

# School

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# Why computer models ?

- ▶ Less work than building actual detectors.
- ▶ Cheaper:
  - ▶ in particular when studying noble gases.
- ▶ Easier to modify the parameters of the model:
  - ▶ makes it e.g. easy to understand how the gas composition influences the transport parameters of electrons in gas mixtures.

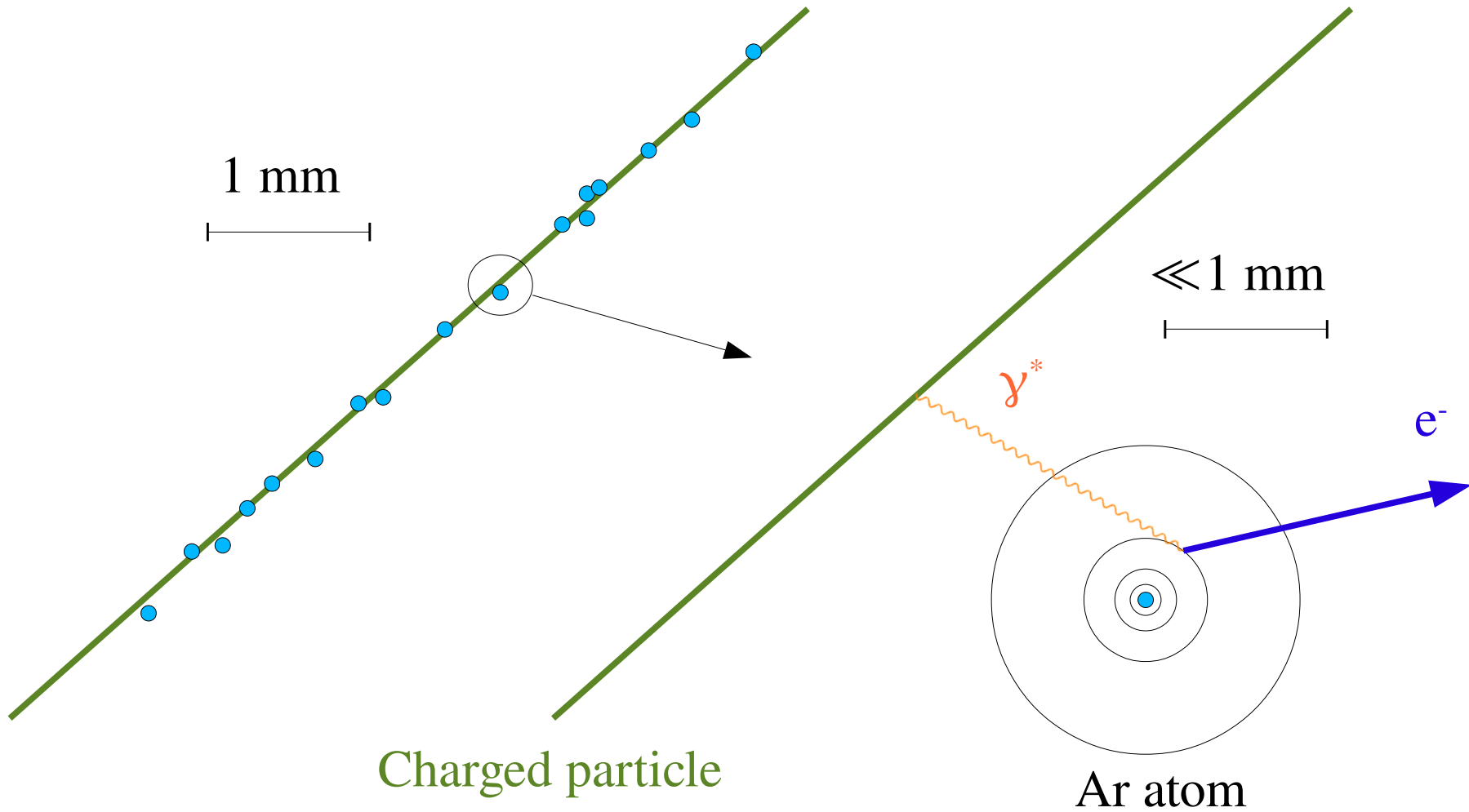
# Which models ?

- ▶ What do we currently model and simulate ?
  - ▶ ionisation trace from charged particles;
  - ▶ electric and magnetic fields, govern motion of ions & electrons;
  - ▶ properties of gas mixtures;
    - ▶ velocity of electrons and ions;
    - ▶ diffusion of electrons (for ions see Mason & McDaniel et al.);
    - ▶ electron attachment (2-body and 3-body);
    - ▶ ionisation and excitation;
    - ▶ electron avalanches;
  - ▶ ion chemistry;
  - ▶ calculation of signals, now also with resistive layers;
  - ▶ wire sagging;
  - ▶ replacement of environment- contaminating gases.

# Ionisation - How

- ▶ SRIM low energy charged particles;
- ▶ dE dx common charged particles;
- ▶ PAI idem, only energy loss;
- ▶ Heed idem, with shell structure.

# Virtual photon exchange



# Basic formulae of the PAI model

► Key ingredient: photo-absorption cross section  $\sigma_y(E)$

$$\frac{\beta^2 \pi}{\alpha} \frac{d\sigma}{dE} = \frac{\sigma_y(E)}{E} \log \left( \frac{1}{\sqrt{(1-\beta^2 \epsilon_1)^2 + \beta^4 \epsilon_2^2}} \right) +$$

Relativistic rise

Cross section to transfer energy E

$$\frac{1}{N \hbar c} \left( \beta^2 - \frac{\epsilon_1}{|\epsilon|^2} \right) \theta +$$

Čerenkov radiation

$$\frac{\sigma_y(E)}{E} \log \left( \frac{2 m_e c^2 \beta^2}{E} \right) +$$

Resonance region

$$\frac{1}{E^2} \int_0^E \sigma_y(E_1) dE_1$$

Rutherford scattering

With:

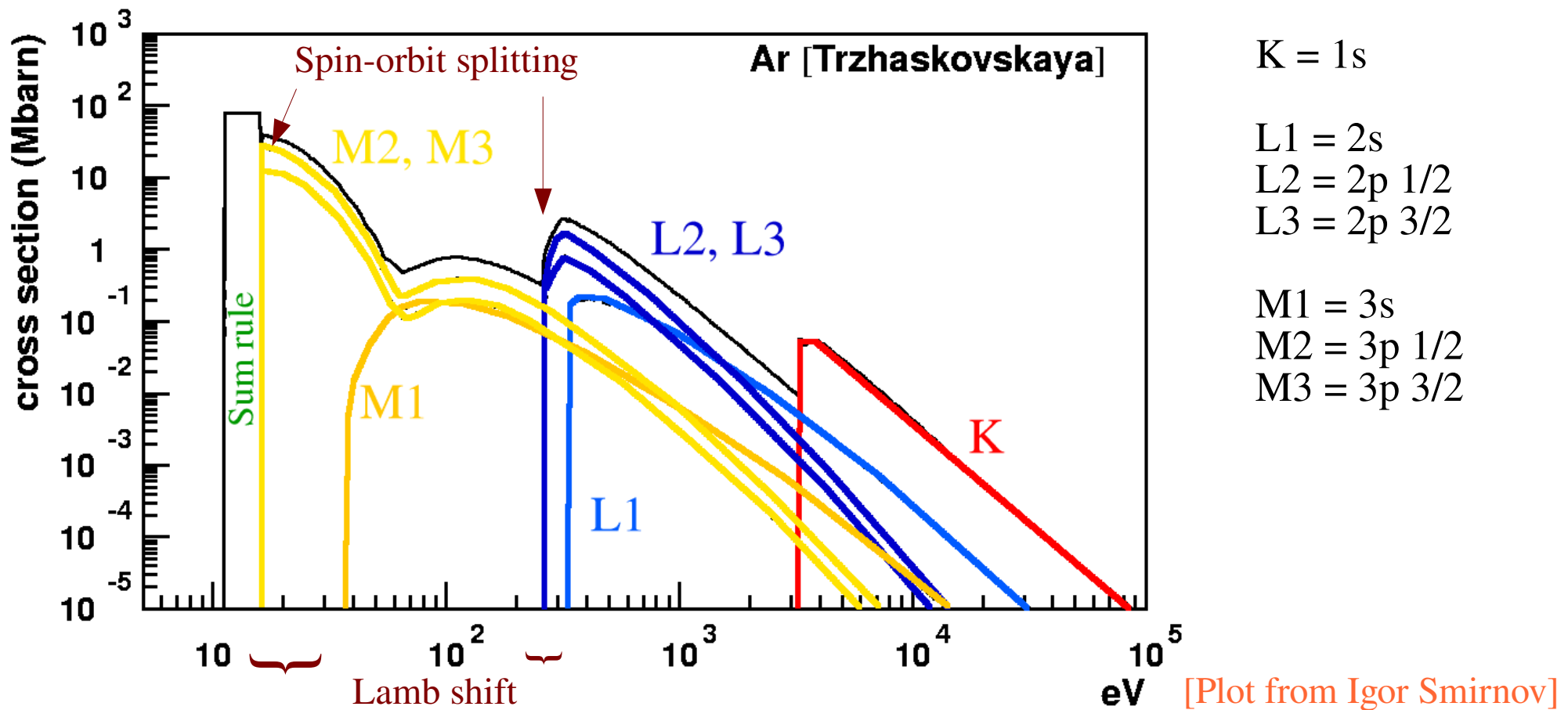
$$\epsilon_2(E) = \frac{N_e \hbar c}{E Z} \sigma_y(E)$$

$$\epsilon_1(E) = 1 + \frac{2}{\pi} \text{P} \int_0^\infty \frac{x \epsilon_2(x)}{x^2 - E^2} dx$$

$$\theta = \arg(1 - \epsilon_1 \beta^2 + i \epsilon_2 \beta^2) = \frac{\pi}{2} - \arctan \frac{1 - \epsilon_1 \beta^2}{\epsilon_2 \beta^2}$$

# Photo-absorption in argon

► Argon has 3 shells, hence 3 groups of lines:



# Transport in gases – How ?

- ▶ Over simplified approach, collision to collision.
- ▶ Traditionally the Boltzmann equation is solved by Legendre polynomial expansion to 2<sup>nd</sup> or 3<sup>rd</sup> order.
- ▶ Around 1962, Art Phelps introduced the MC approach.
- ▶ This is also what Magboltz (Steve Biagi) does.



# Mean free path in argon

- ▶ We know (e.g. from literature) that:
  - ▶ Cross section of 1 atom:  $\sigma \approx 1.5 \cdot 10^{-16} \text{ cm}^2$
  - ▶ Atoms per volume:  $n_0 \approx 2.7 \cdot 10^{19} \text{ atoms/cm}^3$
- ▶ Mean free path for an electron ?
  - ▶ An electron hits all atoms of which the centre is less than a cross section  $\sigma$  radius from its path;
  - ▶ over a distance  $L$ , the electron hits  $n_0 \sigma L$  atoms;
  - ▶ mean free path = distance over which it hits 1 atom;  
$$\lambda_e = 1/(\sigma n_0) \approx 2.5 \text{ } \mu\text{m}$$
  - ▶ much larger than
    - ▶ 4 nm distance between atoms, and
    - ▶ 140-600 pm typical gas molecule diameters.

# MPGDs and the mean free path

- ▶ Recall:
  - ▶ Mean free path of electrons in Ar:  $2.5 \mu\text{m}$ ,
- ▶ Compare with:
  - ▶ Micromegas mesh pitch:  $63.5 \mu\text{m}$
  - ▶ GEM polyimide thickness:  $50 \mu\text{m}$
  - ▶ Micromegas wire thickness:  $18 \mu\text{m}$
  - ▶ GEM conductor thickness:  $5 \mu\text{m}$
- ▶ Hence:
  - ▶ mean free path approaches small structural elements;
  - ▶ such devices should be treated at a molecular level.

# Drift velocity in argon

- ▶ Compare with a Magboltz calculation for pure argon:
  - ▶  $E$  dependence is not too far off (although linear is more common at low fields),

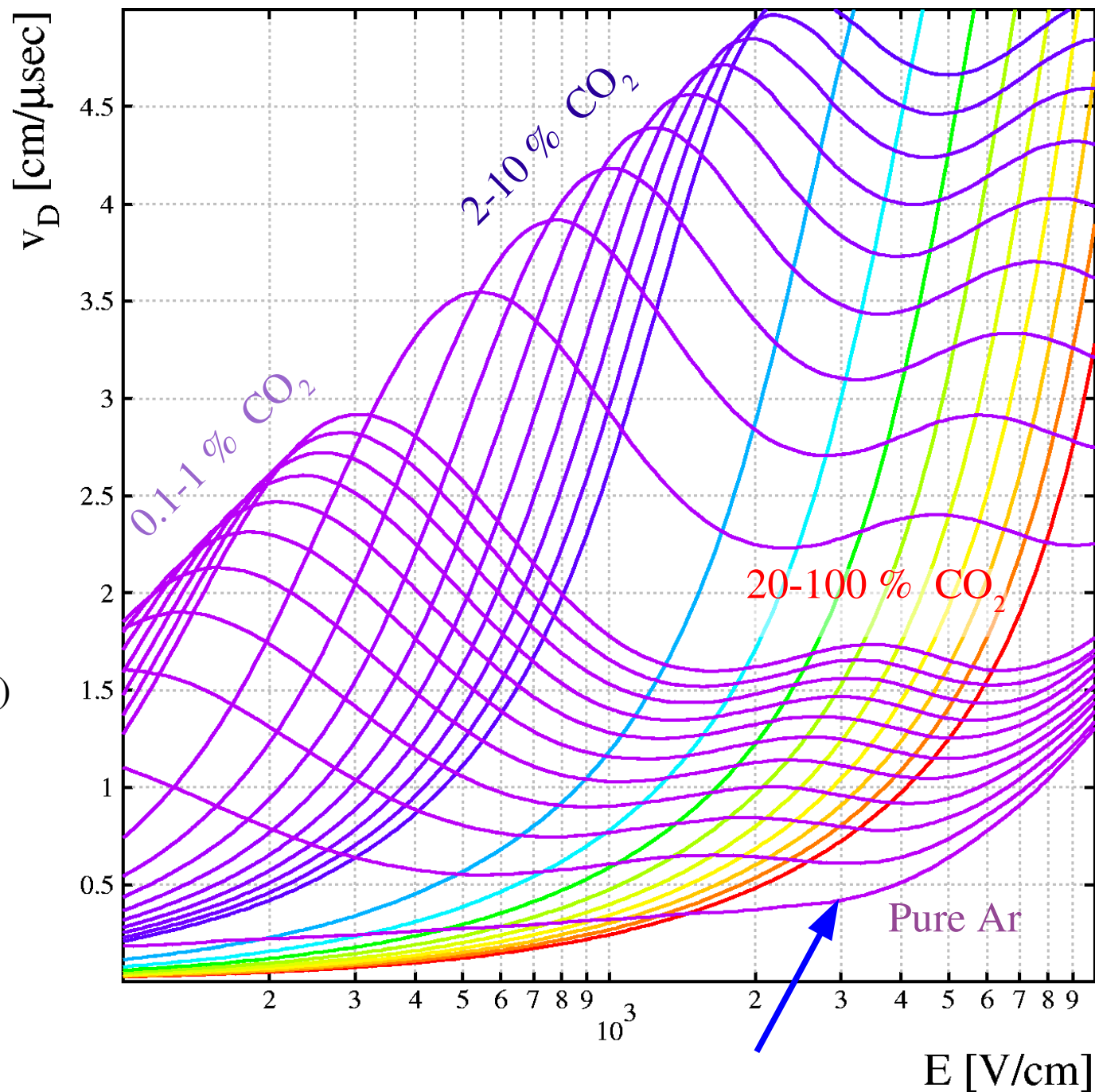
**BUT**

- ▶ the velocity is *vastly* overestimated ! Magboltz finds a velocity that is *30 times* smaller ...

