Basics of ion transport simulation

Yalçın KALKAN
Uludağ University

14th RD51 Collaboration Meeting, VECC-SINP Kolkata, India (27-31 October 2014)

OUTLINE

* Comparison of thermal and kinetic energy of ions
* Models on mobility of ion
* Elastic Scattering of an ion with an gas
* Directions and velocities
* Polarizability
* Generate random numbers for impact parameters
* Radius effect on the impact parameter
* Generate random numbers for impact scattering and azimuthal angle
* Radial velocity distribution spectrum
* Scattering angle distribution spectrum and relation with temperature
* Skullerud Recipe
* Collision Time – Collision Ffequency
* Some tests and results on simulation
* Experimental leg
* Next plans

Thermal Energy of Ions

$$E=\frac{3}{2}k_B T$$

$$k_B=8.6\,10^{-5}\quad\frac{eV}{K}$$

$$T=300\quad K$$

Kinetic Energy of Ions

$$E=\frac{1}{2}m_i v^2$$

$$\mu=1\quad\frac{cm^2}{Vs}\quad,\quad E=100\,\frac{V}{cm}$$

$$Ar^+$$

$$E_T=41.7\,10^{-3}\quad eV$$

$$E_K=2.10^{-7}\quad eV$$

$$E_T\gg E_K$$

Models on mobility

Model 1

T = 0 K

E is high

$$\mu = \frac{1}{\sqrt{2}}\,\frac{q}{\sigma m \mathrm{EN}}$$

Model 2

T $\neq$ 0 K

E is very low

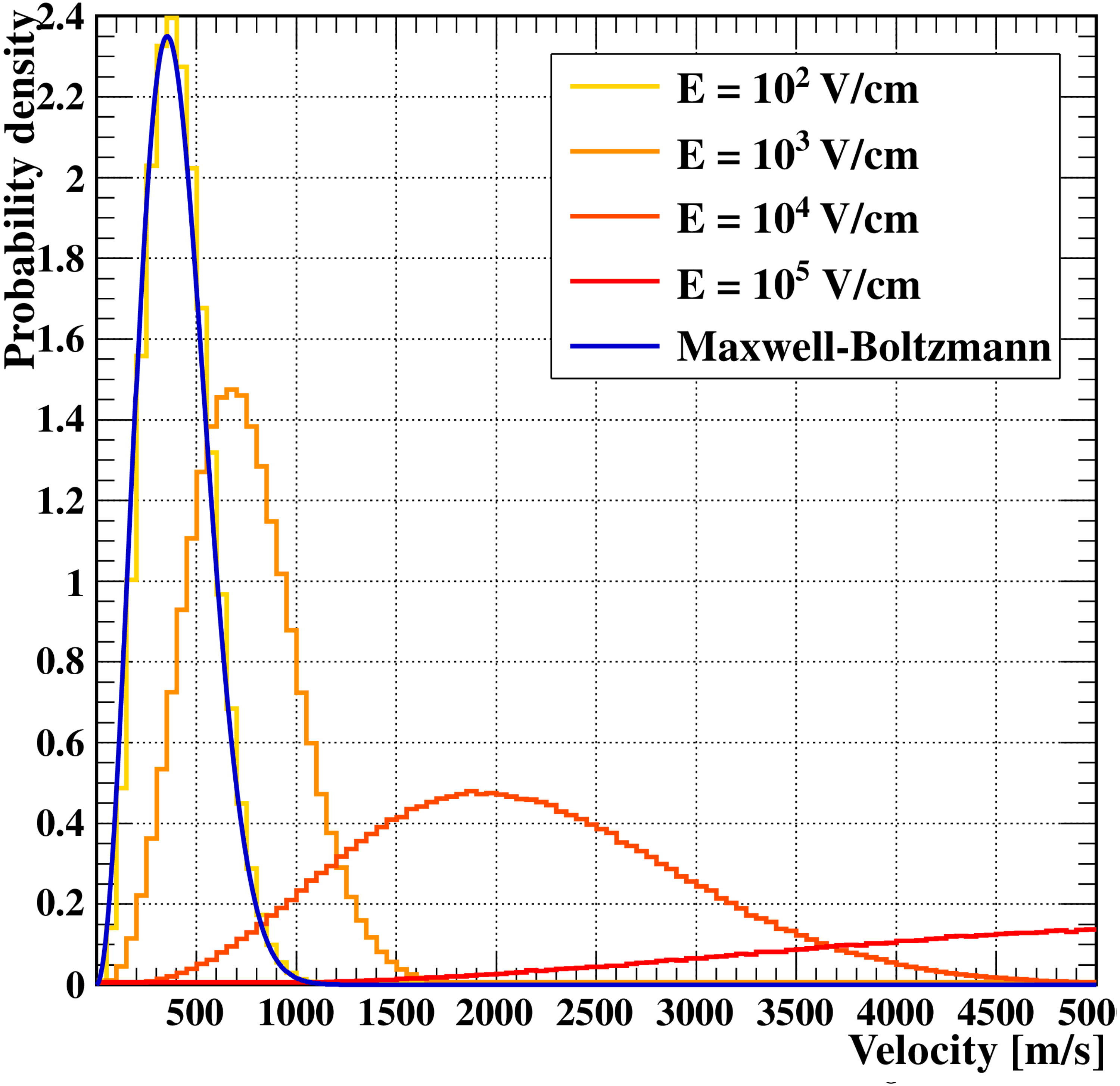
$$\mu = \frac{\sqrt{\frac{\pi}{8}}q}{2\sigma N\sqrt{k_{\mathrm{B}} m T}}$$

A. Effect of Force Law on Mobility

The general expression for the first approximation to K given in Eq. (7) can be rewritten in terms of reduced quantities as follows:

$$[K]_1 = \frac{3e}{16N}\left(\frac{2}{\pi kT}\,\frac{m+M}{mM}\right)^{1/2}\frac{1}{r_m{}^2\Omega^{(1,1)*}}. \qquad (30)$$

Mason, Edward A.; Schamp, Homer W., Jr., Mobility of gaseous Ions in weak electric fields, Annals of Physics, Volume 4, Issue 3, p.233-270.



