structured/coherent scattering:
  - Collision operator is modified to account for coherent elastic scattering
- **Fluid equations (momentum transfer theory)** that includes structured/coherent scattering:
  - Theory is benchmarked against multi term theory for solving the Boltzmann eq.
  - Wannier energy relation and Generalized Einstein relation for diffusion are developed.
- **Monte Carlo simulations**
  - Monte Carlo code is benchmarked using the Percus-Yevic model.

Electron transport in Argon: Gas and Liquid

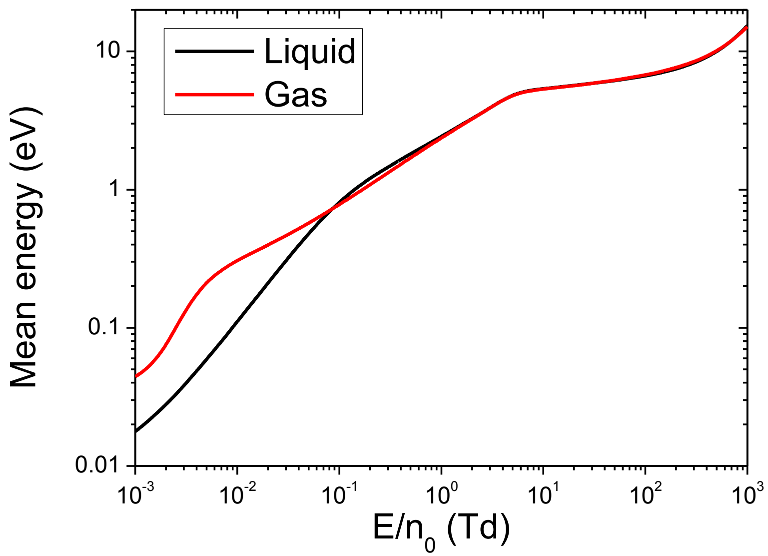


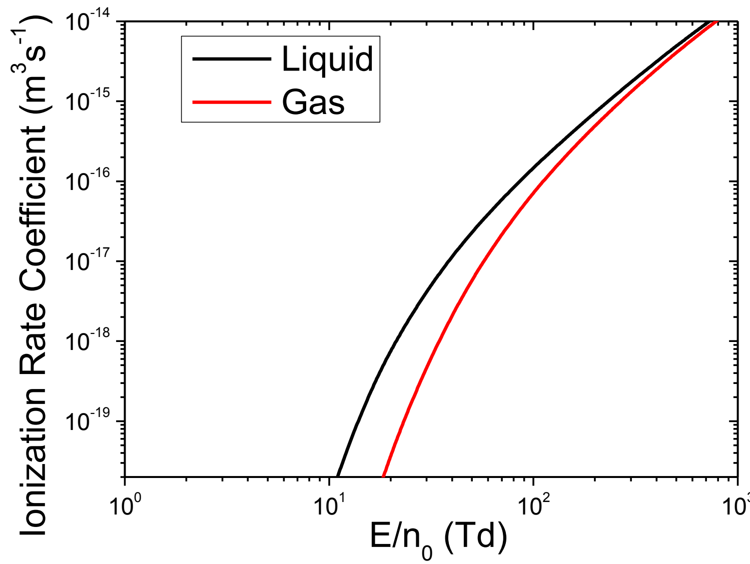
Simulation conditions:
$n_0 = 2.1\times10^{28}m^{-3}$ T = 85K

- For lower E/n_0 drift velocity in liquid Ar is much higher than for the gas phase (the so-called enhanced mobility effect).

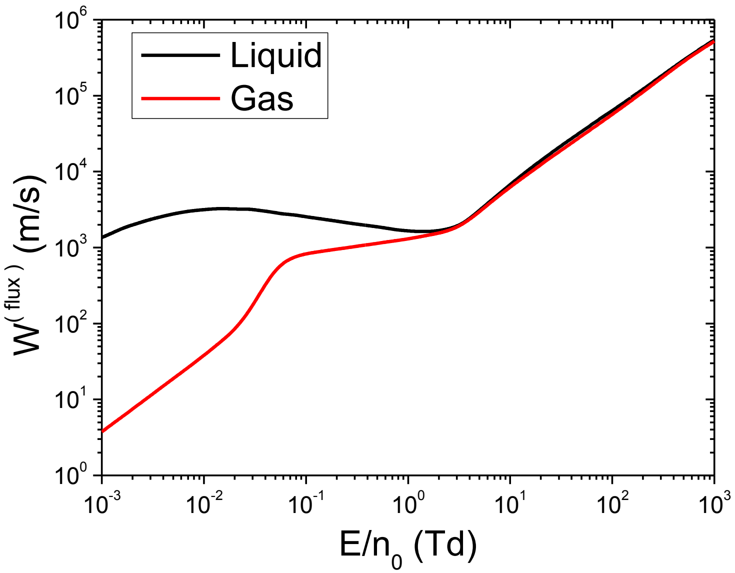
- Structure-induced NDC is clearly evident in the profile of the drift velocity.

- Ionization rate is higher for liquid Ar.



