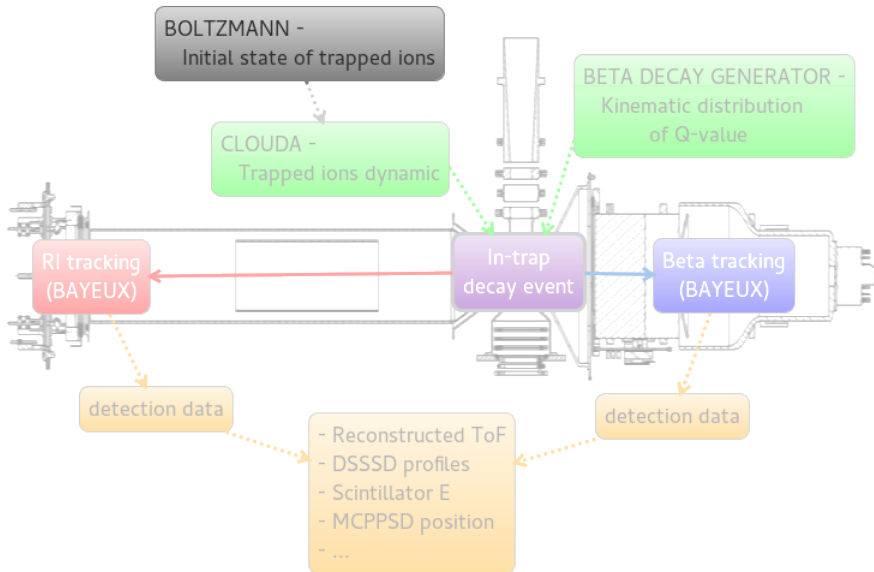# Synopsis

Overview : simulation package

Simulation : initial event

Overview : simulation package

Simulation : initial event

Boltzmann initial state

Simulation : initial event

Buffer gas injected in the trap
$\sim \mathbf{10^{-5}}$ mbar (He or H_2)

$\Downarrow$

Thermalization process kills
all prior information

$\Downarrow$
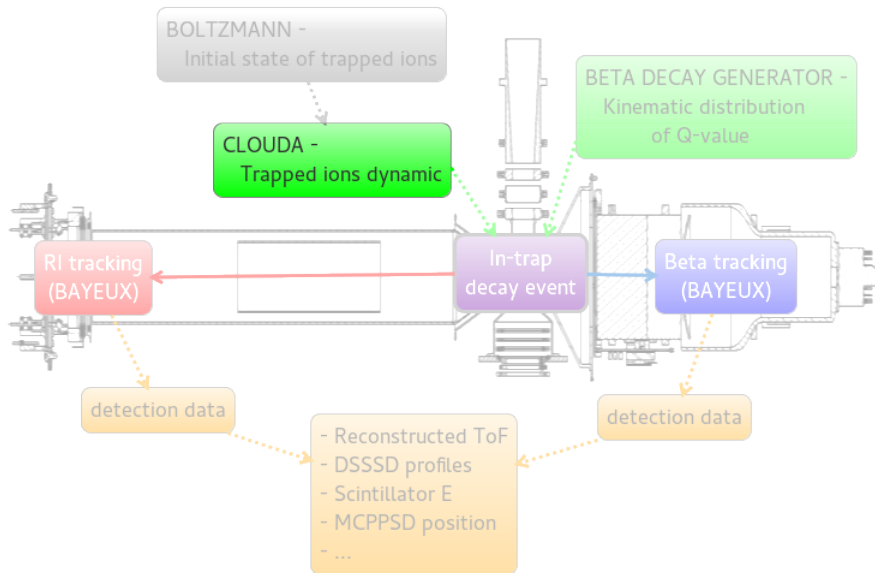
No need to simulate before trap

$\Downarrow$

Any "reasonable" initial state will do
Maxwell-Boltz. Distribution

$T = \mathbf{1000}$ K, $\vec{r}_{\text{init.}} = \mathbf{(0, 0, 0)}$
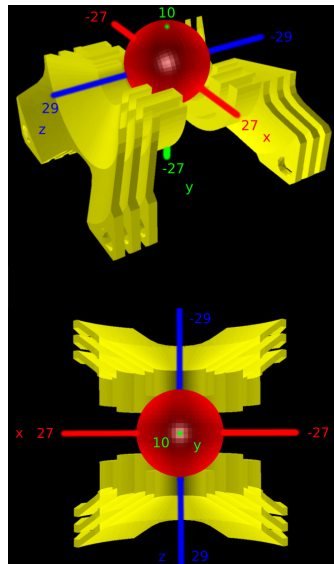
Overview : simulation package

Simulation : initial event

*Trapped ion dynamic : CLOUDA

Simulation : initial event

Trapped ions are subject to :

- Collisions with buffer gas
- Electromagnetic trapping field
- Coulomb N-body repulsion ($\mathcal{O}(N^2)$)

CLOUDA was thus developped :

- GPU based : massive parallelization
  Classic CPU : 4×2 cores, GTX TITAN Black : 2880 CUDA cores
- Steppers : 4th order Runge-Kutta, Leapfrog, Euler (tracking in parallel)
- Timestep $\Delta t = 1$ ns
- Generic : usable for other trap experiments (Paul or Penning)

Objective

Provide a realistic trapped cloud profile $\Rightarrow$ Set β decay in lab. frame.

*CLOUDA – Buffer gas : overview

Simulation : initial event

Issue : simulate buffer gas cooling microscopically $\Rightarrow$ ion-atom collision

Realistic models : collaboration with CELIA (Bordeaux) & Madrid, ion-atom potentials effect

Four models :

- Classical : Hard Spheres (HS), *Classical*
- Quantum : *Cold gas*, *Full*

Global logic applied for any model :

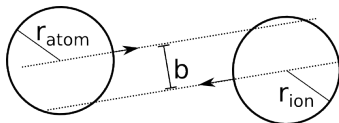1. Check if collision happens $\Rightarrow$ Compute mean free path λ (model dependent)

$$p_{\text{collision}} = 1 - \exp\left(\frac{v_{\text{ion}}.\Delta t}{\lambda}\right)$$