Probability density
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
E = 10^2 V/cm
E = 10^3 V/cm
E = 10^4 V/cm
E = 10^5 V/cm
Maxwell-Boltzmann
500
1000
1500
2000
2500
3000
3500
4000
4500
Velocity [m/s]

Elastic scattering of ion 1/2

Conservation of momentum . . .

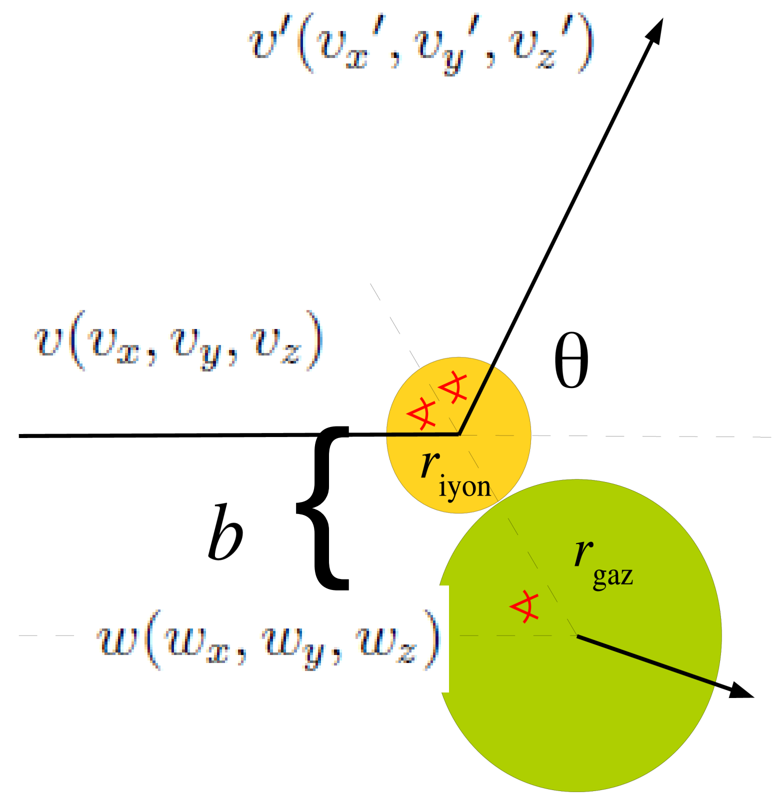
$$m_i v_x + m_g w_x = m_i {v_x}' + m_g {w_x}'$$

$$m_i v_y + m_g w_y = m_i {v_y}' + m_g {w_y}'$$

$$m_i v_z + m_g w_z = m_i {v_z}' + m_g {w_z}'$$

$$0 \leq b \leq r_{gaz} + r_{iyon}$$

$$\frac{1}{2} m_i v^2 + \frac{1}{2} m_g w^2 = \frac{1}{2} m_i v'^2 + \frac{1}{2} m_g w'^2$$



Elastic scattering of ion 2/2

Conversion to center of mass frame . . .

$$v_{(CM)} = -\frac{m_i v_i + m_g v_g}{m_i + m_g}$$

A simple benchmarking . . .

$$|V| = \frac{m_2\,|W|}{m_1}$$

Also momentum conservation . . .

$$m_1 V_x + m_2 W_x = 0$$

$$m_1 V_y + m_2 W_y = 0$$

[in case of the collision on the X-Y plane]

[Capital letters refers to last velocities]

Directions and velocities

Function of velocities . . .

$$f(v) = \left(\frac{m}{2\,\pi\,k_{\mathrm{B}}\,T}\right)^{3} 4\pi\,|v_{\mathrm{g}} - v_{\mathrm{i}}|\,e^{-\frac{mv^{2}}{2\,k_{\mathrm{B}}\,T}}$$

Function of velocities as a result of confirmation . . .

$$\int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dv_l \int_{-\infty}^{+\infty} dx_2 \int_{-\infty}^{+\infty} dv_2 f(x_1) f(v_1) f(x_2) f(v_2) \delta\left(\frac{x}{v} - \left(\frac{x_1}{v_1}, \frac{x_2}{v_2}\right)\right)$$

The latest result is just . . .

$$|v|$$

Polarizability

In $1\ cm^3$ gas volume $d = 6.5\ 10^{-16}\ cm$

Electrical Field . . .

$$E \propto \frac{1}{(r+\epsilon)^2} - \frac{1}{(r-\epsilon)^2} E \propto \frac{-4\epsilon}{r^3}$$

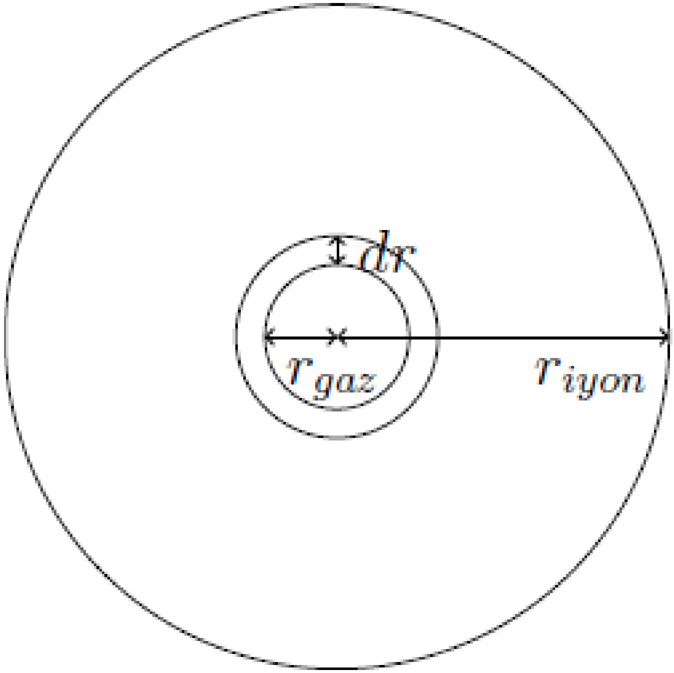
The force between ion and dipole . . .