**WHY ?**

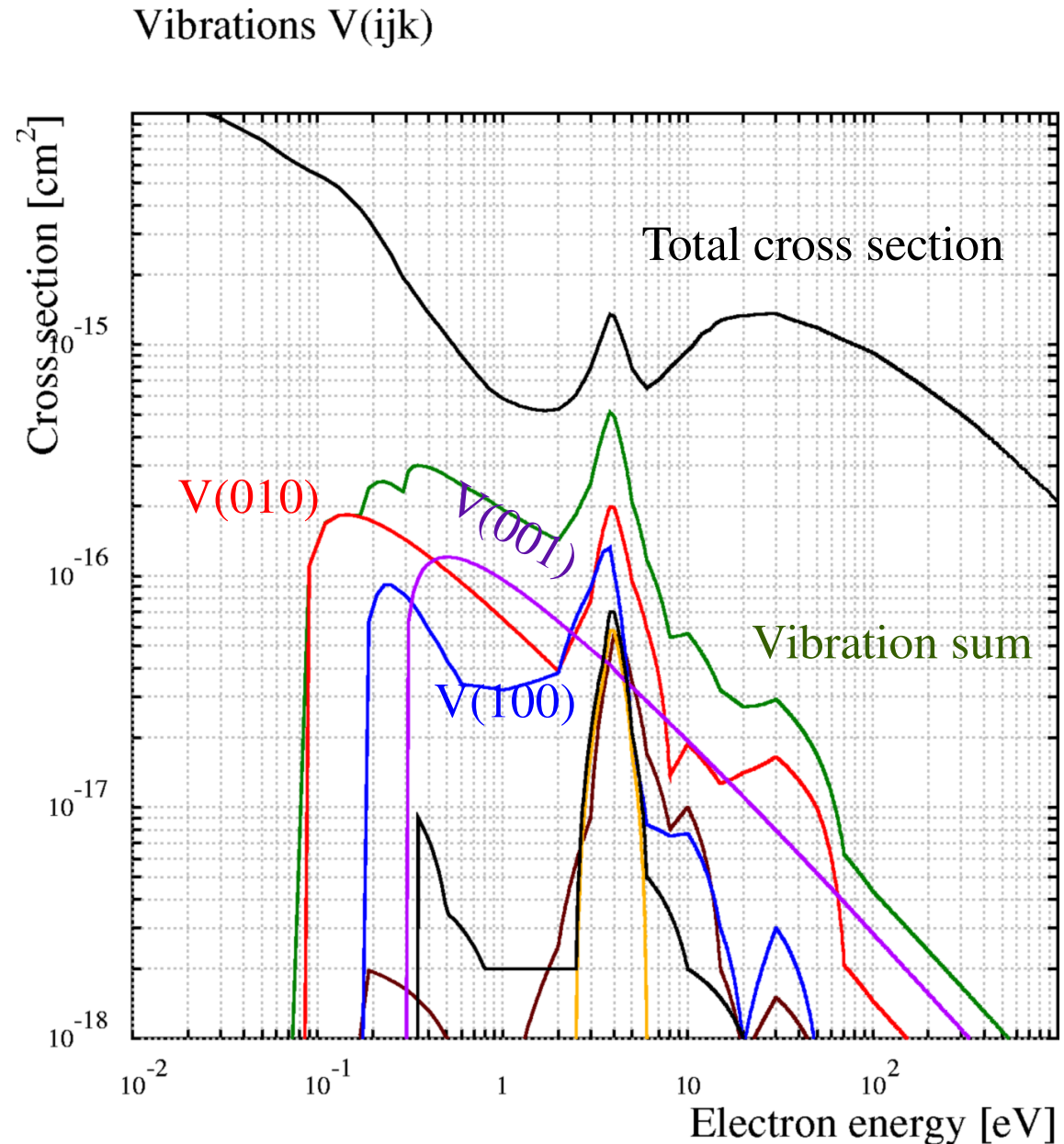
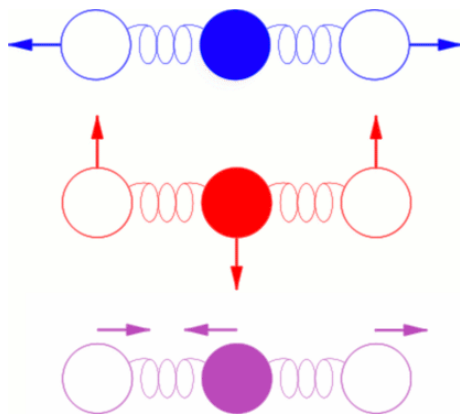
# Adding CO<sub>2</sub>

- ▶ CO<sub>2</sub> makes the gas faster, dramatically.
- ▶ Calculated by Magboltz for Ar/CO<sub>2</sub> at 3 bar.  
(Note where the [arrow](#) is !)

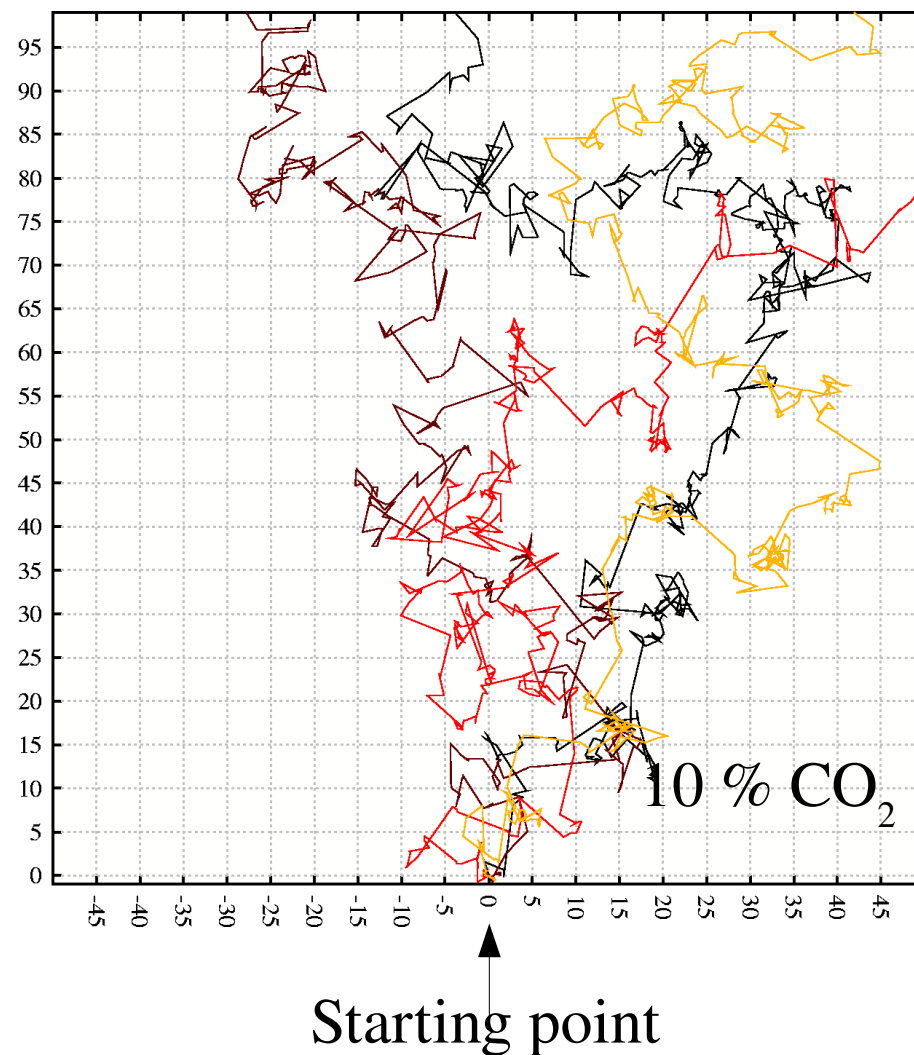
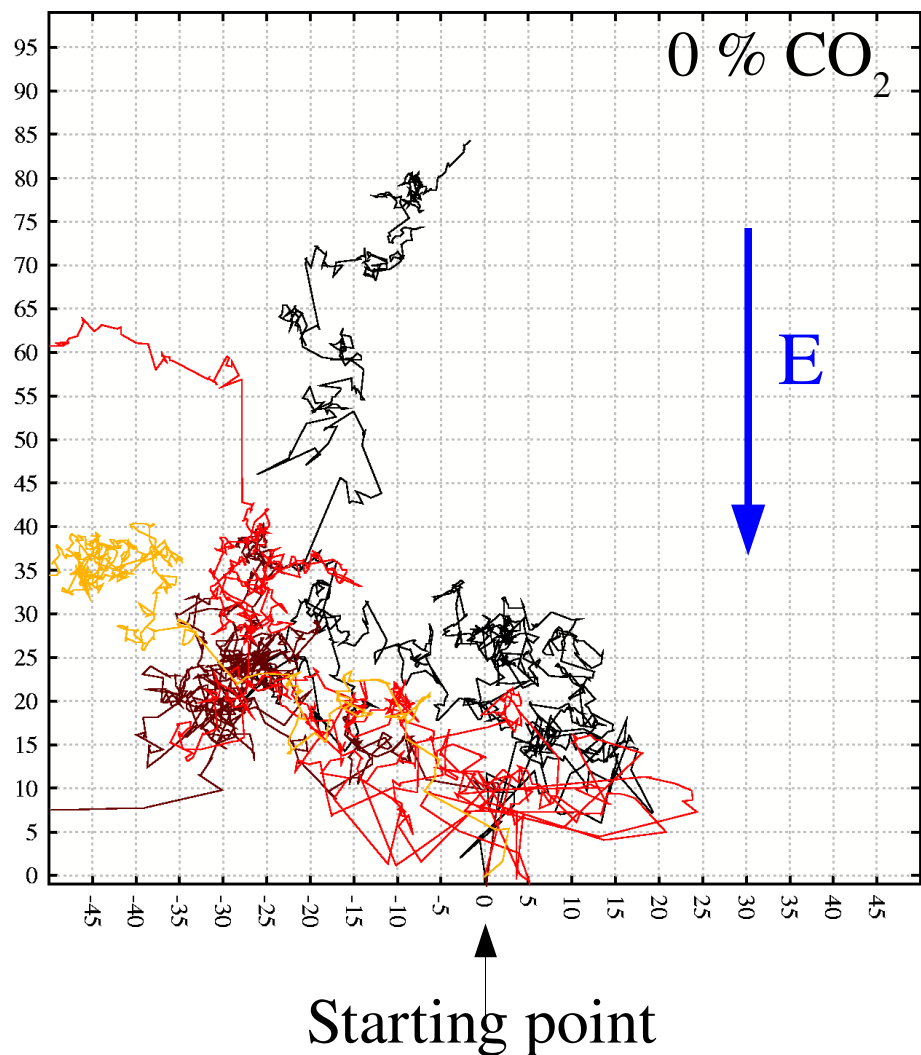


# CO<sub>2</sub> – vibration modes

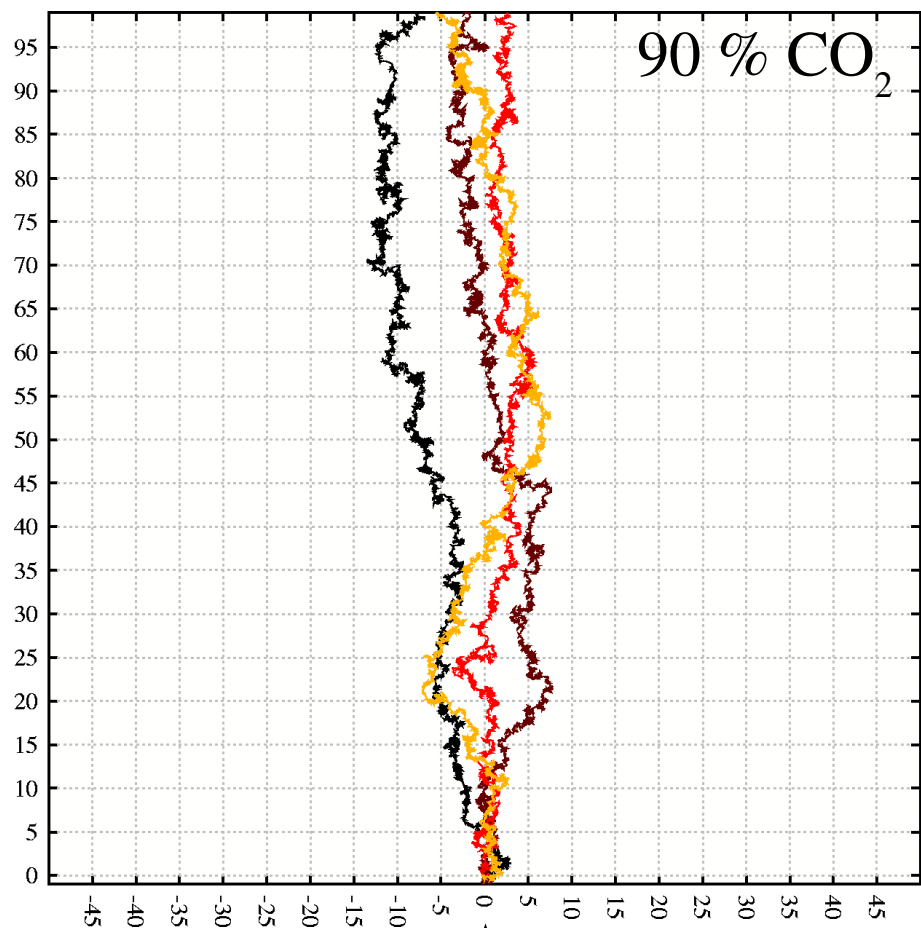
- ▶ CO<sub>2</sub> is linear:
  - ▶ O – C – O
- ▶ Vibration modes are numbered V(*ijk*)
  - ▶ *i*: symmetric,
  - ▶ *j*: bending,
  - ▶ *k*: anti-symmetric.



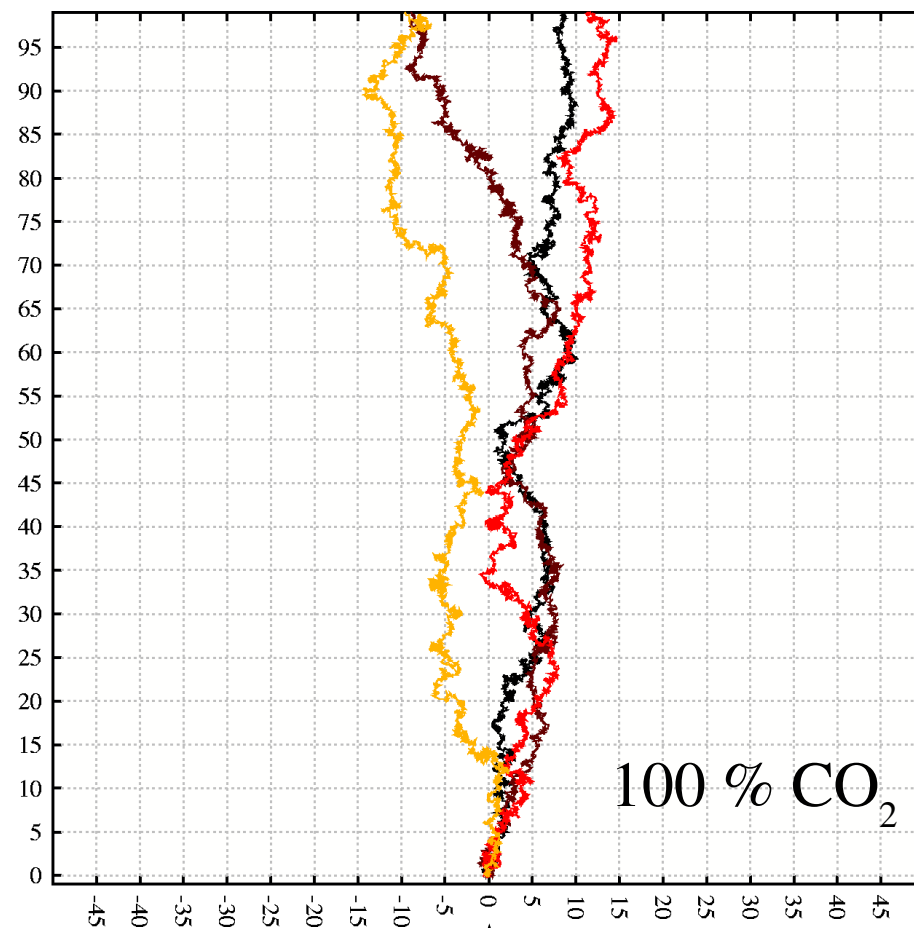
# Electrons in Ar/CO<sub>2</sub> at $E=1$ kV/cm



# Electrons in Ar/CO<sub>2</sub> at $E=1$ kV/cm



Starting point



Starting point

# Calculating transport properties

- ▶ One can of course measure every mixture one needs ...
- ▶ ... but it would be far more efficient if one could compute the transport properties of arbitrary mixtures.



# 1935: Electron energy distribution

- ▶ Calculation of the electron energy distribution
  - ▶ allowing for energy loss in elastic collisions;
  - ▶ detailed balancing of energy and momentum, gain (E-field, diffusion) and loss (elastic collision);
  - ▶ velocity dependent cross section;
  - ▶ use of Legendre expansion (crediting H.A. Lorentz, 1916):

$$\begin{aligned} f(x, v, \omega) &= f_0(x, v) + P_1(\cos \omega) f_1(x, v) \\ &\quad + P_2(\cos \omega) f_2(x, v) + \dots \\ &= f_0(x, v) + (\xi/v) f_1(x, v) + \dots \end{aligned}$$

( $P_1, P_2$ : Legendre polynomials)

The function  $f_0$  determines the random distribution in velocity, and  $f_1$  determines the electron drift. The higher terms in the series are nearly always very small and do not correspond to any simple physical property of the distribution, but serve simply to improve the form of the distribution function.