2. If collision happens, randomize $\vec{v}_{\text{atom}}$ and compute scattering angle θ (model dependent) in center-of-mass frame
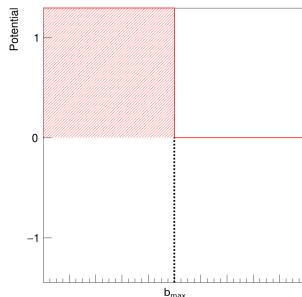
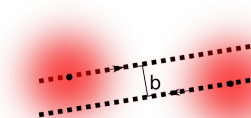# *CLOUDA – Buffer gas : Classical models
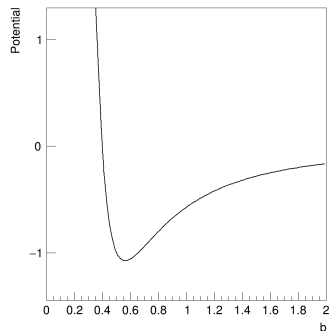
Simulation : initial event

Hard Spheres

$b < b_{max} = r_{atom} + r_{ion}$

Classical

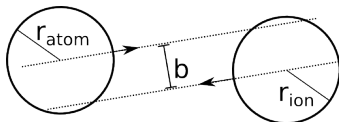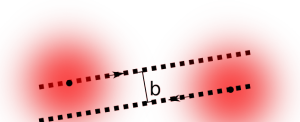$b < b_{max} = $ numerical cut

*CLOUDA – Buffer gas : Classical models

Simulation : initial event

Hard Spheres

Classical

$b < b_{max} = r_{atom} + r_{ion}$

$b < b_{max}$ = numerical cut

Mean free path $\lambda = \boldsymbol{v}_{ion}/\nu$ (ν : collision frequency) :

$$\nu(\boldsymbol{v}_{ion}) = \rho_{gas} \, \pi \, \boldsymbol{b}_{max}^2 \, \boldsymbol{v}_{mp} \left[\left(\frac{\boldsymbol{v}_{ion}}{\boldsymbol{v}_{mp}} + \frac{\boldsymbol{v}_{mp}}{2\boldsymbol{v}_{ion}} \right) \mathrm{erf} \left(\frac{\boldsymbol{v}_{ion}}{\boldsymbol{v}_{mp}} \right) + \frac{1}{\sqrt{\pi}} \exp \left(- \left(\frac{\boldsymbol{v}_{ion}}{\boldsymbol{v}_{mp}} \right)^2 \right) \right]$$
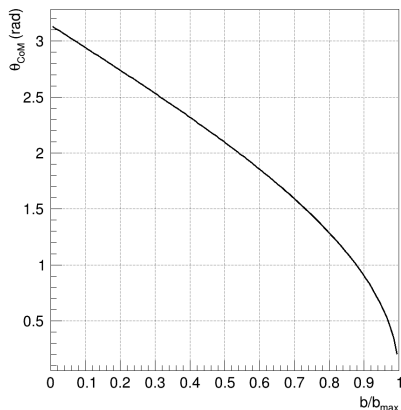
$(\pi \, \boldsymbol{b}_{max}^2)$: constant cross section

*CLOUDA – Buffer gas : Classical models

Simulation : initial event

Hard Spheres

HS θ distribution

$$\theta = \pi - 2\arcsin(b/b_{max})$$

Classical

Realistic classical model scattering

Legend:
- E = 0.005 eV
- E = 0.010 eV
- E = 0.015 eV
- E = 0.020 eV
- ...
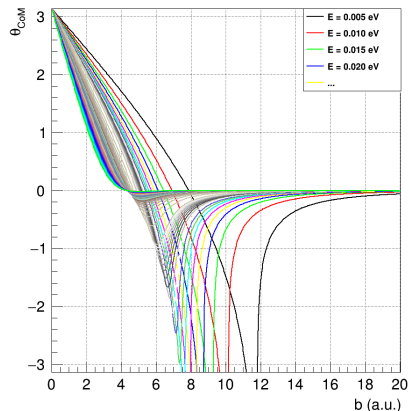
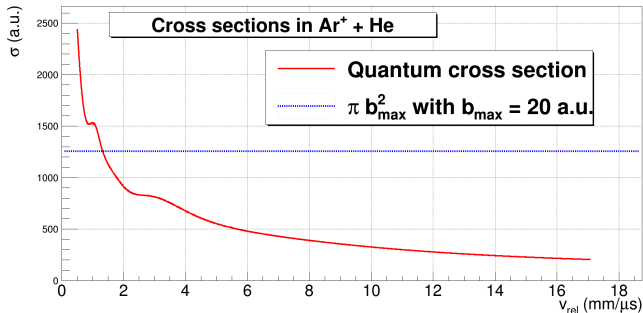$$\theta = f(E_{rel}, b)$$

*CLOUDA – Buffer gas : Quantum models

Simulation : initial event

Mean free path $\lambda = v_{ion}/\nu$ (ν : collision frequency)

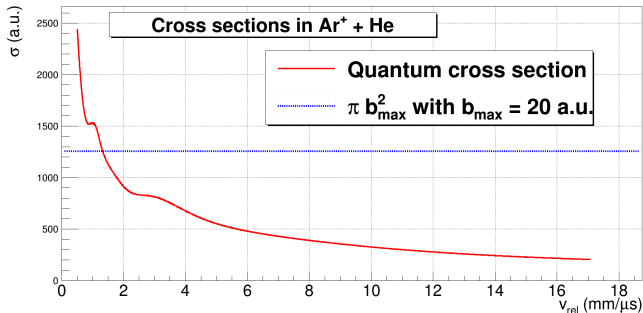- *Cold gas* : $\nu(v_{ion}) = \rho_{gas}\,\sigma(v_{ion})\,v_{ion}$

*CLOUDA – Buffer gas : Quantum models

Simulation : initial event

Mean free path $\lambda = v_{ion}/\nu$ (ν : collision frequency)

- *Cold gas* : $\nu(v_{ion}) = \rho_{gas}\,\sigma(v_{ion})\,v_{ion}$

- *Full* :

$$\nu(v_{ion}) = \frac{\rho_{gas}}{\sqrt{\pi}\,v_{mp}\,v_{ion}} \int_0^{+\infty} dv_{rel}\,\sigma(v_{rel})\,v_{rel}^2 \left\{ \exp\left[-\left(\frac{v_{rel} - v_{ion}}{v_{mp}}\right)^2\right] - \exp\left[-\left(\frac{v_{rel} + v_{ion}}{v_{mp}}\right)^2\right] \right\}$$

Cross sections in Ar$^+$ + He

— Quantum cross section
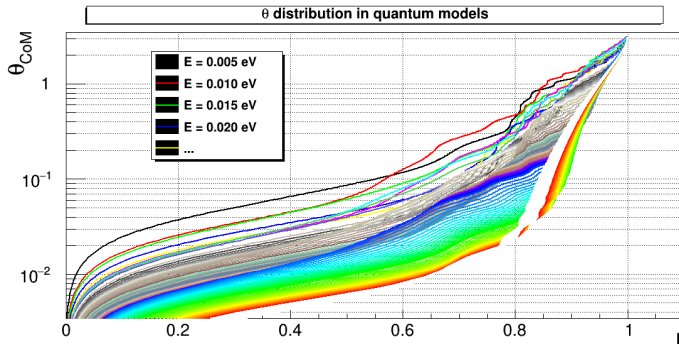···· $\pi\,b_{max}^2$ with b_{max} = 20 a.u.