$$F = \frac{q.\mu}{r^3} = \frac{q.\alpha}{r^5}$$

Generate random numbers for impact parameters

Normalization . . .

$$\int_0^{r_g+r_i} f(r)dr = c\int_0^{r_g+r_i} 2\pi r dr = 1 \quad c = \frac{1}{\pi(r_g+r_i)^2}$$



Probability density . . .

$$f(r) = \frac{2\pi r}{\pi(r_g+r_i)^2} = \frac{2r}{(r_g+r_i)^2}$$

Generation function . . .

$$F(x) = \sqrt{u}(r_g+r_i)$$

Radius effect on the impact parameter

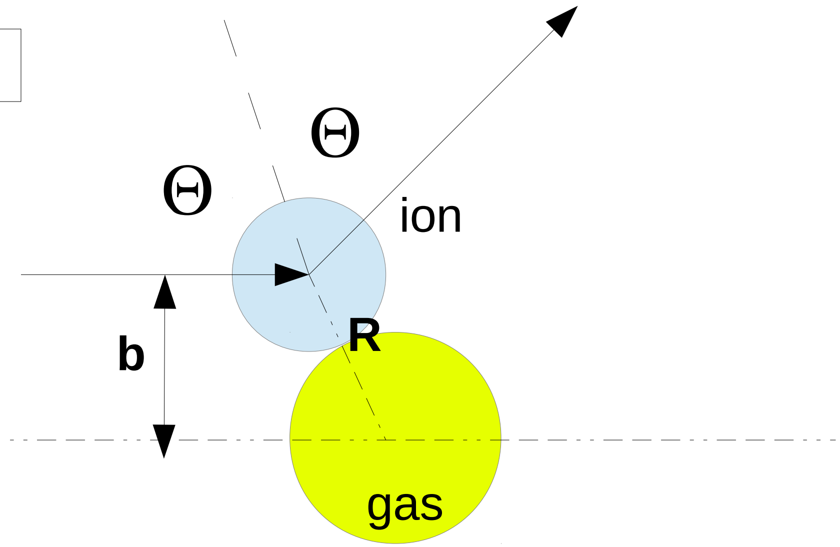
$$cos\ (\theta) = 2cos^2\frac{\theta}{2} - 1$$