# 1962: Numerical $e^-$ transport

- ▶ Iterative approach, allowing for inelastic cross section terms:
  - ▶ educated guess of cross sections (elastic & inelastic);
  - ▶ **numerically** solve the Boltzmann equation (no moments);
  - ▶ compare calculated and measured mobility and diffusion;
  - ▶ adjust cross sections.

“... more than 50,000 transistors plus extremely fast magnetic core storage. The new system can simultaneously read and write electronically at the rate of 3,000,000 bits of information a second, when eight data channels are in use. In 2.18 millionths of a second, it can locate and make ready for use any of 32,768 data or instruction numbers (each of 10 digits) in the magnetic core storage. The 7090 can perform any of the following operations in one second: 229,000 additions or subtractions, 39,500 multiplications, or 32,700 divisions. “ (IBM 7090 documentation)



[L.S. Frost and A.V. Phelps, *Rotational Excitation and Momentum Transfer Cross Sections for Electrons in H<sub>2</sub> and N<sub>2</sub> from Transport Coefficients*, Phys. Rev. **127** (1962) 1621–1633.]

# 1980s: Higher moments, high precision

- ▶ Expansion in spherical harmonics;
- ▶ An accuracy of 1 % (and better) becomes routine.

The starting point for most theoretical work is the Boltzmann equation for the electron velocity distribution function,  $f(\mathbf{r}, \mathbf{v}, t)$ . The latter is formally expanded in a series of spherical harmonics,

$$f(\mathbf{r}, \mathbf{v}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l f_{lm}(\mathbf{r}, v, t) Y_{lm}^*(\hat{\mathbf{v}}), \quad (1)$$

where  $Y_{lm}(\hat{\mathbf{v}}) \equiv Y_{lm}(\theta, \phi) = P_l^{|m|}(\cos\theta) e^{im\phi}$ , and  $\theta, \phi$  denote the polar angles of the unit velocity vector  $\hat{\mathbf{v}}$  in some frame of reference.

S.L. Lin, R.E. Robson and E.A. Mason, *Moment theory of electron drift and diffusion in neutral gases in an electrostatic field*, J. Chem. Phys. **71** (1979) 3483-3498 (the “LRM” paper).

R.E. Robson and K.F. Ness, *Velocity distribution function and transport coefficients of electron swarms in gases: Spherical-harmonics decomposition of Boltzmann's equation*, Phys. Rev. A **33** (1986) 2068–2077.

K.F. Ness and R.E. Robson, *Velocity distribution function and transport coefficients of electron swarms in gases. II. Moment equations and applications*, Phys. Rev. A **34** (1986) 2185–2209.

# Magboltz: microscopic $e^-$ transport

- ▶ A large number of cross sections for 60 molecules...
  - ▶ Numerous organic gases, additives, *e.g.*  $\text{CO}_2$ :
    - ▶ elastic scattering,
    - ▶ 44 inelastic cross sections (5 vibrations and 30 rotations + super-elastic and 9 polyads),
    - ▶ attachment,
    - ▶ 6 excited states and
    - ▶ 3 ionisations.
  - ▶ noble gases (He, Ne, Ar, Kr, Xe):
    - ▶ elastic scattering,
    - ▶ 44 excited states and
    - ▶ 7 ionisations.

# LXcat

- ▶ LXcat (pronounced *elecscat*) is an open-access website for collecting, displaying, and downloading ELECTron SCATtering cross sections and swarm parameters (mobility, diffusion coefficient, reaction rates, etc.) required for modeling low temperature plasmas. [...]"

[<http://www.lxcat.laplace.univ-tlse.fr/>]

# LXcat people

- ▶ Art Phelps,
- ▶ Leanne Pitchford – Toulouse,
- ▶ Klaus Bartschat – Iowa,
- ▶ Oleg Zatsarinny – Iowa,
- ▶ Michael Allan – Fribourg,
- ▶ Steve Biagi
- ▶ ...

Art Phelps



Leanne Pitchford



Michael Allan



Klaus Bartschat

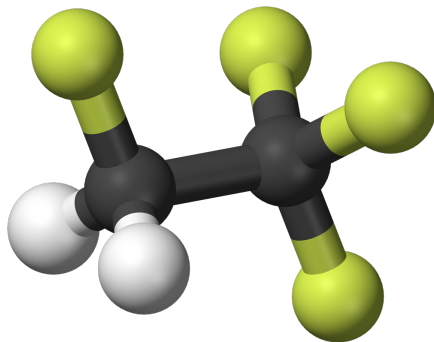


# Greenhouse gases - How

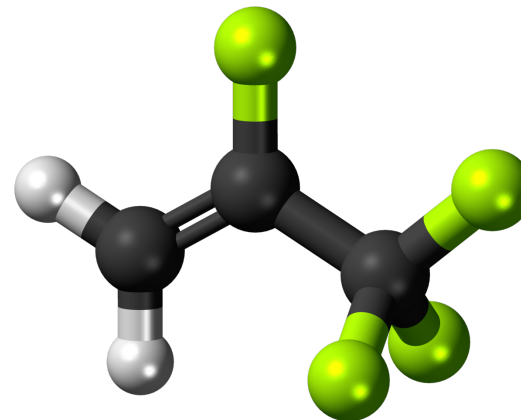
- ▶ Besides Ar and CO<sub>2</sub> other gases are used at present.
- ▶ Some of these have undesirable properties, damaging the atmosphere and groundwater. The Kyoto-7:
  - ▶ carbon dioxide (CO<sub>2</sub>),
  - ▶ methane (CH<sub>4</sub>),
  - ▶ nitrous oxide (N<sub>2</sub>O),
  - ▶ hydrofluorocarbons (HFCs eg R134a),
  - ▶ perfluorocarbons (PFCs),
  - ▶ sulphur hexafluoride (SF<sub>6</sub>), and
  - ▶ nitrogen trifluoride (NF<sub>3</sub>).
- ▶ CF<sub>4</sub> has long life and high GWP.
- ▶ These are being phased out. HFOs are candidates.

# HFO

- ▶ HFO stands for hydrofluoroolefin.
- ▶ They are HFCs which have a double C=C bond.
- ▶ This makes them more reactive and gives them a shorter lifetime.
- ▶ They are slated to replace R134a ( $\text{CH}_2\text{F}-\text{CF}_3$ ):



1,1,1,2-tetrafluoroethane



2,3,3,3-tetrafluoropropene



# Good and bad properties of HFOs

- ▶ HFO-1234yf       $\text{CH}_2=\text{CF}-\text{CF}_3$ 
  - ▶ air conditioning in cars, to replace R134a
- ▶ Good:
  - ▶ low GWP:  $< 1$ ,
  - ▶ short atmospheric lifetime: 10-20 days,
  - ▶ ODP  $\sim 0$  in gases made only with fluorine; a chlorinated gas serves as reference (R11); and ODP is large with brominated substances.
- ▶ Bad:
  - ▶ concern about flammability,
  - ▶ produces HF when burning,
  - ▶ atmospheric decay to trifluoroacetic acid (phytotoxic, aquatic life).

# Lifetime, GWP, ODP

## ► Properties of some common compounds:

Gas	Lifetime [years]	GWP [100 years]	ODP
CO <sub>2</sub>	10-100	reference	0
CCl <sub>3</sub> F (R11)	45	4660	reference
CH <sub>4</sub>	12.4	28	
CH <sub>2</sub> F-CF <sub>3</sub> (R134a)	13.4	1300	0
CHF <sub>2</sub> -CHF <sub>2</sub> (R134)	9.7	1120	0
CH <sub>3</sub> -CF <sub>3</sub> (R143a)	47.1	4800	0
CHF <sub>2</sub> -CF <sub>3</sub> (R125)	28.2	3170	0
CF <sub>4</sub>	50000	6630	0
C <sub>2</sub> F <sub>6</sub>	10000	11100	0
C <sub>3</sub> F <sub>8</sub>	2600	8900	0
SF <sub>6</sub>	3200	23500	0 ?
CF <sub>3</sub> Br (Halon 1301)	65	6290	16
1234yf	10.5 days	<1	0
(Z) 1234ze	10 days	<1	0
(E) 1234ze	16.4 days	<1	0

[from IPCC WG1/AR5]

# Field calculation techniques – How ?

- ▶ Closed expressions, “**analytic** method”:
  - ▶ almost all 2d structures of wires, planes + periodicities;
  - ▶ dielectrics and space/surface charge are laborious;
  - ▶ fast and precise, if applicable.
- ▶ **Finite element method**:
  - ▶ 2d and 3d structures, with or without dielectrics;
  - ▶ several major intrinsic shortcomings.
- ▶ Integral equations or **Boundary element methods**:
  - ▶ equally comprehensive without the intrinsic flaws;
  - ▶ technically challenging and emerging;
  - ▶ consumes more CPU time than FEM, but catching up.
- ▶ Finite differences:
  - ▶ used for iterative, time-dependent calculations.

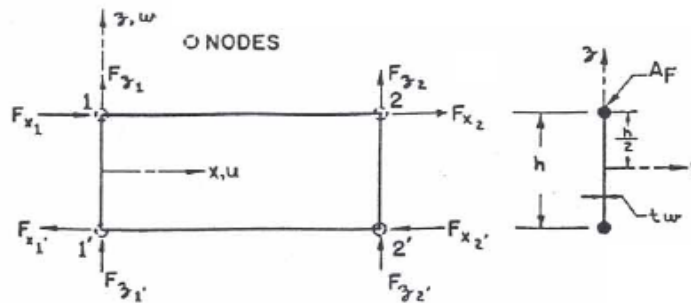
# Analytic field calculations (2d only)

- ▶ Analytic calculations rely on **complex functions** because of two remarkable properties:
  - ▶ Cauchy-Riemann equations:
    - ▶ The real part of *any* complex analytic function is a valid potential function.
  - ▶ Conformal mapping:
    - ▶ Almost *every* analytic geometric transformation of a valid complex potential, is a valid complex potential too.
- ▶ Applicability:
  - ▶ drift chambers, TPCs, MWPCs, drift tubes, hexagonal counters and other 2d detectors.

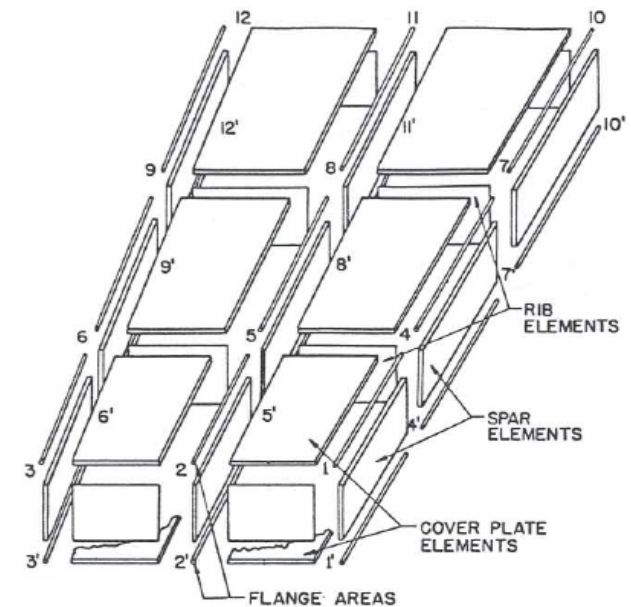


# Aircraft wings – finite elements

- ▶ “*Stiffness and Deflection Analysis of Complex Structures*”, a study in the use of the finite element technique (then called “direct stiffness method”) for aircraft wing design.



$$[K] = \frac{6EI}{Lh^2(1+4n)} \begin{bmatrix} (4/3)(1+n) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -(h/L) & 0 & h^2/L^2 & 0 & 0 & 0 \\ (2/3)(1-2n) & 0 & -(h/L) & (4/3)(1+n) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ h/L & 0 & -(h^2/L^2) & h/L & 0 & h^2/L^2 \end{bmatrix}$$



[M.J. Turner, R.W. Clough, H.C. Martin and L.J. Topp, *Stiffness and Deflection Analysis of Complex Structures*, J. Aero. Sc. **23** (1956), 805-824. MJT & LJT with Boeing.]

# Electron transport – How ?

- ▶ RKF (Runge Kutta with automatic step adjustment).
- ▶ Microscopic – routine for MPGDs.
- ▶ Monte Carlo – deprecated because the step length is not correctly simulated.
- ▶ Can be combined with gas gain.

# Ion transport and chemistry – How ?

- ▶ Using the ion mobility – beware of unphysical approaches, commonly used !
- ▶ E.g.  $\text{Ar}^+$  does not drift long distances in  $\text{CO}_2$ .

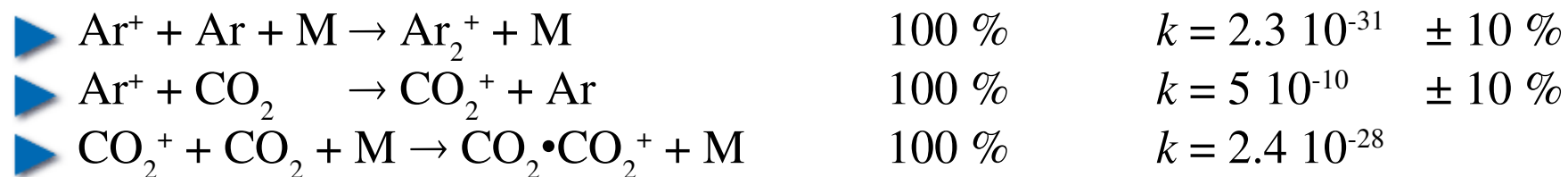
# Avalanche ions in Ar-CO<sub>2</sub> (93-7)

	Ion	Energy [eV]	Rate [GHz]	Fraction
Ar	Ar <sup>+</sup>	15.75961	57.67	93.3 %
CO <sub>2</sub>	CO <sub>2</sub> <sup>+</sup>	13.776	3.234	5.2 %
	CO <sub>2</sub> <sup>+*</sup>	17.314	0.3922	
	CO <sub>2</sub> <sup>+*</sup>	18.077	0.2272	
	O <sup>+</sup>	19.07	0.1374	
	CO <sup>+</sup>	19.47	0.1593	

Magboltz 11.2bis,  
 $E = 100$  kV/cm  
1 atm, 20 C



# Reactions in Ar-CO<sub>2</sub>



[B.M. Smirnov, Cluster Ions and Van Der Waals Molecules]

[V.G. Anicich and W.T. Huntress Jr., Astrophys. J. Suppl. **62** (1986) 553-672.]