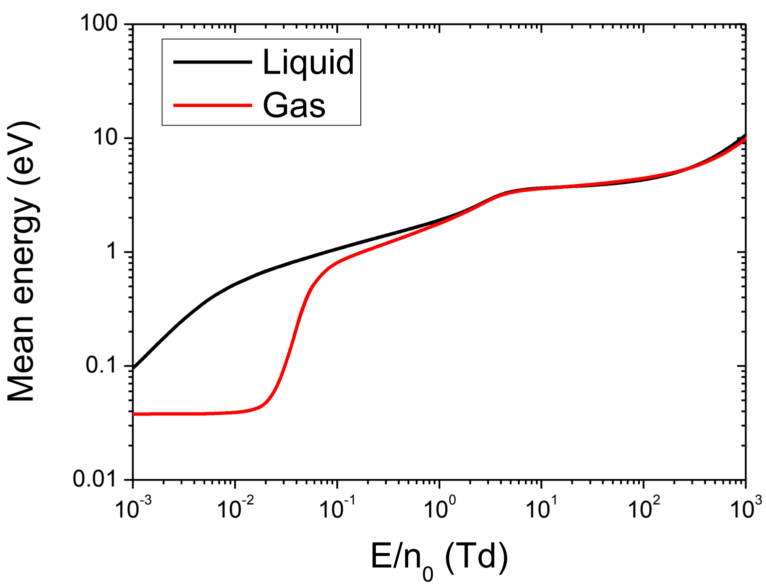


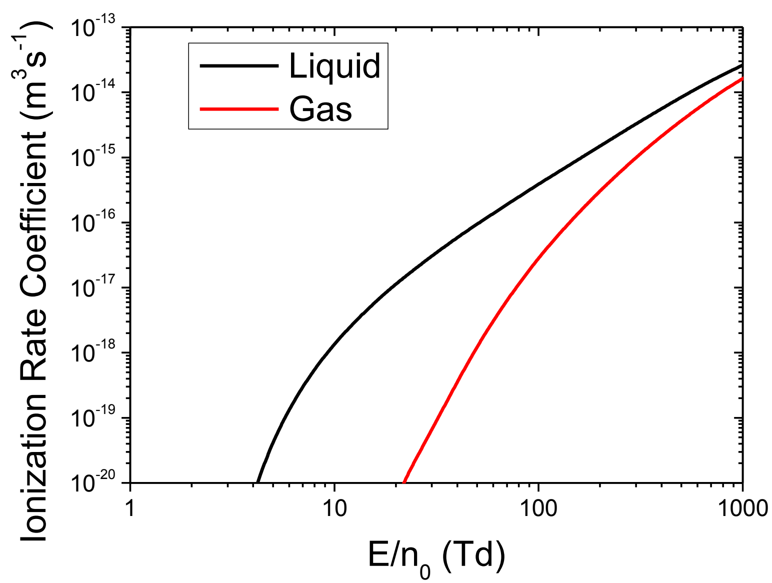
Electron transport in Xenon: Gas and Liquid



Simulation conditions:
$n_0 = 1.4\times10^{28}m^{-3}$ T = 163K

- For lower E/n_0 drift velocity in liquid Xe is much higher than for the gas phase (the so-called enhanced mobility effect).
- Structure-induced NDC is clearly evident in the profile of the drift velocity.
- Ionization rate is higher for liquid Ar.





Development of an electron avalanche and its transition into streamers

• 1D continuity equation for electrons $n_e\,(x,t)$ and ions $n_{p,n}\,(x,t)$

$$\frac{\partial n_e}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial n_e}{\partial x} - w\,n_e\right) + n_e(v_i - v_a)$$

$$\frac{\partial n_p}{\partial t} = n_e v_i \qquad \frac{\partial n_n}{\partial t} = n_e v_a$$

• 2D solution of the Poisson equation where the electric field $E(x,t)$ is calculated along the x-axis, assuming cylindrical distribution of charge with radius R_0 and length d.

$$E(x,t) = \frac{e_0}{2\varepsilon_0}\int_0^d (\mathrm{sgn}(x-x') - \frac{x-x'}{\sqrt{(x-x')^2 + R_0^2}})\,n_e(x',t)\,dx'$$

• Numerical schemes: second-order central finite differences for discretization of spatial derivatives and classical fourth-order Runge–Kutta 4 scheme for integration in time.

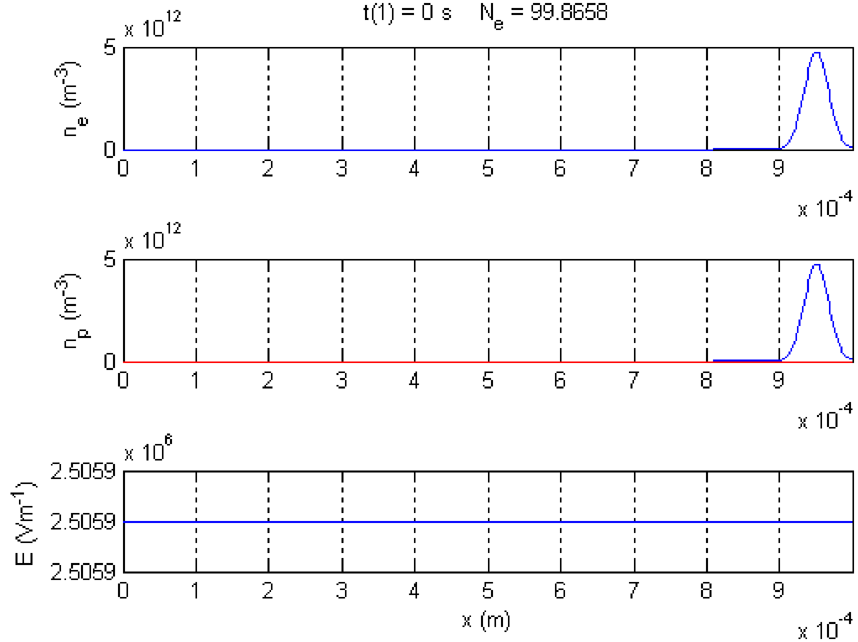
• Initial and boundary conditions:

$$n_e(x=0,t) = n_e(x=d,t) = 0$$

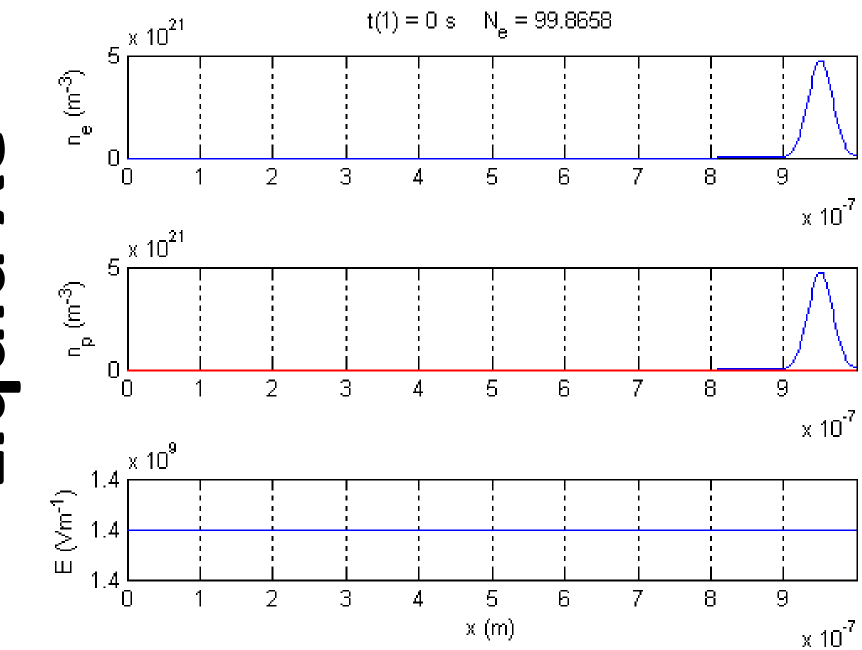
$$n_e(x,t=0) = n_p(x,t=0) = \frac{N_{e0}}{\sigma_0 R_0^2 \pi^{3/2}\sqrt{2}}\exp\left(-\frac{(x-x_0)^2}{2\sigma_0^2}\right)$$