*CLOUDA – Buffer gas : Quantum models

Simulation : initial event

(If collision) Scattering angle : $\theta = f(E_{\text{rel.}}, r)$

$$\frac{\int_0^\theta \frac{d\sigma(v,\theta)}{d\omega} \sin(\theta) d\theta}{\int_0^\pi \frac{d\sigma(v,\theta)}{d\omega} \sin(\theta) d\theta} = r$$

θ distribution in quantum models

E = 0.005 eV
E = 0.010 eV
E = 0.015 eV
E = 0.020 eV
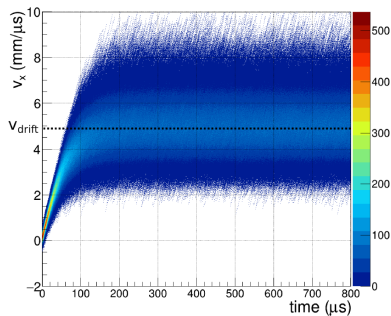...

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

- Constant, uniform, infinite $\vec{E}_x$

*CLOUDA – Buffer gas : Models assessment
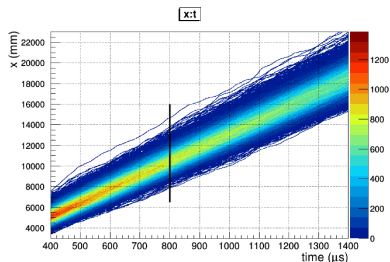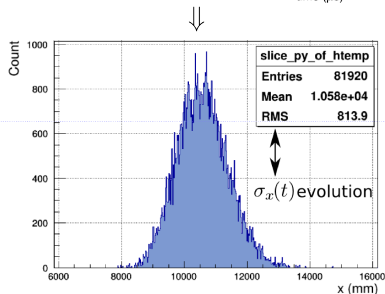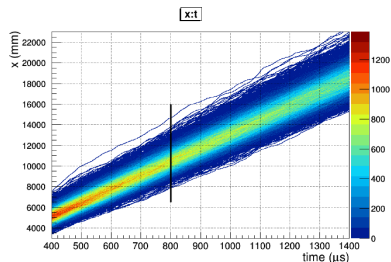
Simulation : initial event

- Constant, uniform, infinite $\vec{E}_x$

- 2 experimental observables for ion-atom collisions :
  - ▶ Drift velocities v_d (^{40}Ar$^+$ + ^{4}He & ^{7}Li$^+$ + ^{4}He)

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

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- 2 experimental observables for ion-atom collisions :
  - ▶ Drift velocities v_d (^{40}Ar$^+$+^{4}He & ^{7}Li$^+$+^{4}He)
  - ▶ Diffusion coefficient D_L, D_T (^{7}Li$^+$+^{4}He only)
    $\sigma_x^2 = \frac{D_L}{2} \times t + b$
    $\sigma_{y,z}^2 = \frac{D_T}{2} \times t + b$

x:t

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

- Constant, uniform, infinite $\vec{E}_x$

- 2 experimental observables for ion-atom collisions :
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  - Diffusion coefficient D_L, D_T (^{7}Li$^+$+^{4}He only)
  $$\sigma_x^2 = \frac{D_L}{2} \times t + b$$
  $$\sigma_{y,z}^2 = \frac{D_T}{2} \times t + b$$

$\Downarrow$

slice_py_of_htemp	
Entries	81920
Mean	1.058e+04
RMS	813.9

$\sigma_x(t)$ evolution

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

- Constant, uniform, infinite $\vec{E}_x$

- 2 experimental observables for ion-atom collisions :
  - Drift velocities v_d ($^{40}Ar^+ + ^4He$ & $^7Li^+ + ^4He$)
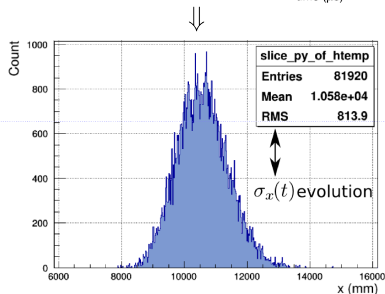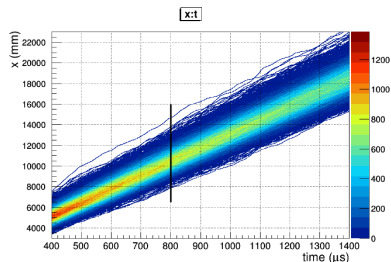 - Diffusion coefficient D_L, D_T ($^7Li^+ + ^4He$ only)
    $$\sigma_x^2 = \frac{D_L}{2} \times t + b$$
    $$\sigma_{y,z}^2 = \frac{D_T}{2} \times t + b$$

- Data will be function of Townsend :

$$(Td) \sim \frac{\text{Electric field}}{\text{Buffer gas density}}$$

Ranging in :
  - 5 – 130 Td for $^{40}Ar^+ + ^4He$
  - 2 – 200 Td for $^7Li^+ + ^4He$