# Reaction rate constant

- ▶ Consider a charge transfer reaction  $A^+ B \rightarrow A B^+$ :
  - ▶ rate  $\propto$  density of B molecules  $N_B$  [1/cm<sup>3</sup>];
  - ▶ The proportionality factor is called **rate constant  $k$** :
    - ▶ rate[1/s] =  $k$  [cm<sup>3</sup>/s]  $N_B$ [1/cm<sup>3</sup>]

# mathematica

- ▶ Start from the number of  $\text{Ar}^+$  and  $\text{CO}_2^+$  produced in the avalanche.
- ▶ Calculate evolution of  $\text{Ar}^+$ ,  $\text{CO}_2^+$ ,  $\text{CO}_2^+\cdot\text{CO}_2$  clusters and  $\text{Ar}_2^+$  dimers.

```
Clear[nAr, nAr2, nCO2, ncl]
evol = DSolve[
  {nAr'[x] == -(rArAr2 + rArCO2) nAr[x],
    nAr[0] == n0Ar,

    nAr2'[x] == rArAr2 nAr[x],
    nAr2[0] == 0,

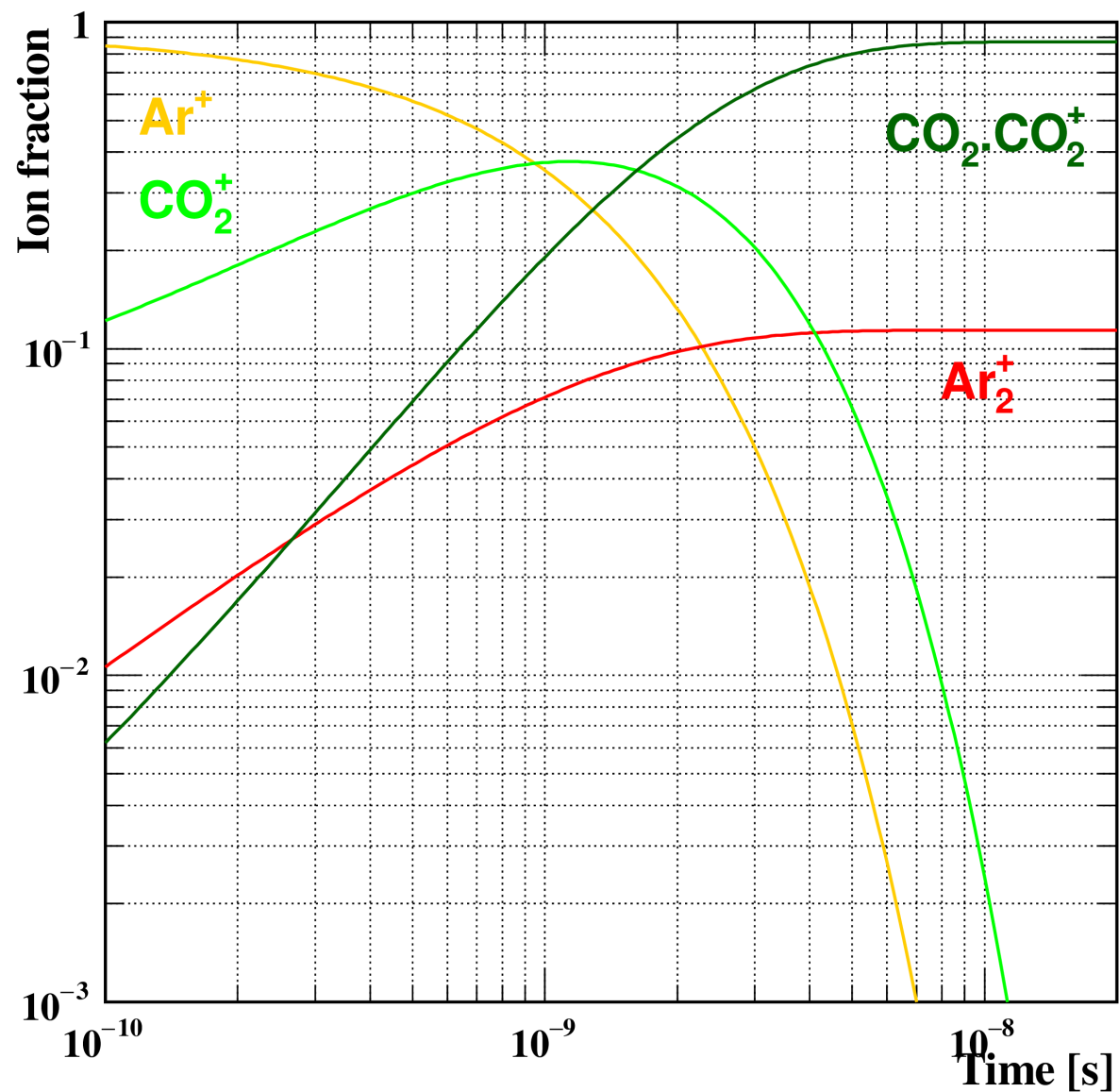
    nCO2'[x] == rArCO2 nAr[x] - rCO2cl nCO2[x],
    nCO2[0] == n0CO2,

    ncl'[x] == rCO2cl nCO2[x],
    ncl[0] == 0},

  {nAr[x], nAr2[x], ncl[x], nCO2[x]},
  x];
CForm[%]
```

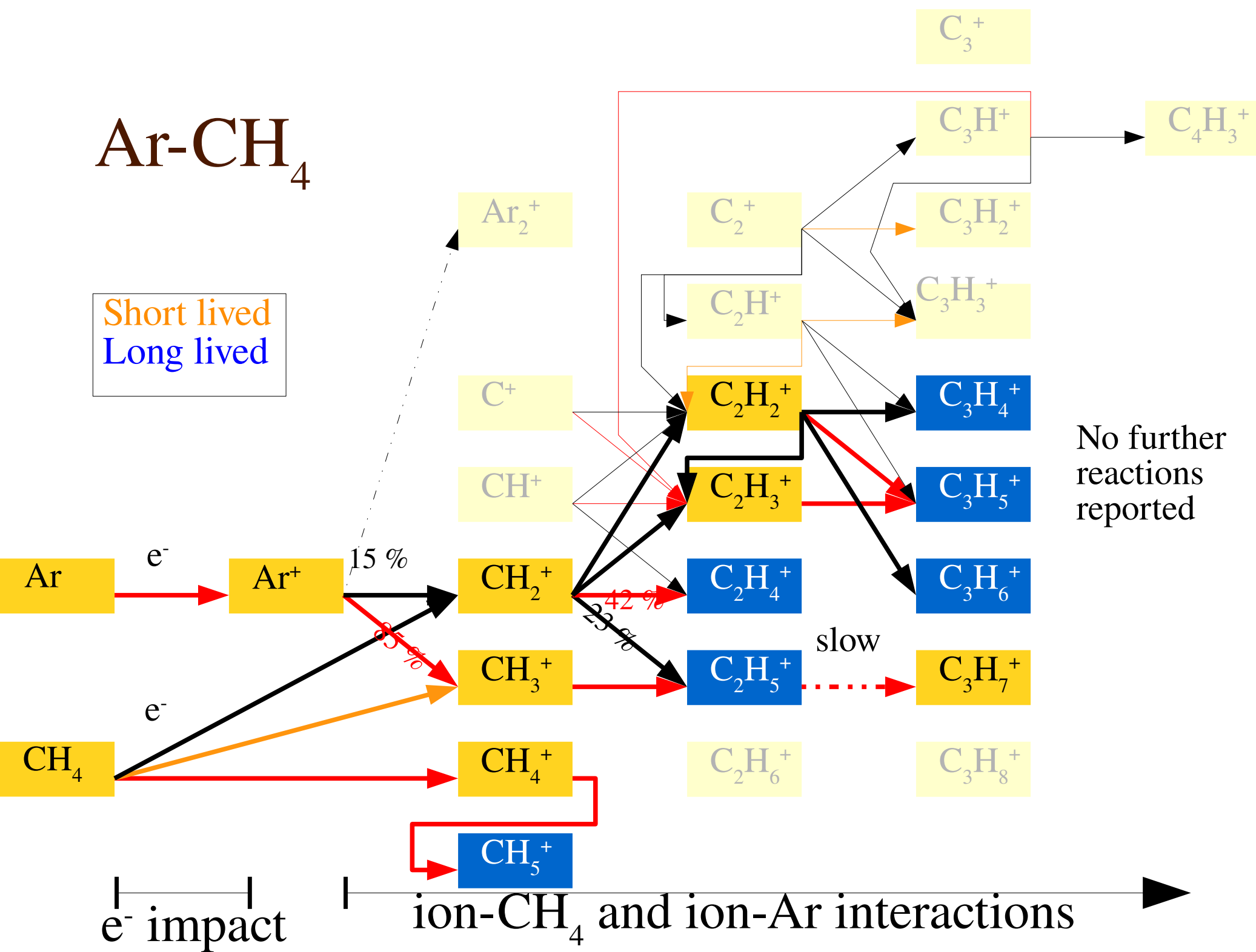
# Evolution in Ar-CO<sub>2</sub> (93-7)

- ▶ Initial ions:
- ▶ Ar<sup>+</sup> →
  - ▶ CO<sub>2</sub><sup>+</sup>
  - ▶ Ar<sub>2</sub><sup>+</sup>
  - ▶ CO<sub>2</sub><sup>+</sup> →
  - ▶ CO<sub>2</sub><sup>+</sup>·CO<sub>2</sub>



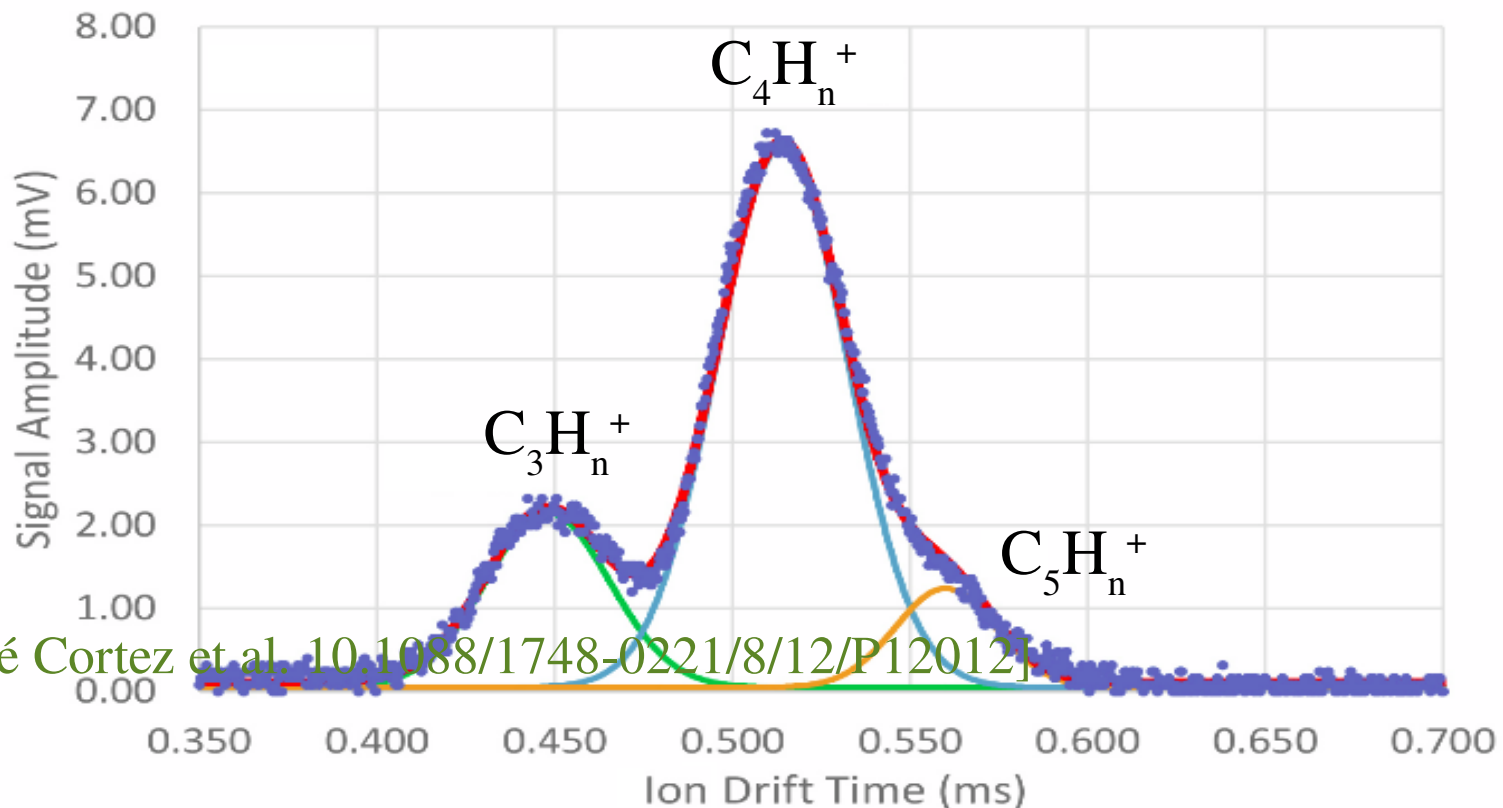


Short lived  
Long lived



# How about alkanes ?

- ▶ Ar 90 % - C<sub>2</sub>H<sub>6</sub> 10 %, at low pressure.
- ▶ Expect Ar<sup>+</sup> or C<sub>2</sub>H<sub>6</sub><sup>+</sup> but ... none are seen – why ?



# Avalanche ions in Ar-CO<sub>2</sub>-CH<sub>4</sub> (90-7-3)

	Ion	Energy [eV]	Rate [GHz]	Fraction
Ar	Ar <sup>+</sup>	15.75961	53.73	88.3 %
CO <sub>2</sub>	CO <sub>2</sub> <sup>+</sup>	13.776	3.119	5.1 %
	CO <sub>2</sub> <sup>+*</sup>	17.314	0.3758	
	CO <sub>2</sub> <sup>+*</sup>	18.077	0.2218	
	O <sup>+</sup>	19.07	0.1324	
	CO <sup>+</sup>	19.47	0.1525	
CH <sub>4</sub>	CH <sub>4</sub> <sup>+</sup>	12.65	1.959	3.2 %
	CH <sub>3</sub> <sup>+</sup>	14.25	1.115	1.8 %
	CH <sub>2</sub> <sup>+</sup>	15.2	0.07018	

Magboltz 11.2bis,  
 $E = 100$  kV/cm  
1 atm, 20 C

# Reactions in Ar-CO<sub>2</sub>-CH<sub>4</sub>

▶ Ar <sup>+</sup> + Ar + M	→ Ar <sub>2</sub> <sup>+</sup> + M	100 %	$k = 2.3 \cdot 10^{-31}$	± 10 %
▶ Ar <sup>+</sup> + CO <sub>2</sub>	→ CO <sub>2</sub> <sup>+</sup> + Ar	100 %	$k = 5 \cdot 10^{-10}$	± 10 %
▶ Ar <sup>+</sup> + CH <sub>4</sub>	→ CH <sub>3</sub> <sup>+</sup> + Ar + H	85 %	$k = 1.1 \cdot 10^{-9}$	± 10 %
▶	→ CH <sub>2</sub> <sup>+</sup> + Ar + H <sub>2</sub>	15 %		
▶ CO <sub>2</sub> <sup>+</sup> + CO <sub>2</sub> + M	→ CO <sub>2</sub> •CO <sub>2</sub> <sup>+</sup> + M	100 %	$k = 2.4 \cdot 10^{-28}$	
▶ CO <sub>2</sub> <sup>+</sup> + CH <sub>4</sub>	→ CH <sub>4</sub> <sup>+</sup> + CO <sub>2</sub>	25 %	$k = 1.1 \cdot 10^{-9}$	± 10 %
▶	→ HCO <sub>2</sub> <sup>+</sup> + CH <sub>3</sub>	75 %		
▶ CH <sub>3</sub> <sup>+</sup> + CH <sub>4</sub>	→ C <sub>2</sub> H <sub>5</sub> <sup>+</sup> + H <sub>2</sub>	100 %	$k = 1.1 \cdot 10^{-9}$	± 10 %
▶ C <sub>2</sub> H <sub>5</sub> <sup>+</sup> + CH <sub>4</sub>	→ C <sub>3</sub> H <sub>7</sub> <sup>+</sup> + H <sub>2</sub>	100 %	$k = 1 \cdot 10^{-14}$	± 10 %
▶ CH <sub>4</sub> <sup>+</sup> + CH <sub>4</sub>	→ CH <sub>5</sub> <sup>+</sup> + CH <sub>3</sub>	100 %	$k = 1.15 \cdot 10^{-9}$	± 10 %
▶ CH <sub>5</sub> <sup>+</sup> + CH <sub>4</sub>	→ products	100 %	$k = 3 \cdot 10^{-11}$	± 30 %
▶ CH <sub>4</sub> <sup>+</sup> + CO <sub>2</sub>	→ HCO <sub>2</sub> <sup>+</sup> + CH <sub>3</sub>	99 %	$k = 9.6 \cdot 10^{-10}$	± 10 %
▶	→ CH <sub>3</sub> CO <sup>+</sup> + OH	1 %		
▶ CH <sub>5</sub> <sup>+</sup> + CO <sub>2</sub>	→ HCO <sub>2</sub> <sup>+</sup> + CH <sub>4</sub>	100 %	$k = 4 \cdot 10^{-11}$	± 10 %
▶ HCO <sub>2</sub> <sup>+</sup> + CH <sub>4</sub>	→ CH <sub>5</sub> <sup>+</sup> + CO <sub>2</sub>	100 %	$k = 6 \cdot 10^{-10}$	± 15 %

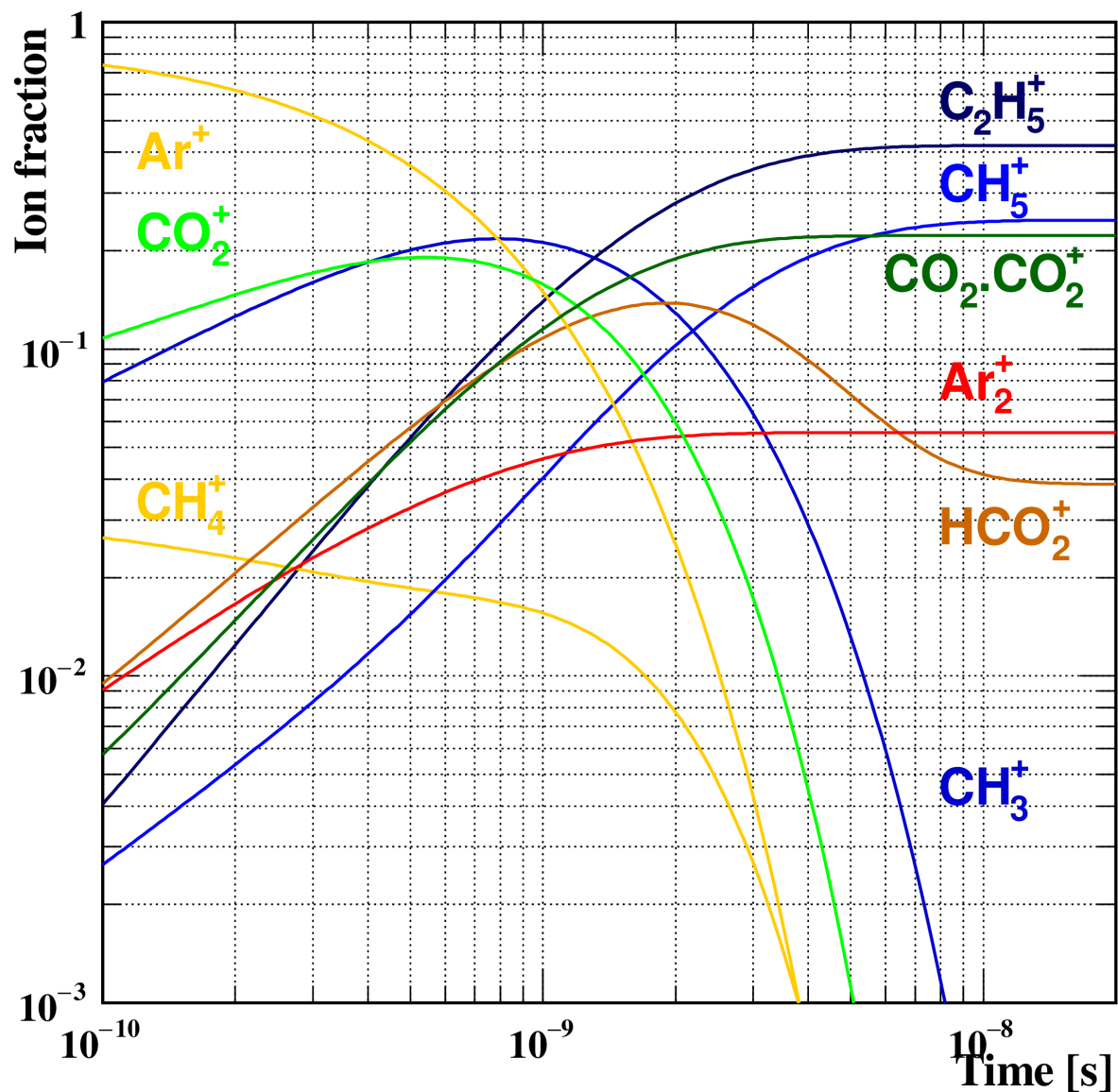
[B.M. Smirnov, Cluster Ions and Van Der Waals Molecules]

[V.G. Anicich and W.T. Huntress Jr., Astrophys. J. Suppl. **62** (1986) 553-672.]