$$F(x) = \sqrt{u}(r_g + r_i)$$

$$cos\ \frac{\theta}{2} = \frac{b}{R}$$

$$cos\ (2\theta) = cos^2(\theta) - sin^2(\theta)$$

$$cos\ (\theta) = 2cos^2\frac{\theta}{2} - 1$$



No relation between R's and b

Generate random numbers for scattering angle and azimuthal angle

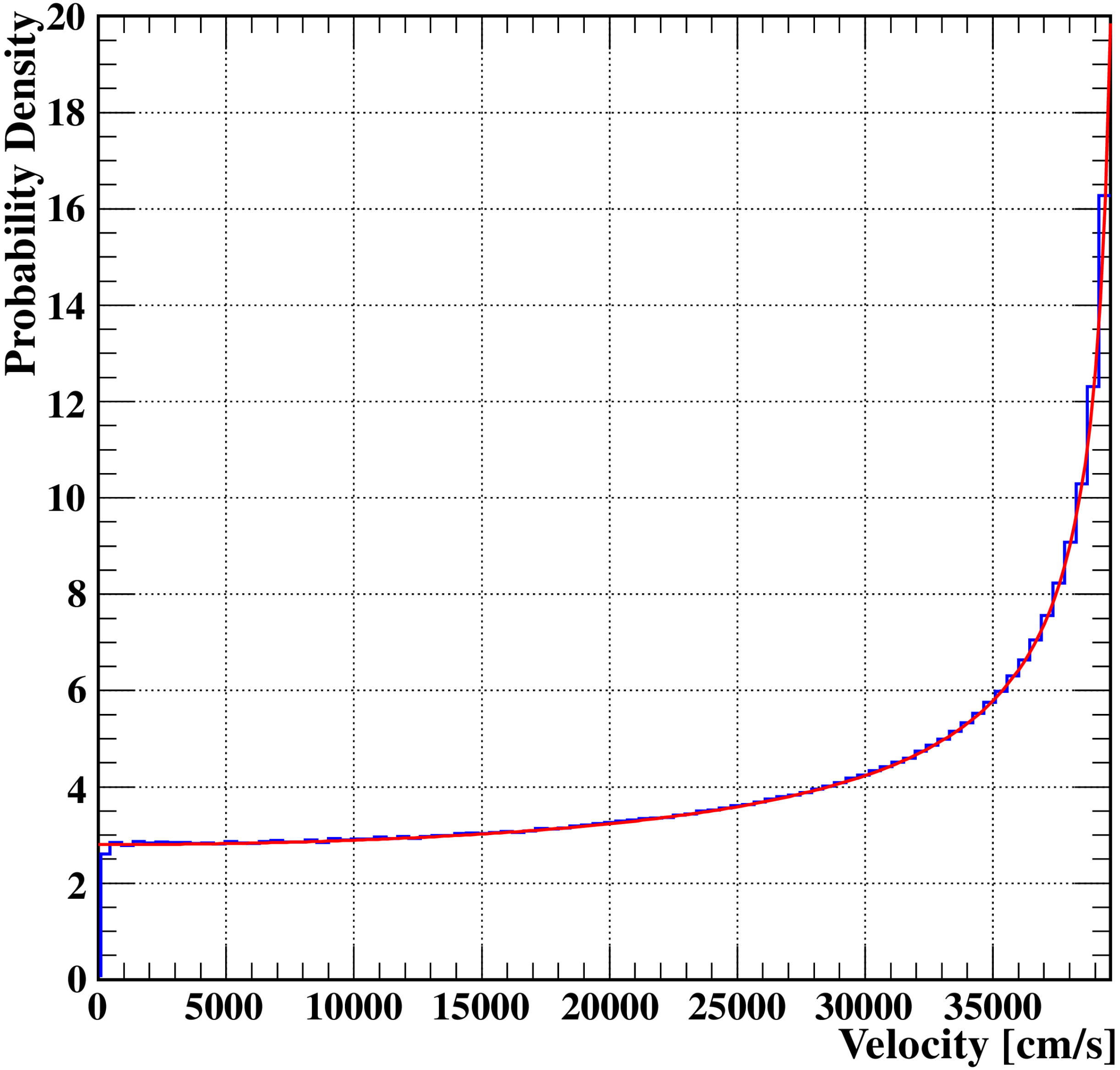
$$\sin\alpha = \frac{b}{r_g + r_i}$$

$$\cos\alpha = \frac{\sqrt{(r_g + r_i)^2 - b^2}}{(r_g + r_i)}$$

$$\sin\theta = 2b\,\frac{\sqrt{(r_g + r_i)^2 - b^2}}{(r_g + r_i)}$$

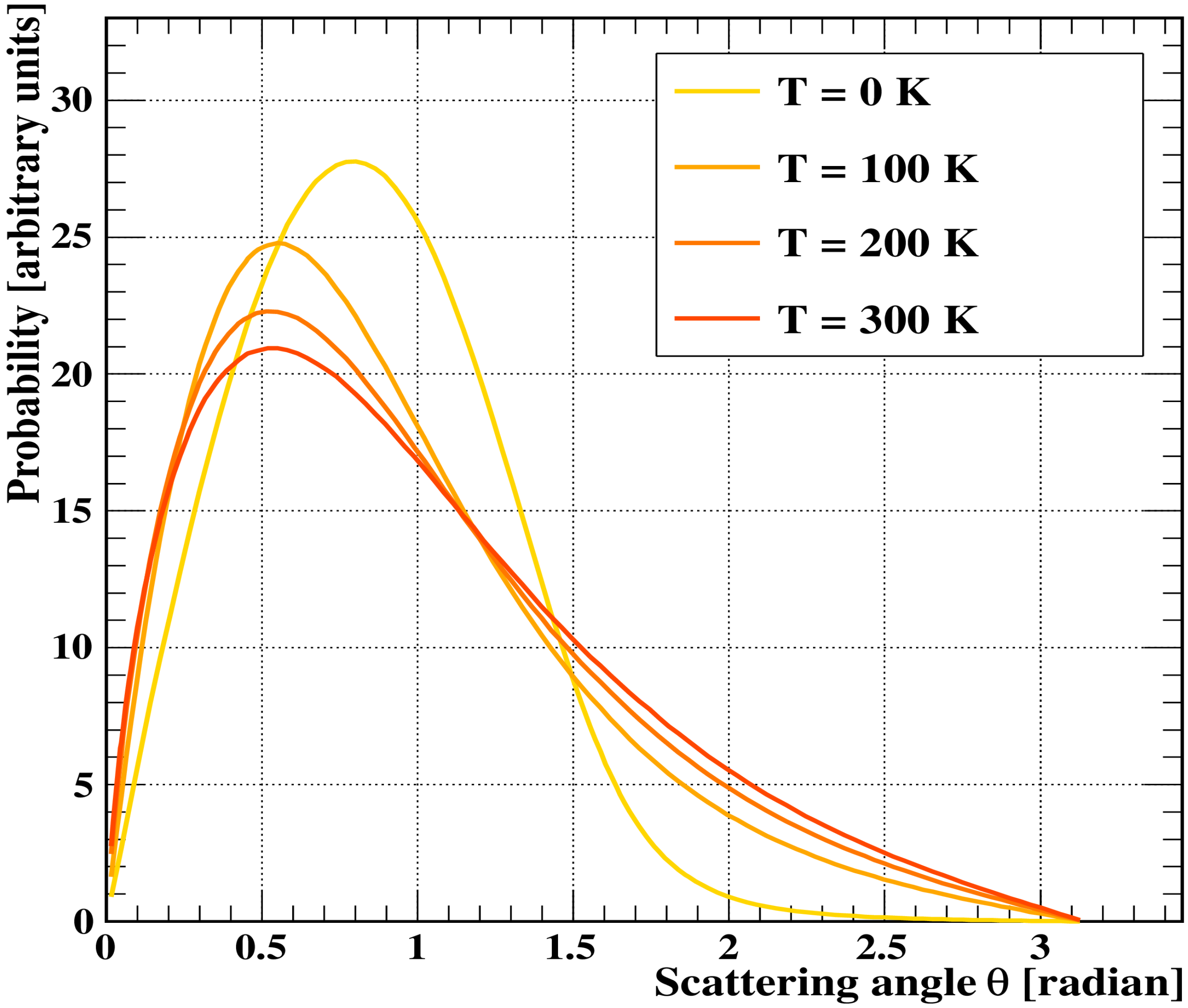
- Random number for azimuthal angle is uniform between [0,2π]

Radial velocity distribution spectrum



$$v_{termal} = \frac{3\ k_{\mathrm{B}}\ T}{m}$$ (Red line)

