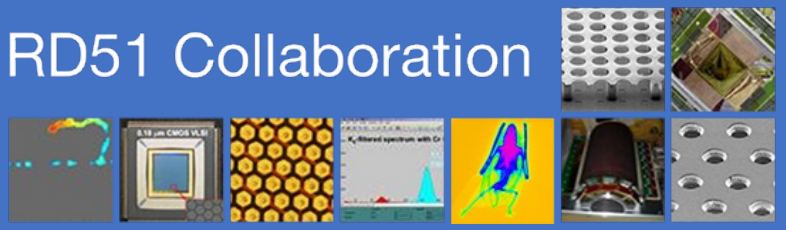
RD51 Collaboration



WG4

Modelling of Physics Processes and Software Tools

Rob Veenhof, Ozkan Sahin, Heinrich, Piet Verwilligen

RD-51 Mini Week, February 27th 2023

Discussion on future of Simulations & SW Development

DRD1 Community meeting on March 1-3
1h time-slot to discuss possible common software developments (Wires, TPC, RPC, MPGD)
We would like to start the discussion already today

I have asked to a selection of colleagues to make a set of slides
concerning future developments or future directions in Software & Simulation
3-4 slides for a 5' presentation, with 5' for discussion and questions

- Future Garfield++ developments - *Heinrich Schindler*
- NeBEM & COMSOL possibilities - *Supratik Mukhopadhyay*
- Simulation of Resistive Elements - *Djunes Janssens*
- Discharge modeling and simulation - *Piotr Gasik*
- Ion Drift, Ion Clustering and Penning - *Ozkan Sahin*
- Simulation of negative Ions in Garfield++ - *Elisabetta Baracchini*
- Fast simulation for MPGDs - *Riccardo Farinelli*
- Scintillation simulation in Garfield++ - *Diego Gonzalez Diaz*
- Charge recombination modelling - *Faustino Gomez*

Primary ionisation

Heed

- Based on (an extended version of) the PAI model.
- Widely used for simulating ionisation by fast charged particles.
- A feature that is currently missing is the simulation of multiple scattering.
- Other potential refinements include
  - using molecular instead of atomic photoabsorption cross-sections,
  - implementing a more detailed simulation of atomic relaxation.

Degrade

- Degrade (S. Biagi) simulates ionisation by electrons, using the same set of cross-sections as Magboltz.
- Interface to Garfield++ to be developed.
- One could also use the cross-sections available in Degrade and port the Monte Carlo simulation to C++.

Other projectiles

- For simulating heavy ions, interfaces to SRIM/TRIM are available but have limitations. Are there alternative packages with a similar scope?
- Additional examples for interfacing Geant4 and Garfield++ and/or wrappers could also be useful.

Electric fields

Field maps

- MPGD simulations typically use field maps exported from FEM solvers (Ansys, Comsol, Elmer, ...).
- If needed, similar interfaces to other solvers (*e. g.* Maxwell) and support for additional element types could be implemented.
- Interpolation in the field map is usually a significant contributor to the CPU time of a simulation program. Could profit from performance optimization.
- For iterative calculations, a direct interface with a field solver would be very useful.
- Is there interest in magnetic field maps?

Wire chambers

- Some features available in "classic" Garfield like the `SET` instruction in the `&OPTIMISE` section have not been ported yet.
- Computation of wire sag, multipole terms have been translated but should be validated/tested more extensively.

Electron avalanches

- Microscopic[a] tracking (Monte Carlo simulation based on electron-atom/molecule cross-sections à la MAGBOLTZ) has become standard for MPGDs.
  - The method used in `AvalancheMicroscopic` corresponds to the one in MAGBOLTZ with background gas motion switched off.
  - For some cases (*e. g.* low pressure), the stepping algorithm might need to be improved.
- Easy to use and important for simulating stochastic effects, but can become slow when dealing with high gain and/or large distances.
- Could profit from code optimisation to better exploit modern CPUs or GPUs and clever ideas for dealing with large avalanche sizes (super particles, transition to hydrodynamic methods, . . .).
- We usually assume that the electrons (and ions) move in a static field, independently from each other. Simulation of scenarios where that assumption is not valid (space charge, recombination, . . .) is currently not (at all) straightforward.

[a] As opposed to calculating the average drift path based on macroscopic transport coefficients.

Charge transport

Excitation transfer

- At present, Penning effects are simulated based on effective transfer probabilities determined from fits to measured gain curves.
- In principle, Penning transfer could also be simulated microscopically. This requires however a wealth of input data:
  - radiative transition rates, lineshapes, photoabsorption cross-sections and ionization yields,
  - rate constants and ionization yields for collisional quenching, ...
- These sets of data are also needed for a microscopic modelling of electroluminescence (*e. g.* in optical TPCs).

Ion transport

- Ion drift lines are simulated macroscopically, with a drift velocity $v_D = KE$ calculated from literature values for the (reduced) mobility $K_{(0)}$ – if available.
- One usually uses a single set of mobilities for all ions in the mixture.
- A first major improvement would be to have a recommended/default set of mobility data for commonly used mixtures.
- Development of a "microscopic" method (including charge transfer, formation of clusters, ...) would require a lot of work (and input data).
- Basic functionality for drifting negative ions exists, but detachment is not yet implemented.

Signals

- At present, time-dependent weighting potentials (see Djunes' talk) can be calculated analytically (for simple geometries) or using COMSOL. Are there other field solvers with which this can be done?
- Function for adding white noise to a signal pulse exists. Should be extended to support $1/f$ noise (and, more generally, arbitrary frequency spectra).

Other

- Code refactoring for concurrency/parallelism.
- Make interfaces more Python-friendly.
- Overhaul "event displays" and other viewers.
- Improve documentation.
- ...

Possibilities related to COMSOL and neBEM

Supratik Mukhopadhyay

on behalf of

Detector Applications Laboratory, SINP

COMSOL

Present status

- Works in a hybrid mode in which primary ionization details are obtained from Heed / Geant4 and transport properties are computed using Magboltz.
- Hydrodynamic simulation of basic detector parameters such as gain, energy resolution was carried out. The Transport of Diluted Species (TDS) module was found to be very useful for this purpose.
- Discharge simulation including preliminary assessment of discharge probability was possible.
- Space charge simulation illustrating its effects on electric field and detector parameters such as gain was performed.
- Detailed computation of electric field considering the effects of surface and volume currents in resistive components of RPCs has been performed.

Future projections

- Use of Charged Particle Tracking (CPT) module to improve simulations that require particle description.
- Implement improved boundary conditions for more realistic simulations.
- Study the applicability and limitations of deterministic simulations.
- Improve representation of statistical processes.
- Further exploration of effects of space charge, charging up and resistive components.

neBEM

Present status:

- Very precise potential and electric field values are obtained for any 2D / 3D geometry.
- Competitively accurate w.r.t any other commercial FEM / BEM package.
- Parallelized using OpenMP.
- Field maps and reduced order modeling crudely implemented.
- Preliminary implementation of space charge and charging up simulations.
- Open source, available from CERN website. Released along with Garfield++ since 2019.

Future projects:

- Orders of magnitude improvement in speed is possible:
  - FMM / GMRES or similar algorithms.
  - Improved parallelization (OpenMP, GPU, other technologies).
  - Smaller data storage and faster flow.
  - Use of lookup tables to replace time-consuming mathematical functions.
- Improvements in geometry modeler, surface mesh generation, adaptive mesh.
- Space charge and charging up simulation to be improved significantly. Charge transport through dielectrics is another important area to be explored.
- Magnetostatics to be incorporated.
- Limited electrodynamics, e.g., problems related to surface and volume currents to be included.
- Poisson equation is generic – other areas of application need to be explored.
- GUI, if possible.

Space charge

- **Present status**
- COMSOL based studies for GEM and RPCs.
  - Influence of space charge on electric field, gain and formation of discharge.
- “Garfield++-Heed-Magboltz-neBEM” based studies on space charge in RPCs.
  - Influence of space charge on the growth and saturation of an avalanche.
  - Introduction of a new Garfield++ class that carried out parallelized avalanche computation and considered line charges (and their reflections) to represent space charge.

Future projections

- Enrich the present studies. Extend investigations for other detectors.
- Improve space charge computation in neBEM. Surface distribution (rather than line) can be more realistic representation of space charge.

Thank you!

RD51 Mini-Week

DRD1 Preparation - Simulation of Resistive Detectors

Djunes Janssens

djunes.janssens@cern.ch

Supervisors: J. D'Hondt , E. Oliveri, W. Riegler, H. Schindler and R. Veenhof.

February 27th, 2023


Overview

Detectors with resistive elements become increasingly more popular in our community to improve the performance and stability of our detectors.

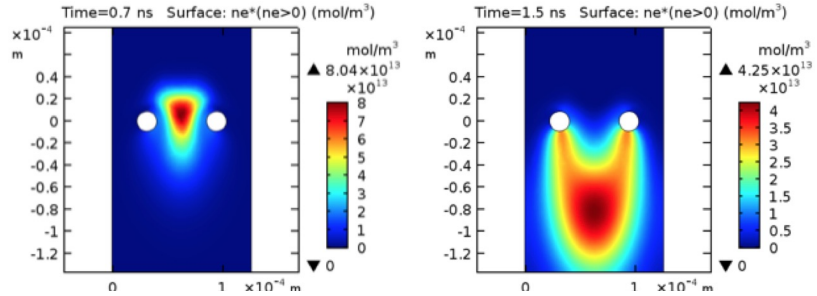
Signal formation:

- Importing 2D COMSOL solutions into Garfield++
- Inclusion of non-uniformities and defects in resistive electrodes
- General form of the Ramo-Shockley theorem

Quenching of sparks:

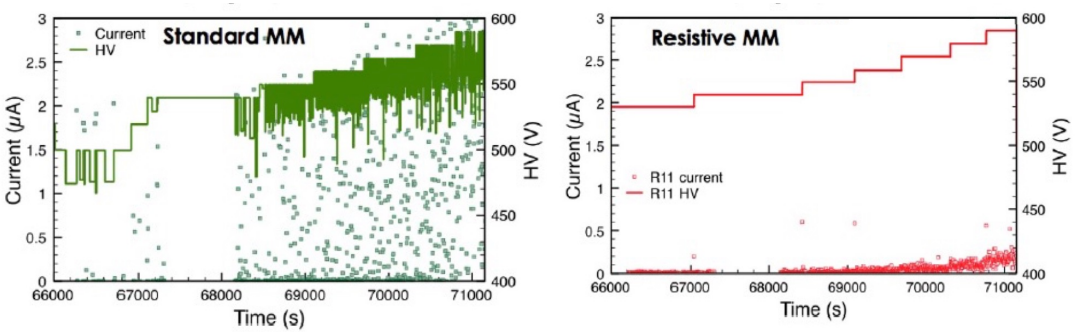
- Possible synergy with P. Gasik suggestions.

Simulation:



D. S. Bhattacharya et al., J. Phys. Conf. Ser. 1498 (2020) 012032

Measurments:

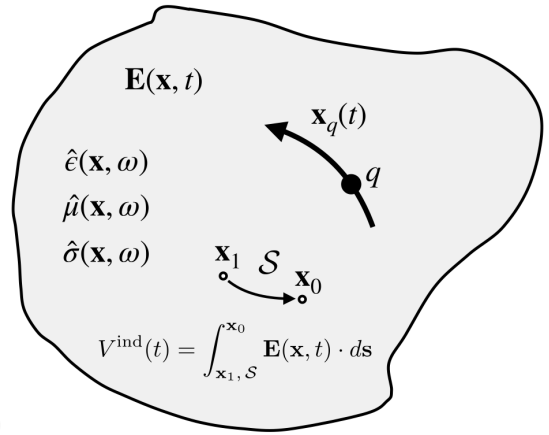


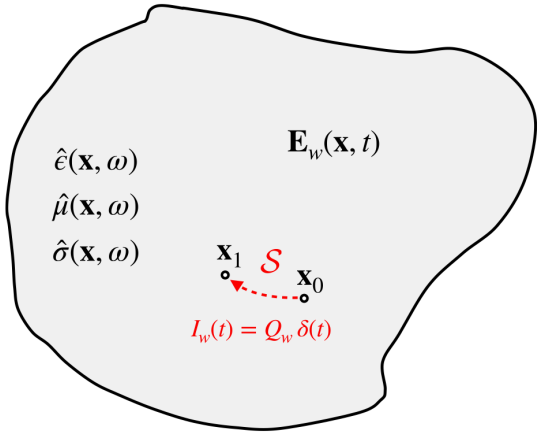
T. Alexopolous et al., NIM A 640 (2011) 110.

Ramo-Shockley theorem and its extensions

Currently we are not able to calculation signals in detectors where signal propagation times and radiation effects are not negligible, like transmission lines and antennas.

- Geometries including space-charge
  G. Cavalleri, E. Gatti et al., NIM 92 (1971), 137-140
- Signals on electrodes connected with impedance elements
  E. Gatti, G. Padovini and V. Radeka, NIM 193 (1982) 651-653
- Permittivity and non-linear materials
  L. A. Hamel, M. Julien, Proceedings of SPIE vol. 4507 (2001), 255-263
  L. A. Hamel, M. Julien, NIMA 597 (2008), 207-211
- Geometries that contain material of finite resistivity
  W. Riegler, NIMA 491 (2002), 258-217
  W. Riegler, NIMA 535 (2004), 287-293
  W. Riegler, NIMA 940 (2019) 453-461
- General Maxwell compliant form using Lorentz-reciprocity
  W. Riegler and P. Windischhofer, NIMA 980 (2020) 164471





$$V^{\mathrm{ind}}(\omega) = \int_{\mathbf{x}_1,\mathcal{S}}^{\mathbf{x}_0} \mathbf{E}(\mathbf{x},\omega)d\mathbf{s} = -\frac{1}{I_w(\omega)}\int_V \mathbf{E}_w(\mathbf{x},\omega)\mathbf{J}^e(\mathbf{x},\omega)dV$$

Overview

Alongside these desirable effects, other "secondary" processes play a role in the performance of resistive detectors.

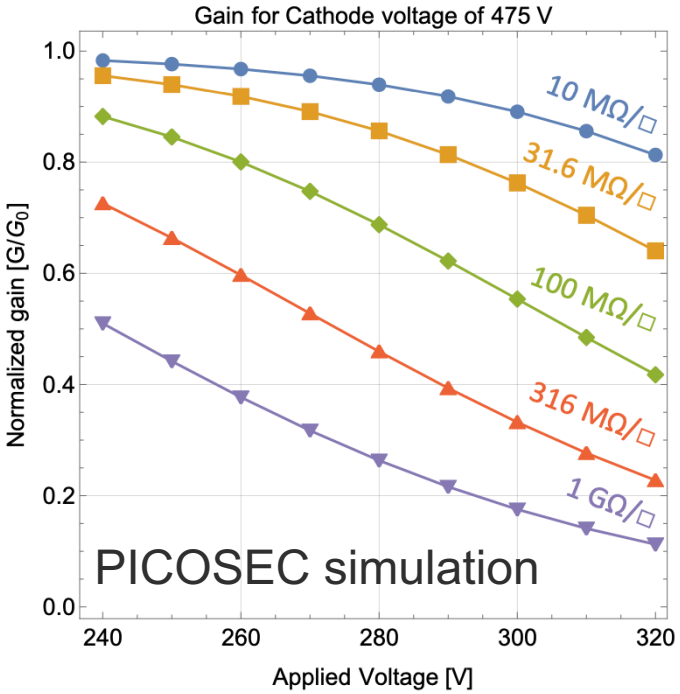
Rate capability studies:

- Already great progress in the form of equivalent circuits:
  Zhujun Fang et al., Nucl. Instrum. Meth. A 1032 (2022) 166615
- This could be extended using finite element solvers, the solution of which can be imported into Garfield++

Thermal or Johnson Noise:

- Simulate noise contribution based on the power spectrum of of a detector with impedance Z(iω).

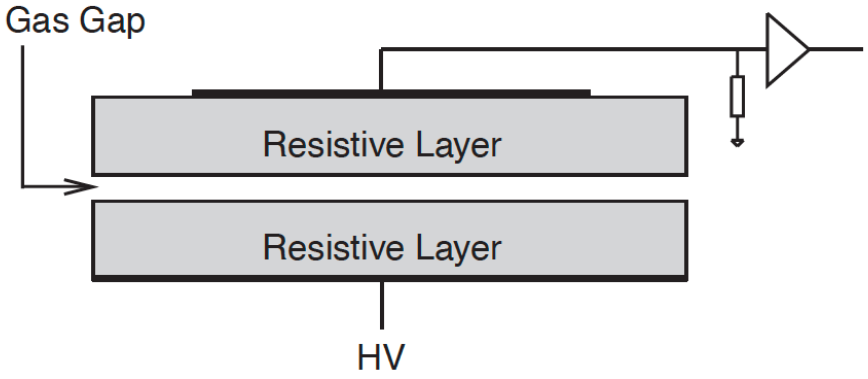
$$w_i(f) = 4k_B T \,\mathrm{Re}\left(\frac{1}{Z(i\omega)}\right)$$



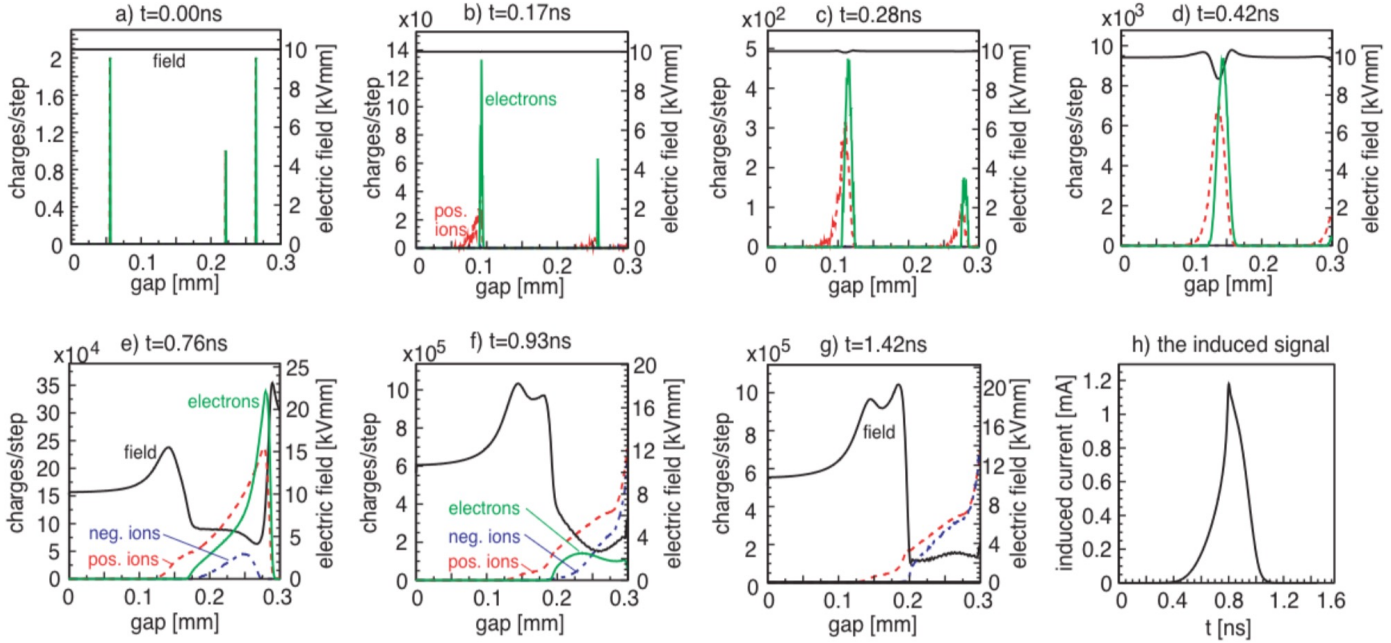
Space-charge effects and resistive elements

Resistive materials that collect electrons need time to spread and evacuate their charge from the collection area.