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event
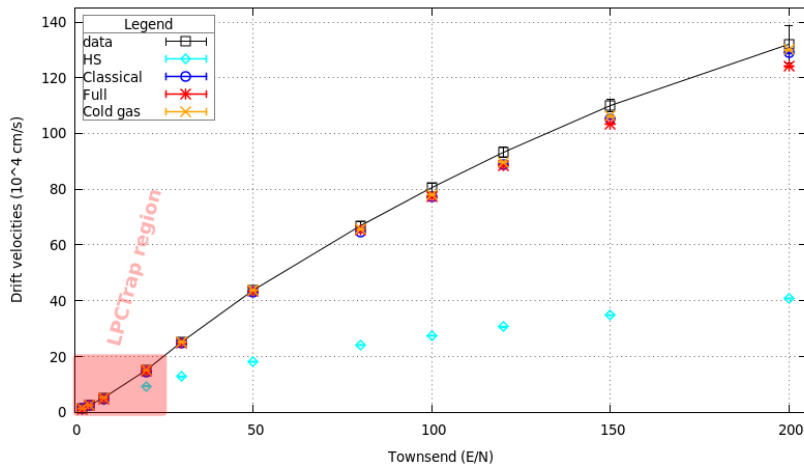
Drift velocitites v_d – $^{40}Ar^+ + {}^4He$
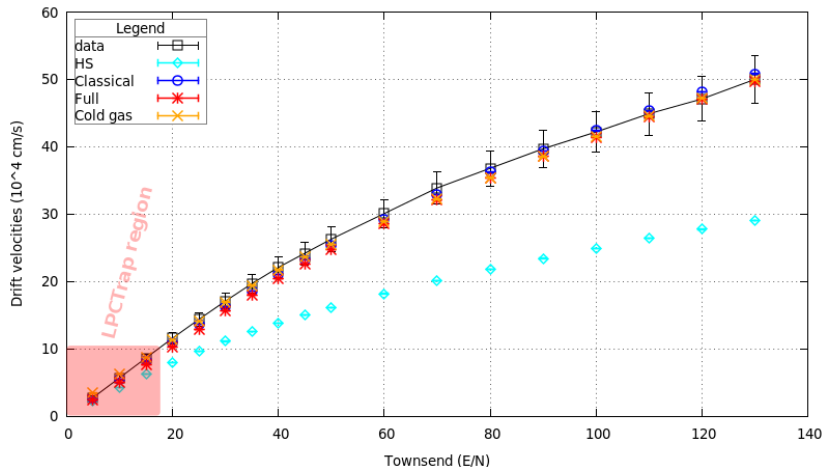
⇒ Good agreement, except for Hard Spheres

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event
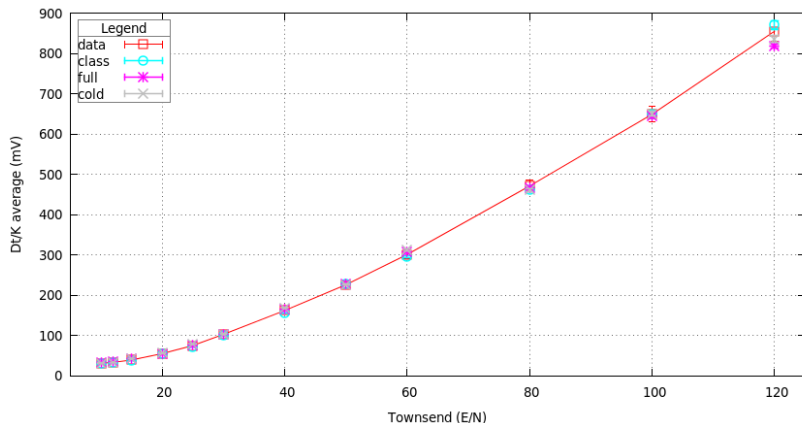## Drift velocitites v_d – $^7Li^+ + ^4He$

⇒ Good agreement, except for Hard Spheres

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

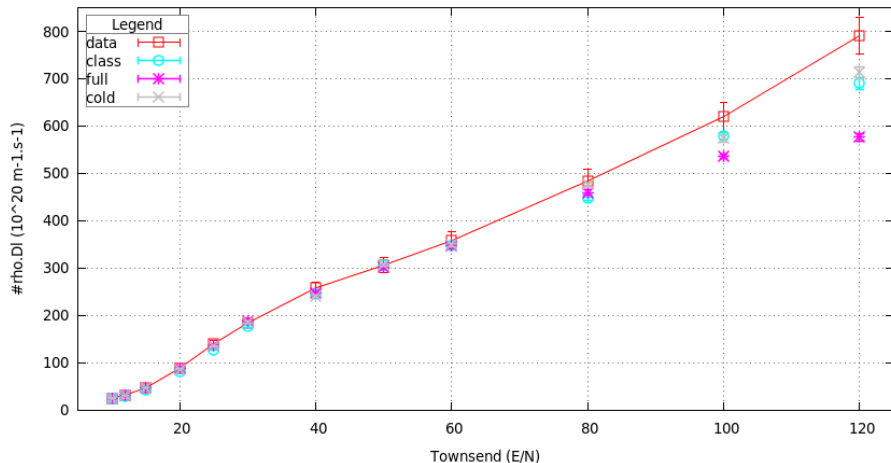Transverse diffusion coefficient D_T – ^{7}Li$^+$ + ^{4}He

$\Rightarrow$ Good agreement

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

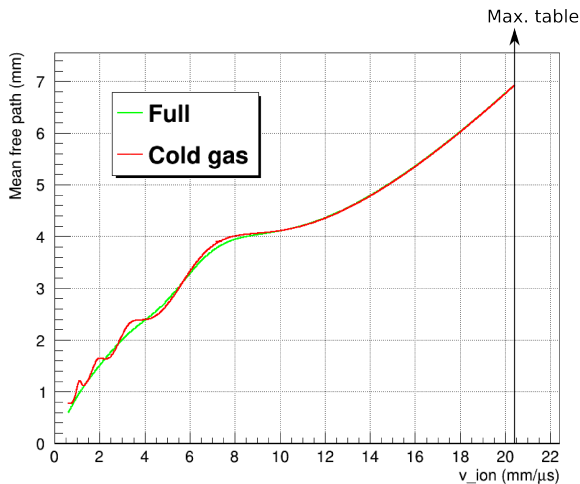Longitudinal diffusion coefficient D_L – ^{7}Li$^+$ + ^{4}He

$\Rightarrow$ Good agreement until 80 Td, then discrepancies (espc. *full*...)