Scattering angle distribution spectrum and relation with temperature



Skullerud Recipe

$$\nu(v) = N v_i \sigma(v)$$

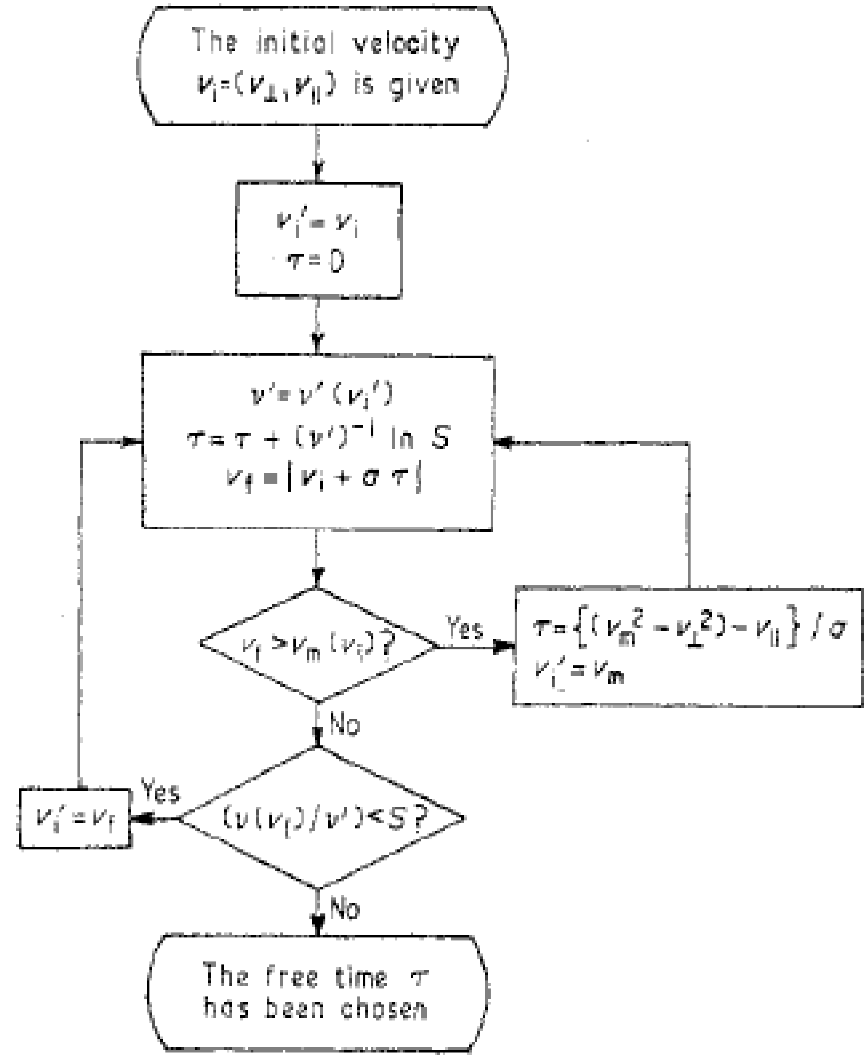
$$v = v_i + at$$

$$P(t) = exp\left(- \int_{t=0}^{\tau} \nu(|v_i + at|)dt \right)$$

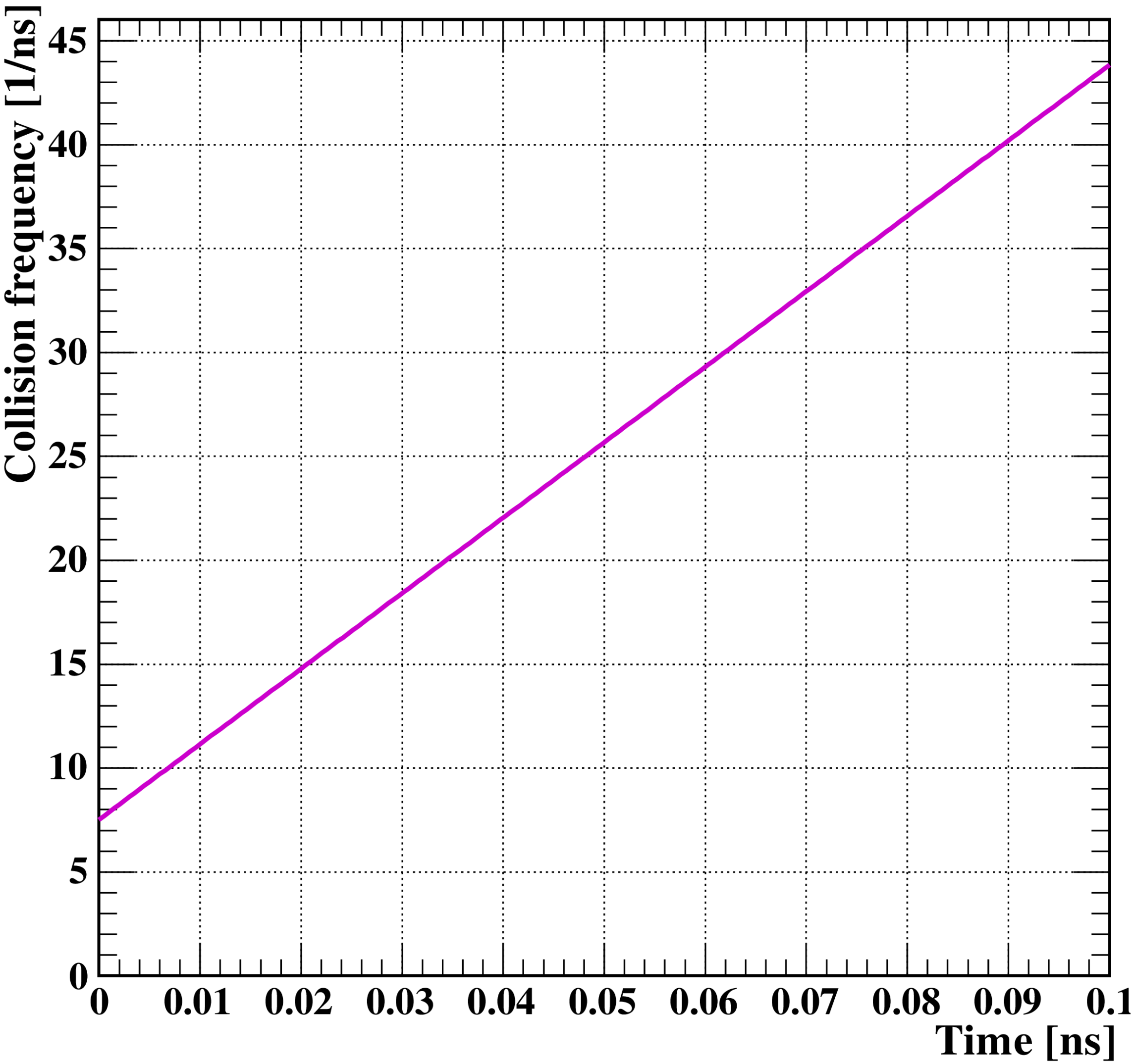
$$P(t) = S$$

$$\tau = \nu^{-1} \log S$$

$$K = \int_0^{\tau} \nu(t)dt$$