Locally this can result in the collapsing of the amplification field, limiting the growth of the avalanches of subsequent clusters.



Simulation work:

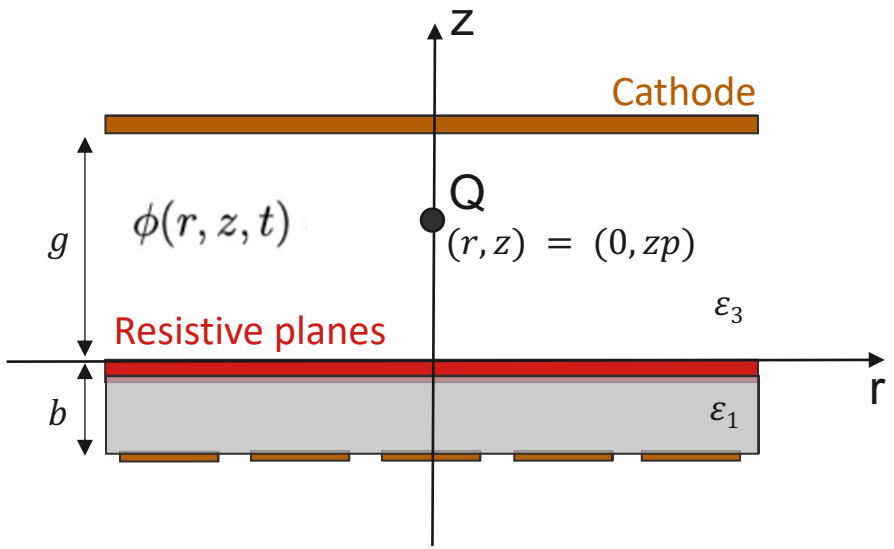


C. Lippmann and W. Riegler, Nucl. Instrum. Meth. A 517 (2004) 54–76

Space-charge effects and resistive elements

A way of implementing this is to include the analytical dynamic potential of the charge in a parallel plate type geometry.

$$\phi(r,z,t) = \frac{Q}{2\varepsilon_3\pi}\int_0^\infty dk\, J_0(kr) f(k,z,t)$$



For those who like equations

$$f(k,z,t) = \frac{e^{-k(b+z_<)}(1-\coth(gk))\sinh(k(g-z_>))\left(h_1 - h_2 e^{-\frac{t}{\tau(k)}}\right)}{D(k)}$$

$$D(k) = 2\varepsilon_3\left(\varepsilon_1\left(e^{2bk}+1\right)\left(e^{2gk}-1\right) + \varepsilon_3\left(e^{2bk}-1\right)\left(e^{2gk}+1\right)\right)$$

$$\tau(k) = \frac{R}{k}\left(\varepsilon_1\coth(bk) + \varepsilon_3\coth(gk)\right)$$

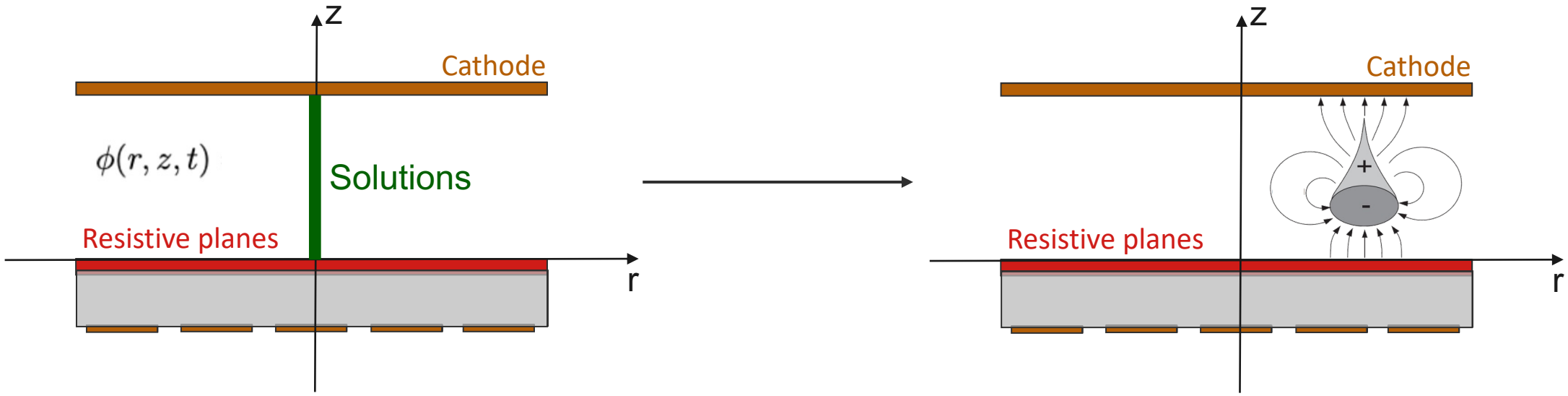
$$h_1 = \left(e^{k(b+g)} - e^{k(b+g+2z_<)}\right)\left((\varepsilon_1+\varepsilon_3)\left(e^{2k(b+g)}-1\right) - 2(\varepsilon_1-\varepsilon_3)e^{k(b+g)}\sinh(k(b-g))\right)$$

$$h_2 = 8\varepsilon_3\sinh(bk)\sinh(k(g-z_<))\exp\left(k\left(+2b+2g+z_<\right)\right)$$

Space-charge effects and resistive elements

This potential, which only needs to be evaluated once over all possible z positions, needs to integrated over the drifting particles.

The resulting field will then be a corrention factor to the applied static field inside the geometry.



DRD1 WG4 preparation:

Discharge modelling & simulation

RD51 mini-week

27.02.2023

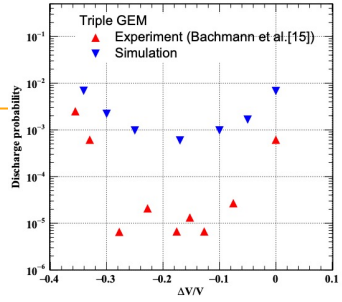
P. Gasik

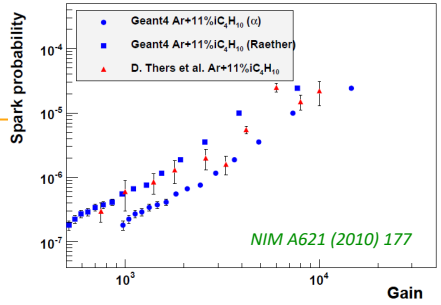
(personal view)

What we can (Geant)

- Reproduce discharge curves obtained with different MPGDs
- Predict discharge rate with different sources and geometries
- Predict gas effects (more discharges with heavier gases)
- Evaluate discharge limits, incl. discharge dev. time
- Understand the effects related to charge density
  - Stacks (GEMs, GEM+MMG)
  - Magnetic field influence
  - Electric field influence
  - Emission angle, track length, drift lengths
  - Drift and diffusion

JINST 16 (2021) P09001





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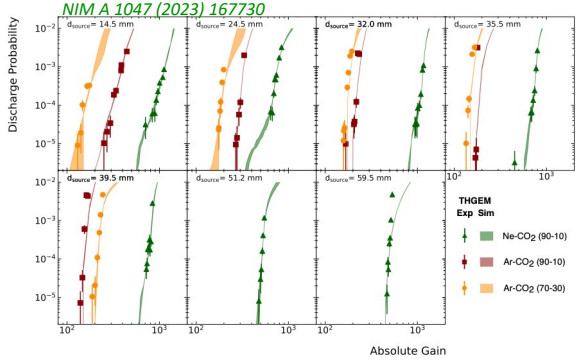
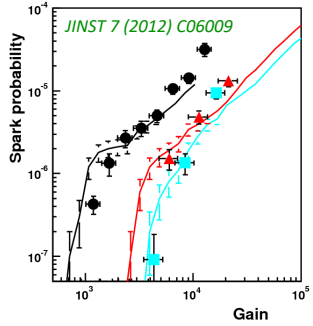
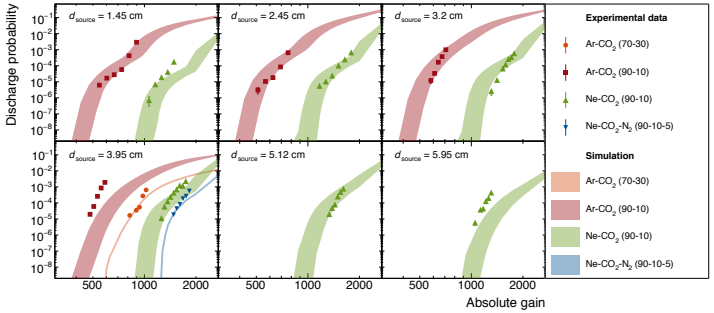
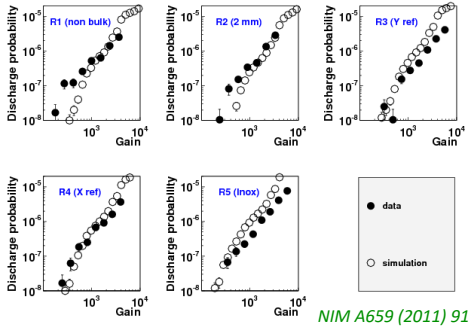


JINST 7 (2012) C06009



NIM A 870 (2017) 116

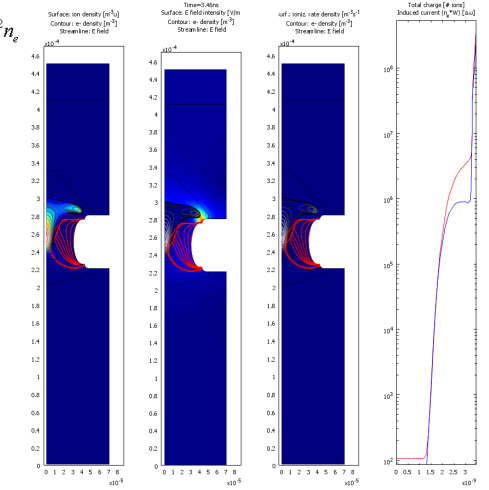




NIM A659 (2011) 91

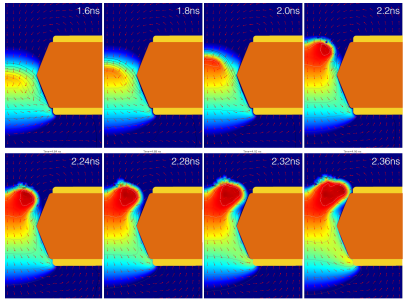
What we can (FEM)

$$\begin{cases} \dfrac{\partial n_e}{\partial t} + \vec{\nabla}\cdot(\vec{W}_e n_e) = \alpha\left|\vec{W}_e\right| n_e + D_e \nabla^2 n_e \\ \dfrac{\partial n_{i+}}{\partial t} = \alpha\left|\vec{W}_e\right| n_e \\ \nabla^2 V = -\dfrac{e}{\varepsilon_0}(n_{i+} - n_e) \end{cases}$$



- We can simulate streamer formation using a simplified hydrodynamic model (no photoionization, diffusion-assisted streamers).

IEEE (2015) 1



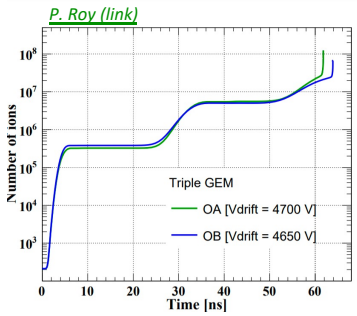
P. Fonte, MPGD Stability workshop, TUM 2018 (link)

- The model:
  - Seems to describe qualitatively fast breakdown in MPGDs
  - Gives correct breakdown limit for GEM
  - Seems to reproduce SQS in needles
  - Allows to simulate space charge effects, and their time development

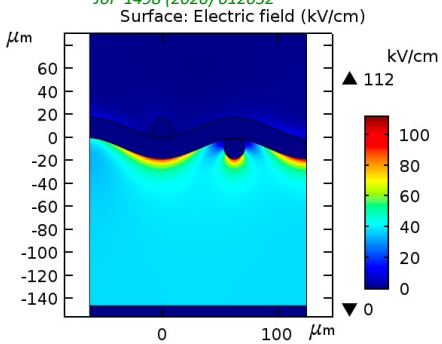
P. Fonte, TUM 2018

- We can optimize geometry, simulate hot spots, etc.

P. Roy (link)



JoP 1498 (2020) 012032



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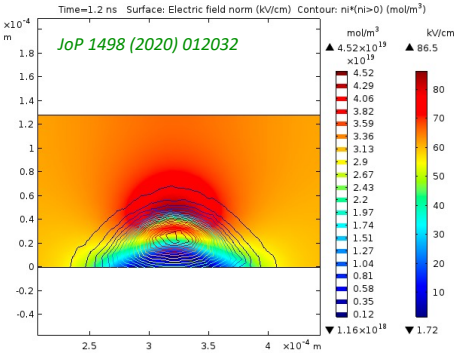
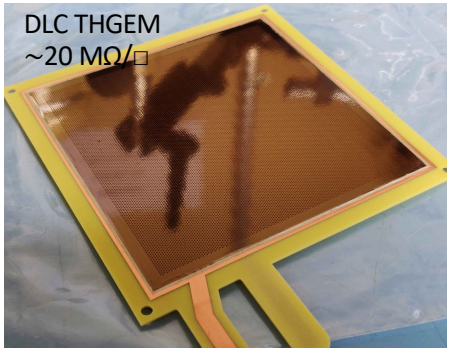
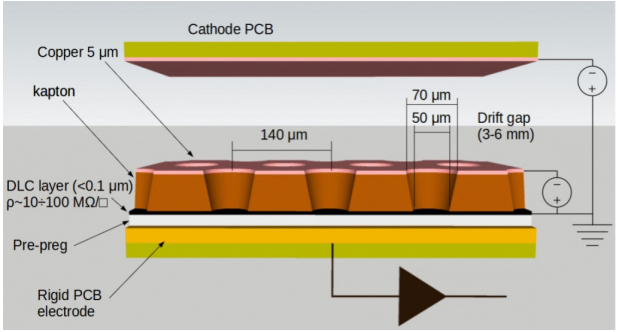


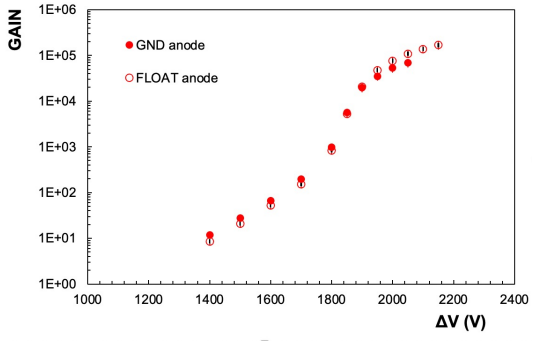
The effort needs to continue

- Continue discharge simulations in new MPGD structures with currently available tools/models
- Update the tools/models ☺
- Discharge development with resistive layers

  (more and more experimental data available, see e.g. JINST 17 P11004)



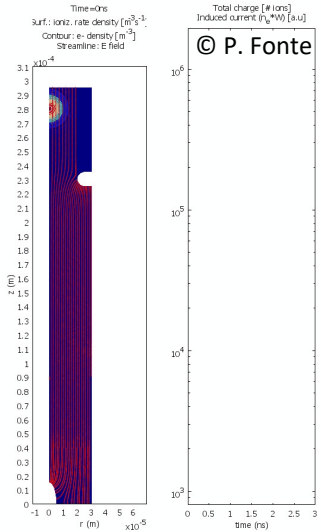




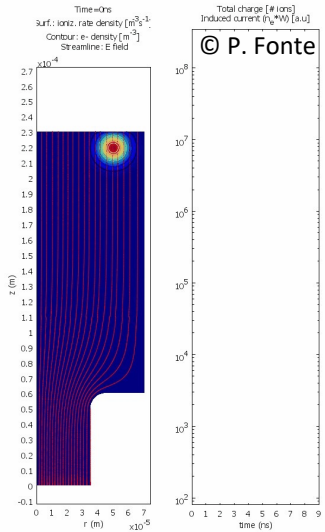
MPGDs in SQS mode?

P. Fonte, “Simulations of discharge phenomena”, RD51 Meeting, TU Munich 2018 (link)

- Discharge probability could be reduced if a radial shape E-field is formed in the MPGD avalanche gap
- Both simulation and R&D effort. Still need for optimization, but ideas on the market!

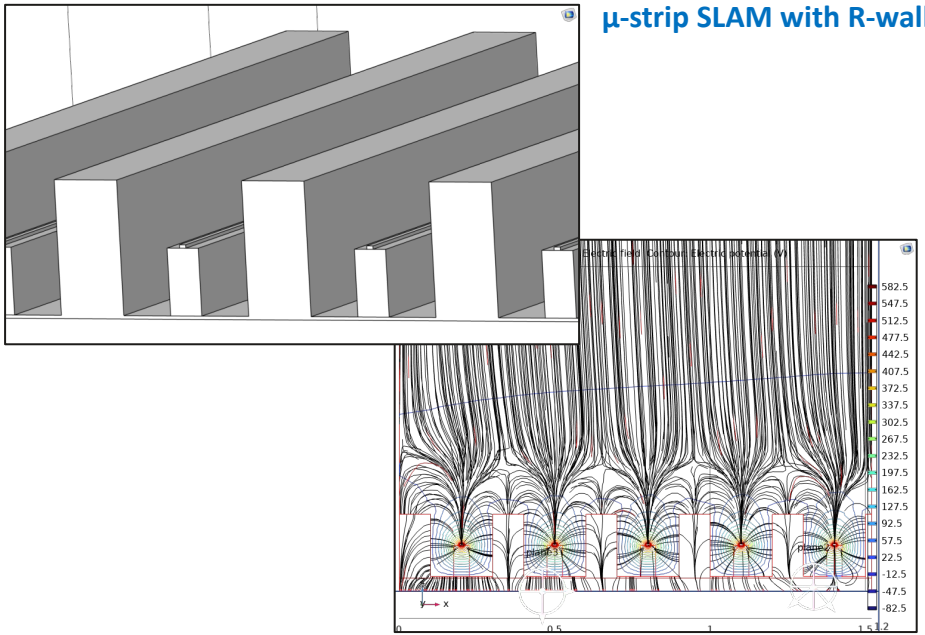


Needle + InGrid



Cathodeless CAT

µ-strip SLAM with R-walls



- RD51 Common Project: “***Discharge Consortium in quest for Spark-Less-Avalanche-Microstructures***”

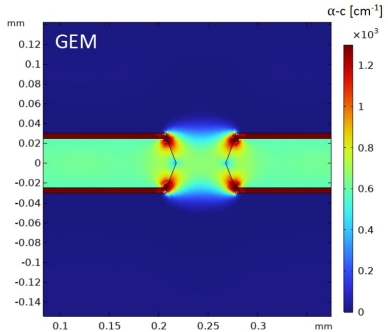
What would be good to have/answer?