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

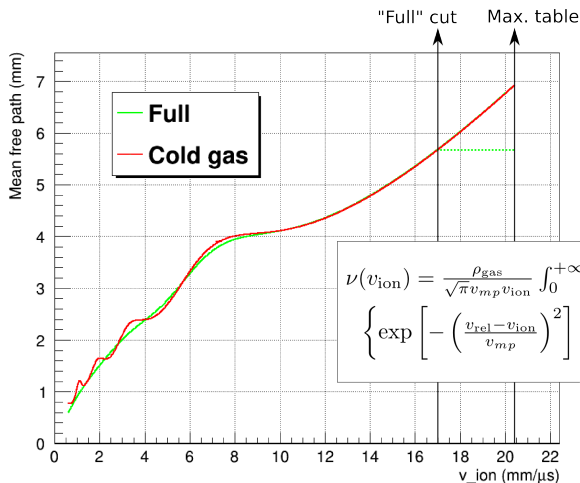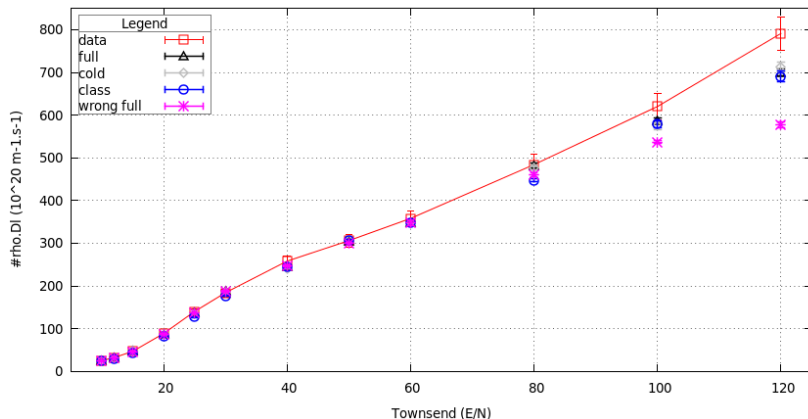Longitudinal diffusion coefficient D_L – ^{7}Li$^+$ + ^{4}He

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

Longitudinal diffusion coefficient D_L – $^7Li^+$ + ^4He

*CLOUDA – Buffer gas : Models assessment

Simulation : initial event

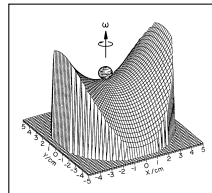Longitudinal diffusion coefficient D_L – $^7Li^+ + {}^4He$

- Discrepancies source (probably) found
- Computations with wider tables on the way. . .

*CLOUDA – EM fields description

Simulation : initial event

Implemented fields :

- Penning trap : Ideal
- Paul trap : Ideal
  - $\vec{E} = -\frac{2}{r_0^2}(\Phi_0 + \Phi_1 \cos(2\pi f_{RF} t))(\vec{x} + \vec{y} - 2\vec{z})$
  - "Radio-Frequency Phase (RFP)" = $(2\pi f_{RF} t) \bmod (2\pi)$
- Paul trap : Realistic
  - Include : real geometry, real potential applied on electrodes
  - Use a Boundary Element Method (BEM) to compute the field in all space
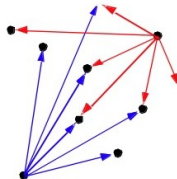 - Parametrize realistic field using harmonic synthesis :

$$\Phi(r, \theta, \varphi) = \sum_{\ell=0}^{\infty} \left(\frac{r}{r_0}\right)^{\ell} \sum_{m=0}^{\ell} \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}}$$
$$\times P_{\ell}^{m}(\cos\theta)\,(\mathcal{A}_{\ell m}\cos(m\varphi) - \mathcal{B}_{\ell m}\sin(m\varphi))$$

Typically, $\ell_{max} = 12$

*CLOUDA – N-body space charge

Issue : compute the N^2 Coulomb repulsions at each timestep

Multiple algorithms possible :

- Exact computation ($\mathcal{O}(N^2)$) :
    - **Tile Calculation**
    - Chamomile Scheme
- Faster methods (approximate long range interactions) :
    - Barnes-Hut $\Rightarrow \mathcal{O}(N \log N)$
    - Fast Multipole Methods (FMM), *e.g. ExaFMM* $\Rightarrow \mathcal{O}(N)$
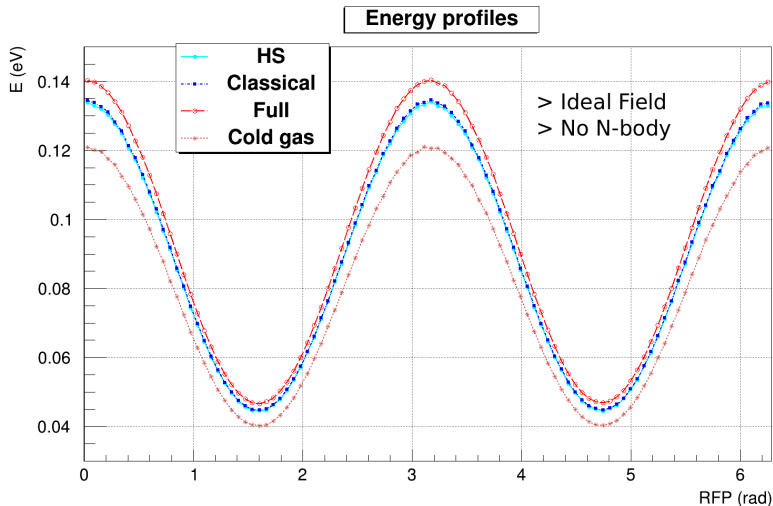
*Trapped ion dynamic : CLOUDA – Summary

We have :

- Buffer gas collisions :
  - ► Hard Spheres (HS)
  - ► *Classical*
  - ► *Full*
  - ► *Cold gas*
- EM fields :
  - ► Ideal Paul trap
  - ► Realistic Paul trap (Harmonic Synthesis)
- N-body : Tile Calculation. Either On or Off.