Collision Time – Collision Frequency

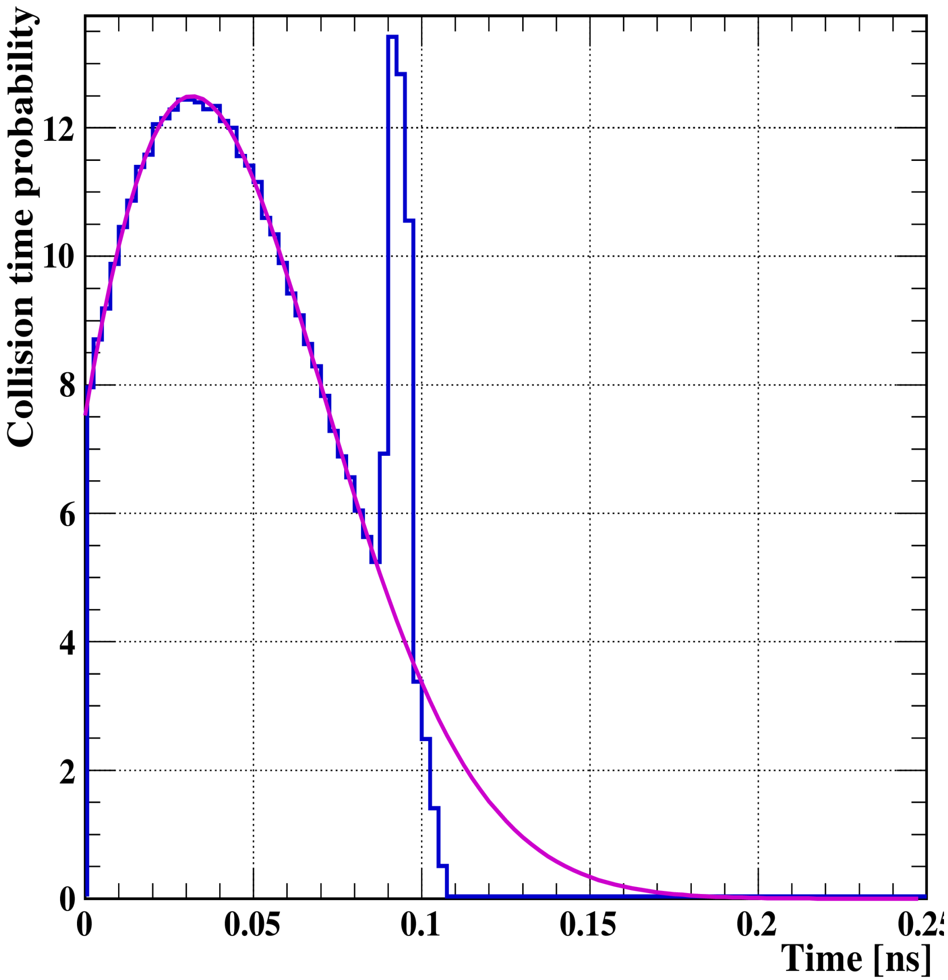


Ar^+ in Ar

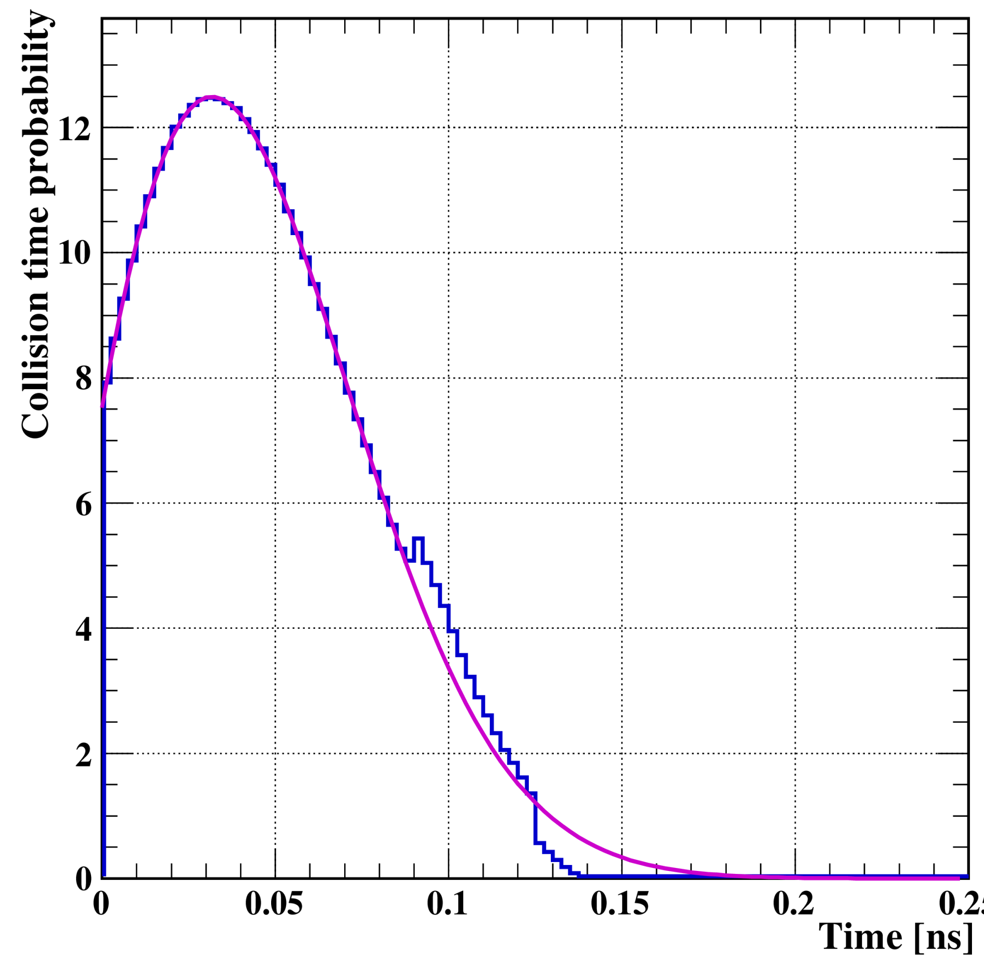
Cross Section : 615 Mb
Temperature : 300 K
Pressure : 101.225 Torr
Initial velocity of Ion : 5 μm/ns
Electric Field : 10^6 V/cm
Skullerud is purple line.
Reference temperature and pressure also number density of gas from NIST.