$$n_n(x,t=0) = 0$$

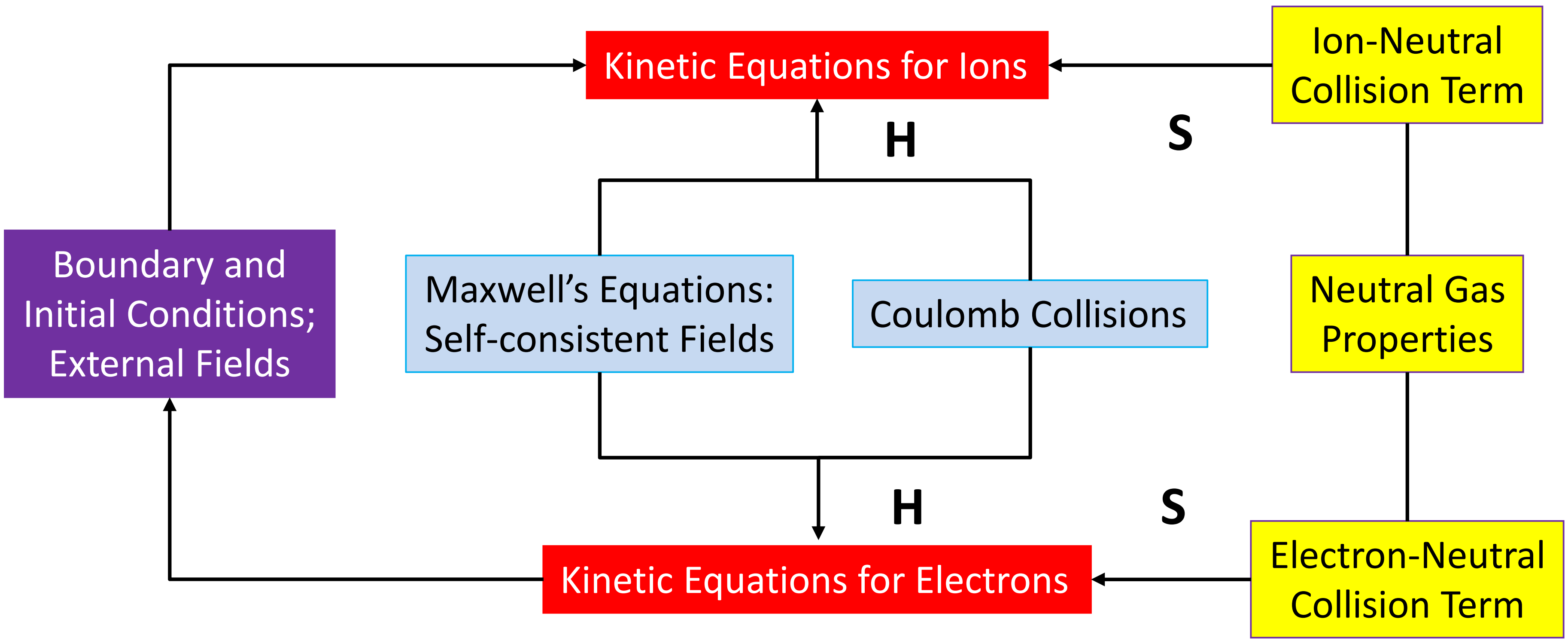
Gaseous Xe



Liquid Xe



Kinetic and fluid models of avalanches and discharges – Big picture



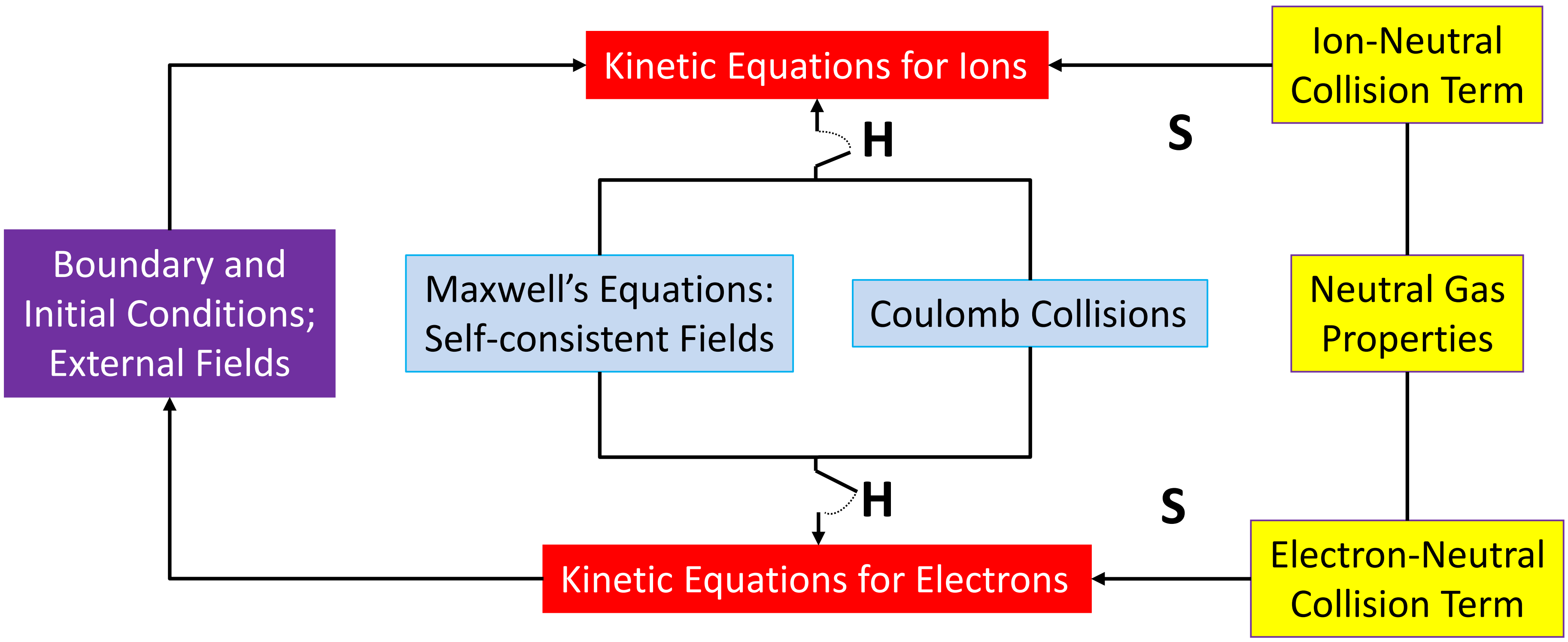
General problem of kinetic theory for detectors where discharges take place (switches H and S closed)

$$\frac{\partial f_i}{\partial t} + \mathbf{c}\cdot\frac{\partial f_i}{\partial \mathbf{r}} + \frac{q_i}{m_i}\left(\mathbf{E} + \mathbf{c}\times\mathbf{B}\right)\cdot\frac{\partial f_i}{\partial \mathbf{c}} = -J\left(f_i, F_0\right) - \sum_{i'} J\left(f_i, f_{i'}\right)$$

+ Maxwell's equation

+ Boundary and Initial Conditions

Kinetic and fluid models of avalanches and discharges – Big picture



General problem of swarm kinetic theory (switches H open, switches S closed)

$$\frac{\partial f_i}{\partial t} + \mathbf{c} \cdot \frac{\partial f_i}{\partial \mathbf{r}} + \frac{q_i}{m_i}\left(\mathbf{E} + \mathbf{c} \times \mathbf{B}\right) \cdot \frac{\partial f_i}{\partial \mathbf{c}} = -J\left(f_i, F_0\right)$$

Swarm limit:
provision of benchmarks for discharges in particle detectors in the free diffusion limit!