Cloud profile
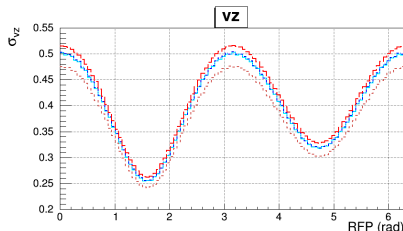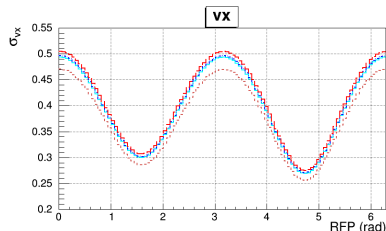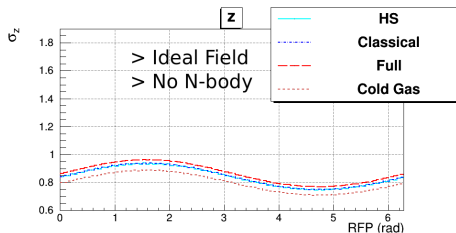
⇒ What effect all models have on the final cloud ?
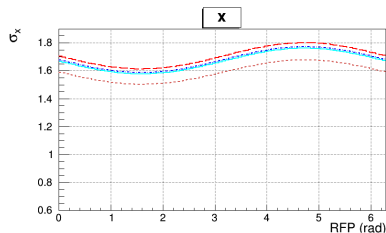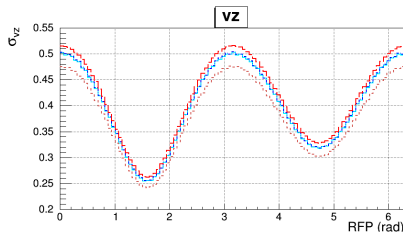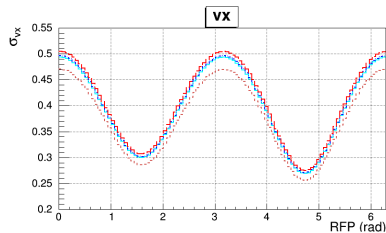
*C LOUDA – Buffer gas effect
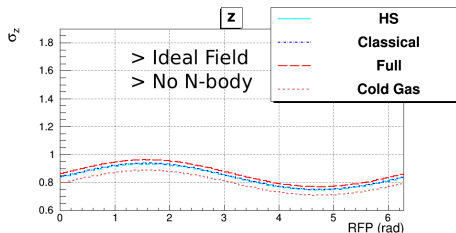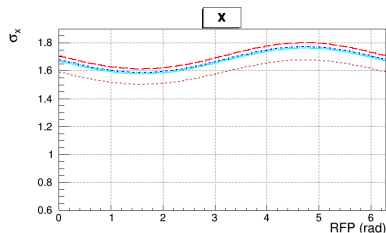
Simulation : initial event

*CLOUDA – Buffer gas effect

Simulation : initial event
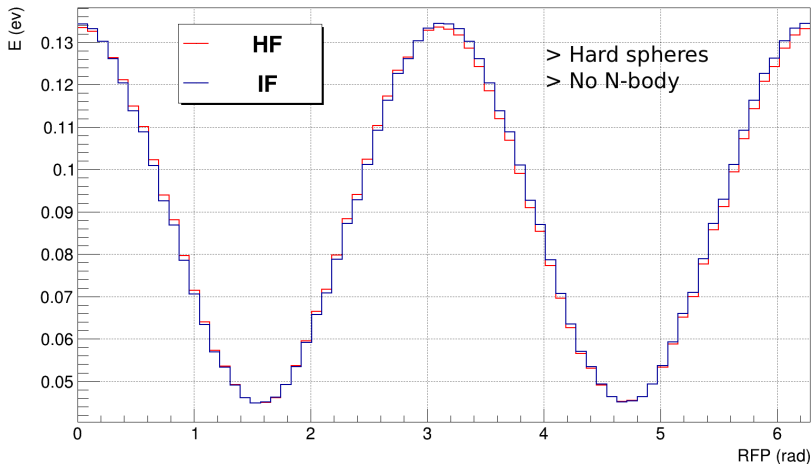
*CLOUDA – Buffer gas effect

Simulation : initial event

$\Rightarrow$ Chosen buffer gas model has an important impact
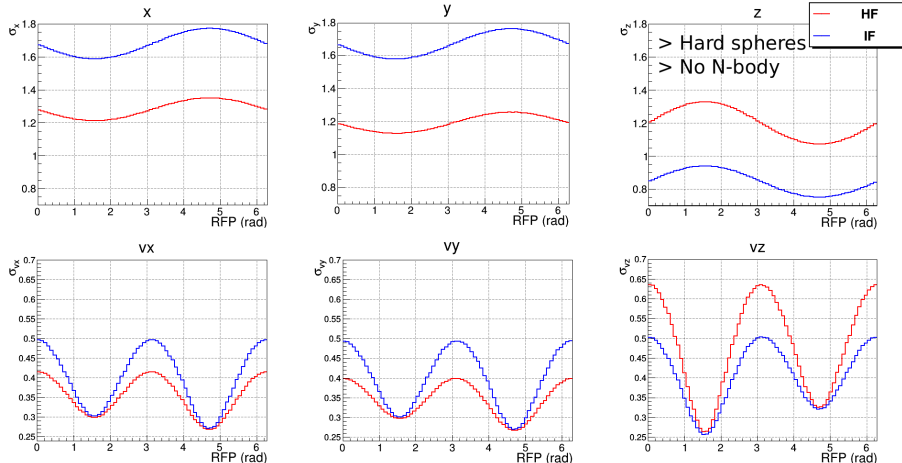
*CLOUDA – EM fields effect