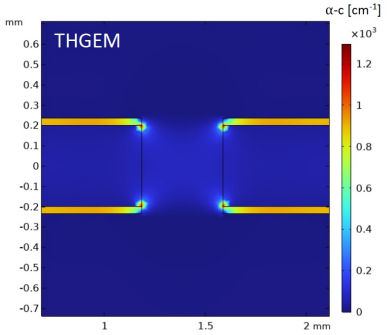
- Simulation of an avalanche process and its transition to a streamer (Garfield++)
  - Q_{crit} dependency on the gas mixture → fundamental transport properties of a given gas?
  - Detailed simulations to describe and explain the observed differences

NIM A 1047 (2023) 167730

Gas	THGEM		GEM	
	$\langle Q_{crit} \rangle$ [$\times 10^6\, e$]	t_{int} [ns]	Q_{crit} [$\times 10^6\, e$]	t_{int} [ns]
Ne-CO_2 (90-10)	7.1 ± 2.2	30–210	7.3 ± 0.9	20–90
Ar-CO_2 (90-10)	4.3 ± 1.5	20–110	4.7 ± 0.6	15–50
Ar-CO_2 (70-30)	2.5 ± 0.9	40–310	–	–

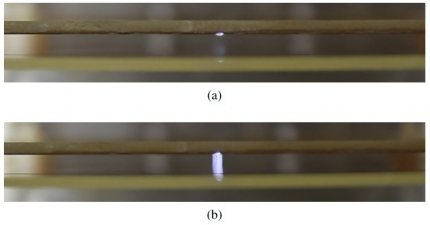
- Understand discharge probability and Q_{crit} values obtained with different geometries
  - Q_{crit} for both GEM and THGEM structures agree with each other, in spite of geometrical differences!
  - The “effective volume” for a streamer creation in a THGEM may be comparable to the size of a GEM
  - Detailed simulations of streamer formation are necessary!



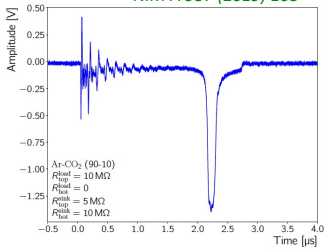


What would be good to have/answer?

- Simulation model describing secondary (propagated, delayed) discharges developing in the gaps between subsequent foils in a stack.
  - Mechanism ⇀ still a topic of a debate.
  - Need to understand the entire process and, if possible, to eliminate the cause of these violent events completely.
  - Model development of a primary discharge in a GEM hole and its subsequent transition to a gap discharge, taking into account:
    - Space-charge densities
    - Drift and amplification of charges, ion bombardment
    - Heating of the electrodes …
    - … and thermionic emission from the latter.



NIM A 937 (2019) 168



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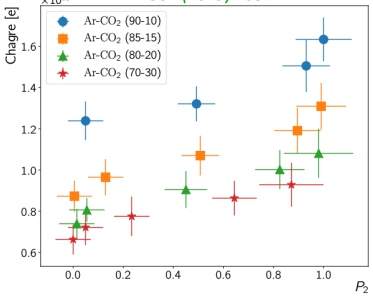
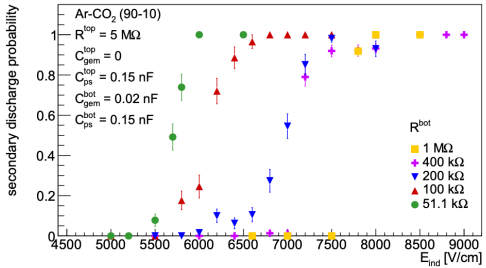
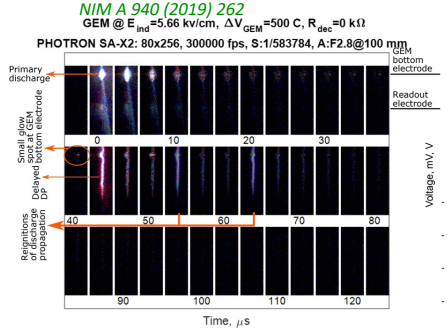


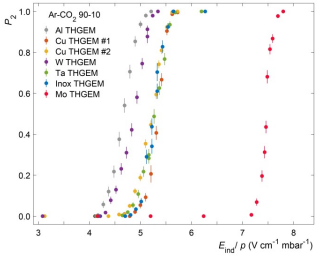
JINST 14 (2019) P08024



NIM A 940 (2019) 262



NIM A 1019 (2021) 165829



Penning Energy Transfers

$e^- + A \rightarrow A^+ + 2e^-$: ionisation → Townsend coefficients

$e^- + A \rightarrow A^*$: excitation → **what happens ? Michel Penning explains**

1. F.M. Penning, *The starting potential of the glow discharge in neon argon mixtures between large parallel plates: II. Discussion of the ionisation and excitation by electrons and metastable atoms*, Physica, Volume **1** (1934).
2. M.J. Druyvesteyn and F.M. Penning, *The Mechanism of Electrical Discharges in Gases of Low Pressure*, Rev. Mod. Phys., **12** (1940).

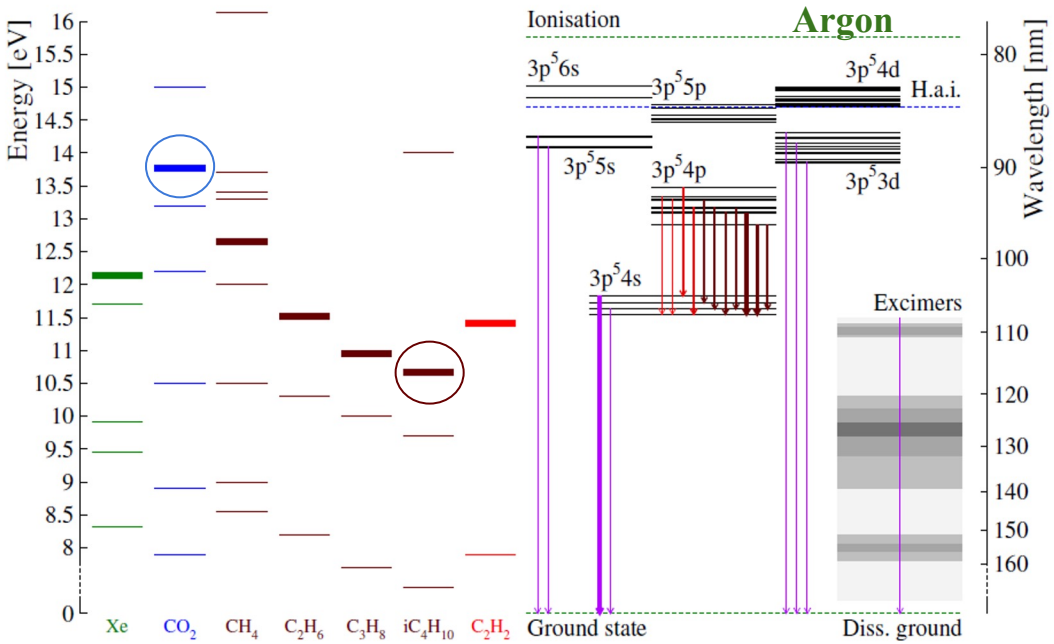
❖ **$Ar^* + CO_2 \rightarrow Ar + CO_2^+ + e^-$**

➢ Ar^* $3p^5 3d$ (13.8 eV) and higher excitations can ionise CO_2 (IP: 13.77 eV)

❖ **$Ar^* + iC_4H_{10} \rightarrow Ar + iC_4H_{10}^+ + e^-$**

➢ All excited Argon atoms can ionise iC_4H_{10} (IP: 10.67 eV)

➢ The lowest excited Argon 11.55 eV

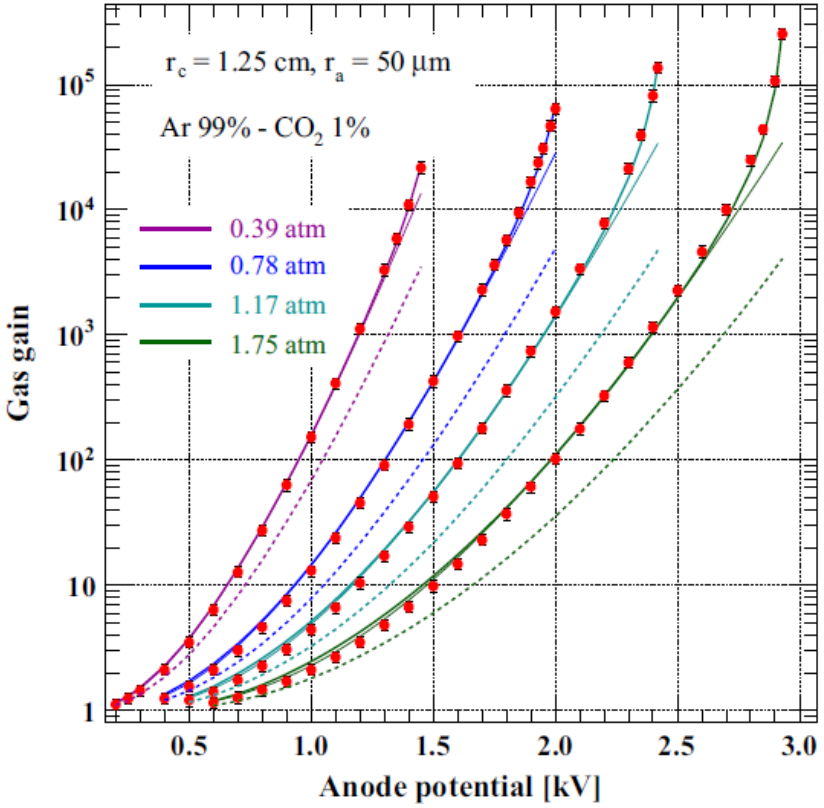


- Penning energy rates ($\mathbf{r_{Pen}}$) can be extracted from the measured gas gain by using transport parameters of Magboltz!

$$\alpha_{Pen} = \alpha\left(1 + r_{Pen}\frac{\nu^{exc}}{\nu^{ion}}\right) \Rightarrow G = e^{\int \alpha_{Pen}(E(r))\,dr}$$

Penning corrected gas gain

Calculation Method



$$\alpha_{Pen} = \alpha\left(1 + r_{Pen}\frac{\nu^{exc}}{\nu^{ion}}\right) \Rightarrow G = e^{\int \alpha_{Pen}(E(r))\,dr}$$

Penning corrected gas gain

without any correction

with Penning transfer

with Penning and **feedback corrections**

$$G_{Total} := G/(1-\beta G)$$

$A^* \rightarrow A + \gamma$

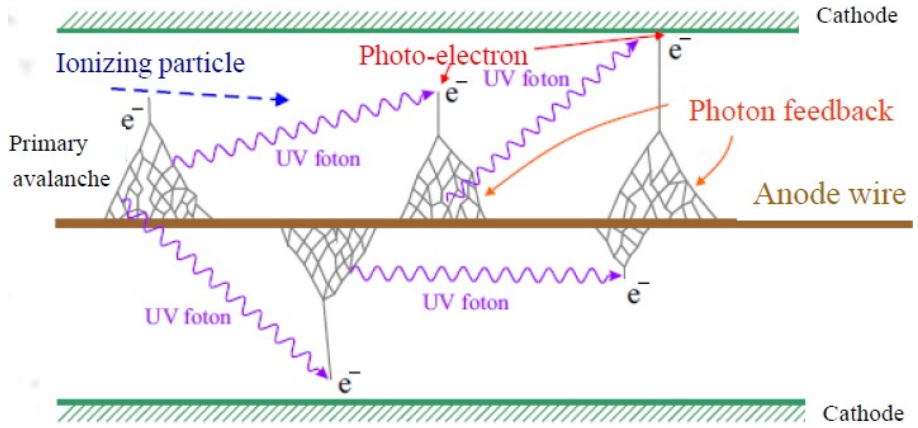


Photo-electrons:

in gas itself

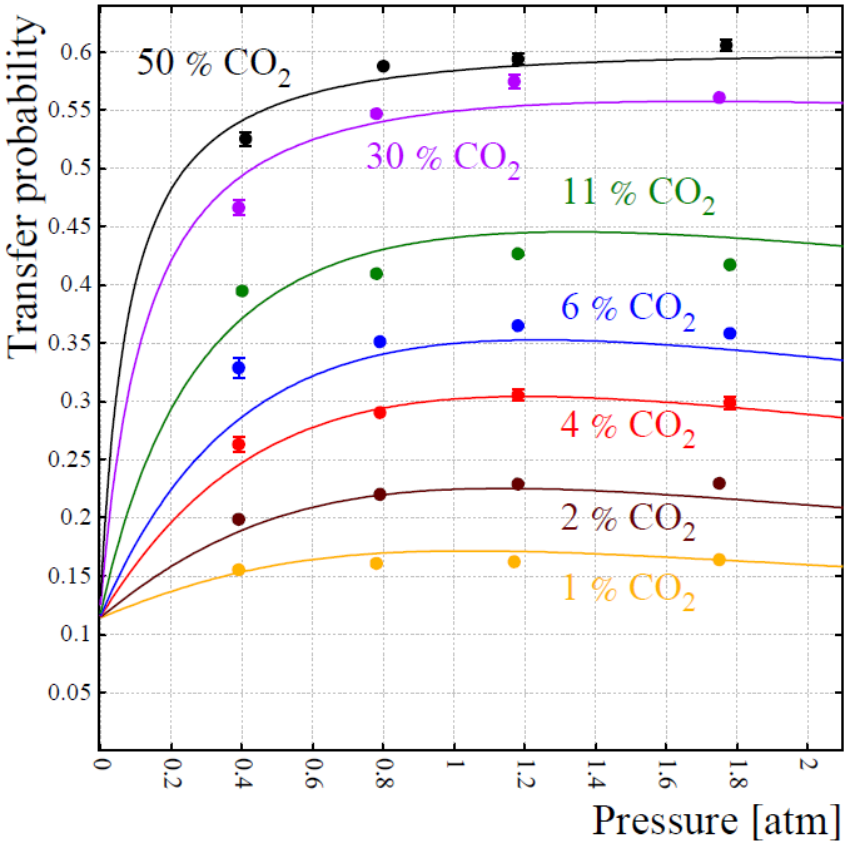
from cathode

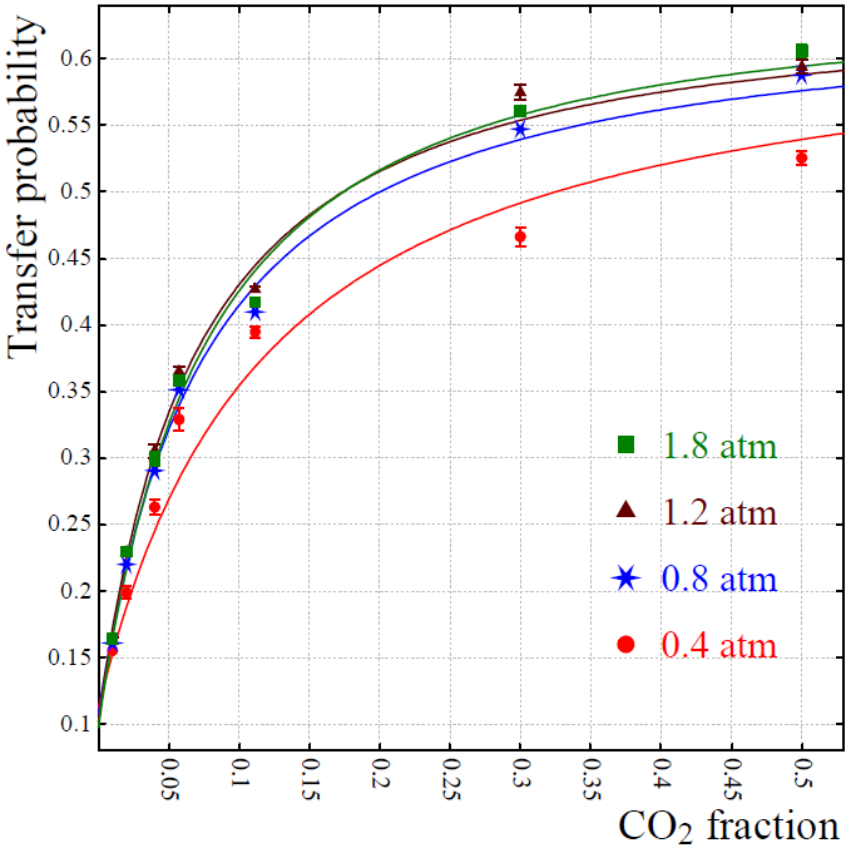
insufficiant absorption in gas

Secondary, delayed avalanches

over exponential increases at high gas gains

Model of the energy transfer probabilities (Ar-CO_2)





$$r_{Pen}(p,c) = \frac{a_5 p^2 (1-c)^2 + a_1 pc + a_4 c + a_3}{a_6 p^2 (1-c)^2 + pc + a_2}$$

- ❖ **Numerator: increase the ionizations**
- ❖ **Denominator: excitation loses**

Ar_2^* - CO_2 Ar^* - CO_2 Ar^* - γ

1) **Excimers**
2) **Collosional ionizations**
3) **Radiative energy transfers**

Some outputs

Investigated Penning Mixtures

1) Ar – Xe
2) Ar – CO_2
3) Ar – CH_4
4) Ar – C_2H_2
5) Ar – C_2H_6
6) Ar – C_3H_8
7) Ar – iC_4H_{10}
8) He – iC_4H_{10}
9) Ne – iC_4H_{10}
10) Ne – CO_2
11) Ne – CO_2 – N_2
12) Ne – N_2
13) Xe – TMA
14) Xe – CO2 (not finished)

- The Penning effect cannot be ignored in gas gain simulations
- Penning energy transfer rates can be derived from the measured gas gains
  - They have a wide application area for all **gas detectors**
- Transfer rate models can be used to separate the efficiency of the different physical processes playing a role in avalanche multiplications.
  - Each gas mixture has its own unique and interesting combination of avalanche properties.
- Gain fits also provides feedback parameters

Investigated Non-Penning Mixtures

1) C_3H_8 – CO_2 – N_2 : Propane-based tissue equivalent (TEG) mixture
2) CH_4 – CO_2 – N_2 : Methane-based tissue equivalent (TEG) mixture
3) Pure CO_2 : proves that the cross sections in Magboltz are correct

- **Medical applications:** correct dose determination
- Learn about dissociations like CH3, CH2, CH, C, CO, O, O2, N

Penning Transfer Implementation for Garfield++

Garfield++ Installation Examples Documentation

Penning transfer

https://garfieldpp.web.cern.ch/examples/penning/

If one of the components in a gas mixture (typically a noble gas) has excited states above the ionisation energy of another component (typically a quencher), the transformation of excitation energy into ionisations (known as Penning transfer) can contribute significantly to the gas gain. This effect can be described in terms of a probability r_P that an excited state eventually results in ionisation. The transfer probability for a given gas mixture and pressure can be determined by comparing measured gain curves with Magboltz simulations. Provided that sufficient experimental data are available, r_P can be parameterised as function of the concentration c of the admixture and the pressure p. The following table lists the gas mixtures for which r_P values have been determined from gain curve fits in recent years and the publications in which they can be found.