Fluid models of avalanches and discharges in the gaseous particle detectors

1. Classical or first-order fluid model

$$\frac{\partial n}{\partial t} = \nabla \cdot (\mu n \mathbf{E} + \mathbf{D} \cdot \nabla n) + n(\nu_I - \nu_A)$$

$$\frac{\partial n_p}{\partial t} = n\nu_I, \quad \frac{\partial n_n}{\partial t} = n\nu_A$$

$$\nabla^2 \phi = \frac{e}{\varepsilon_0}(n - n_p - n_n), \quad \mathbf{E} = -\nabla\phi$$

- Developed on purely phenomenological grounds.
- Requires the knowledge of the FLUX transport coefficients as a function of local electric field.
- Stochastic and undirected motion is included in an ad hoc manner through the diffusion term.

2. First – order model based on the hydrodynamic approximation

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{W}_F n - \mathbf{D}_F \cdot \nabla n) = S^{(0)} n - \mathbf{S}^{(1)} \cdot \nabla n + \mathbf{S}^{(2)} : \nabla\nabla n$$

or equivalently:

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{W}_B n - \mathbf{D}_B \cdot \nabla n) = S^{(0)} n - \nabla \mathbf{S}^{(1)} n + \nabla \mathbf{S}^{(2)} \nabla n$$

- Developed assuming hydrodynamic approximation.
- Requires the knowledge of the FLUX/BULK transport coefficients and corrections $S^{(k)}$ of the source terms as a function of local electric field.
- The contributions of electron attachment and ionization must be separated.
- Eqs. are closed in local field approximation.

Fluid models of avalanches and discharges in the gaseous particle detectors

3. High-order fluid model

$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{v} = -n\left(\tilde{\nu}_A - \tilde{\nu}_I\right)$$

$$\frac{\partial}{\partial t}(n\mathbf{v}) + \frac{2}{3m}\nabla(n\varepsilon) - n\frac{e}{m}\mathbf{E} = -n\mathbf{v}\left(\tilde{\nu}_m + \tilde{\nu}_I + \frac{2}{3m}\varepsilon\tilde{\nu}_A{}'\right)$$

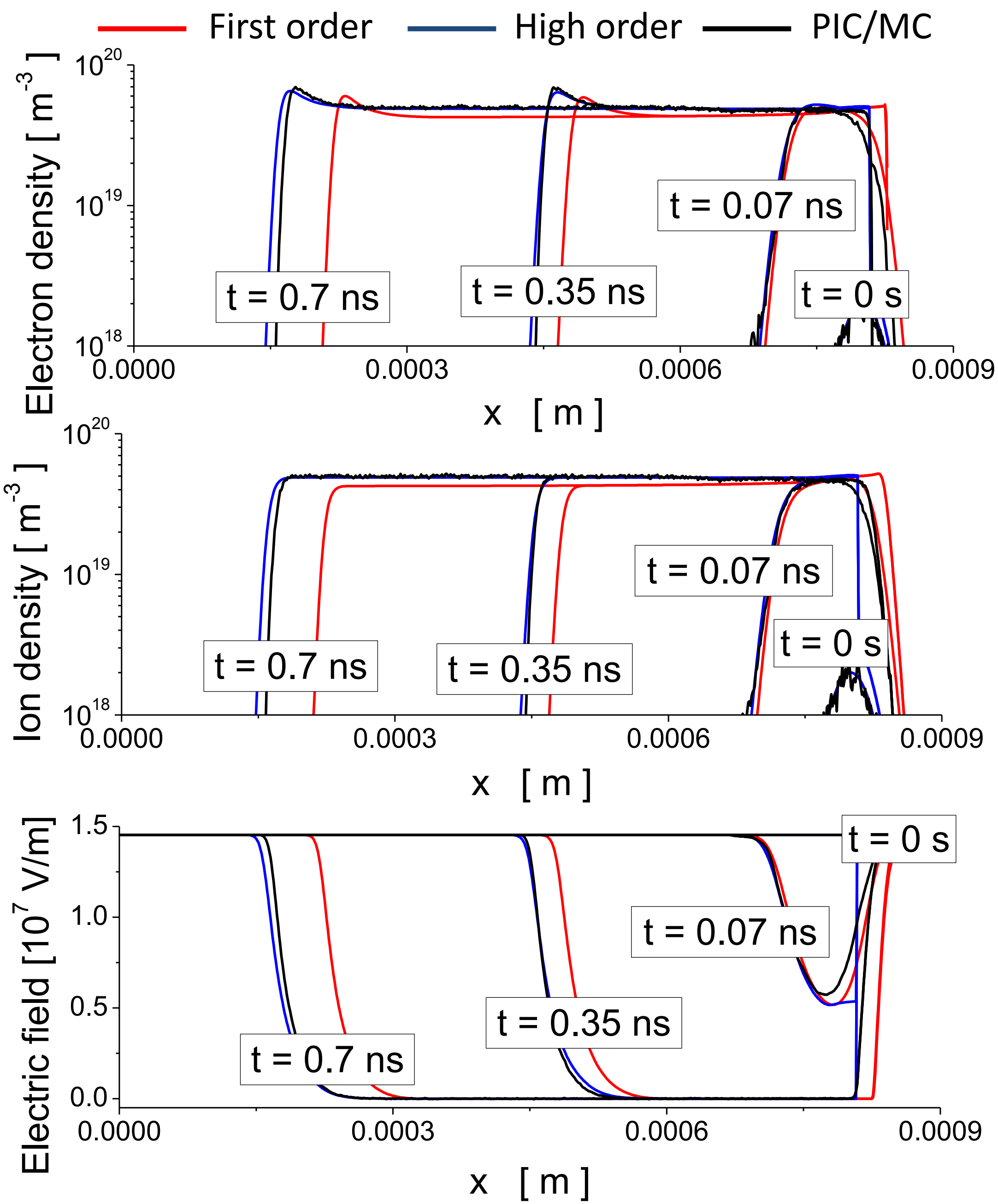
$$\frac{\partial}{\partial t}(n\varepsilon) + \nabla \cdot (n\boldsymbol{\xi}) - e\mathbf{E}\cdot(n\mathbf{v}) = -n\tilde{\nu}_e\left(\varepsilon - \frac{3}{2}kT_0\right) - n\sum_i\left(\tilde{\nu}_i - \tilde{\nu}_i^s\right)\varepsilon_i - n\varepsilon\tilde{\nu}_A - n\sum_i \tilde{\nu}_i^{(i)}\Delta\varepsilon_i^{(i)}$$