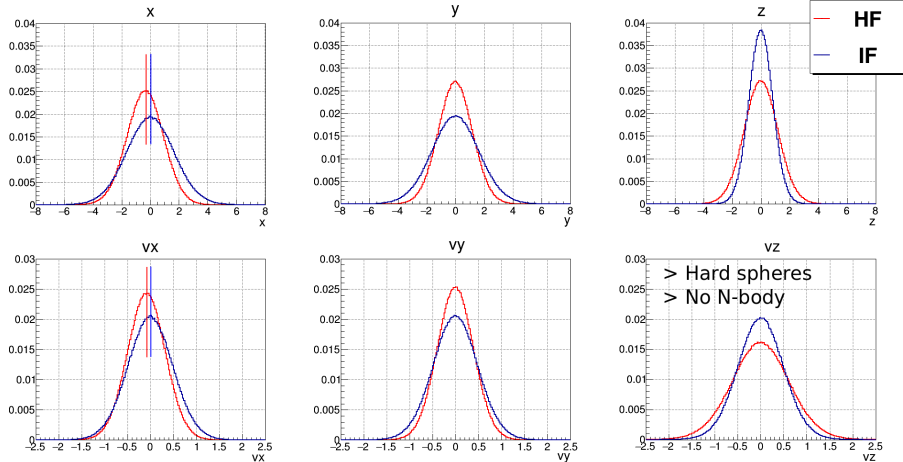Simulation : initial event

Energy profile

> Hard spheres
> No N-body

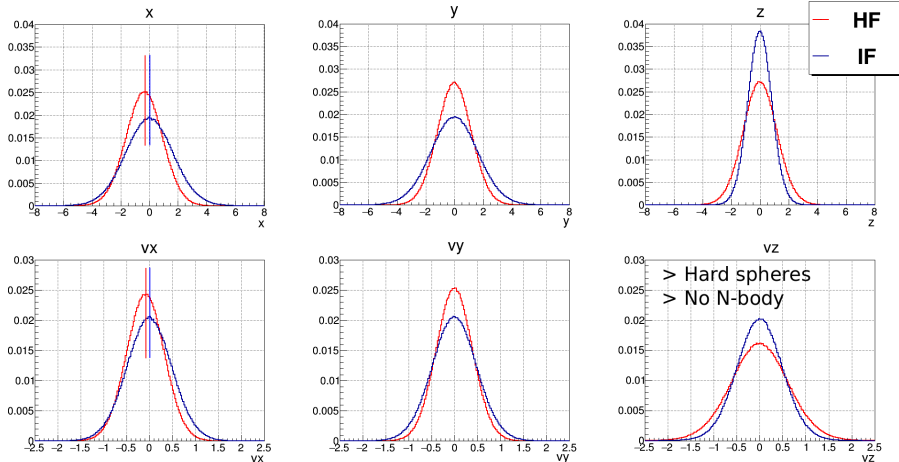# *CLOUDA – EM fields effect

Simulation : initial event

*CLOUDA – EM fields effect

Simulation : initial event

> Hard spheres
> No N-body

*CLOUDA – EM fields effect

Simulation : initial event

> Hard spheres
> No N-body

⇒ Trapping EM field must be properly described

*CLOUDA – N-body effect

Simulation : initial event

> Ideal field
> Hard spheres

LPCTrap: up to
10^5 trapped ions

*CLOUDA – N-body effect

Simulation : initial event

Cloud profile at thermal equilibrium

> Ideal field
> Hard spheres

LPCTrap: up to 10^5 trapped ions
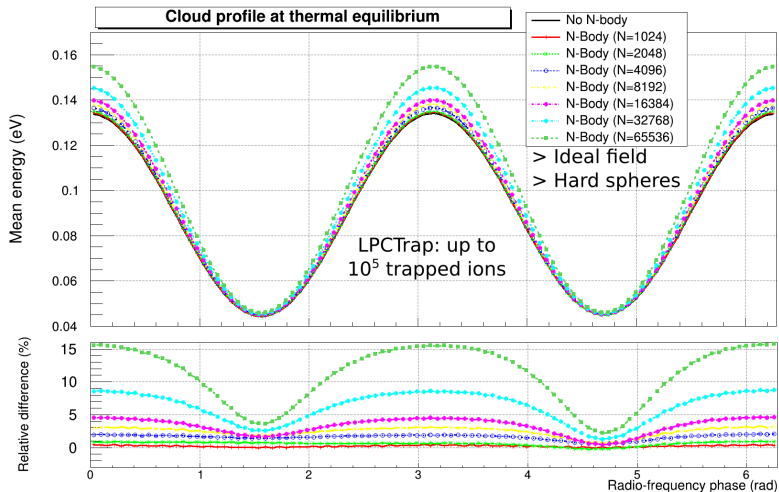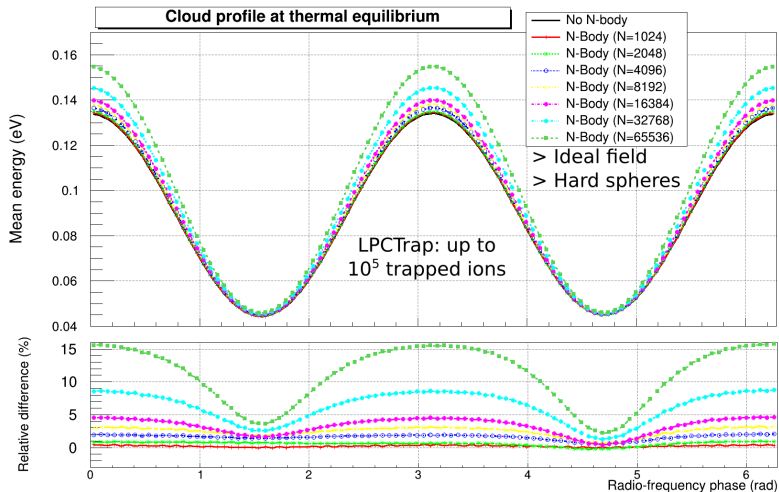
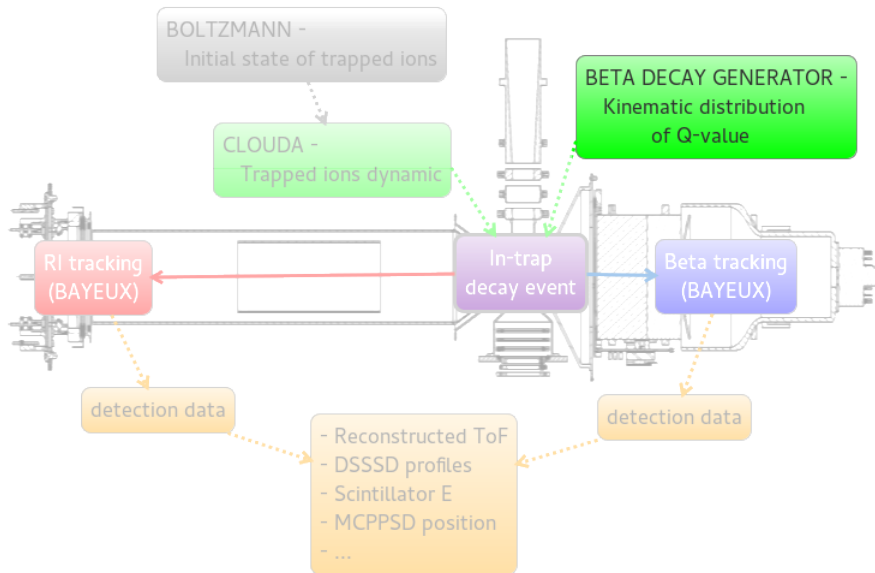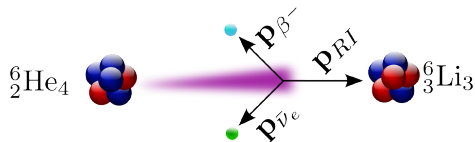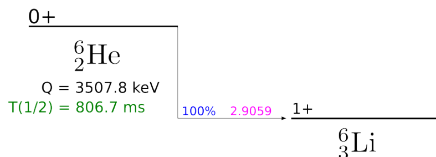$\Rightarrow$ N-body has an important impact