- Many Garfield++ users have inquired about the energy transfer rates to be utilized and where to obtain these numbers before performing calculations

➢ Indeed, the rates can be accessed from the literature, but more practical method would be helpful

➢ **An automated** version of Penning transfer rate calculation has been added to Garfield++ with the available data in the literature

➢ The users have had access to the implementation since Oct 2nd of 2021

➢ **Models are still needed for many gas mixtures !!!**

Available models

Ar/CO_2	NIM A 768 (2014), 104	$r_P(c)$ at atmospheric pressure
Ar/CO_2	JINST 12 (2017), C01035	$r_P(c, p)$
Ar/CH_4	JINST 5 (2010), P05002	$r_P(c, p)$
Ar/C_2H_6	JINST 5 (2010), P05002	r_P for 10% C_2H_6 at atmospheric pressure
Ar/C_3H_8	JINST 5 (2010), P05002	$r_P(c)$ at atmospheric pressure
Ar/iC_4H_{10}	JINST 5 (2010), P05002	r_P for 10% iC_4H_{10} at atmospheric pressure
Ar/C_2H_2	JINST 5 (2010), P05002	r_P at atmospheric pressure
Ar/Xe	JINST 5 (2010), P05002	$r_P(c)$ at atmospheric pressure
Ne/CO_2	JINST 16 (2021), P03026	$r_P(c, p)$
Ne/N_2	JINST 16 (2021), P03026	$r_P(c, p)$
Xe/TMA	JINST 13 (2018), P10032	$r_P(p)$ for 5% TMA

NEXT

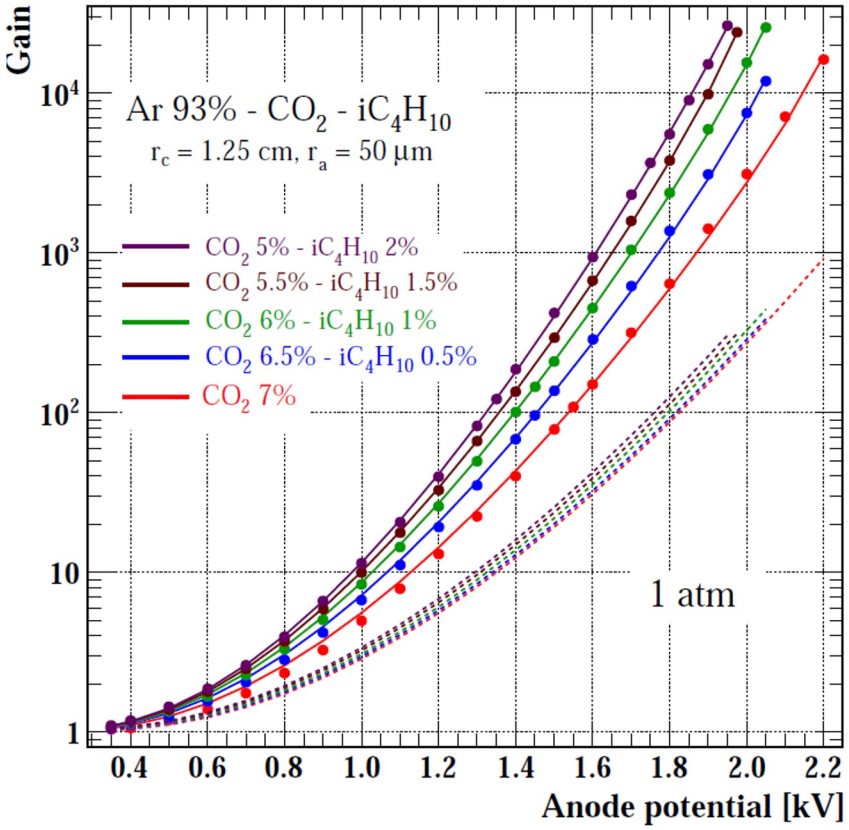
- New investigations for other mixtures are needed:
  - There are still **missing $r_{Pen}(p,c)$ models** for Garfield++ users,
  - They can be constructed by extracting Penning rates from the systematic gas gain measurements (pressure and concentration dependences).

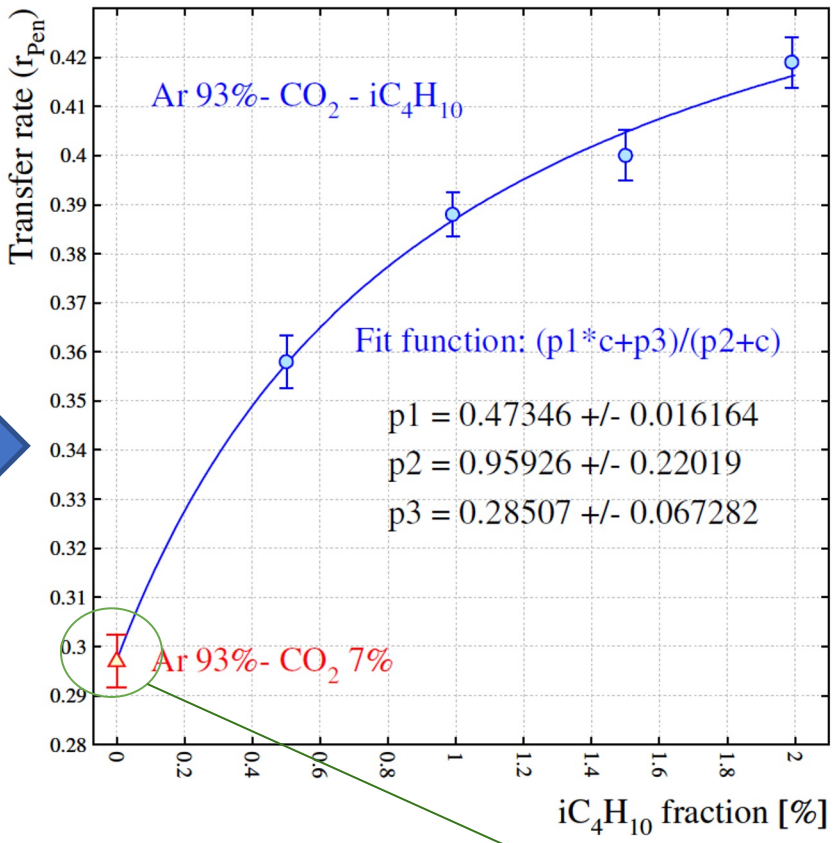
- Penning extraction and modelling for **Ternary mixtures**. Examples:
  - $Ar/CO_2/CF_4$ 40/15/45 **(LHCb GEM)**
  - $Ar/CO_2/iC4H_{10}$ **(Atlas MM): in progress**

- **Non-equilibrium** effects, especially at high e-field gradients, should be carefully worked (**in progress**).
  - Very interesting effect in the avalanche formations.

- The **feedback** processes in gas gains should be extensively researched.
  - As a start, it can be useful to model the available parameters.

Ar-CO_2-iC_4H_{10} mixtures (ongoing work)





1) Collosional ionizations (p1 ≈ 47 %)

➢ $Ar^* + B \rightarrow Ar + B^+ + e^-$

■ B: CO_2 or CO_2 + iC_4H_{10}

2) c = 0 refers to transfer rate in Ar 93 %-CO_2 7 %

p3/p2 ≈ 30 % is comparable with earlier data

$$r_{Pen}(c) = \frac{p1 \cdot c + p3}{c + p2}$$

Negative ion drift simulation

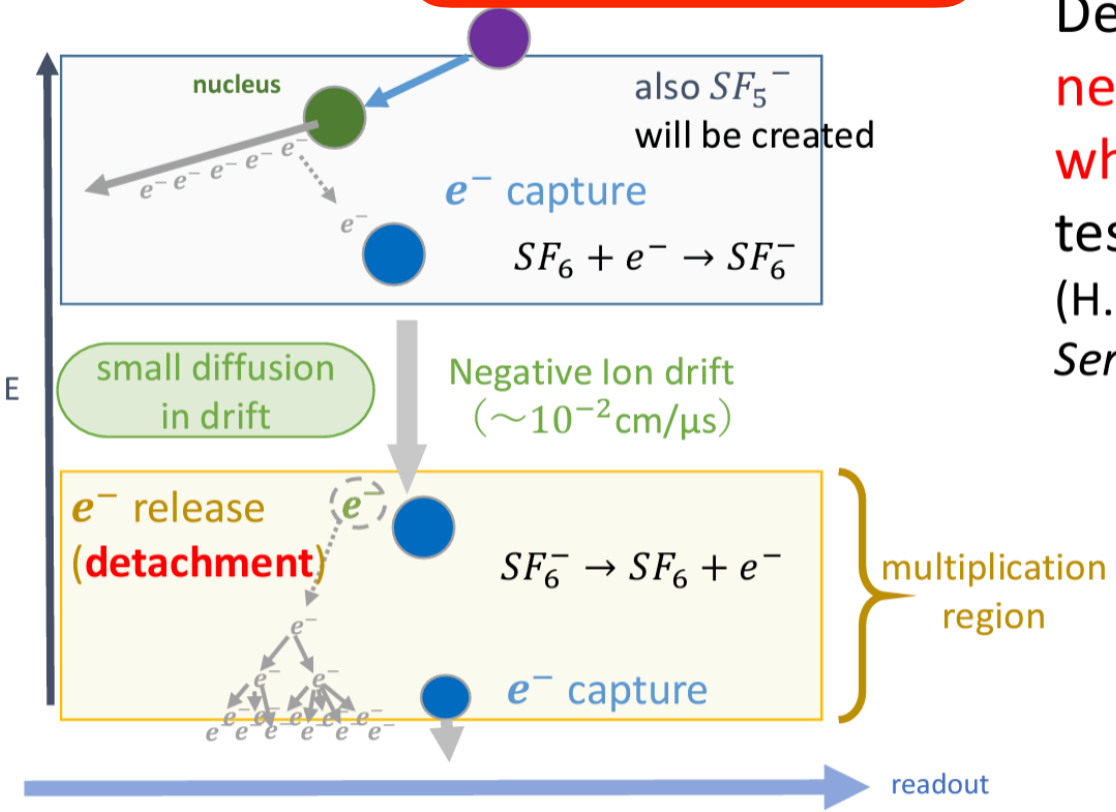
What exists and what we dream for

E. Baracchini, Gran Sasso Science Institute

Negative ion drift amplification simulation of pure SF_6

From H. Ishiura talk at RD51 workshop Nov 2021

➢Key feature: Detachment model



Detachment model :
negative ion releases electron while in strong electric field
tested In previous work
(H.Ishiura *et al* 2020 *J. Phys.: Conf. Ser.* **1498** 012018

a). Threshold model
Electric field as threshold

b). cross section model
calculate probability
and detach or not

NEW: This model was implemented as
"AvalancheNIMicroscopic" class for model verification(T.Shimada)

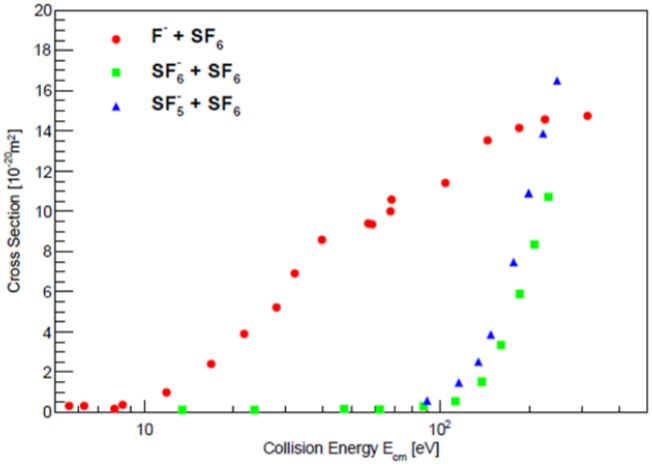
Published on *J.Phys.Conf.Ser.* 1498 (2020) 1, 012018

Negative ion drift GEM amplification simulation: results

Main e⁻ detachment processes

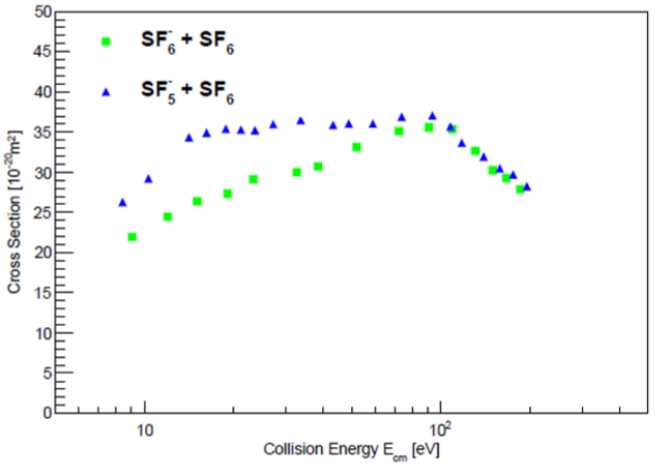
$$SF_6^- + SF_6 \rightarrow e^- + SF_6 + SF_6$$
$$SF_5^- + SF_6 \rightarrow e^- + SF_5 + SF_6$$
$$F^- + SF_6 \rightarrow e^- + F + SF_6$$

Last process dominates due to cross section threshold

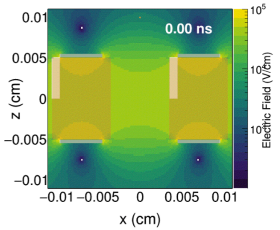


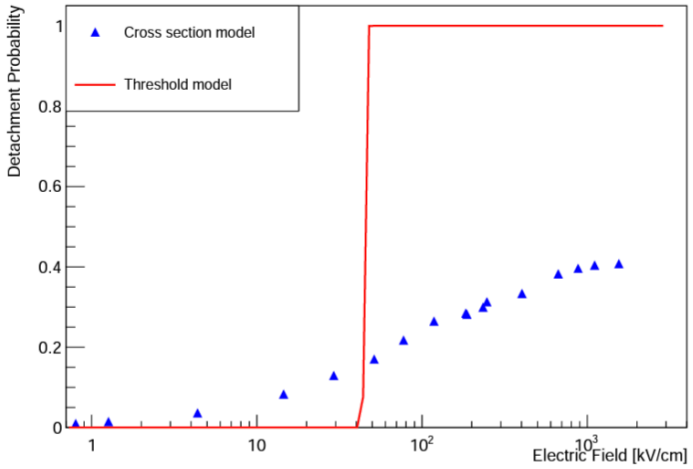
Main mechanisms for F⁻ production

$$SF_6^- + SF_6 \rightarrow F^- + SF_5 + SF_6$$
$$SF_5^- + SF_6 \rightarrow F^- + SF_4 + SF_6$$

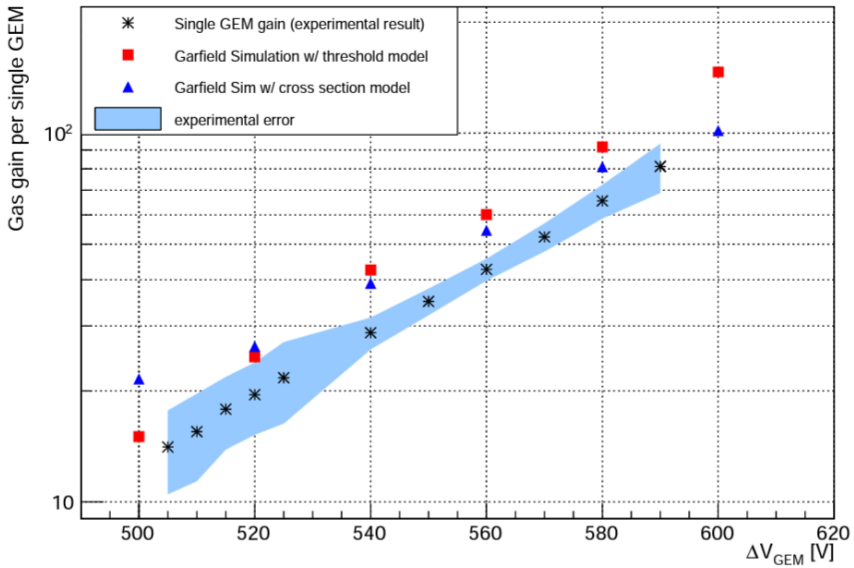


Cross section and threshold model dependence on electric field





From *J.Phys.Conf.Ser.* 1498 (2020) 1, 012018



Cross section model reproduces data within a factor 2

NEED TO KNOW cross sections for simulation

Amplification simulation nearly works..for pure SF_6

From *Astropart.Phys.* 33 (2010) 216-220

resulting expression relating gain to applied voltage is cast in terms of two parameters: E_{min}, the electric field where the avalanche starts (referred to as the "starting field"), and ΔV, the potential difference through which the avalanche charge doubles:

$$\frac{ln(G)\ ln(\frac{b}{a})}{V} = \frac{ln2}{\Delta V} \cdot ln\left(\frac{V}{ln(\frac{b}{a})aE_{min}}\right) \quad (1)$$

The approximate constancy of E_{min}/P for pure CS_2 and the semi-quantitative agreement of the collisional estimate given above with the measured E_{min} values, supports the conclusion that avalanches in CS_2 are initiated by collisional detachment of electrons from ions, followed by a normal Townsend avalanche of the free electrons.

A similar analysis of CH_3NO_2:CO_2 mixtures shows that the simplified collisional detachment model predicts values of E_{min} of the same order as the experimental results. However the values do not scale with pressure as predicted by the model. It is suggested that the extremely high fields needed for detachment in these mixtures, along with the capture of energetic electrons by CO_2, may account for these effects.

Take away message: multiple components (especially if poliatomic) in a gas mixture significantly complicates the picture given the many possible interaction/processes that can take place (not only in terms of e- detachment, see later)

- What about mixtures? i.e. He:SF_6 as the foreseen gas for CYGNUS
- What about mixtures with poliatomic gases? i.e. He:SF_6:CF_4 as in CYGNO
- Pure SF_6 cross sections have been measured….but what about SF_6 - X cross sections?
  - Is it possible to measure such cross sections?
  - Need a dedicated cross section measurements campaing?

And what about diffusion in drift?

everybody is thinking thermal….but it might not be so trivial!

From the original NID paper
Nucl.Instrum.Meth.A 440 (2000) 355-359

R.m.s. diffusion of negative ions measured in noble gas mixtures with CS_2. Drift length was 15 cm. The diffusion values reported are corrected for the finite sizes of apertures and for electric field mismatch between drift and proportional counter regions

Gas	Pressure (Torr)	E (kV/m)	Transverse diffusion (mm r.m.s.)
Ar mix	40	47.0	$0.12\ ^{+0.05}_{-0.1}$
Ar mix	40	35.3	$0.21\ ^{+0.02}_{-0.1}$
Ar mix	40	23.5	0.38 ± 0.02
Xe mix	40	47.0	$0.13\ ^{+0.05}_{-0.1}$
Xe mix	16.5	23.5	0.33 ± 0.03

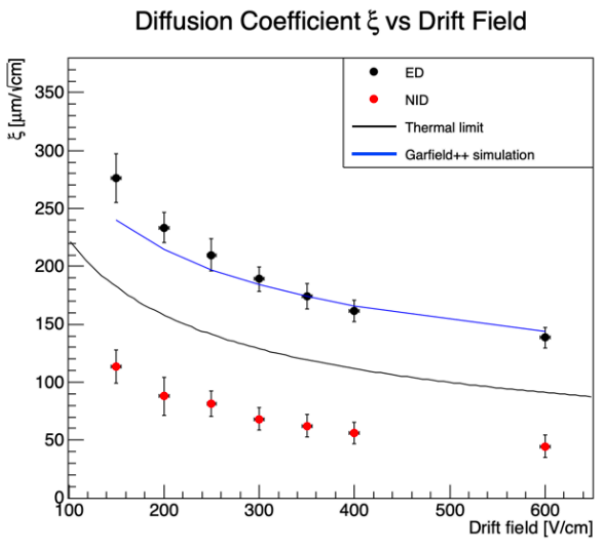
Even though thermal behaviour is claimed in the text, working out the numbers factor 2-3 below thermal is found + falling faster than 1/sqrt(E) expected from thermal

Nucl.Instrum.Meth.A 555 (2005) 55-58

Gas Mixture	Slope	Temperature
$100\%CS_2$	0.16 ±0.02 Vmm/Torr	360 ±40 K
$90\%CS_2$-10%Ar	0.13 ±0.03 Vmm/Torr	300 ±80 K
$50\%CS_2$-50%Ar	0.11 ±0.02 Vmm/Torr	260 ±40 K
$25\%CS_2$-75%Ar	0.10 ±0.02 Vmm/Torr	240 ±50 K

Effective diffusion temperature dependence on amount of Ar, going below the thermal limit

E. Baracchini talk at MPGD 2022



He:CF_4:SF_6 59/39.4/1.6 @ 650 mbar factor 4 below thermal

Chemical Physics
Volume 54, Issue 3, 15 January 1981, Pages 341-364

A simple physical interpretation can be given to eq. (72). Energy is fed into the internal degrees of freedom of the ions by collisions with the structureless neutrals; the source of the internal energy is thus the translational motion. Energy leaks out of both the internal and translational degrees of freedom of the ions only through the translational (recoil) motion of the neutrals. Since the leak is the same for both forms of energy, and since the internal energy is fed by the translation, it is not surprising to find a relation like eq. (72) at steady state. In contrast, with molecular neutrals the internal and translational energies of the ions can leak into the internal degrees of freedom of the neutrals at different rates, depending on the details of the inelastic cross sections. The steady-state energy balance will thus depend on the cross sections, and no general relation like eq. (72) can be obtained.