$$\frac{\partial}{\partial t}(n\boldsymbol{\xi}) + \nabla\left(\beta\frac{2n}{3m}\varepsilon^2\right) - \frac{5}{3}n\varepsilon e\mathbf{E} = -\tilde{\nu}_m(n\boldsymbol{\xi})$$

- Fluid eqs. are developed as velocity moment of the BE.
- Requires the knowledge of the collision frequencies for transfer of momentum, energy as well as for attachment and ionization.
- Eqs. are closed in the local mean energy approximations.

4. Fluid equations based on a two term theory for solving the BE and many others …

High order fluid model for streamer discharges: 1D models in pure N_2



Transition of an electron avalanche into a streamer

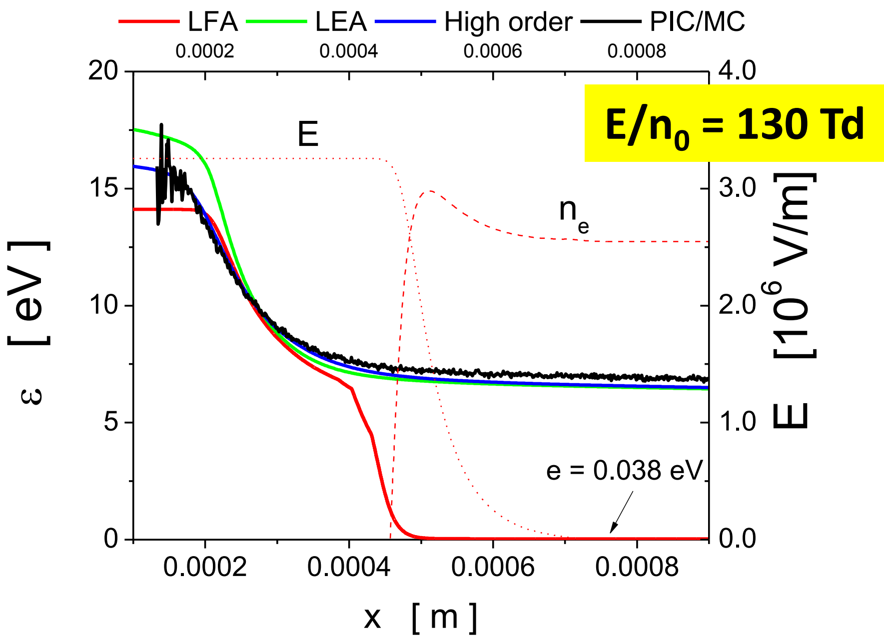
- The initial Gaussian grows due to the ionization processes;

- Electrons are more mobile than ions and charge separation process occurs and initial spatially homogeneous **E** field is distorted;