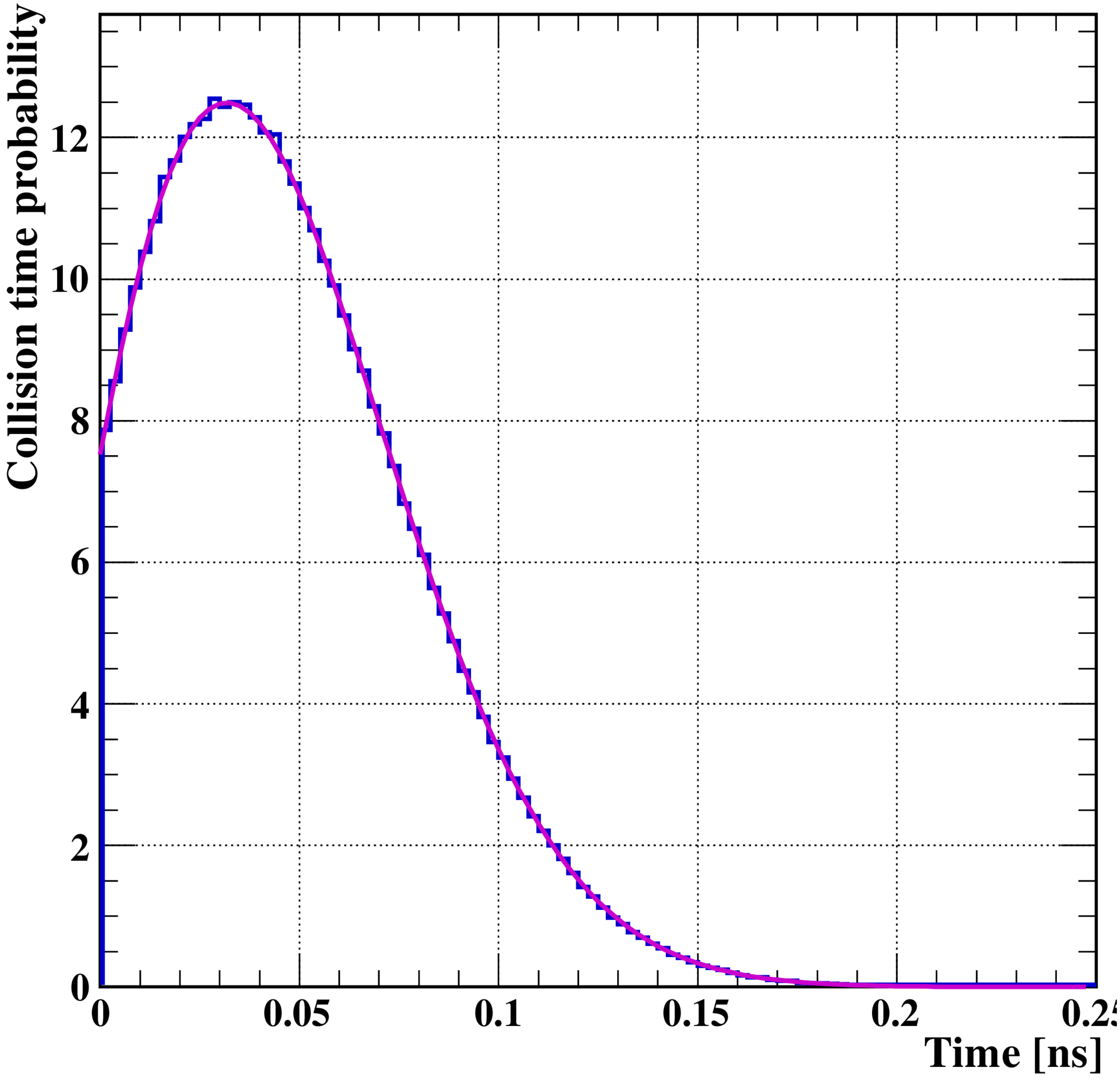
Ar+ in Ar …
Max Coll. Freq = 40 GHz
Purple → Skullerud
Blue → MC