To my understanding, polyatomic gases allow for the possibility of loosing energy in many more ways than single atomic species drifting in same species gases and therefore inelastic collisions needs to be properly taken into account in the diffusion. Exact calculation of inelastic collision between polyatomic atoms are very difficult (impossible?) to solve

Wishlist

from reasonable to dreams

- Gain simulation for multiple amplification structures:
    - GEMs, Micromegas, MMTHGEM, MWPC…
- Gain simulation for gas mixtures, including polyatomic
- More measurements with more diverse drift fields/pressures/ gases/gas mixtures/amplification structures to compare with and on which optimise simulations
- Diffusion simulation for polyatomic gas mixtures with elastic and inelastic collision integrals calculation
    - …just a guess of what is missing from the thermal picture behaviour, need to be verified

Parametrization of a MPGD

Ionization

Electron drift

Amplification

Resistive

Induction

Readout

We know, Garfield++ is an excellent tool to simulate a MPGD. It can take care of many parameters involved.

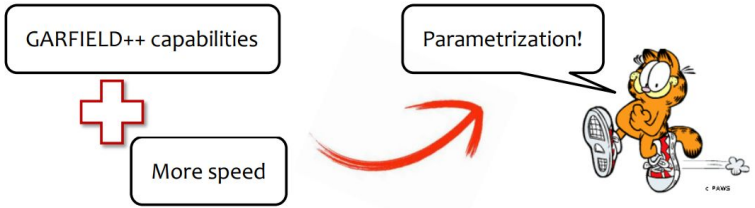
This approach is fine if we want to simulate a single event from the ionization to the readout.

We know also that the events are statistically different and then to evaluate the proper performance of a detector large statistic is needed.

Now, is the Garfield approach valid for large statistic? The detector parameters do not change (geometry, gas, HV) but it changes only the ionization and (of course) the signal induced on the readout.

Could we think about a tool to parametrize inside Garfield++ electron diffusion and amplification with dedicated simulation to speed-up large statistic simulation?

e.g. I simulate the GEM gain with 1M events and I create a gain distribution then if I have to do this simulation, I can sample from the distribution.
We could create repository and speed-up most of the simulation performed in the MPGD community.



Repositories

About repositories, we could share the code related to many simulation used for reproduce a MM, a GEM, a μRWELL.

There is an amazing User Guide for Garfield++ but we could create a guide also for application of Garfield++ for MPGD

e.g. extend the already existing pages [1] [2] with a “distributed code” to speed-up the knowledge sharing and the upgrades of the community

Resistive simulation

In literature there are several approaches to this problem [1] [2].

What about a **new class** inside Garfield++ to “filter” the induced current through the resistive layer?

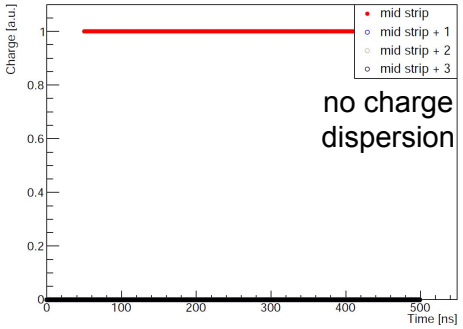
ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Nuclear Instruments and Methods in Physics Research A 566 (2006) 281–285
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima

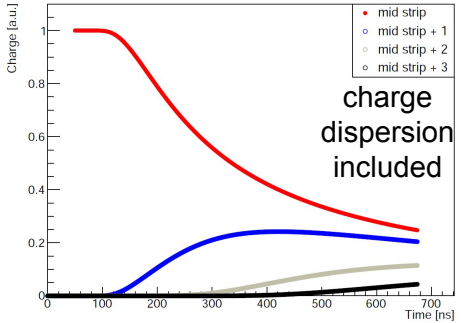
Simulating the charge dispersion phenomena in Micro Pattern Gas Detectors with a resistive anode

M.S. Dixit[a,b,*], A. Rankin[a]

customized for strip 1D

$$
\begin{aligned}
Q(t) &= \int_{x_1}^{x_2} \rho(x,t)\mathrm{d}x \\
&= \frac{q}{\sqrt{2\pi}\left[\sigma_0\left(1+\frac{t-t_0}{\tau}\right)\right]} \int_{x_1}^{x_2} \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2\left(1+\frac{t-t_0}{\tau}\right)^2}\right] \Theta\left(t-t_0\right)\mathrm{d}x \\
&= \frac{q}{2}\left[\mathrm{erf}\left(\frac{x_2-x_0}{\sqrt{2}\sigma_0\left(1+\frac{t-t_0}{\tau}\right)}\right) - \mathrm{erf}\left(\frac{x_1-x_0}{\sqrt{2}\sigma_0\left(1+\frac{t-t_0}{\tau}\right)}\right)\right] \Theta\left(t-t_0\right)
\end{aligned}
$$





Garfield++,Geant4 and digitization

Garfield++ is used by the detector community for R&D.

Geant4 is used the experiment community for physics performance.

Existing works already interface the two tools [1] [2].
Is there any official solution to use to energy deposited in Geant4 and transform it in primary electron to be used in Garfield++?

This is a question from FCC/CEPC communities where the detector digitization is needed and a simple smearing of the Geant4 track is not sufficient.

Readout segmentation

Now Garfield++ can simulate the induced signal and the electronics with the Sensor class.

This is an amazing results but, as far I know, inside a simulation only one sensor/pad/strip can be defined.

A segmented readout would allow to reproduce several electronic channels, similarly to a real detector.

modelling scintillation in gases (microscopically)

D. González-Díaz (IGFAE-USC)

with C. Azevedo (Univ. Aveiro), S. Biagi, M. Kuzniak (Astrocent, Warsaw), A. Saá-Hernández (IGFAE-USC)

scintillation in gases

State of the art

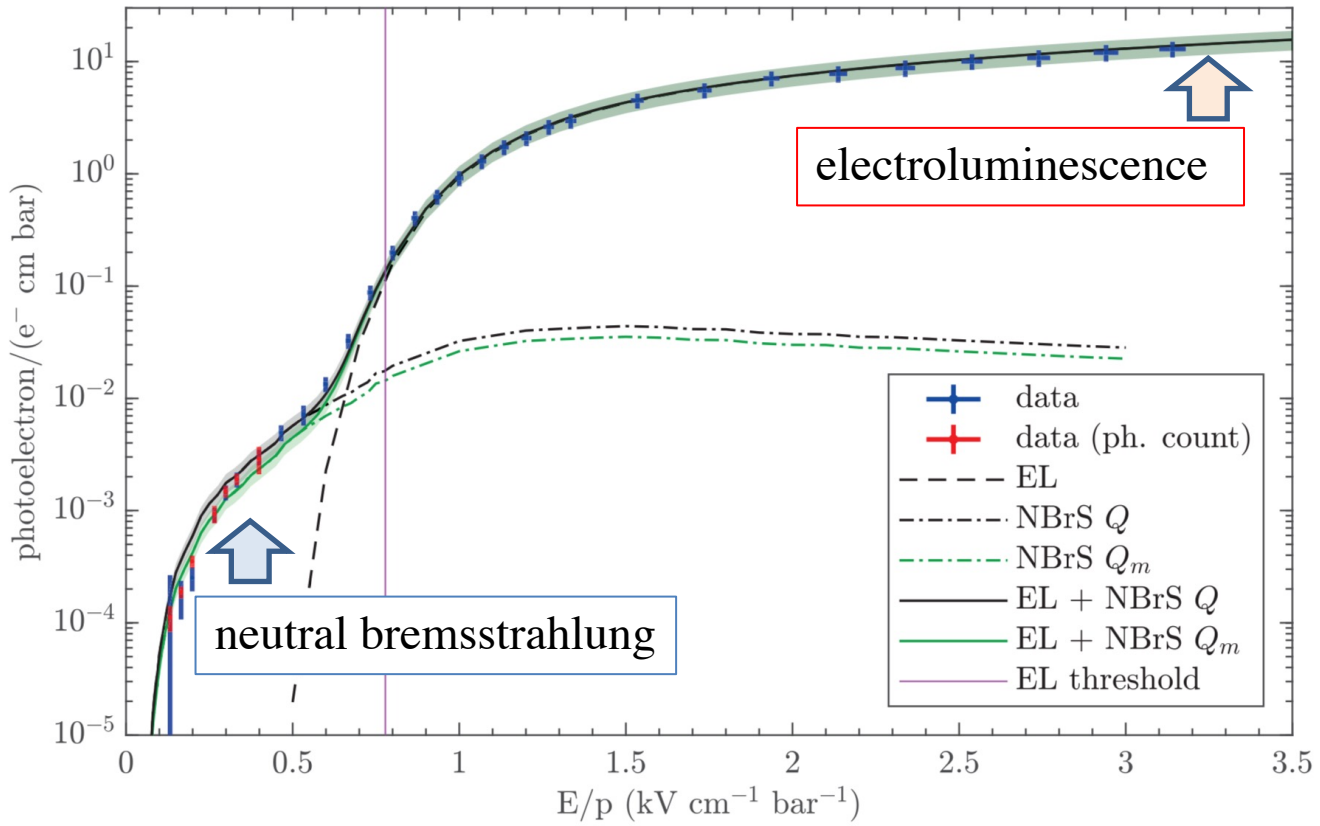
PHYSICAL REVIEW X **12,** 021005 (2022)

Neutral Bremsstrahlung Emission in Xenon Unveiled

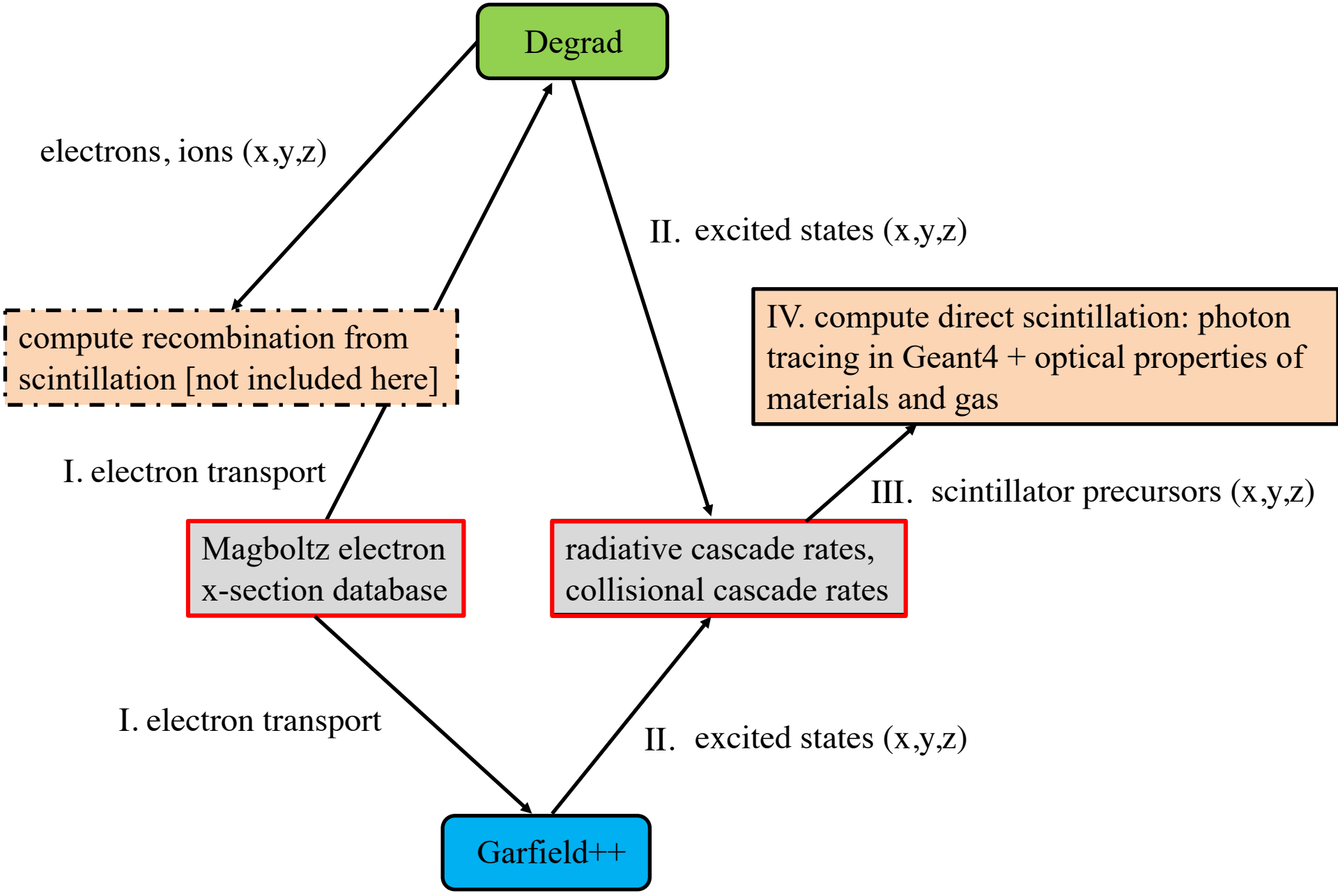
C. A. O. Henriques,[1,†] P. Amedo,[2] J. M. R. Teixeira,[1] D. González-Díaz,[2] C. D. R. Azevedo,[3] A. Para,[4] J. Martín-Albo,[5]

xenon scintillation in uniform fields

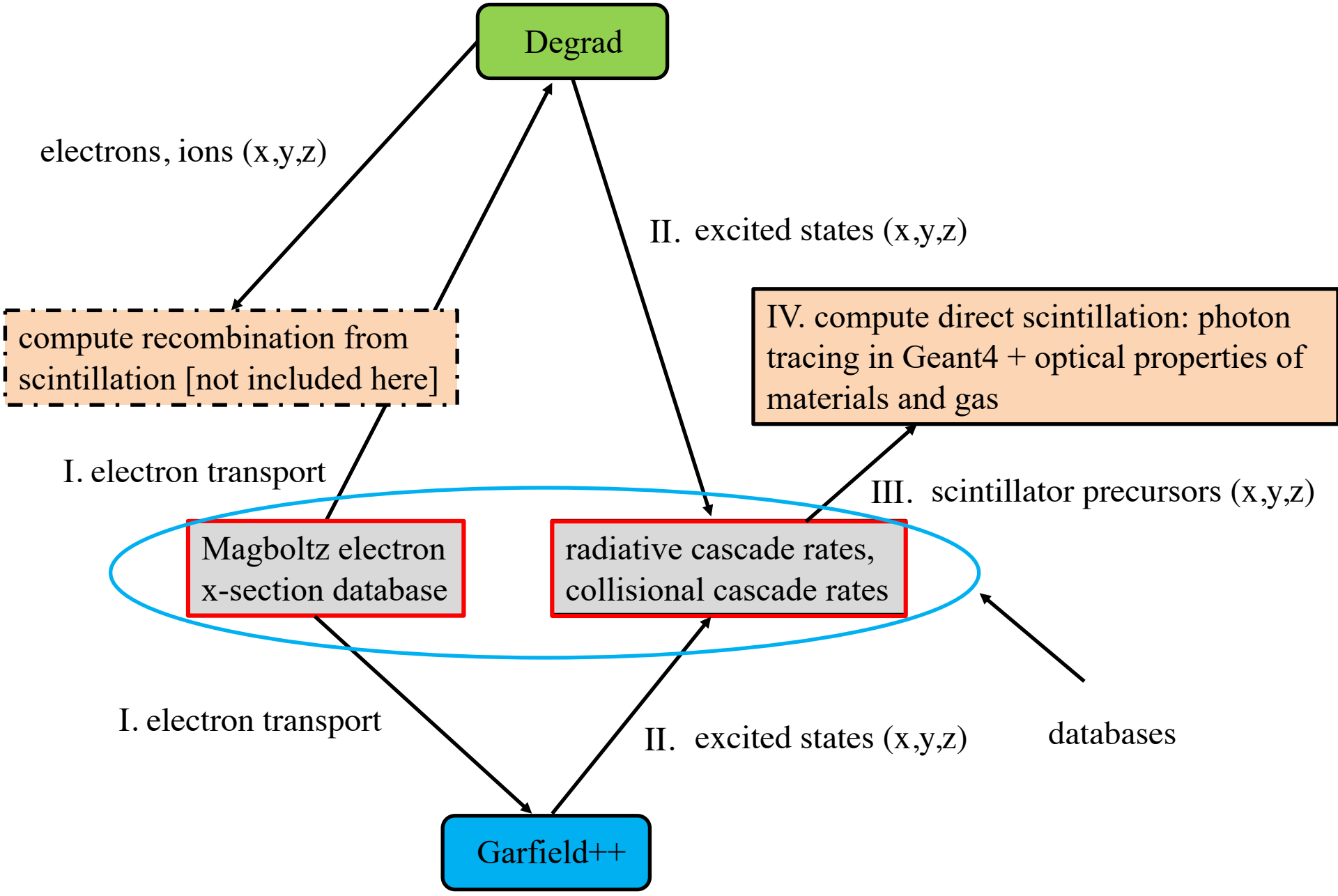
6 orders of magnitude!