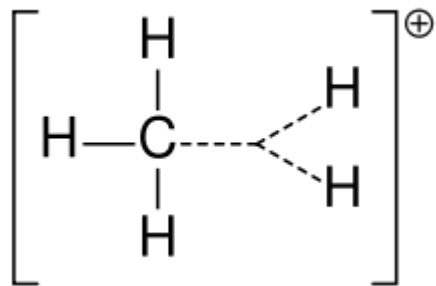
# Evolution in Ar-CO<sub>2</sub>-CH<sub>4</sub> (90-7-3)

- Initial ions:
- ▶ Ar<sup>+</sup> →
  - ▶ CO<sub>2</sub><sup>+</sup>,
  - ▶ CH<sub>3</sub><sup>+</sup>,
  - ▶ Ar<sub>2</sub><sup>+</sup>
  - ▶ CO<sub>2</sub><sup>+</sup> →
  - ▶ CH<sub>4</sub><sup>+</sup>
  - ▶ CO<sub>2</sub><sup>+</sup>·CO<sub>2</sub>
  - ▶ HCO<sub>2</sub><sup>+</sup>
  - ▶ CH<sub>4</sub><sup>+</sup> →
  - ▶ CH<sub>5</sub><sup>+</sup>,
  - ▶ HCO<sub>2</sub><sup>+</sup>
  - ▶ CH<sub>3</sub>CO<sup>+</sup>
  - ▶ CH<sub>3</sub><sup>+</sup> →
  - ▶ C<sub>2</sub>H<sub>5</sub><sup>+</sup>

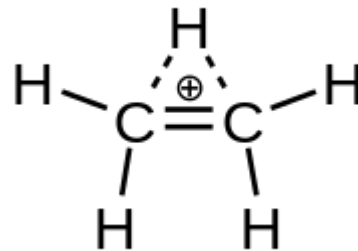


# Products after 10 ns

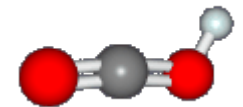
- ▶  $\text{C}_2\text{H}_5^+ \rightarrow \text{C}_3\text{H}_7^+$       slow reaction,  $k = 1 \cdot 10^{-14}$   
 [Hiraoka & Kebarle <https://doi.org/10.1063/1.431116>]
- ▶  $\text{CH}_5^+ \rightarrow$  “products”      slow reaction,  $k = 3 \cdot 10^{-11}$
- ▶  $\text{CO}_2 \cdot \text{CO}_2^+ \rightarrow$  grows to  $n = 3-4$ , reacts with  $\text{CH}_4$  to  $\text{HCO}_2^+$  ?  
 [Y. Kalkan et al. 2015 JINST 10 P07004]
- ▶  $\text{Ar}^+ \rightarrow \text{Ar}_2^+$       drifts faster than  $\text{Ar}^+$
- ▶  $\text{HCO}_2^+ \rightarrow \text{CH}_5^+$        $\text{HCO}_2^+$  decays at  $k = 6 \cdot 10^{-10}$



methanium



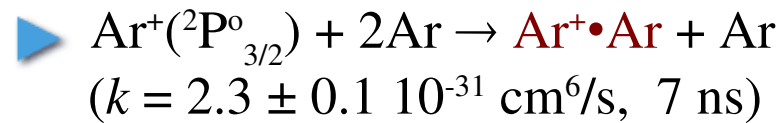
ethenium



protonated  
carbon dioxide

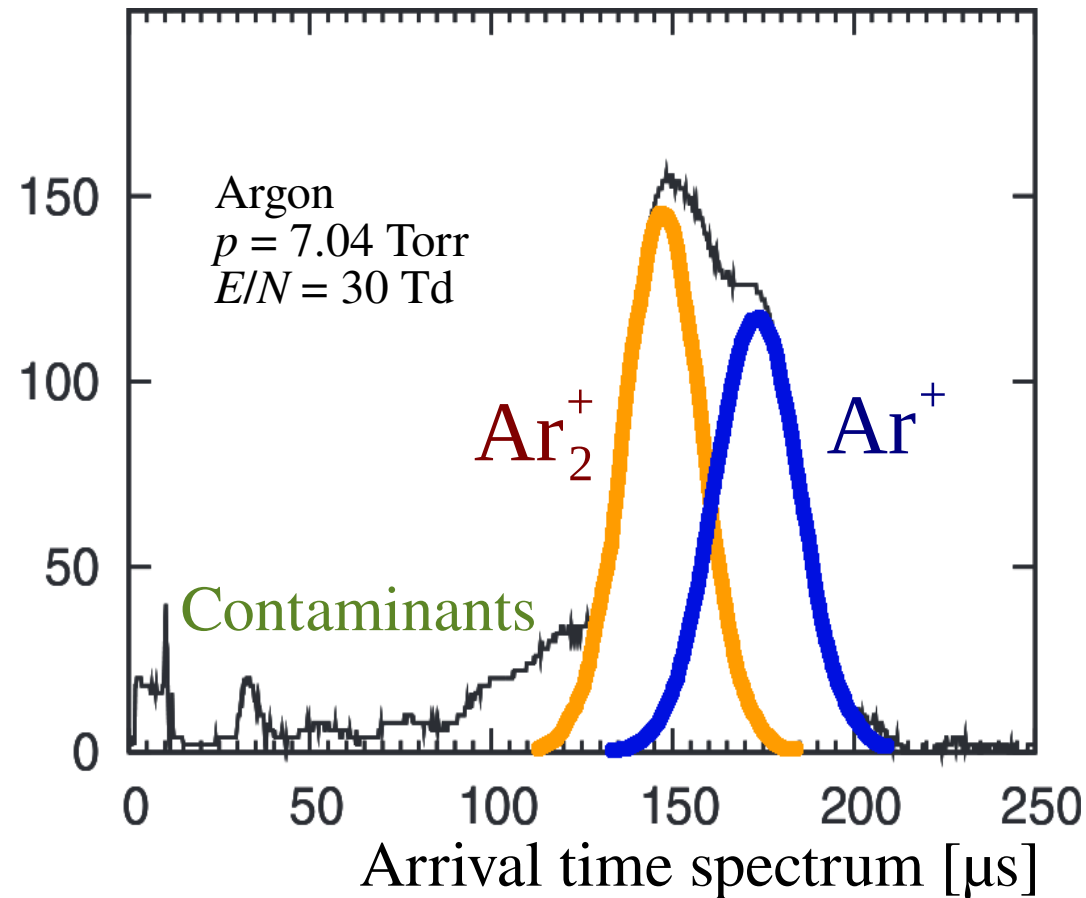
# Ions drifting in pure Ar

▶ In pure argon, dimers are formed:



▶ Note: dimers move *faster* than ions due to  $\text{Ar} \leftrightarrow \text{Ar}^+$  resonant charge exchange

[PNB Neves et al. 10.1063/1.3497651]



# Gain – How ?

- ▶ Take into account:
  - ▶ ionisation, and also
  - ▶ excitation;
  - ▶ Penning effect.
  
- ▶ Study:
  - ▶ fluctuations;
  - ▶ hump.



# 1901: Gas multiplication

## ► John Townsend:

Let a force  $X$  be applied to  $N_0$  negative ions in a gas at pressure  $p$  and temperature  $t$ . Let  $N$  be the total number of negative ions after the  $N_0$  ions have travelled a distance  $x$ . The new negative ions travel with the same velocity as the original  $N_0$  ions, so that all the negative ions will be found together during the motion. The number of negative ions produced by  $N$  ions travelling through a distance  $dx$  will be  $\alpha N dx$ ; where  $\alpha$  is a constant depending on  $X$ ,  $p$ , and  $t$ .

Then

$$dN = \alpha N dx.$$

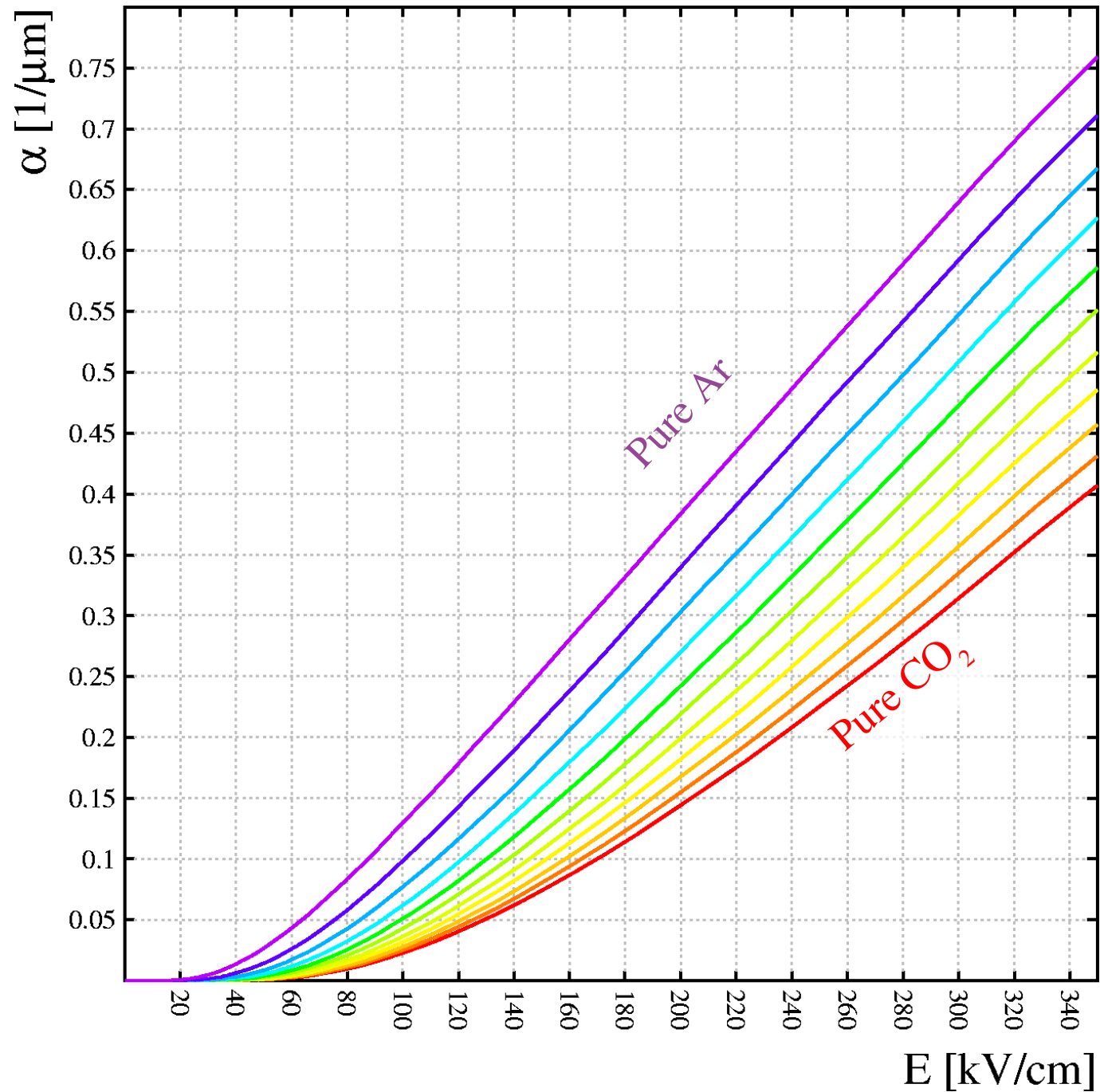
Hence

$$N = N_0 e^{\alpha x}$$

[J.S. Townsend, “*The conductivity produced in gases by the motion of negatively charged ions*”, *Phil. Mag.* **6-1** (1901) 198-227. If access to the *Philosophical Magazine* is restricted, then consult a German-language abstract at <http://jfm.sub.uni-goettingen.de/>.]

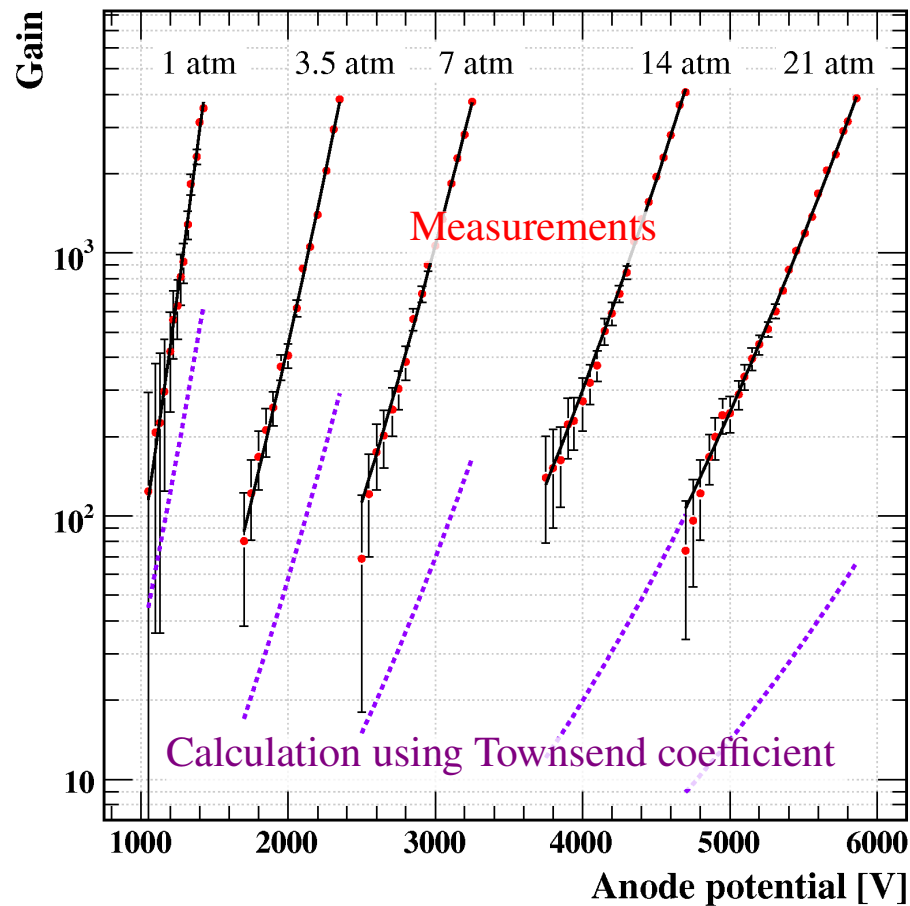
# $\alpha(\text{Ar-CO}_2)$

- ▶  $\alpha$  = number of  $e^-$  an avalanche  $e^-$  creates per cm.
- ▶ Adding  $\text{CO}_2$  reduces the gain.
- ▶ Calculated by Magboltz for Ar/ $\text{CO}_2$  at 3 bar.