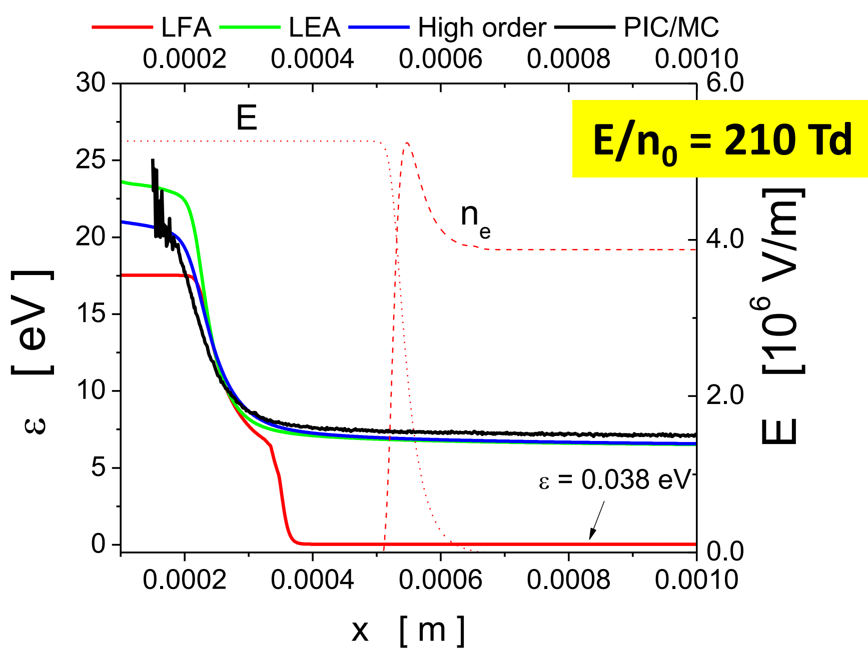
- When the screening of the field is almost complete, the ionization stops in the ionized region;

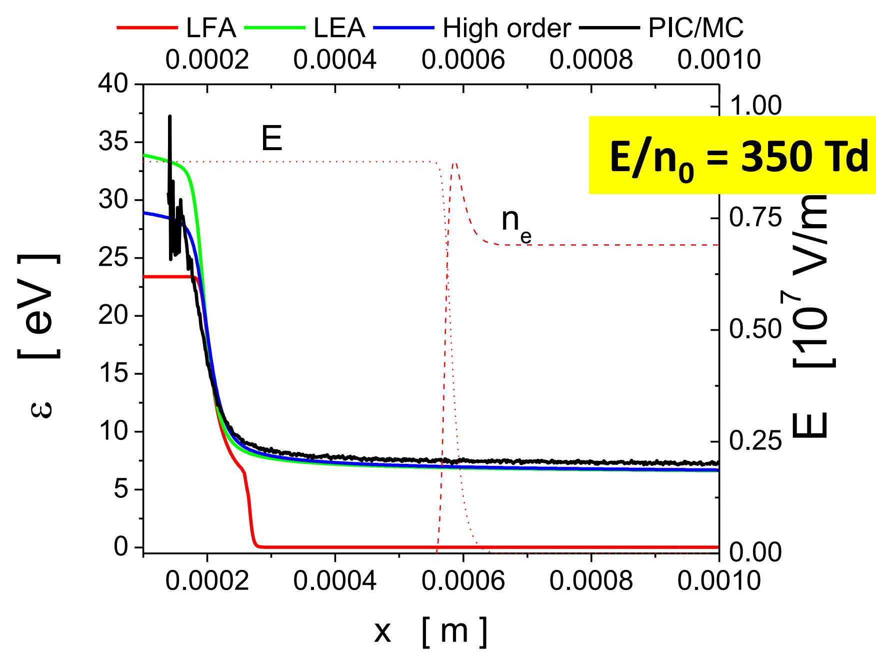
- Typical profiles of the electron density and electric field of a streamer are established.

High order fluid model for streamer discharges: 1D models in pure Ne



- Non-local effects in the profile of the average energy in the streamer interior are clearly evident!
- Surprisingly good agreement between our high order and LEA model!
- In the highly non-equilibrium region ahead of the streamer front there is an excellent agreement between our high order fluid model and PIC-MC!