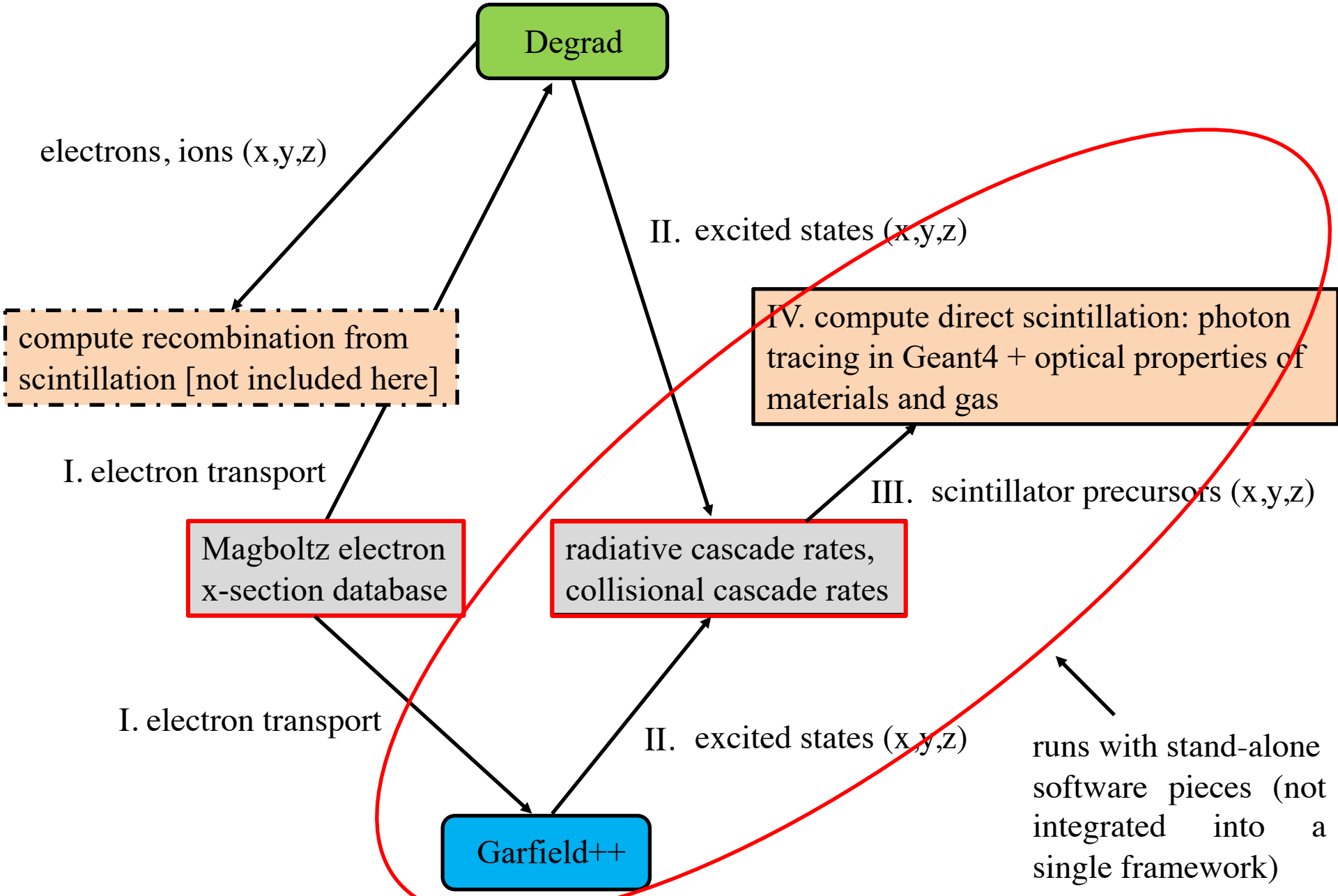
A microscopic code for computing scintillation



A microscopic code for computing scintillation



A microscopic code for computing scintillation



Example and history-line

scintillation in gases

II. Compute excited states

Physics Letters B 703 (2011) 217–222

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

A simulation toolkit for electroluminescence assessment in rare event experiments

C.A.B. Oliveira [a,*], H. Schindler [b], R.J. Veenhof [c,d], S. Biagi [e], C.M.B. Monteiro [f], J.M.F. dos Santos [f], A.L. Ferreira [a], J.F.C.A. Veloso [a]

III. Compute scintillation precursors

Nuclear Inst. and Methods in Physics Research, A 877 (2018) 157–172

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Microscopic simulation of xenon-based optical TPCs in the presence of molecular additives

C.D.R. Azevedo [a], D. González-Díaz [b,*], S.F. Biagi [c], C.A.B. Oliveira [d], C.A.O. Henriques [f],

Nuclear Inst. and Methods in Physics Research, A 935 (2019) 121–134

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Interfacing Geant4, Garfield++ and Degrad for the simulation of gaseous detectors

Dorothea Pfeiffer [a,b,*], Lennert De Keukeleere [c,**], Carlos Azevedo [d], Francesca Belloni [e], Stephen Biagi [f], Vladimir Grichine [g], Leendert Hayen [c], Andrei R. Hanu [h], Ivana Hřivnáčová [i], Vladimir Ivanchenko [b,j], Vladyslav Krylov [k,l], Heinrich Schindler [b], Rob Veenhof [b,m]

Eur. Phys. J. C (2021) 81:609
https://doi.org/10.1140/epjc/s10052-021-09316-0

THE EUROPEAN PHYSICAL JOURNAL C

Letter

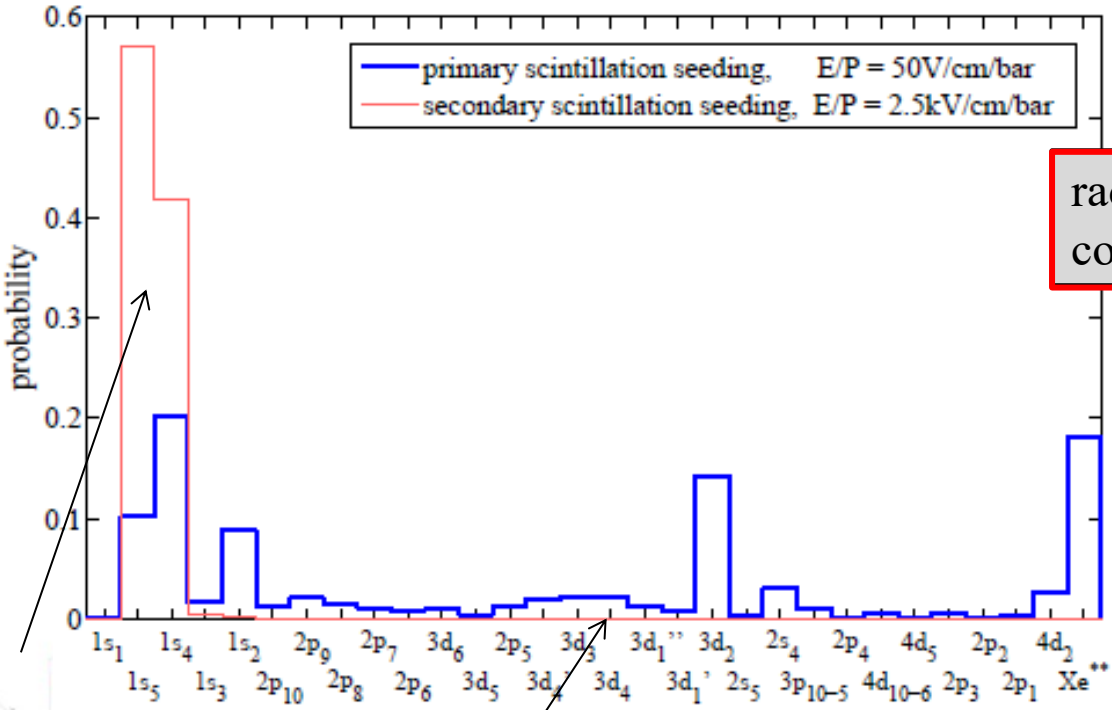
Development of very-thick transparent GEMs with wavelength-shifting capability for noble element TPCs

M. Kuźniak [1,a], D. González-Díaz [2,b], P. Amedo [2], C. D. R. Azevedo [3], D. J. Fernández-Posada [2], M. Kuźwa [1], S. Leardini [2], A. Leonhardt [8], T. Łęcki [5], L. Manzanillas [6], D. Muenstermann [7], G. Nieradka [1], R. de Oliveira [4], T. R. Pollmann [8,9], A. Saá Hernández [2], T. Sworobowicz [1], C. Türkoğlu [1], S. Williams [4]

IV. Integrate Geant4 and Garfield++

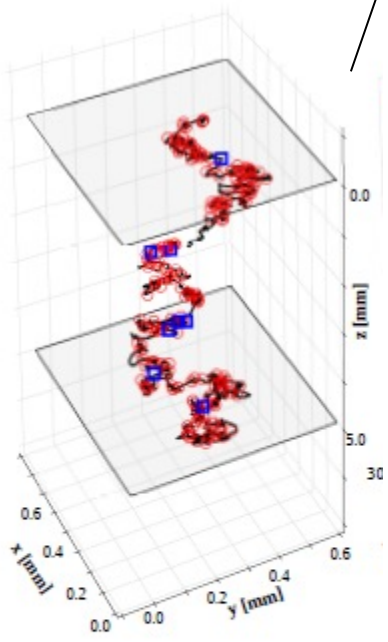
IV. Simulate optical response of MPGD structure

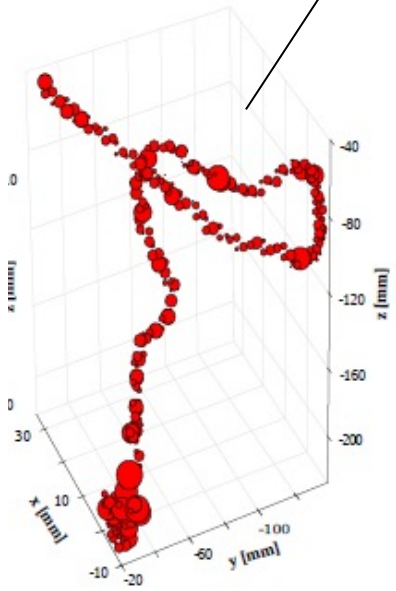
IIa. Computation of probability distribution of excited states



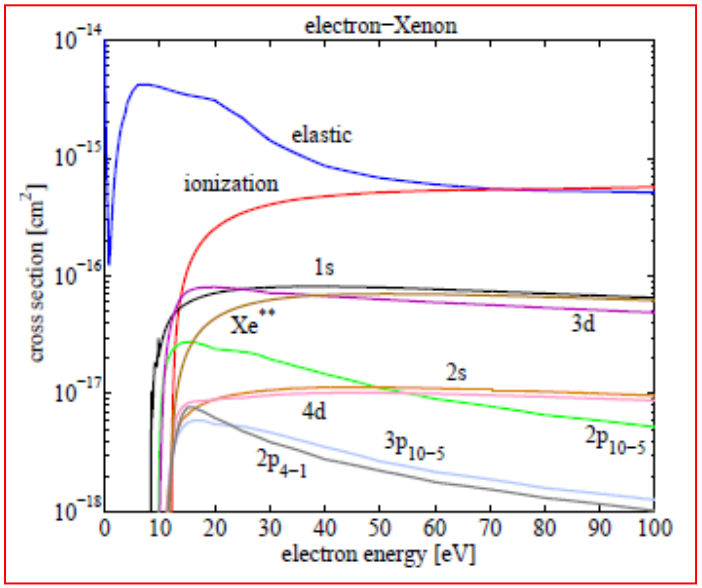
radiative cascade rates,
collisional cascade rates

Garfield++





Degrad



IIb. Computation of atomic cascade, including quenching

decay constant

2-body collision rates

3-body collision rates

radiative cascade rates,
collisional cascade rates

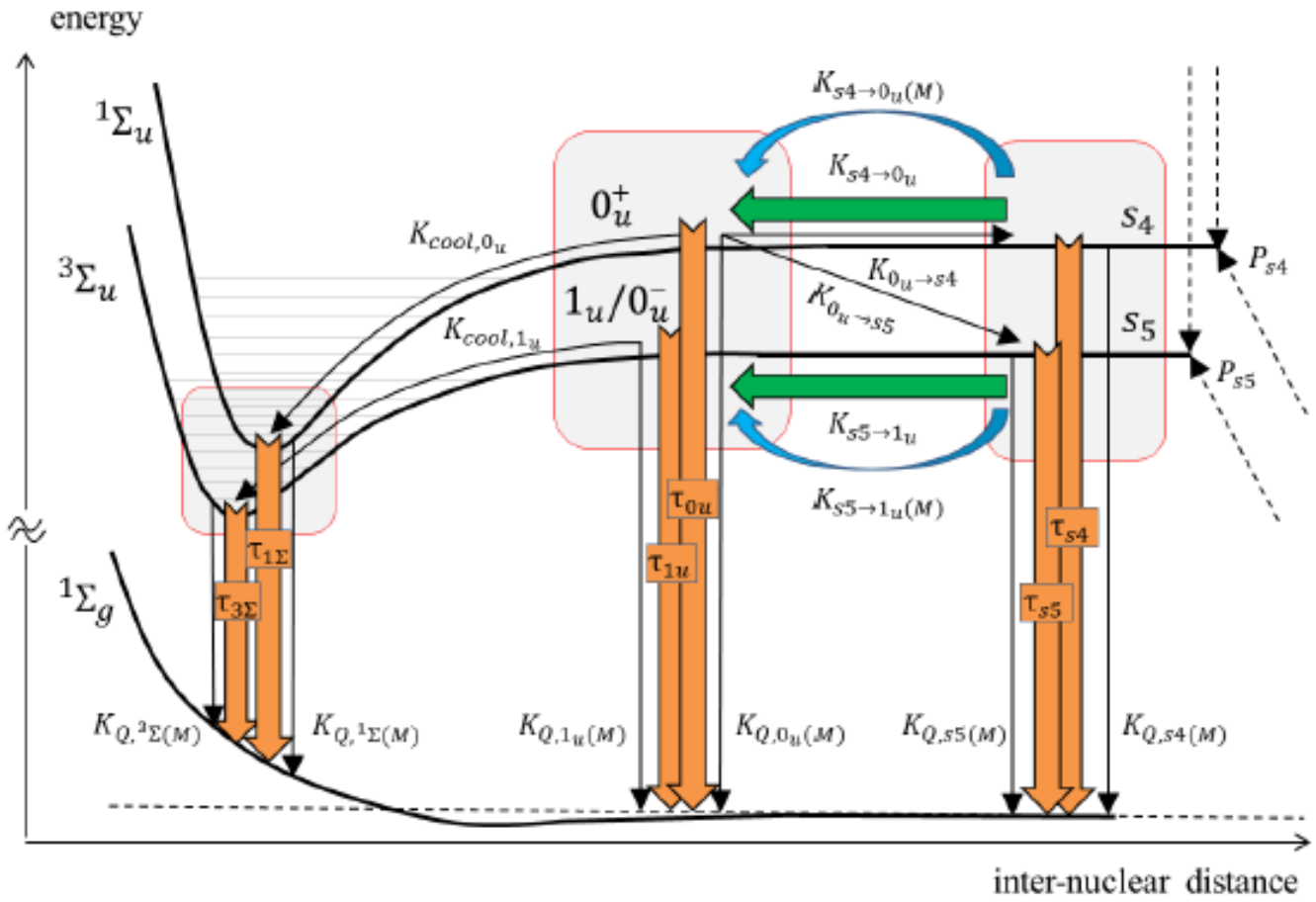
each value represents a vector!

state (Paschen)	state (Racah)	energy [eV]	$\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]	K_3@1bar [ns^{-1}]
$1s_1$	-	0.000	-	-	-
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}	0.1465
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	-	0.0855
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224	-
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	2.4954	-
$2p_{10}$	$6p[1/2]_1$	9.580	0.026	3.7802	-
$2p_9$	$6p[5/2]_2$	9.686	0.027	2.7425	-
$2p_8$	$6p[5/2]_3$	9.721	0.031	1.8036	-
$2p_7$	$6p[3/2]_1$	9.789	0.028	4.3979	-
$2p_6$	$6p[3/2]_2$	9.821	0.036	2.0062	-
$3d_6$	$5d[1/2]_0$	9.890	4.36×10^{-3}	9.7649	-
$3d_5$	$5d[1/2]_1$	9.917	$0.015/n_H$	4.8328	-
$2p_5$	$6p[1/2]_0$	9.933	0.031	0.1599	0.4273
$3d'_4$	$5d[7/2]_4$	9.943	4.34×10^{-3}	4.8676	-
$3d_3$	$5d[3/2]_2$	9.959	8.16×10^{-3}	4.8664	-
$3d_4$	$5d[7/2]_3$	10.039	7.34×10^{-3}	4.8510	-
$3d''_1$	$5d[5/2]_2$	10.157	1.21×10^{-3}	4.8649	-
$3d'_1$	$5d[5/2]_3$	10.220	1.39×10^{-3}	4.8639	-
$3d_2$	$5d[3/2]_1$	10.401	$3.04\times10^{-3}/n_H$	1.3637	-
$2s_5$	$7s[3/2]_2$	10.562	0.018	4.9415	-
$2s_4$	$7s[3/2]_1$	10.593	$0.178/n_H$	4.9415	-
$3p^*_{10-5}$	-	10.902	0.010	12.6008	-
$2p_4$	$6p[3/2]_1$	10.958	0.024	10.3277	-
$4d^*_{10-6,4,3}$	-	10.971	0.014	5.9298	-
$4d_5$	$6d[1/2]_1$	10.979	0.018	4.8426	-
$2p_3$	$6p[3/2]_2$	11.055	0.036	11.6125	-
$2p_2$	$6p[1/2]_1$	11.069	0.033	10.3277	-
$2p_1$	$6p[1/2]_0$	11.141	0.027	10.4018	-
$4d_2$	$6d[3/2]_1$	11.163	$0.716/n_H$	4.8674	-
Xe^{**}	-	11.7	-	12.35	-

-	$1s_1$	$1s_5$	$1s_4$	$1s_3$	$1s_2$	$2p_{10}$	$2p_9$	$2p_8$	$2p_7$	$2p_6$
$1s_1$	-	0	0	0	0	0	0	0	0	0
$1s_5$	$1^{(1)}$	-	0	0	0	0	0	0	0	0
$1s_4$	0	0	-	0	0	0	0	0	0	0
$1s_3$	0	$0.11^{(2,3)}$	$0.89^{(2,3)}$	-	0	0	0	0	0	0
$1s_2$	0	$0.010^{(2,3)}$	$0.079^{(2,3)}$	$0.247^{(3)}$	-	$0.663^{(4)}$	0	0	0	0
$2p_{10}$	0	$0.014^{(3)}$	$0.116^{(3)}$	$0.216^{(4)}$	$0.654^{(4)}$	-	0	0	0	0
$2p_9$	0	0	0	$0.3604^{(4)}$	$0.1351^{(3)}$	$0.405^{(4)}$	-	$0.099^{(4)}$	0	0
$2p_8$	0	0	0	$0.178^{(3)}$	$0.110^{(3)}$	$0.245^{(3)}$	$0.466^{(3)}$	-	0	0
$2p_7$	0	0	0	$0.348^{(3)}$	$0^{(2)}$	$0.011^{(2)}$	$0.067^{(2)}$	$0.539^{(2)}$	-	$0.034^{(3)}$
$2p_6$	0	0	0	$0.234^{(3)}$	$0.001^{(2)}$	$0.001^{(2)}$	$0.345^{(3)}$	$0.259^{(3)}$	$0.161^{(3)}$	-

it is mostly a parameter matrix
and a cascade software
(stand-alone)

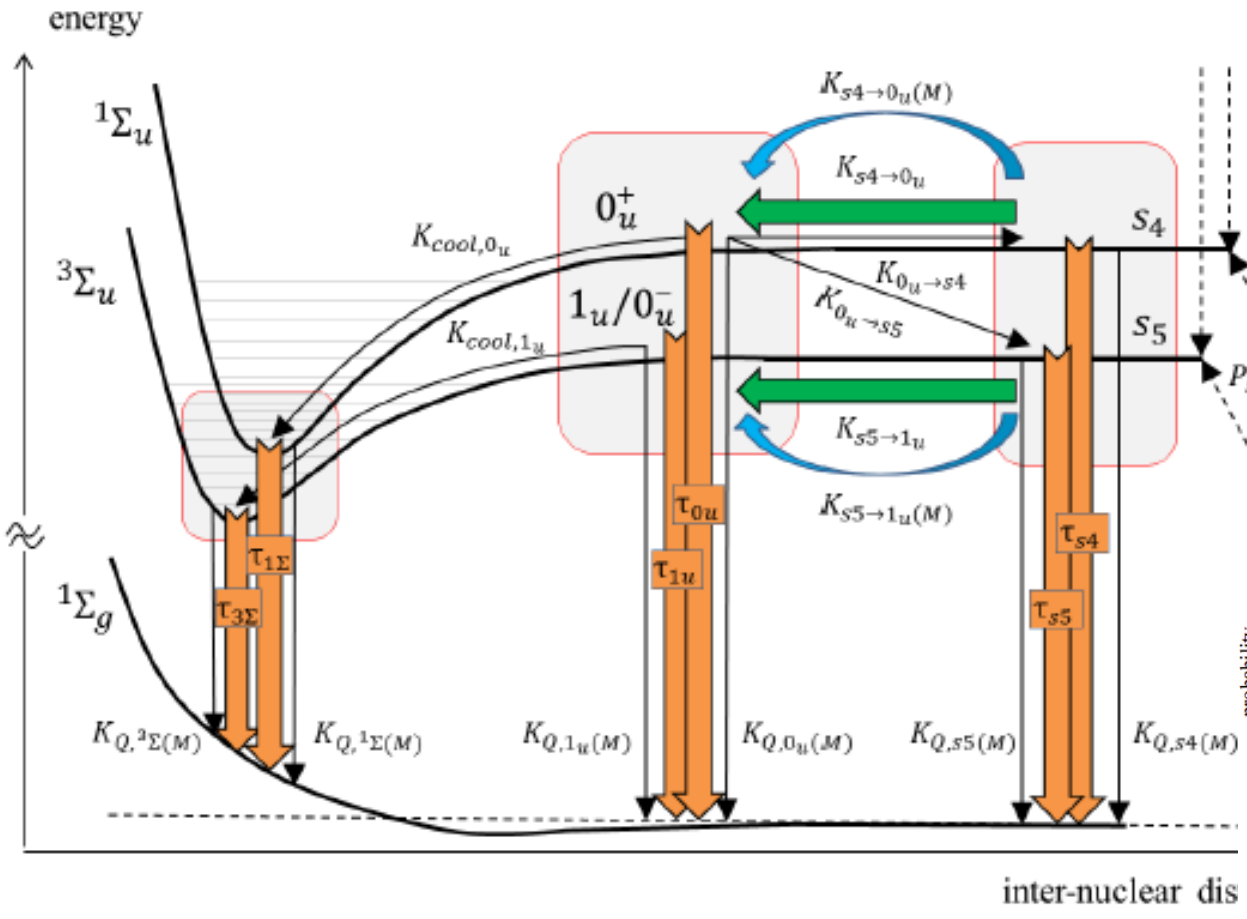
IIc. Formation of scintillation precursors (excimers), including quenching