Overview : simulation package

Simulation : initial event

β decay generator

Simulation : initial event

- Distribution of Q-value between decay products

$0+$

^6_2He

Q = 3507.8 keV
T(1/2) = 806.7 ms

100%   2.9059

$1+$

^6_3Li

$^6_2\text{He}_4$ P_{β^-} P_{RI} $^6_3\text{Li}_3$

$P_{\bar{\nu}_e}$

β decay generator

Simulation : initial event
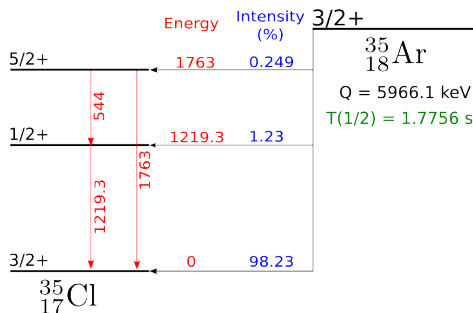
- Distribution of Q-value between decay products
- Take $a_{\beta\nu}$ into account
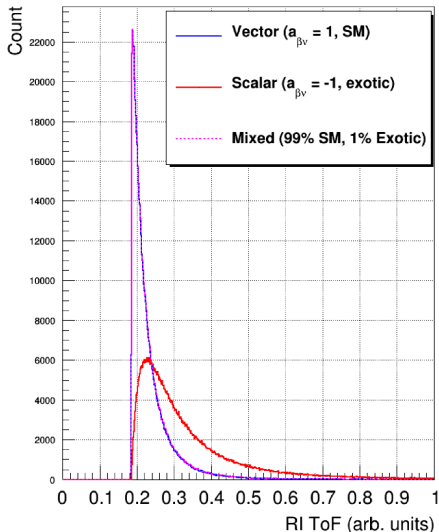
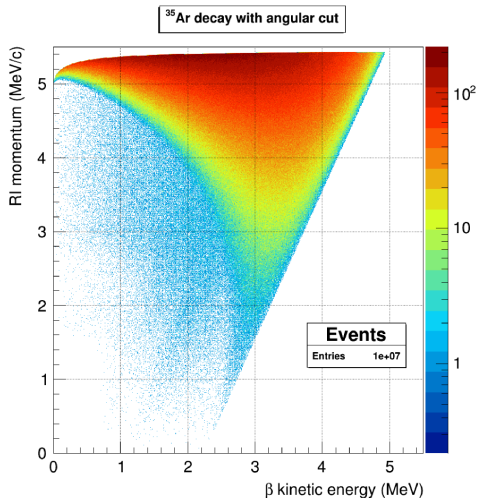# β decay generator

Simulation : initial event

- Distribution of Q-value between decay products
- Take $a_{\beta\nu}$ into account
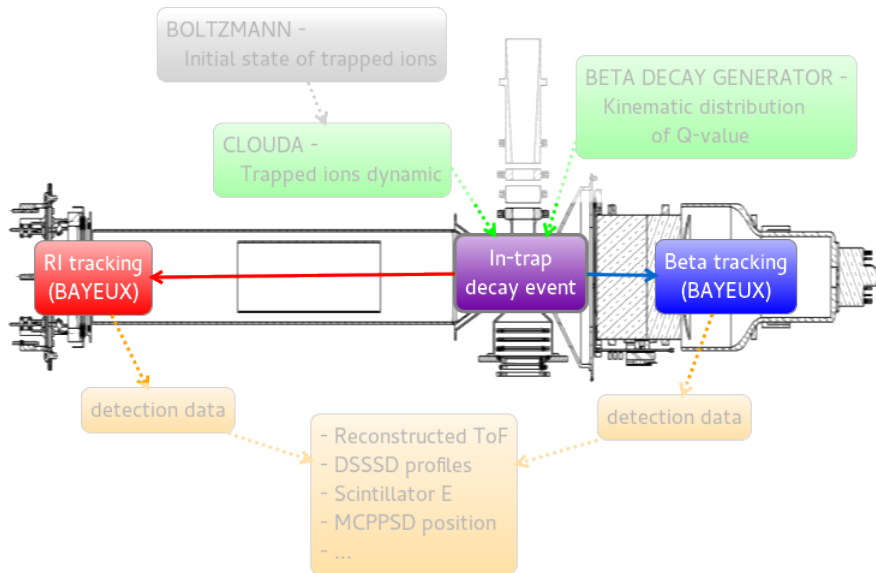- γ de-excitation

β decay generator

Simulation : initial event

- Distribution of Q-value between decay products
- Take $a_{\beta\nu}$ into account
- γ de-excitation
- Fermi function
- Other corrections to consider : radiative, recoil, . . .

^{35}Ar decay with angular cut

Events

Entries   1e+07

Overview : simulation package

Simulation : initial event

Bayeux

Simulation : tracking

- β scattering : important systematic effect
- RI and β tracking requires :
  - ▶ Fine geometry description
  - ▶ Realistic EM fields
    (Paul trap, free flight tube)
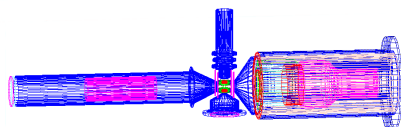 - ▶ Data filtering tools

Bayeux

Simulation : tracking

- β scattering : important systematic effect
- RI and β tracking requires :
  - ▶ Fine geometry description
  - ▶ Realistic EM fields (Paul trap, free flight tube)
  - ▶ Data filtering tools

  $\Rightarrow$ Done using BAYEUX :
- *Geomtools* to control geometry
- Wraps GEANT4 for β scattering
- Able to inject field maps in the Monte Carlo engine

Thanks to Ph. Velten !

Bayeux

Simulation : tracking

- β scattering : important systematic effect
- RI and β tracking requires :
  - ▶ Fine geometry description
  - ▶ Realistic EM fields (Paul trap, free flight tube)
  - ▶ Data filtering tools

  $\Rightarrow$ Done using BAYEUX :
- *Geomtools* to control geometry
- Wraps GEANT4 for β scattering
- Able to inject field maps in the Monte Carlo engine
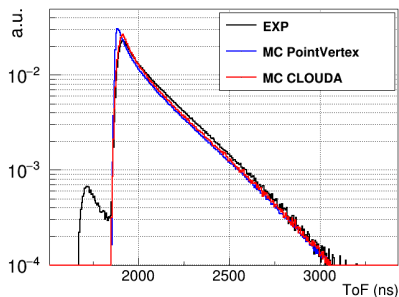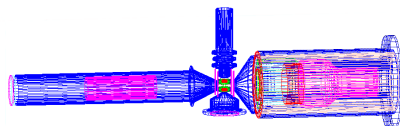

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