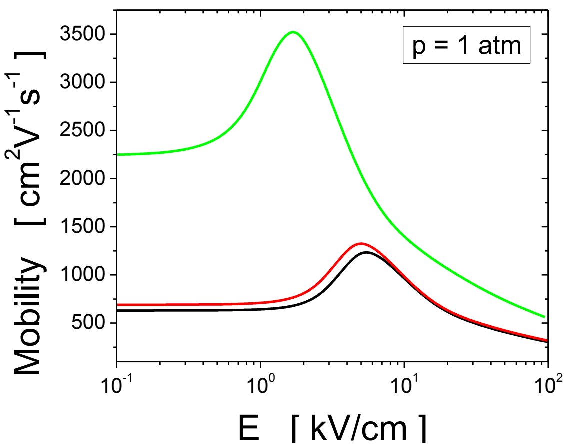


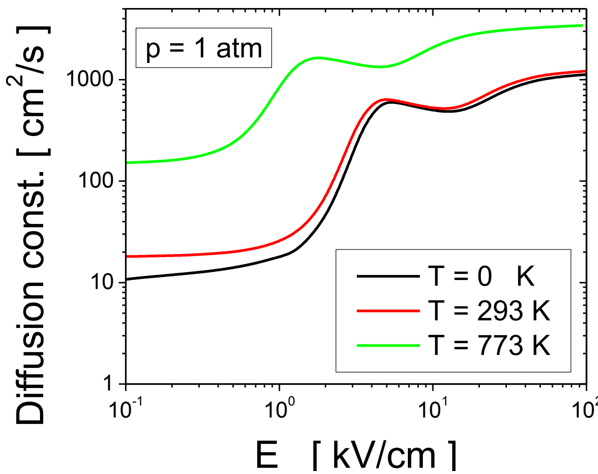


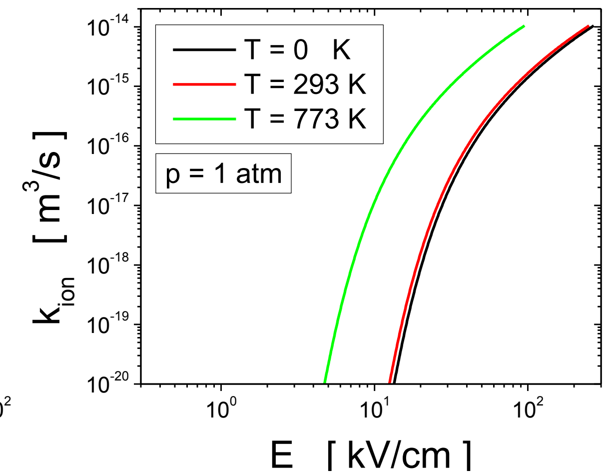
Simulations of positive streamers in the mixtures of CO_2 and N_2

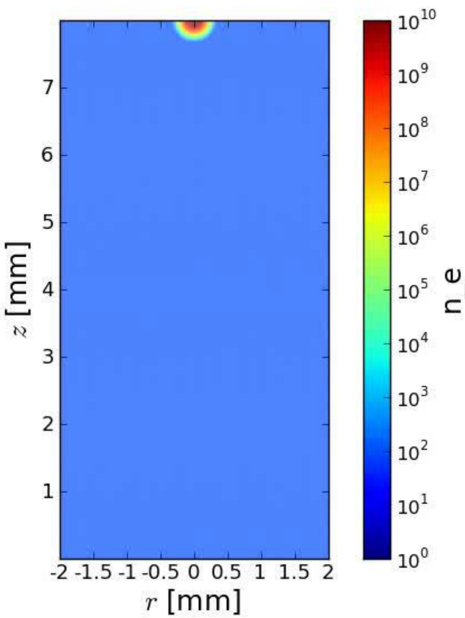
We have simulated positive streamers in the mixtures of CO_2/N_2=95%/5%.

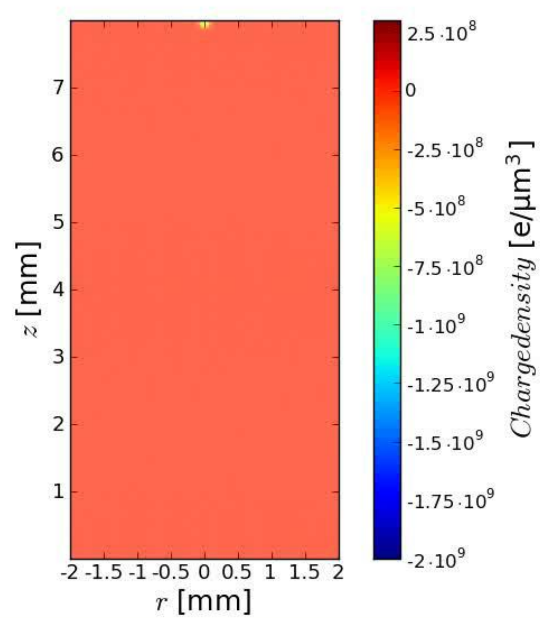
Simulation conditions: plane-to-plane geometry, 8mm gap with 24 kV/cm, p = 1 atm, no photo-ionization .

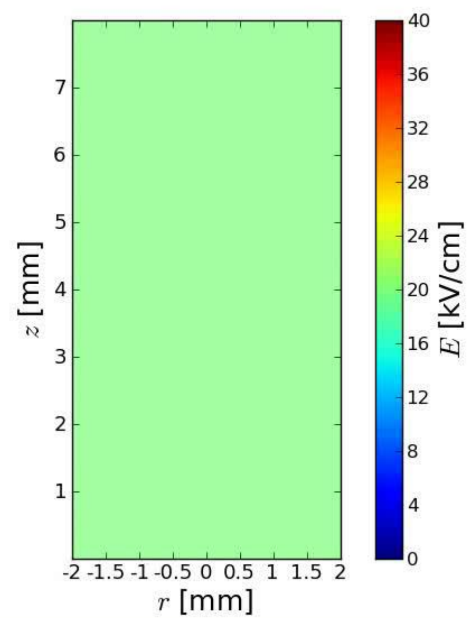












Concluding remarks

• There is a big overlap between transport theory of swarms and modeling of particle detectors.

• However, there is a big gap between swarm and particle detector literature.

• What need to be done to overcome this gap?

Swarm physics has a lot to offer to the particle detector community in its quest for accuracy.

- Only normalized set of cross sections can be used in modeling.
- Care must be taken about the nature of transport data to be used in modeling.
- Care must be taken about the existing symmetry properties of the EDF in velocity space and how to solve the Boltzmann equation.
- When electron transport is greatly affected by attachment care must be taken how to compensate electrons in MC simulations.
- High-order transport coefficients are required for conversion of experimental to rigorously defined bulk and flux data. They can be negative!
- Care must be taken how to derive, truncate and close the system of fluid equations. Correct implementation of transport data and cross sections for charged particle scattering is also important part of modeling.