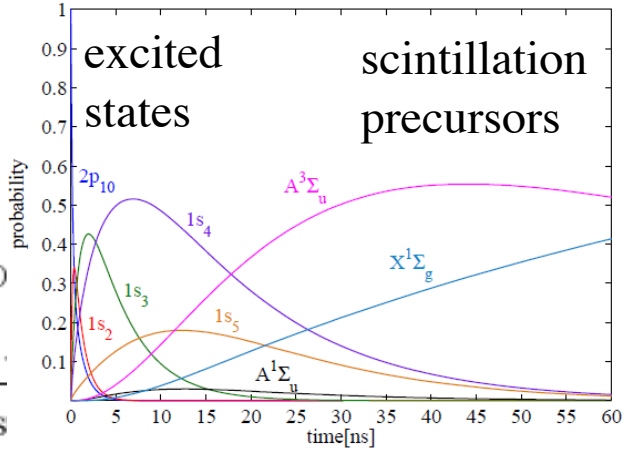
radiative cascade rates,
collisional cascade rates

$\tau_{^3\Sigma}$	100 ns$^{(1)}$	$K_{Q,^3\Sigma(M)}$	11.12 ns^{-1}	$K_{s_5\to 1_u}$	0.1465 ns$^{-1\,(1)}$	$K_{s_5\to 1_u(M)}$	116 ns^{-1}
$\tau_{^1\Sigma}$	4.55 ns$^{(1)}$	$K_{Q,^1\Sigma(M)}$	12.85 ns^{-1}	$K_{s_4\to 0_u}$	0.0855 ns$^{-1\,(1)}$	$K_{s_4\to 0_u(M)}$	116 ns$^{-1\,(6)}$
τ_{1_u}	40 ns$^{(1)}$	$K_{Q,1_u(M)}$	11.12 ns^{-1}	$K_{0_u\to s_4}$	1.43 ns$^{-1\,(1)}$		
τ_{0_u}	5 ns$^{(1)}$	$K_{Q,0_u(M)}$	12.85 ns^{-1}	$K_{0_u\to s_5}$	6.42 ns$^{-1\,(1)}$		
τ_{s_5}	42 s$^{(2)}$	$K_{Q,s_5(M)}$	11.12 ns$^{-1\,(4)}$	$K_{cool,0_u}$	1.72 ns$^{-1\,(1)}$		
τ_{s_4}	$3.56 \times n_H$ ns$^{(3)}$	$K_{Q,s_4(M)}$	12.85 ns$^{-1\,(5)}$	$K_{cool,1_u}$	1.72 ns$^{-1\,(1)}$		

IIc. Formation of scintillation precursors (excimers), including quenching



radiative cascade rates,
collisional cascade rates



$\tau_{3\Sigma}$	100 ns$^{(1)}$	$K_{Q,^3\Sigma(M)}$	11.12 ns^{-1}	$K_{s_5\to 1_u}$	0.1465 ns$^{-1\,(1)}$	$K_{s_5\to 1_u(M)}$	116 ns^{-1}
$\tau_{1\Sigma}$	4.55 ns$^{(1)}$	$K_{Q,^1\Sigma(M)}$	12.85 ns^{-1}	$K_{s_4\to 0_u}$	0.0855 ns$^{-1\,(1)}$	$K_{s_4\to 0_u(M)}$	116 ns$^{-1\,(6)}$
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τ_{0_u}	5 ns$^{(1)}$	$K_{Q,0_u(M)}$	12.85 ns^{-1}	$K_{0_u\to s_5}$	6.42 ns$^{-1\,(1)}$		
τ_{s_5}	42 s$^{(2)}$	$K_{Q,s_5(M)}$	11.12 ns$^{-1\,(4)}$	$K_{cool,0_u}$	1.72 ns$^{-1\,(1)}$		
τ_{s_4}	$3.56 \times n_H$ ns$^{(3)}$	$K_{Q,s_4(M)}$	12.85 ns$^{-1\,(5)}$	$K_{cool,1_u}$	1.72 ns$^{-1\,(1)}$		

III. Photon tracing (Geant4)

scintillation in gases

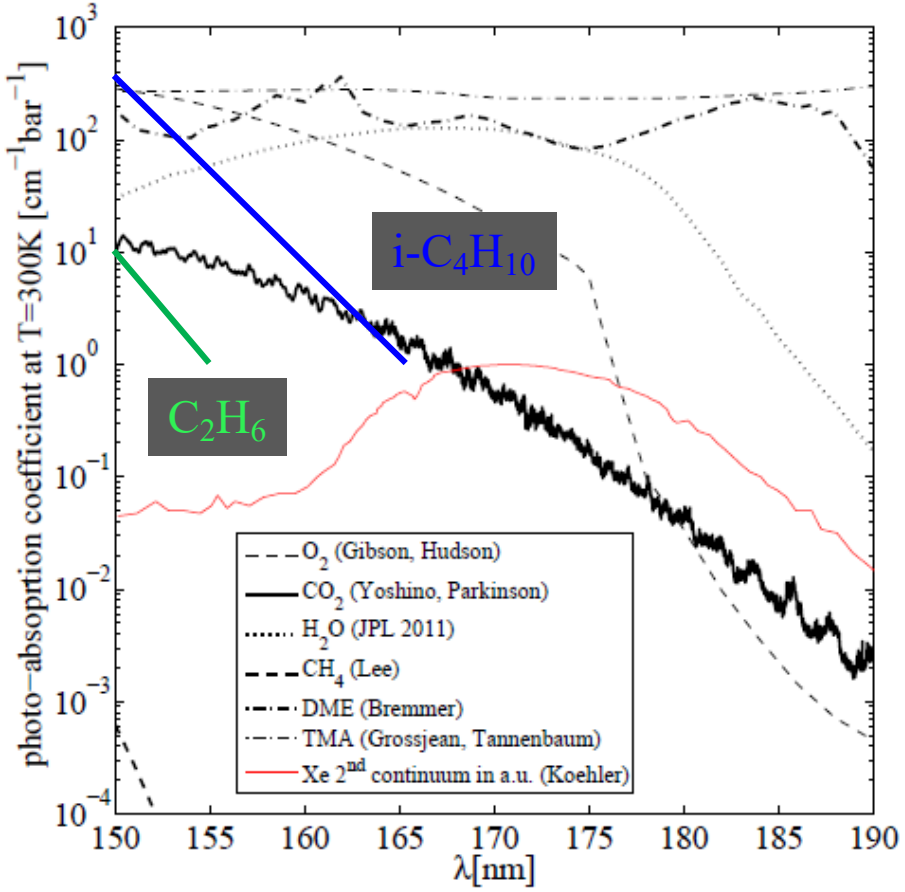
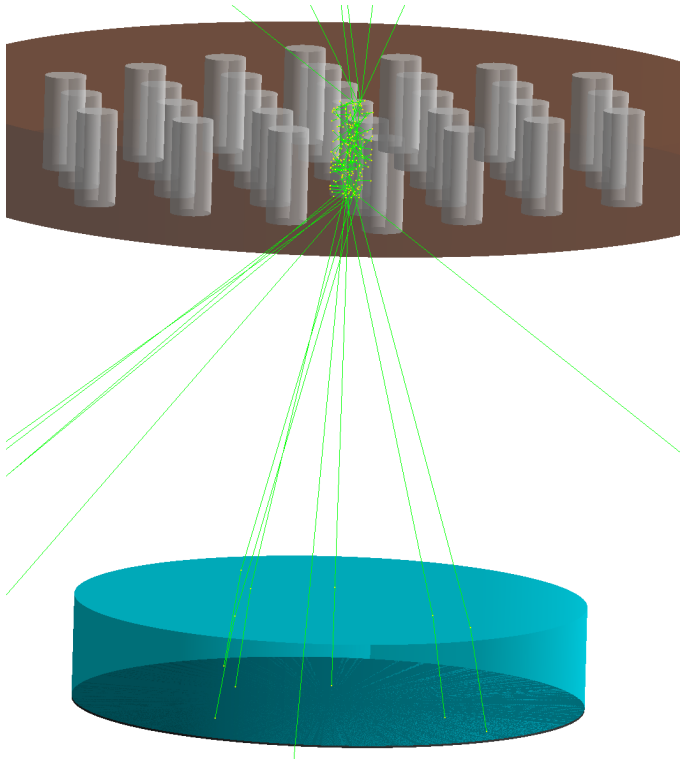
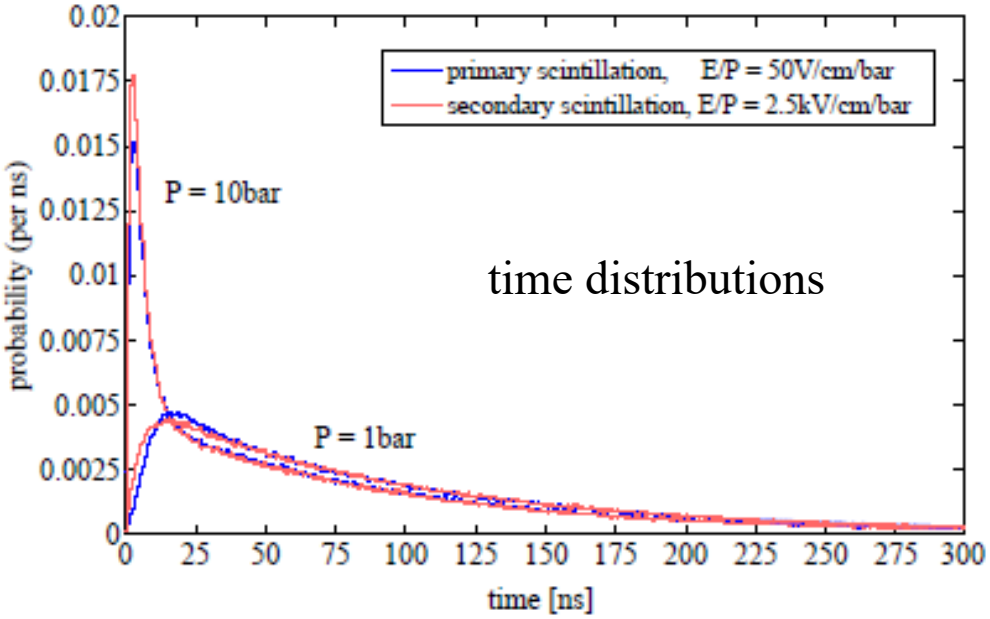


Fig. 1. Compilation of photo-absorption coefficients of some relevant TPC admixtures at around $T = 300$K in the region corresponding to the Xenon 2nd continuum, [9–18]. The reference spectrum from Koehler has been overlaid as a thin continuous line [2]. For H_2, N_2 and CF_4 there is no data in the region shown, and their cross-sections are plausibly orders of magnitude below that of CH_4.

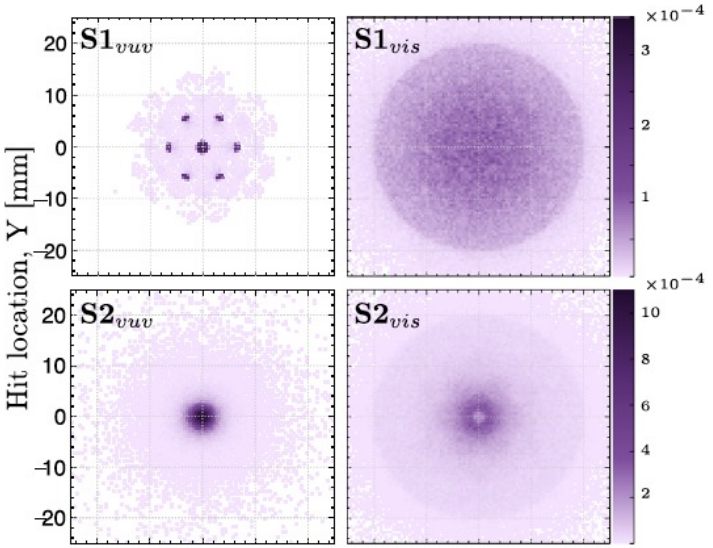


$$\Pi = \frac{1}{P_o} N_o \sigma_a(\lambda)$$

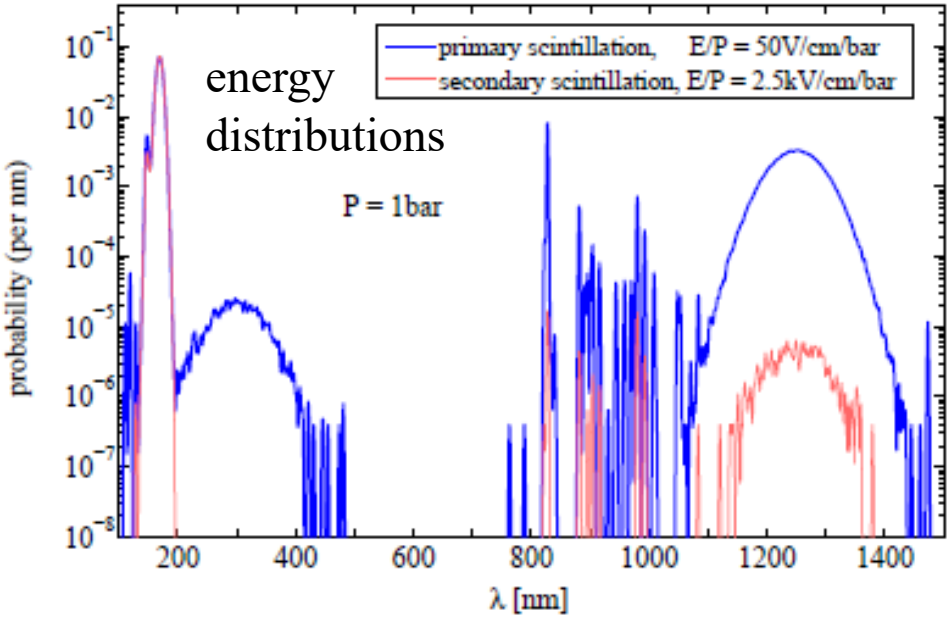
Illustrative photon outputs



time distributions



spatial distributions



Nuclear Inst. and Methods in Physics Research, A 877 (2018) 157–172

Eur. Phys. J. C (2021) 81:609
https://doi.org/10.1140/epjc/s10052-021-09316-0

Status

- Tools for computing primary and secondary scintillation for pure gases and mixtures exist.
- They allow obtaining (λ, t, x, y, z).
- Big effort done for xenon.

- Argon started but stopped due to lack of manpower.
- Integration with Garfield++ started but stopped due to lack of manpower.
- Integration with Pyboltz started but stopped due to lack of manpower.

Outlook

- In the absence of additional funds or manpower, wait for an opportunity to develop the above items.

Attachment and recombination in gaseous detectors
Medical Physics Applications

Faustino Gómez , José Paz, Diego González-Castaño,
Nicolás Gómez-Fernández

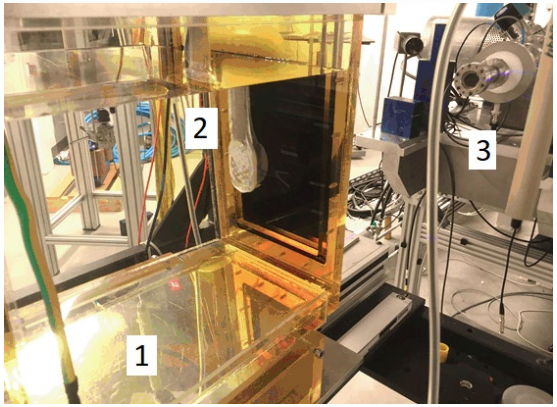
Dpt. Particle Physics
Radiation Physics Laboratory
University of Santiago de Compostela, Spain

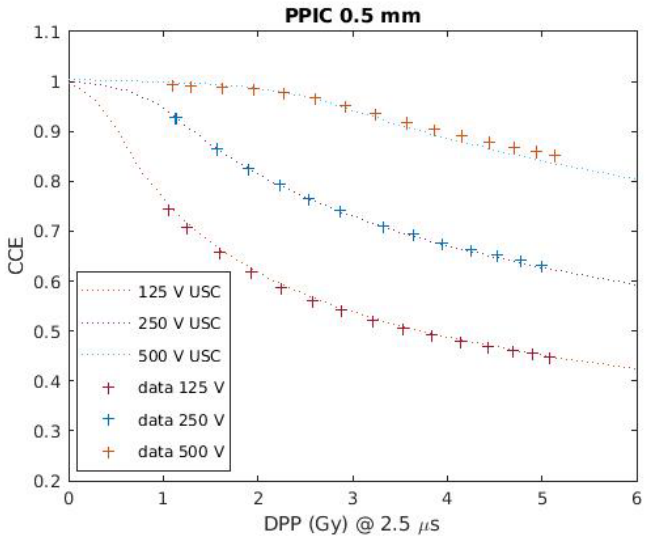
RD51 February 2023 collaboration meeting

USC
UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

The recombination problem

- FLASH radiotherapy has challenged the use of ionization chambers as secondary standard for dosimetry (especially electron beams).
- Current knowledge of recombination is poor and analytical models do not describe correctly the effect.
- Electron deliveries can produce an instantaneous dose rate of 3 MGy/s





USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

The recombination problem

Considering symmetry along the transverse dimensions (y and z), the system of differential equations can be written as a one-dimensional effective problem along the coordinate (x) perpendicular to the electrode planes,

$$
\begin{aligned}
\frac{\partial n_+(x,t)}{\partial t} &= I(x,t) - \alpha\, n_+(x,t)\, n_-(x,t) - \theta\, n_+(x,t)\, n_e(x,t) + g(x,t)\, v_e(x,t)\, n_e(x,t) + \\
&\quad + \frac{\partial}{\partial x}\left[D_+(x,t)\,\frac{\partial n_+(x,t)}{\partial x}\right] - \frac{\partial}{\partial x}\left[E(x,t)\,\mu_+\, n_+(x,t)\right], \\
\frac{\partial n_-(x,t)}{\partial t} &= \gamma\, n_e(x,t) - \alpha\, n_+(x,t)\, n_-(x,t) + \\
&\quad + \frac{\partial}{\partial x}\left[D_-(x,t)\,\frac{\partial}{\partial x} n_-(x,t)\right] + \frac{\partial}{\partial x}\left[E(x,t)\,\mu_-\, n_-(x,t)\right], \\
\frac{\partial n_e(x,t)}{\partial t} &= I(x,t) - \gamma\, n_e(x,t) - \theta\, n_+(x,t)\, n_e(x,t) + g(x,t)\, v_e(x,t)\, n_e(x,t) + \\
&\quad + \frac{\partial}{\partial x}\left[D_e(x,t)\,\frac{\partial}{\partial x} n_e(x,t)\right] + \frac{\partial}{\partial x}\left[v_e(x,t)\, n_e(x,t)\right],
\end{aligned}
\tag{1}
$$