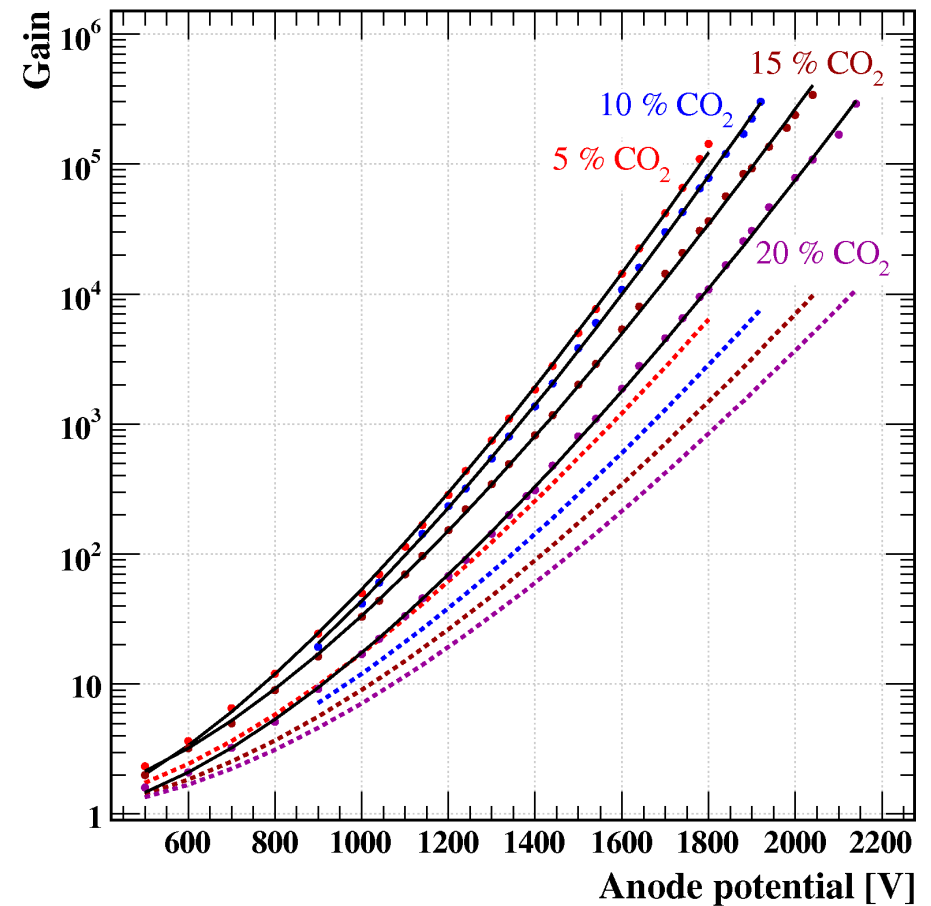


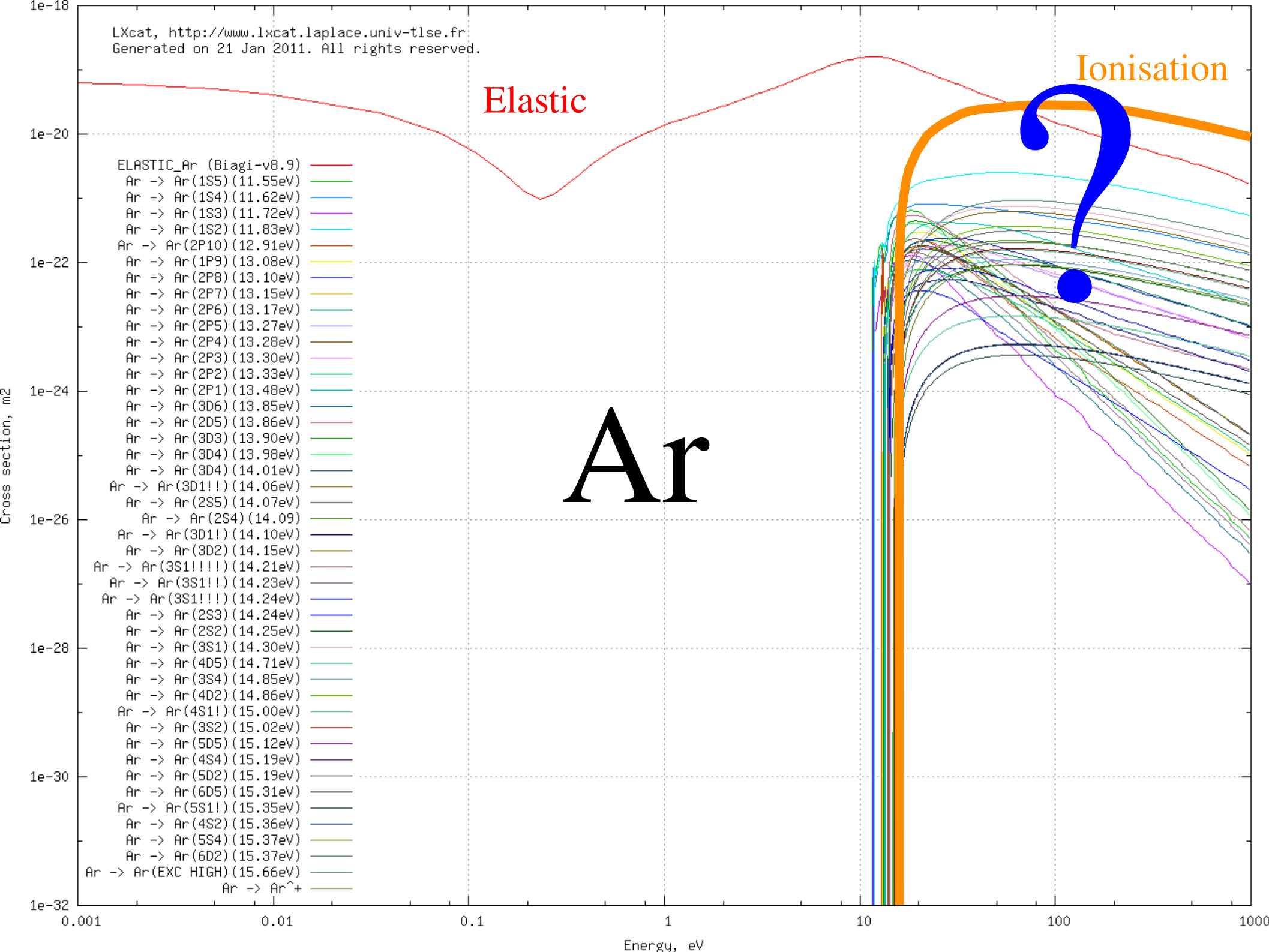
# Does this reproduce the measurements ?

► Ar - CH<sub>4</sub>



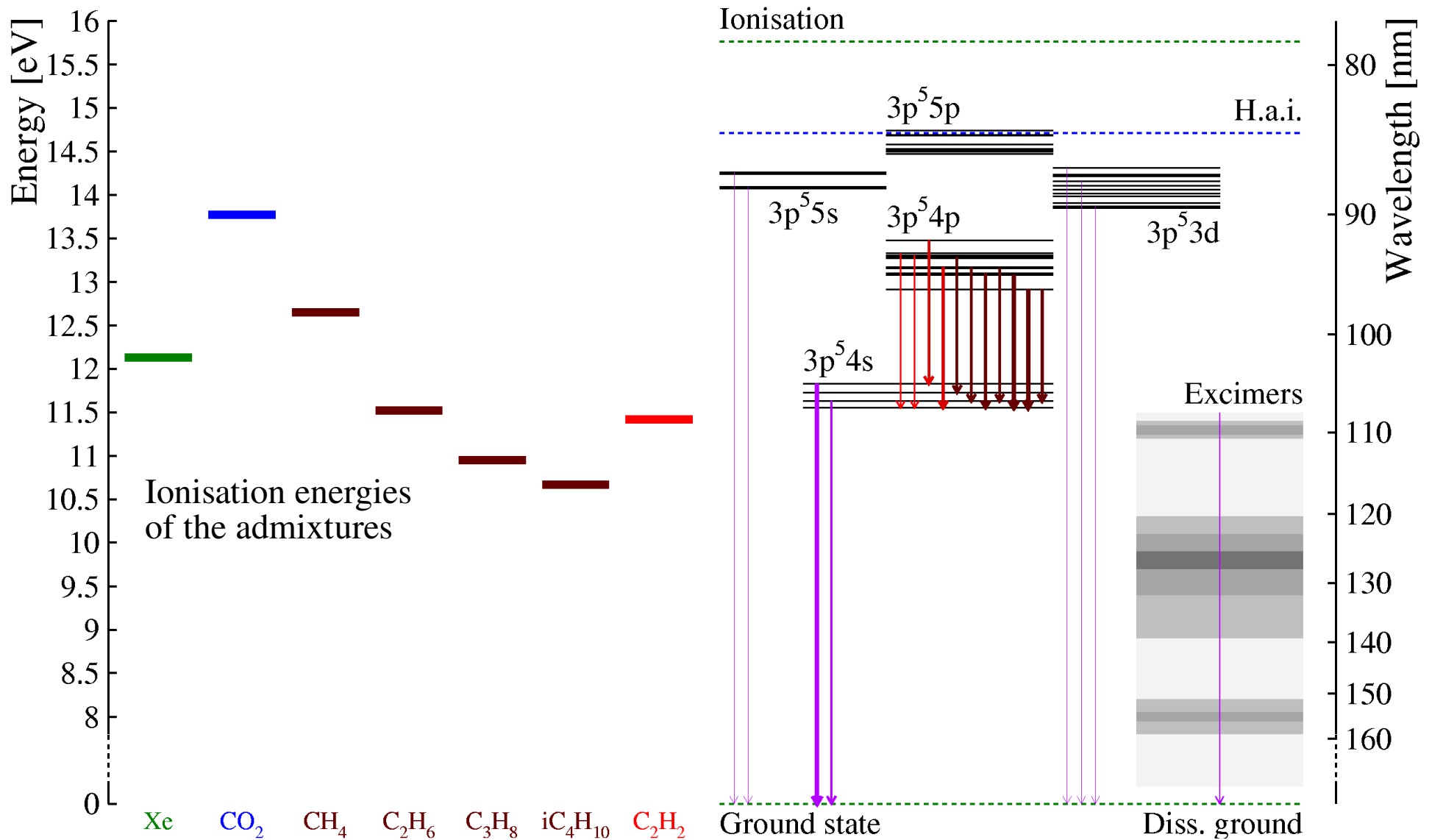
► Ar - CO<sub>2</sub>







# Level diagram argon and admixtures



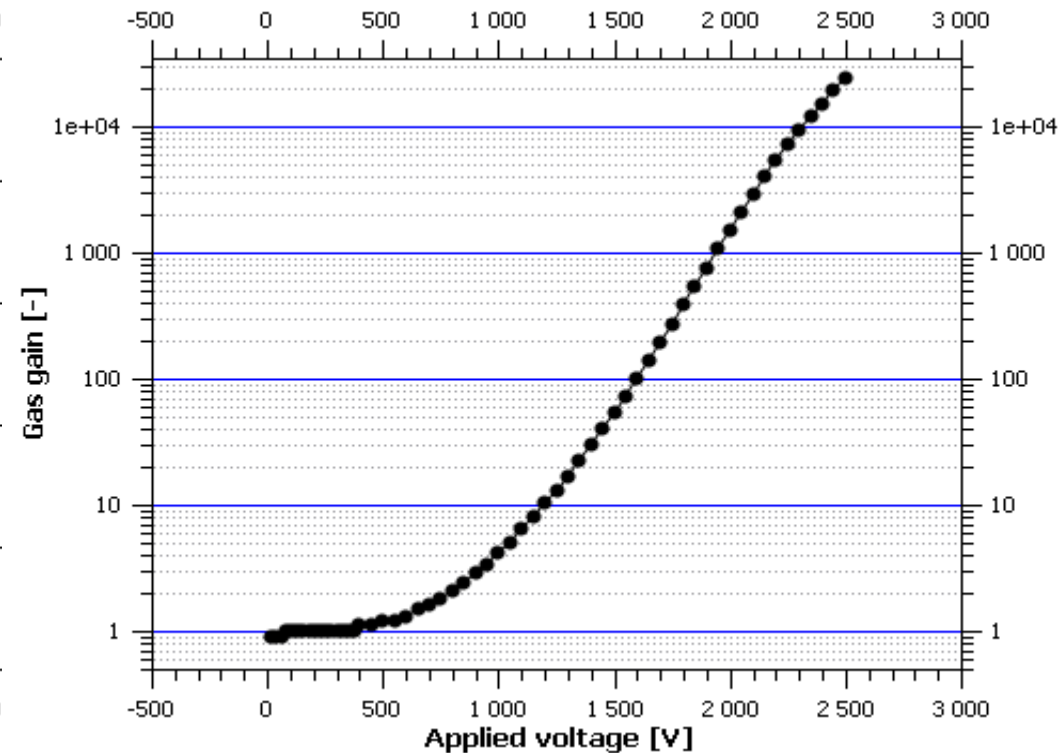
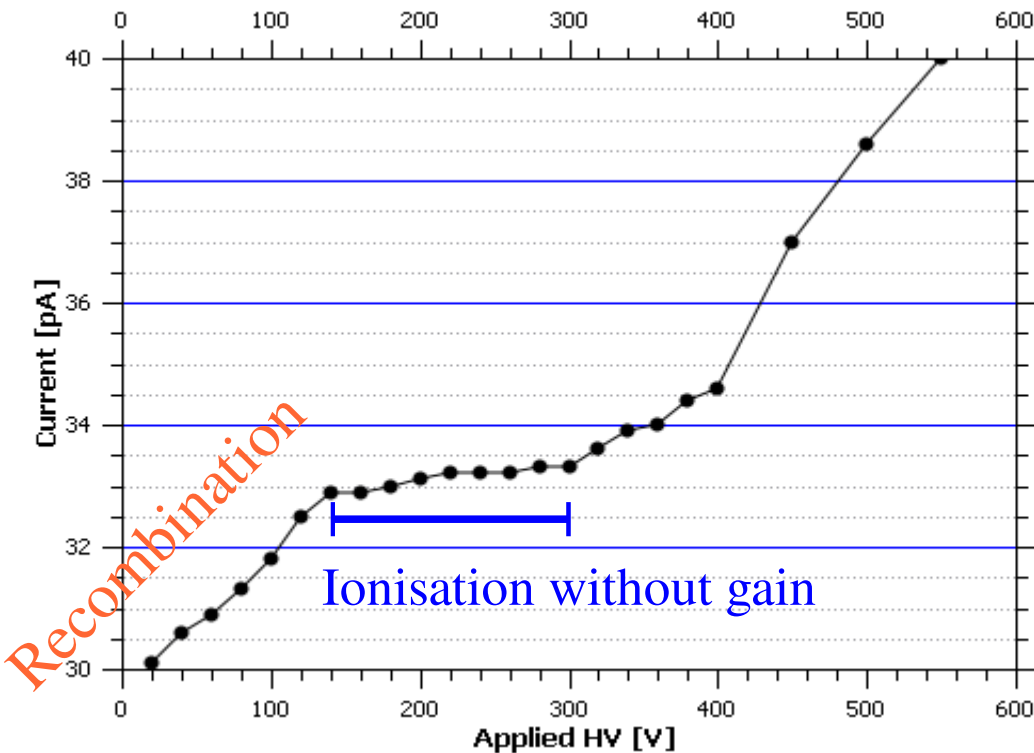


# Penning effect

- ▶  $\text{Ar}^* 3p^5 4s$  can transfer to  $\text{iC}_4\text{H}_{10}$ ,  $\text{C}_3\text{H}_8$  and  $\text{C}_2\text{H}_6$ ;
  - ▶ two  $4s$  are metastable, the two others live 2.6 ns and 8.6 ns;
- ▶  $\text{Ar}^* 3p^5 4p$  can also ionise  $\text{CH}_4$ ;
  - ▶  $4p$  decays to  $4s$  with a lifetime of 20-40 ns;
- ▶  $\text{Ar}^* 3p^5 3d$  can in addition transfer to  $\text{CO}_2$ ;
  - ▶ radiative  $3d$  decays take  $\sim 3.5$  ns, the others  $\sim 50$  ns.
- ▶ For comparison, collision frequencies of  $\text{Ar}^*$  in pure quencher are  $\sim 100$  ps.

# Data covers 5 orders of magnitude !

- ▶ Current reference is taken at the ionisation level.
- ▶ Main source of error: ~5 %.