10^6 event



10^7 event

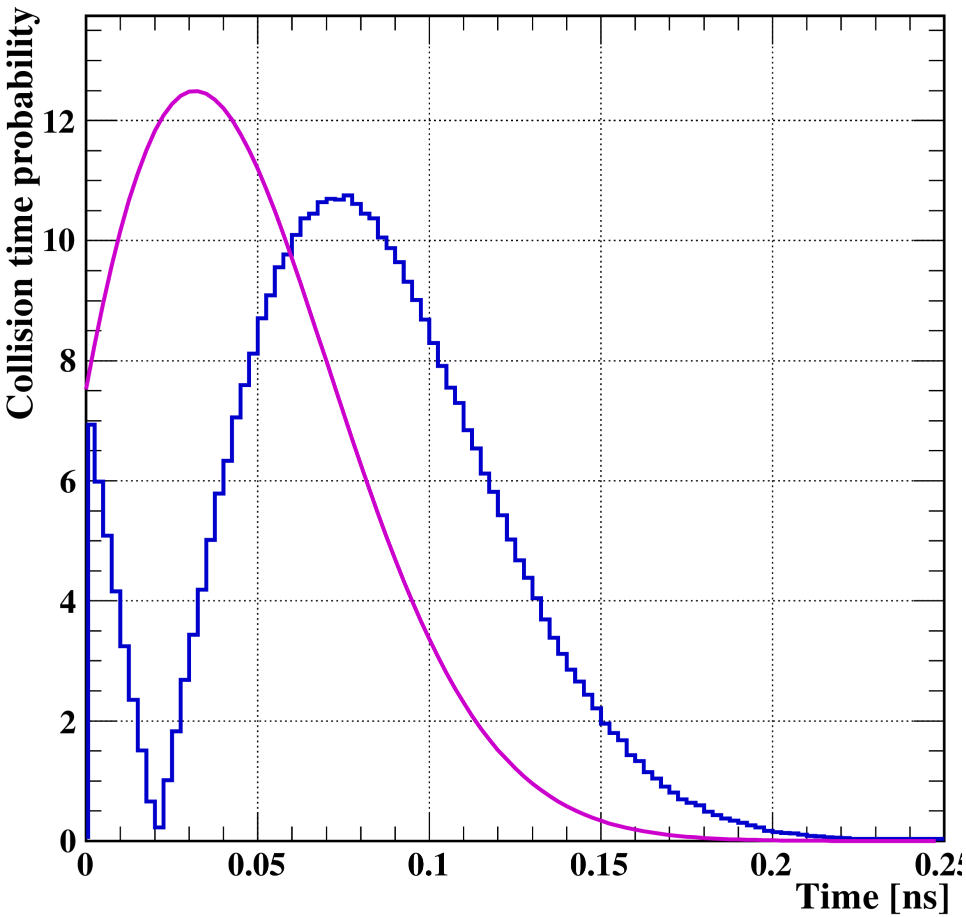


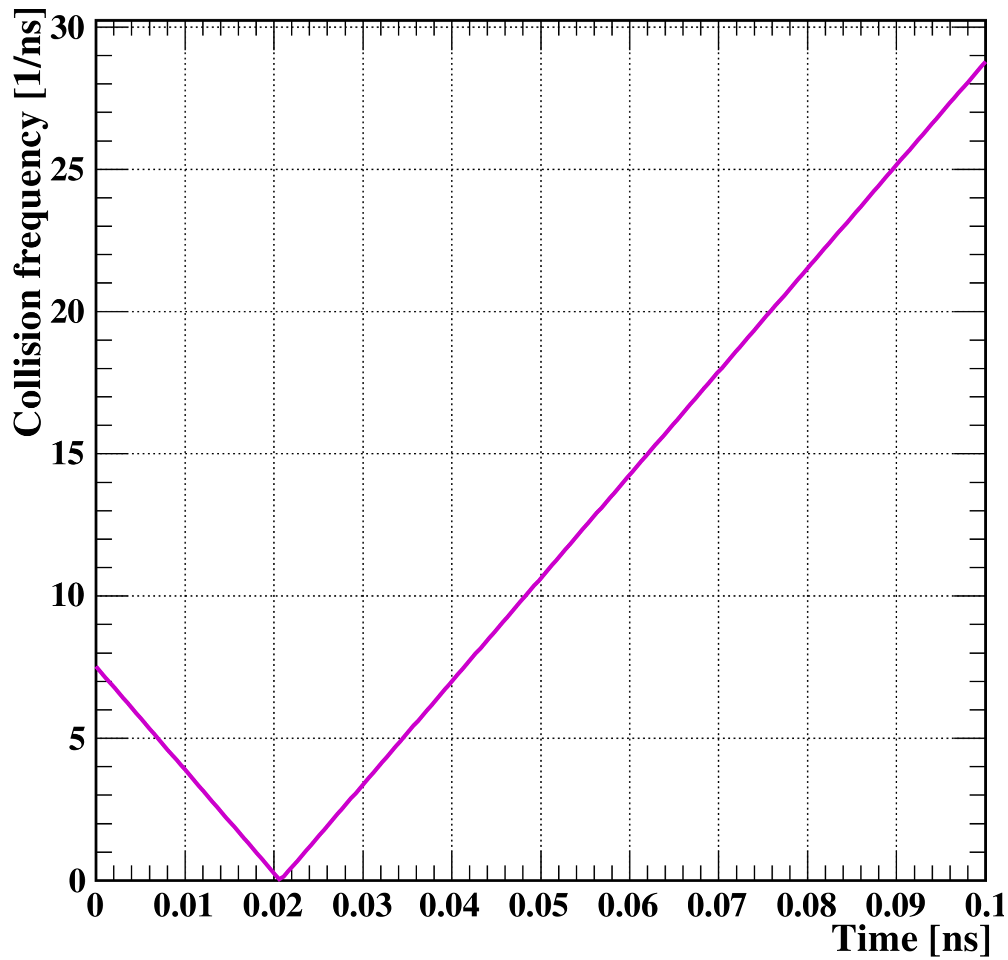


Ar+ in Ar …
Max Coll. Freq = 40 GHz
Purple → Skullerud
Blue → MC

Ar+ in Ar …
Purple → Skullerud
Blue → MC

for negative ion velocity ...





Experimental leg

- Coimbra University has visited.
- Uludağ University Gas Detector Laboratory is preparing.

Next plans

- Finish the tests of simulation
- Compare with simulation and experimental data for Ar+ in Ar also CO2+ in CO2
- Look complex ions

Acknowledges

- Plots and discussions with Rob Veenhof
- Some discussions with André Cortez and Pedro Encarnação