Symbol	Unit	Definition
n_+, n_-, n_e	m^{-3}	Positive ion, negative ion ane electron density, respectively
I	$m^{-3}\,s^{-1}$	Charge liberated per unit time and volume that escapes initial recombination
α	$m^3\,s^{-1}$	Volume recombination coefficient between ions
θ	$m^3\,s^{-1}$	Volume recombination coefficient between electron and positive ions
g	m^{-1}	First Townsend coefficient
γ	s^{-1}	Electron attachment coefficient
μ_+, μ_-	$m^2\,V^{-1}\,s^{-1}$	Positive and negative ion mobility, respectively
v_e	$m\,s^{-1}$	Electron drift velocity
D_+, D_-, D_e	$m^2\,s^{-1}$	Positive, negative ion and electron diffusion coefficient
E	$V\,m^{-1}$	Electric field across the ionization chamber
V	V	Voltage applied to the ionization chamber
d	m	Distance between electrodes
e	C	Elementary charge
ϵ	$C\,V^{-1}\,m^{-1}$	Air permittivity

The recombination problem

Mathematical description of charge carrier transport

The electric field dependence across the chamber can be computed solving the one dimensional *Poisson* equation:

$$\frac{\partial E(x,t)}{\partial z} = \frac{e}{\epsilon}\left[n_+(x,t) - n_-(x,t) - n_e(x,t)\right], \tag{2}$$

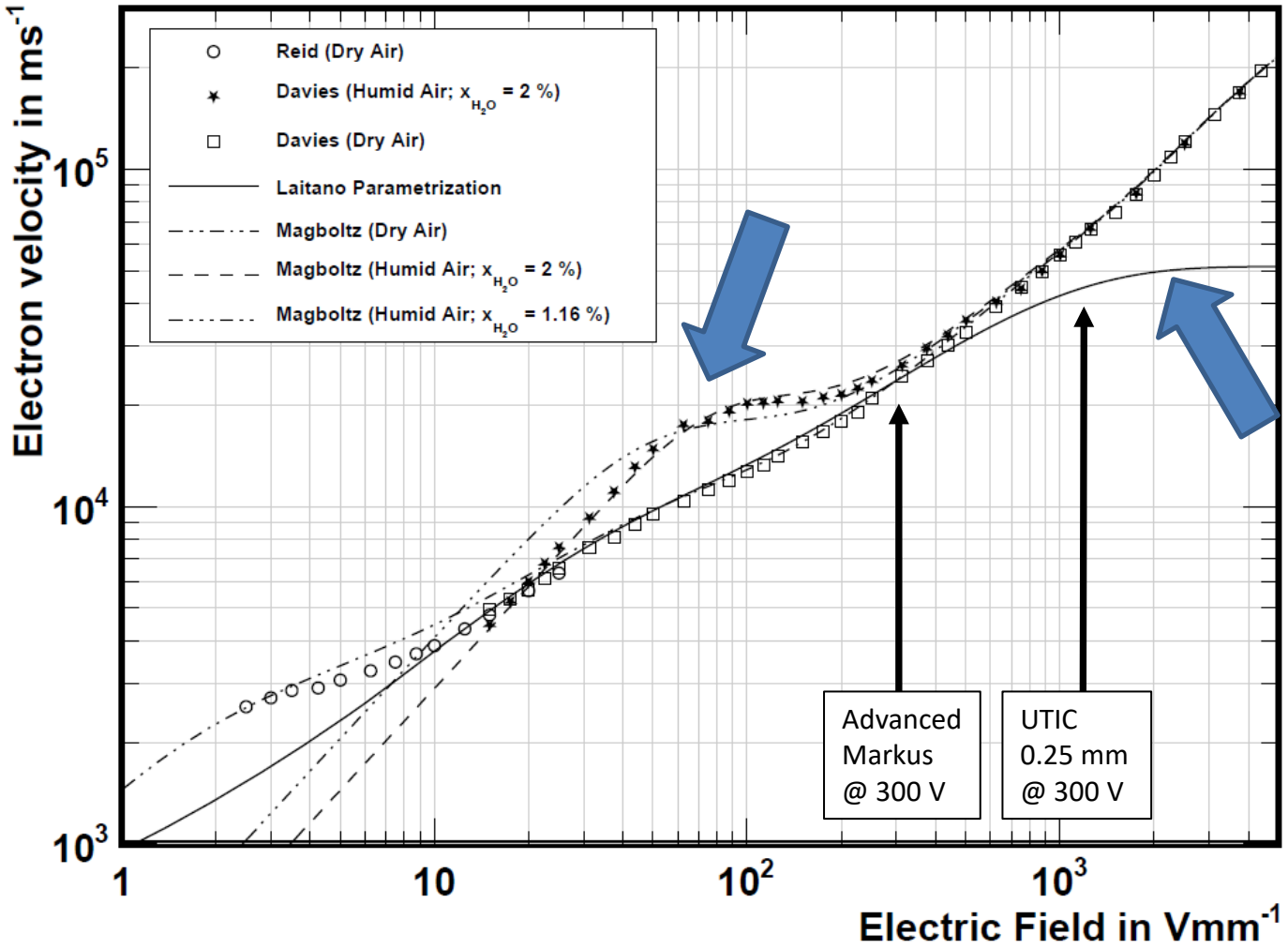
If we assume that the behaviour of high voltage supply do not disturb the ideal potential between the electrodes separated by the distance d, then

$$\int_0^d E(x,t)\, dz = V \quad \forall t \tag{3}$$

The instantaneous current produced at any time may be calculated using the Shockley-Ramo theorem

$$I_{IC}(t) = \frac{e}{d}\,\Delta x \sum_{i=0}^{N}\left[\mu_+ E(x_i,t) n_+(x_i,t) + \mu_- E(x_i,t) n_-(x_i,t) + v_e(x_i,t) n_e(x_i,t)\right]. \tag{4}$$

Humidity matters



Electron drift velocity as a function of electric field is substantially different in humid air respect to dry air for moderate electric field (~100 V/mm)

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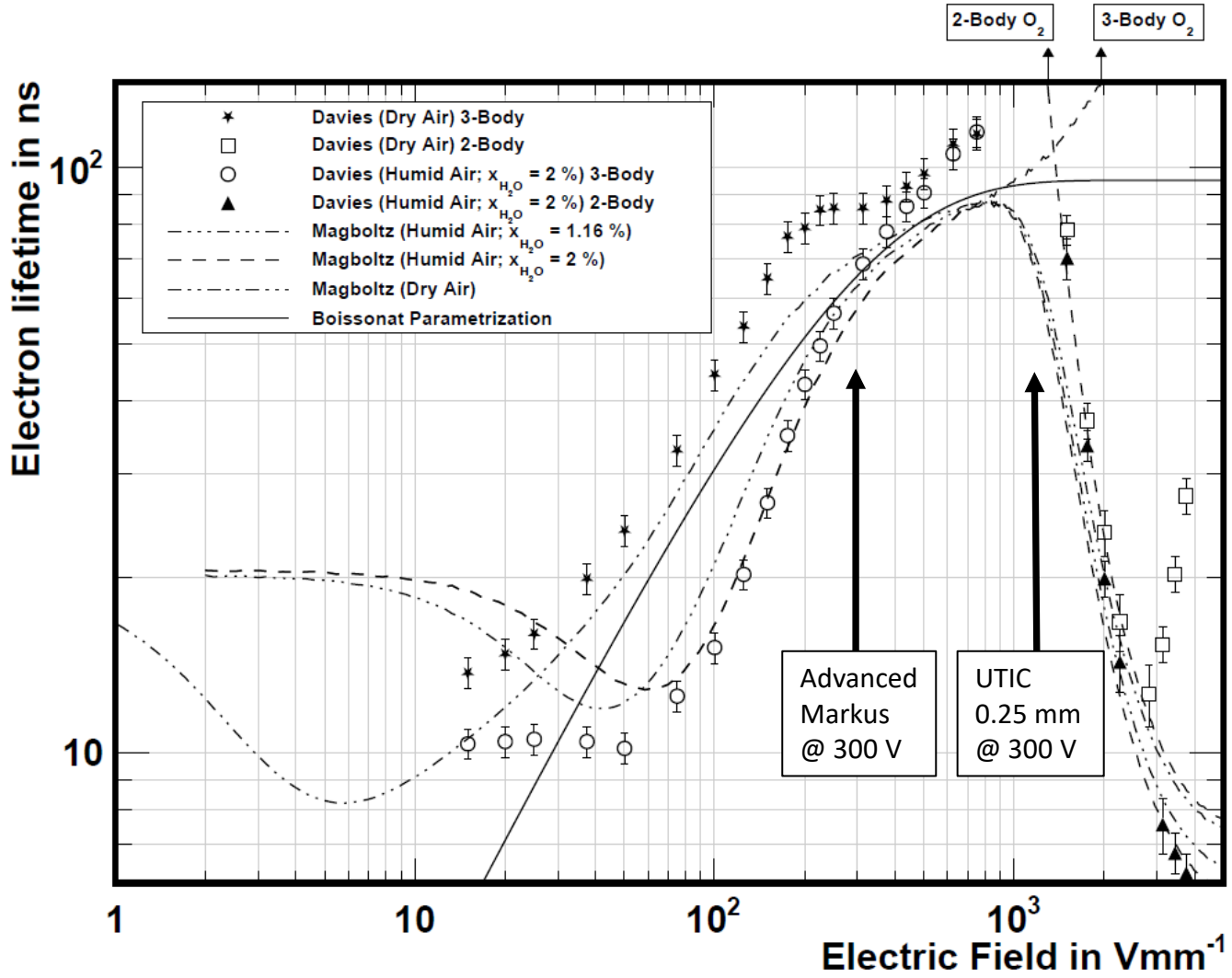
Electron attachment



The use of electric fields in excess of ~1500 V/mm will enhance the two-body attachment processes and can yield an effective reduction of electron lifetime.

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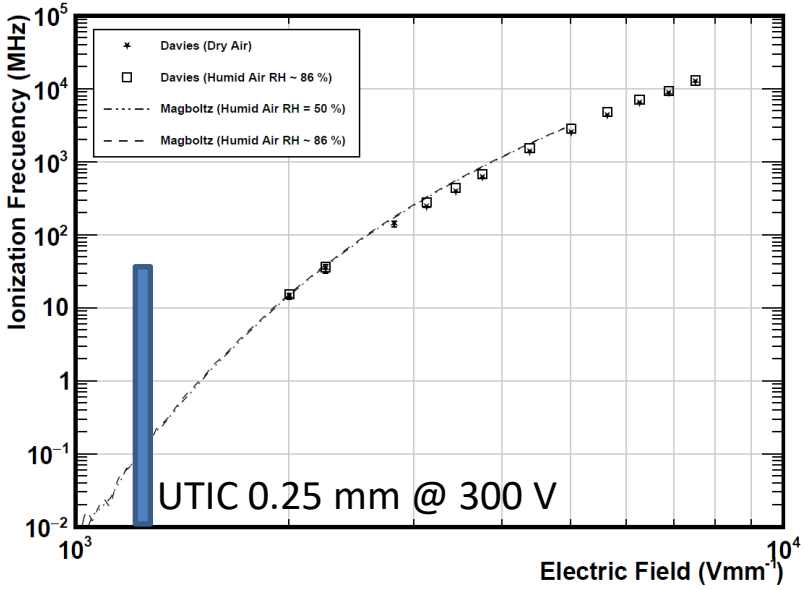
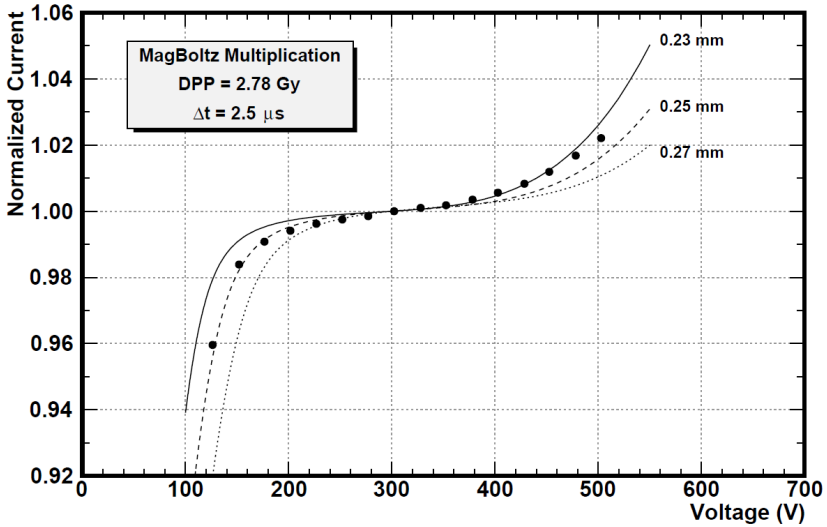
Charge multiplication



First Townsend coefficient has very limited experimental data in the region of electric field used in ICs. Figure shows MonteCarlo method results from Magboltz.



Simulation of charge multiplication for the Ultra Thin Ionization Chamber (0.25 mm) chamber. Data from Rafael Kranzer (PTW).

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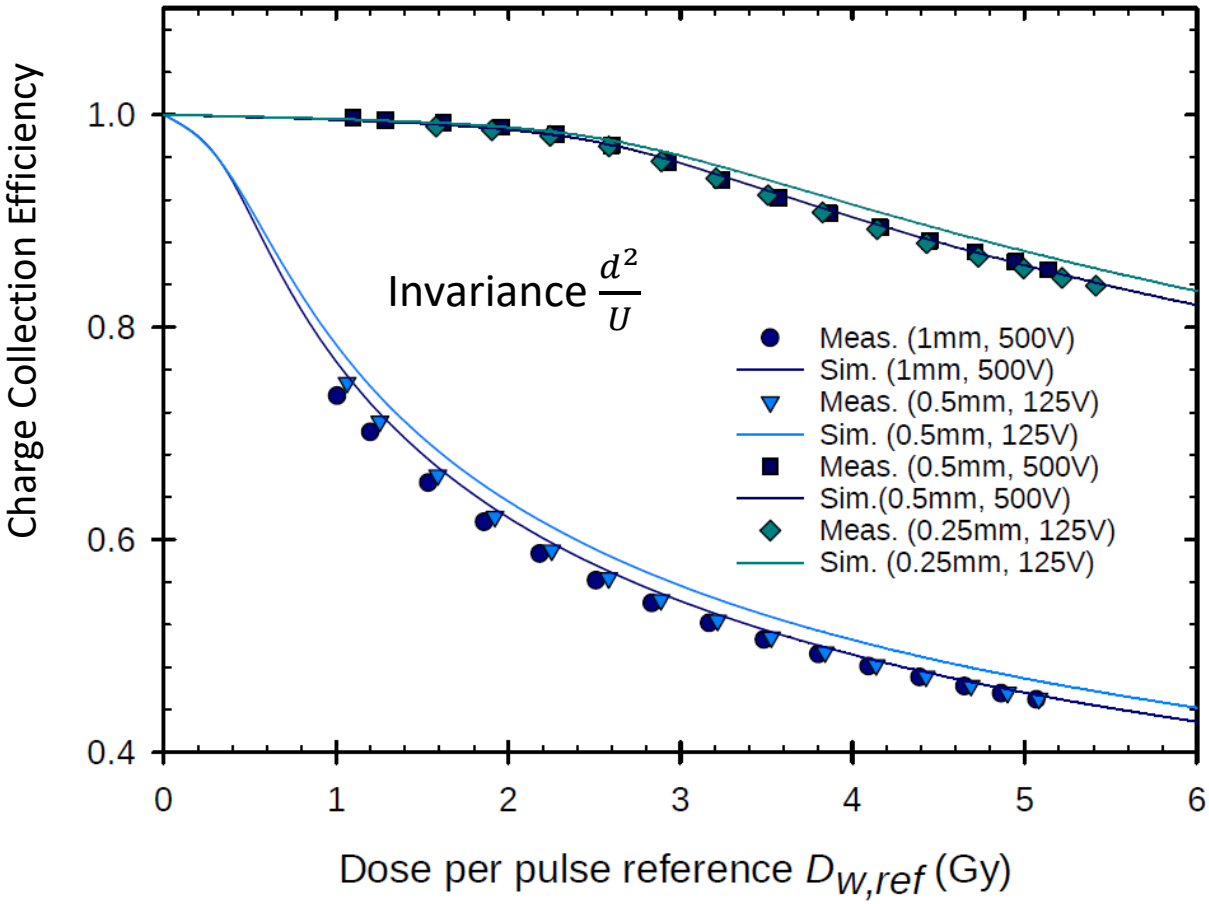
Numerical models



Limited agreement between models and data.
Data from Rafael Kranzer (PTW) and Andreas Schüeller (PTB).

UHDpulse

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Conclusions

- We need a better knowledge of ion and electron mobilities in air and their dependence with ambient conditions.
- Electron attachment (lifetime) through 2 and 3 body processes is poorly parametrized in many of the dosimetry articles.
- Ion-ion and electron-ion recombination coefficients has a large uncertainty (>10%). We even do not know if they have a dependence on the electric field and ambient conditions.
- Current work has lead to a probable modification of the DIN protocol for dosimetry and the international Code of Practice.

Missing Topics

- **Ion clustering and ion drift velocity**
  - Measurements of the clusters (laser)
  - Solve differential equations – Model drifting ions
  - Include drift velocities for different ions in Garfield++

- **Other missing topics?**
  - Please raise your hand – or write email

At the end some personal thoughts

- **Enlarge group of knowledgable people → create group of future SW developers**
  - **Simulation school** … *one afternoon is good start … but for simulations students need a project they can work on for a month … conveners can provide support (often supervisor at home institute cannot help debugging … creating group for mutual help*
- **Make tools more easy to use – *especially interface with other SW***
- **Make people contributing to the same project / same framework**
  - *Maximalize impact of mainting this software centrally / by the collaboration*
  - *Magboltz is FORTRAN, one-man project, need to decide how to move in future*
- ***Bring the software into the 21st century***
  - *Parallelize: MPI, openMP*
  - *Accellerators: GPU, FPGA,*
  - *New techniques: Neural networks, Machine learning, …*
  - *Modern code base for Garfield++ with automatic tests of pull requests etc …*
  - *Need help/input from software engineers … knowledge of CPU Architecture, CUDA programming, advanced programming skills, …*
  - *Example: ourobouros software developed, but developer moved on … include space-charge effects with BEM method inside Garfield++*
- ***Make SW work more attractive and more visible, give right recognition!***
  - *Stimulate mix of Hardware & SW work – only few examples*
- **Get dedicated funding**
  - *Knock on the door … and keep knocking … SW development is in ECFA Roadmap*
  - *For EU funding need to reach out to industry (Plasma SW, SiPM simulations, …) need your HELP*

WG4 and Work Packages (WP) ?

- **Disclaimer:**
  - *I am not fully updated on the idea of WP – very busy week … often working during meetings*
- **Not sure how WPs can fit best into WG4:**
  - *We should avoid at all costs that work ongoing right now in WG4 gets blocked or hurdled because of not finding the right WP, not passing review of Funding Agencies*
  - *Should have a low-level entry ticket to individuals / small-size institutes*
- **Two Possibilities:**
  - *Encourage all proponents submitting WPs to include a task in simulation and trying to maximize what can be done for SW Development*
    - *All people working in various WPs on simulation can then meet in WG4 sessions*
    - Pro: groups tend to work more on Simulation & SW when they have direct benefit of the SW they are developing
    - Neg: continuity, de-centralized work on SW, maybe not well coordinated, … ?
  - *One or few WG4 dedicated WPs:*
    - E.g. maintenance and development of Garfield++
    - Will allow to have funding for PhD, Postdoc, Experts to work on SW
    - Pro: centralized, WG/WP should keep an eye on all players in DRD1 and make sure usefulness
  - *Likely we end up with a mix of the above?*
- **Questions – Suggestions?**