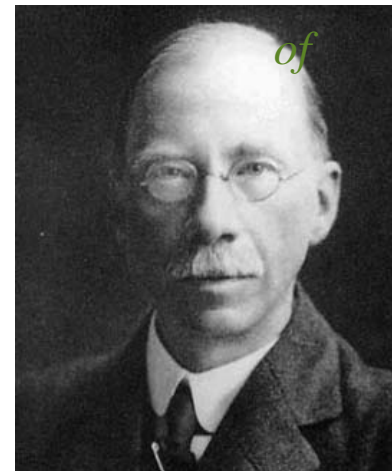
# G.U. Yule (1923), W.H. Furry (1937), R.A. Wijsman (1949) & others

- ▶ If the distance between ionisations fluctuates exponentially with a mean of  $1/\alpha$  (reciprocal of the Townsend coefficient),
- ▶ then, the avalanche size fluctuates (nearly) exponentially:

$$p(n) = \frac{1}{\bar{n}} \left(1 - \frac{1}{\bar{n}}\right)^{n-1}$$

[G. Udney Yule, *A Mathematical Theory of Evolution, based on the Conclusions Dr. J.C. Willis, F.R.S.*, Phil. Trans. Roy. Soc. London B **213** (1925) 21-87.  
W.H. Furry, *On Fluctuation Phenomena in the Passage of High Energy Electrons through Lead*, Phys. Rev. **52** (1937) 569-581.  
Robert A. Wijsman, *Breakdown Probability of a Low Pressure Gas Discharge*, Phys. Rev. **75** (1949) 833-838.]

George Udney Yule (1871-1951)



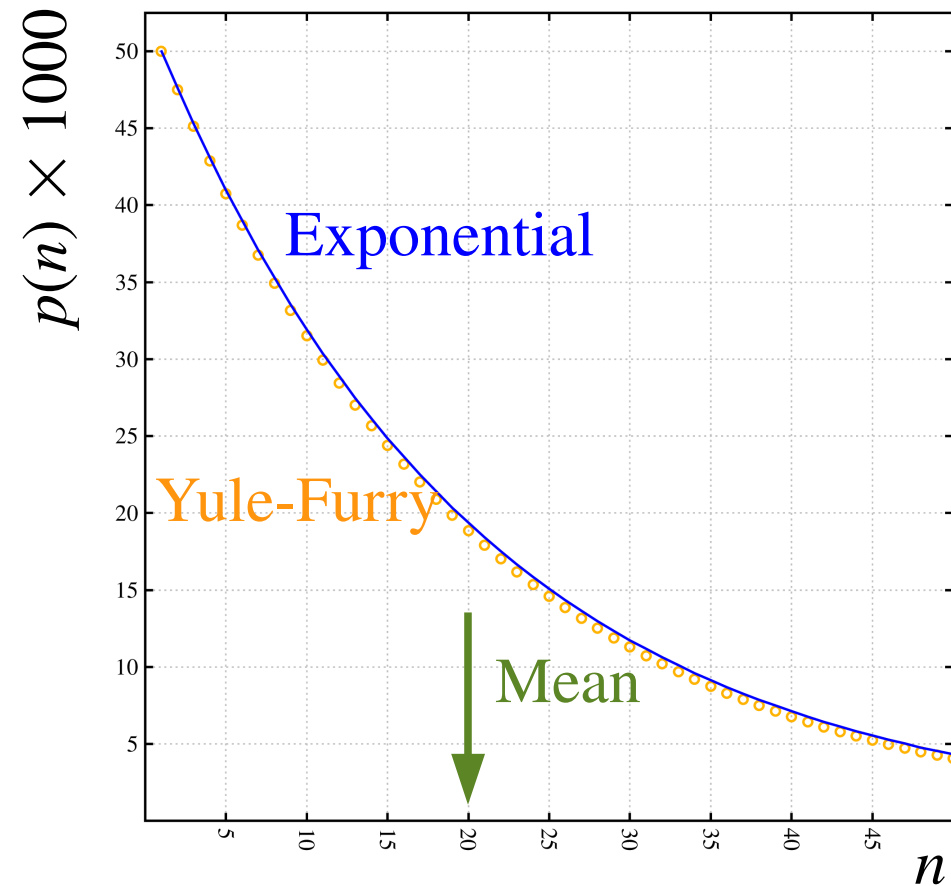
# Statistics Yule-Furry

- ▶ Yule-Furry is exponential for large mean avalanche sizes:

$$\begin{aligned} p(n) &= \frac{1}{\bar{n}} \left(1 - \frac{1}{\bar{n}}\right)^{n-1} \\ &= \frac{1}{\bar{n}} \frac{1}{1 - 1/\bar{n}} \left(1 - \frac{1}{\bar{n}}\right)^{\bar{n} \frac{n}{\bar{n}}} \\ &\approx \frac{e^{-n/\bar{n}}}{\bar{n} - 1} \end{aligned}$$

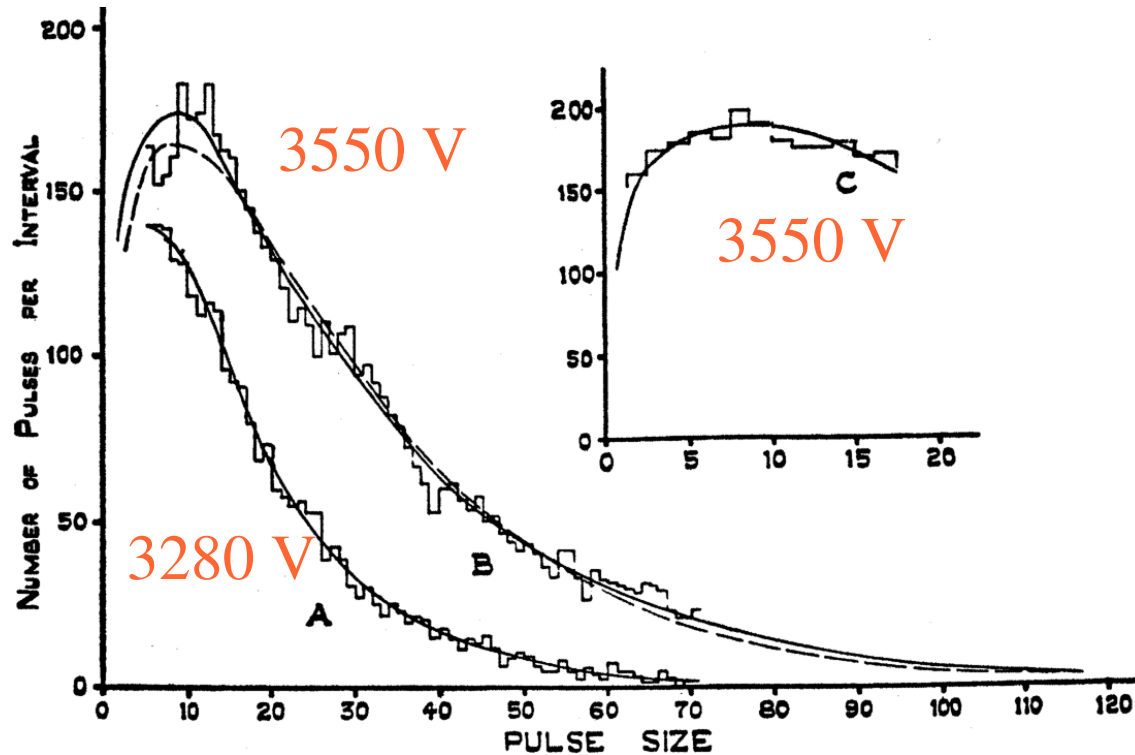
Mean:  $\bar{p}$

RMS:  $\bar{p} \sqrt{1 - 1/\bar{p}} \approx \bar{p}$



# S.C. Curran (1949)

- ▶ S.C. Curran *et al.* measure the pulse height distribution in a cylindrical counter ( $d = 150 \mu\text{m}$  wire, Ar 50 % CH<sub>4</sub> 50 %,  $p = 670$  mbar) at  $G \sim 10^4$ - $10^5$ :



Fit curve:

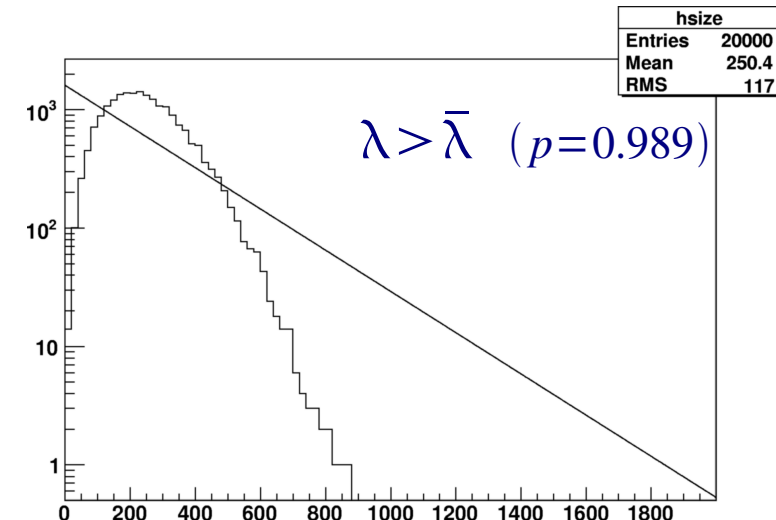
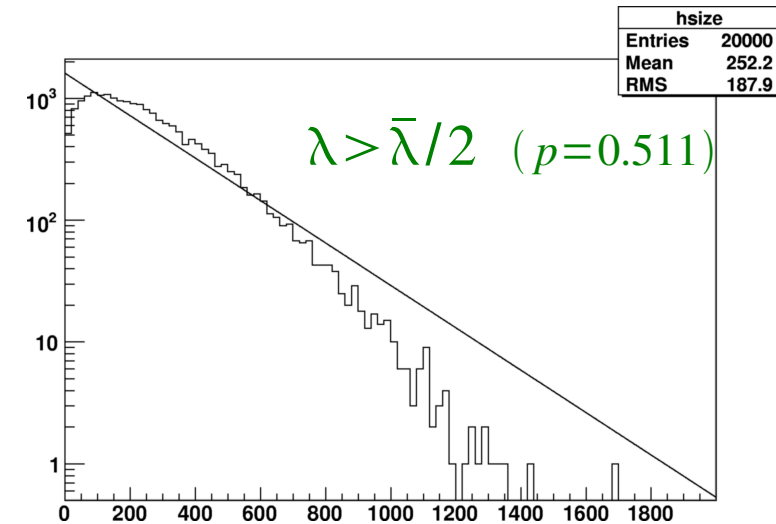
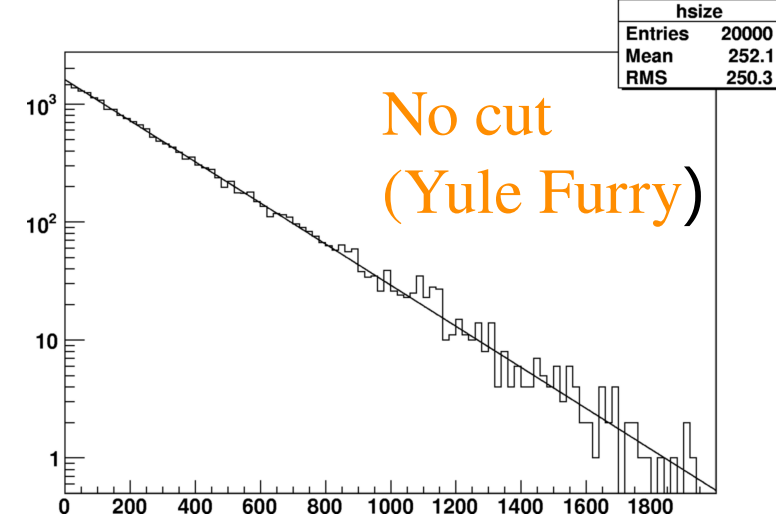
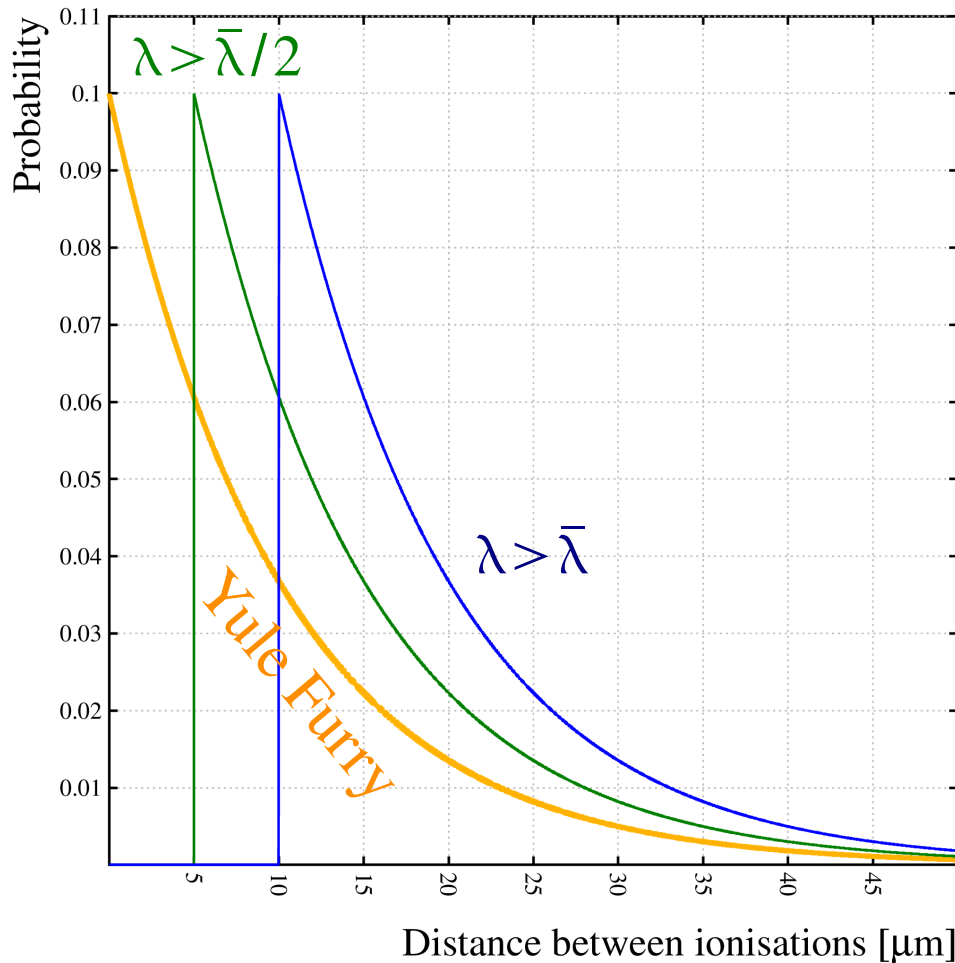
$$p(n) = \sqrt{n} e^{-n}$$
$$\left(\frac{\sigma}{\mu}\right)^2 \approx \frac{2}{3}$$

# Two schools of thought ...

- ▶ The distance between ionisations does not simply vary exponentially (e.g. *the Raether group*).
- ▶ The Townsend coefficient is not constant (e.g. *Byrne, Lansiaart & Morucci*).

# Minimum step length

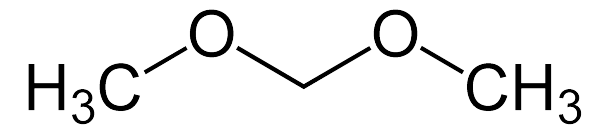
- ▶ Imposing a minimum distance between ionisations adds a hump to the avalanche size spectrum.



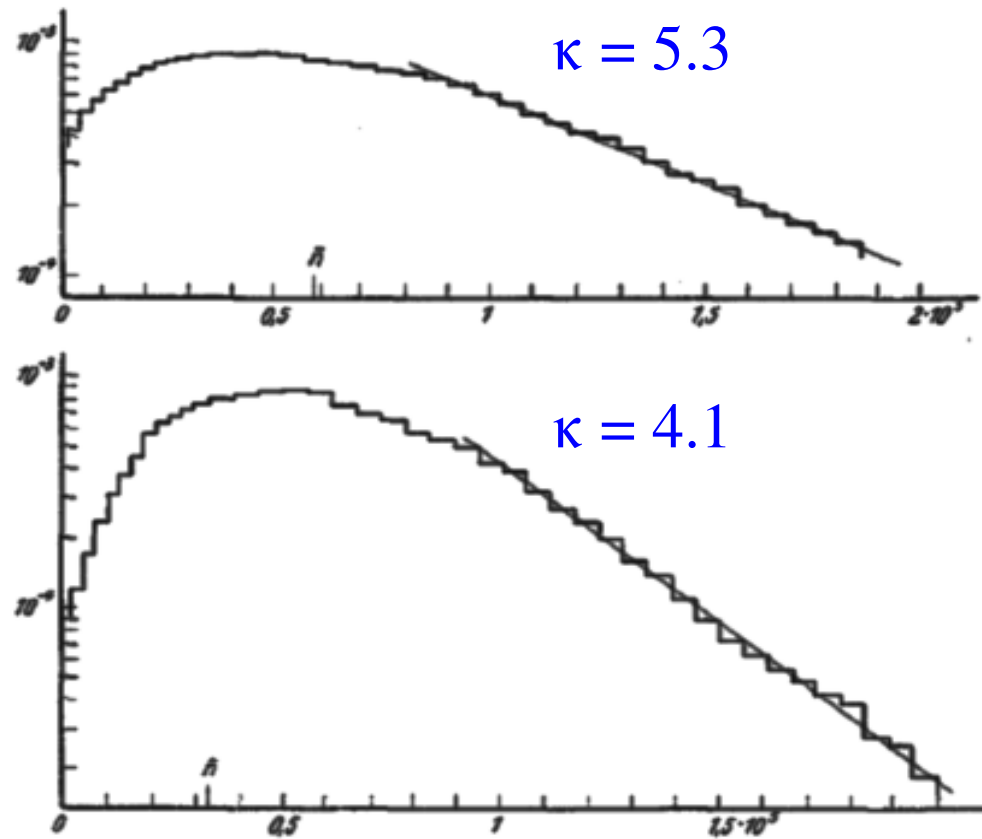
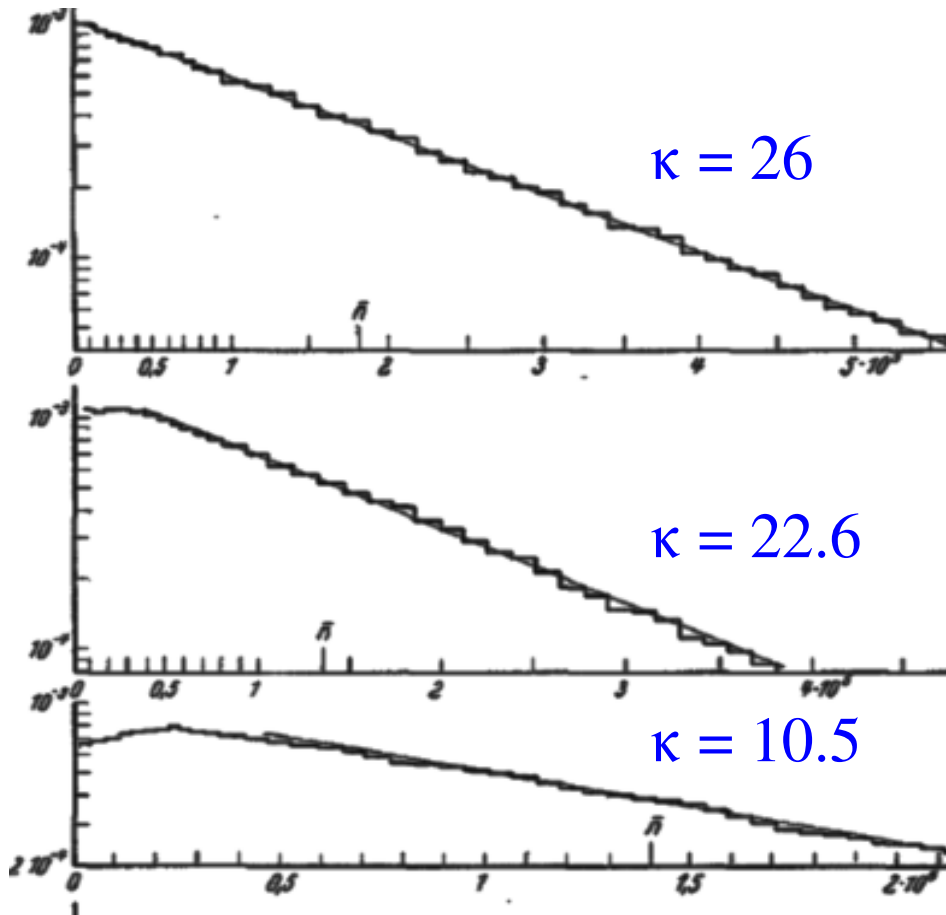




# Hans Schlumbohm (1958)



- ▶ Dimethoxymethane gain spectra: increasing  $E$ , decreasing  $p d$  and  $\sim$  equal mean gain.



# A. Lansiant & J.P. Morucci (1962)

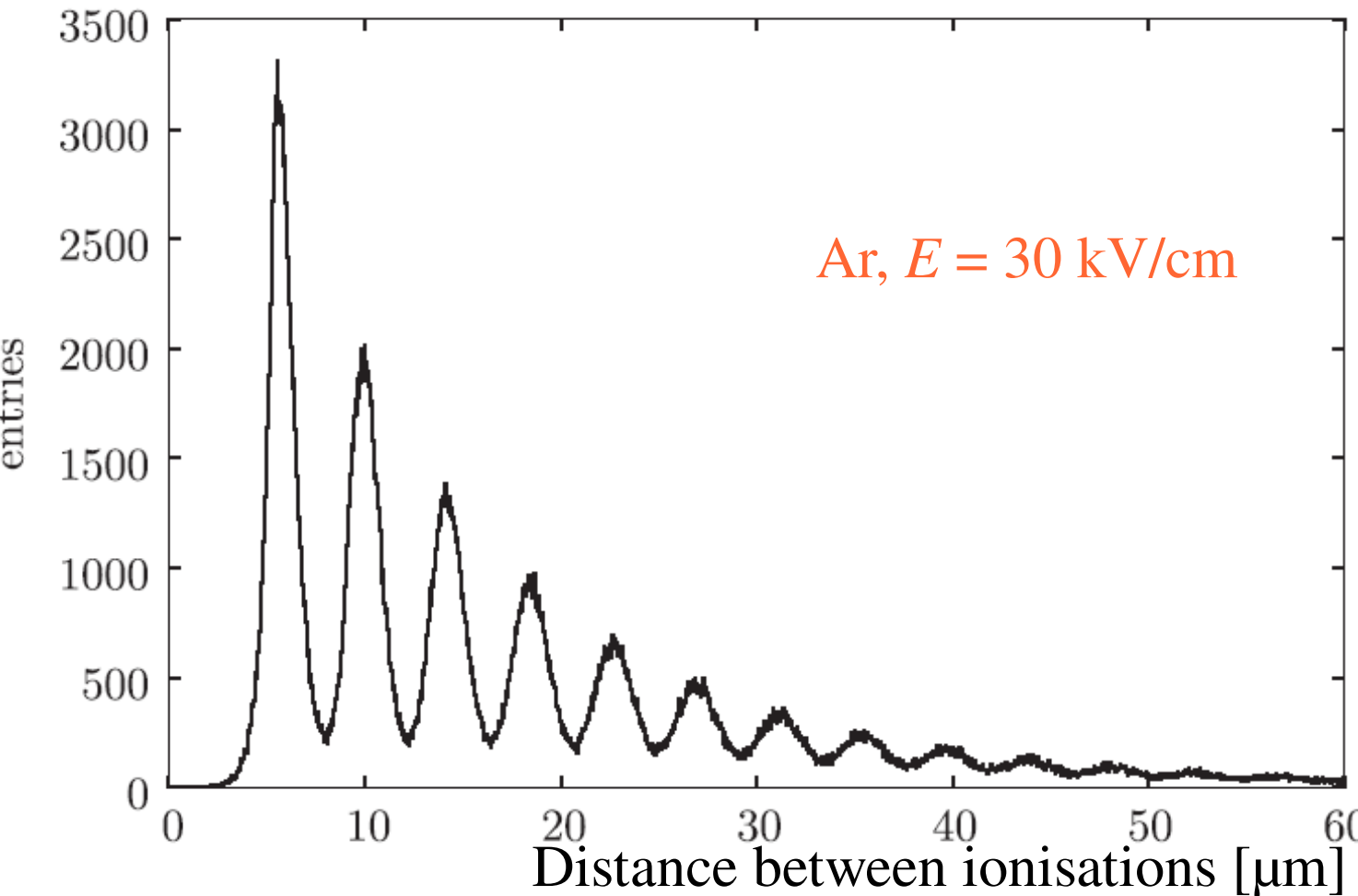
- ▶ Small avalanches are composed of electrons that
  - ▶ have ionised less, hence
  - ▶ have more energy, hence
  - ▶ will ionise more easily
- ▶ They modeled this with an avalanche size-dependent  $\alpha$ :
$$\alpha(n) = \alpha(0) \left( 1 + \frac{k}{n} \right)$$
- ▶ Implies that  $(\sigma/\mu)^2 = 1/(1+k) < 1$ , in agreement with Curran's measurements.
- ▶ In such a mechanism, the electron energy distribution continues to decrease, without reaching an equilibrium.

# Monte Carlo approach

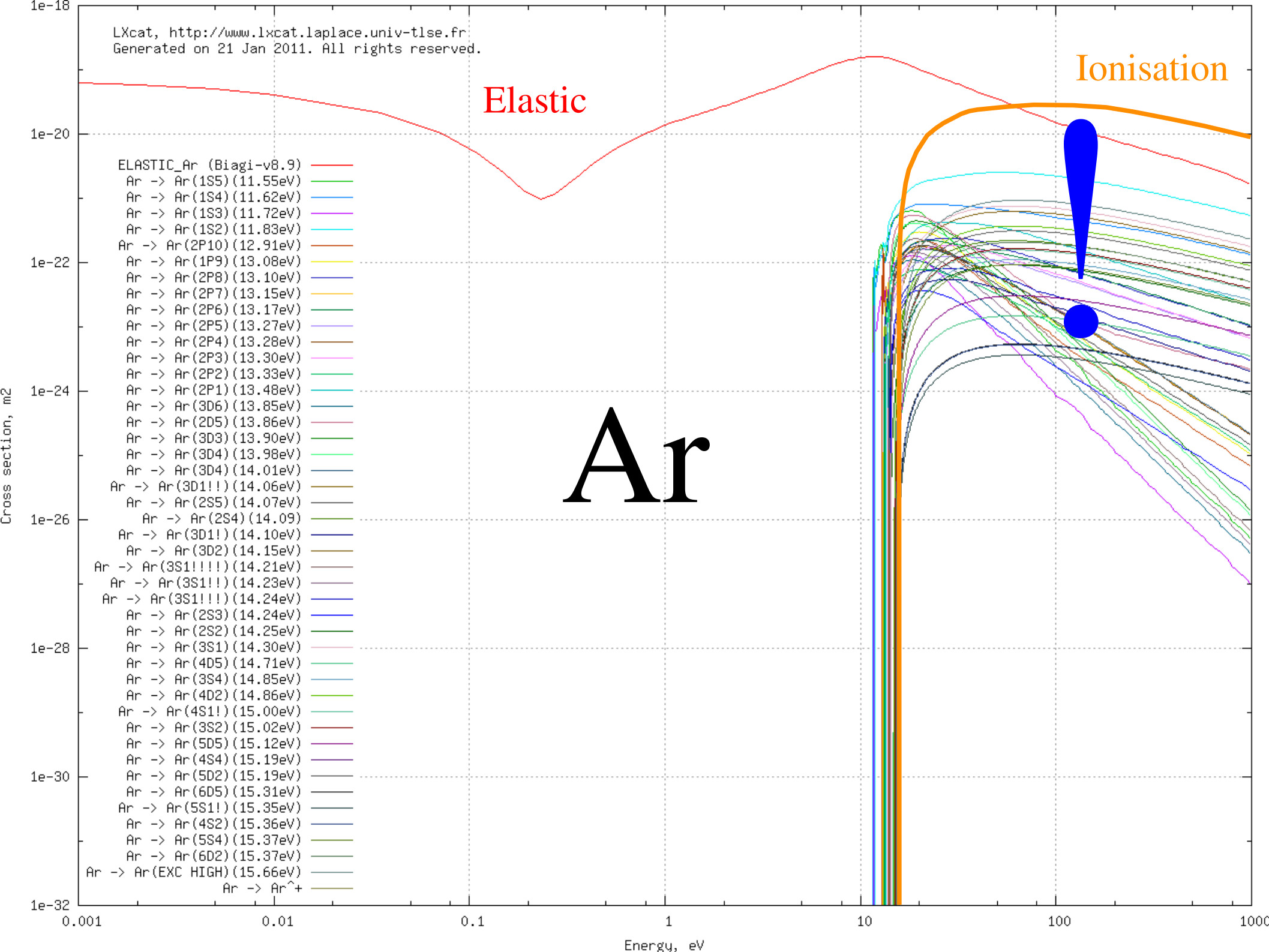
- ▶ Analytic models are precious for the insight they afford.
- ▶ But ... the complexity of real gases and electric fields in real detectors, make realistic models unwieldy:
  - ▶ inelastic collisions (vibrations, rotations, polyads);
  - ▶ excitations and Penning transfers;
  - ▶ attachment;
  - ▶ intricate, position-dependent  $E$  and  $B$  fields.
- ▶ Predictions for experiments are more practical using a Monte Carlo approach, here based on Magboltz.

# Distance between ionisation: MC

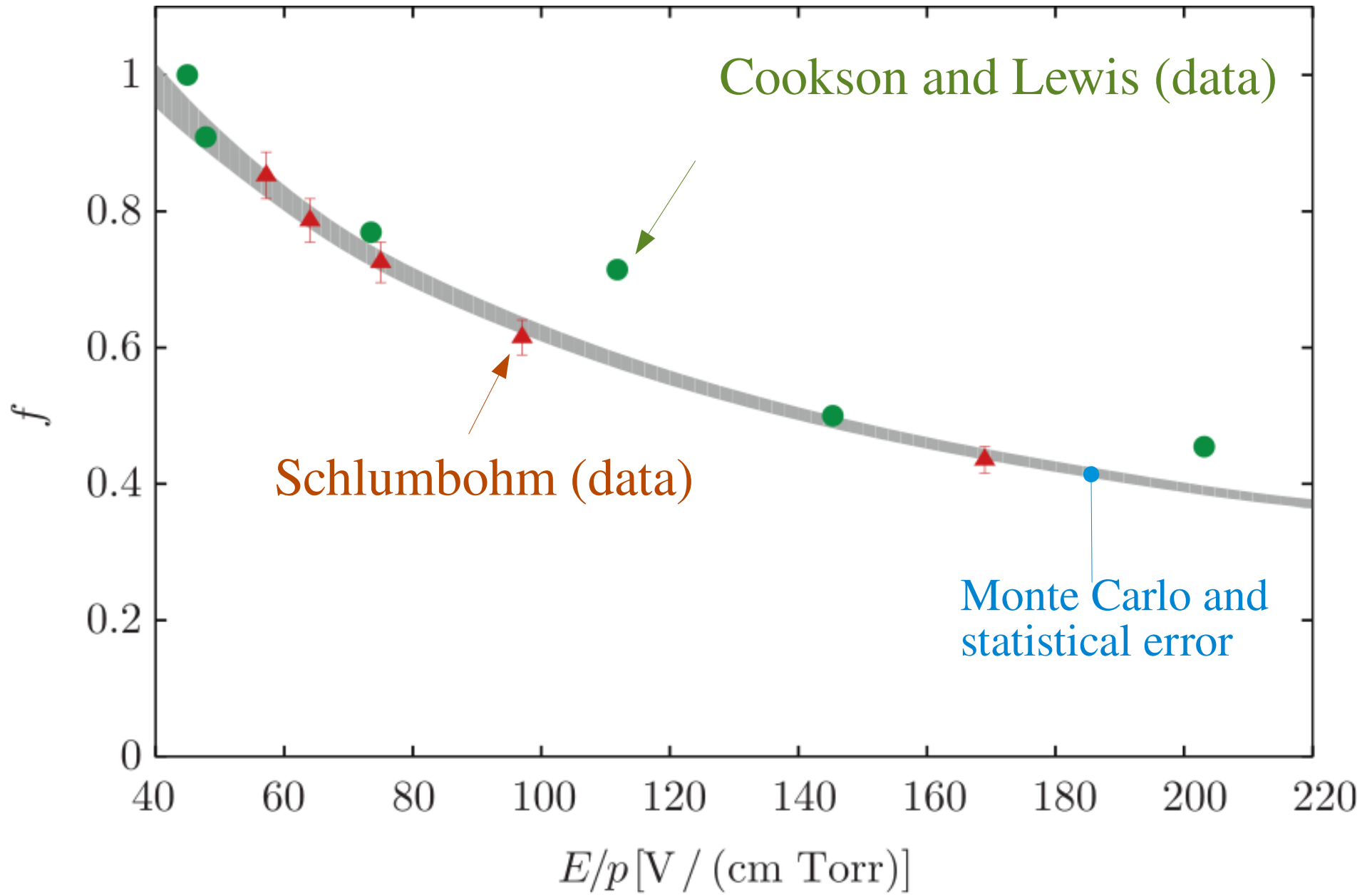
- ▶ The distance between successive ionisations oscillates, shown here for Ar (also happens in e.g. CH<sub>4</sub>). Why ?



[Magboltz calculations  
by Heinrich Schindler]



# MC verification: methane



# Signals – How ?

- ▶ Weighting field
- ▶ quasi-static