Implementation of cross-species ionization in PyECLOUD

L. Mether, G. Iadarola

Acknowledgements: K. Poland, G. Rumolo

e-cloud meeting
14 August, 2019

Outline

- Introduction
- Cross-species ionization model and implementation
- First simulation results

Motivation

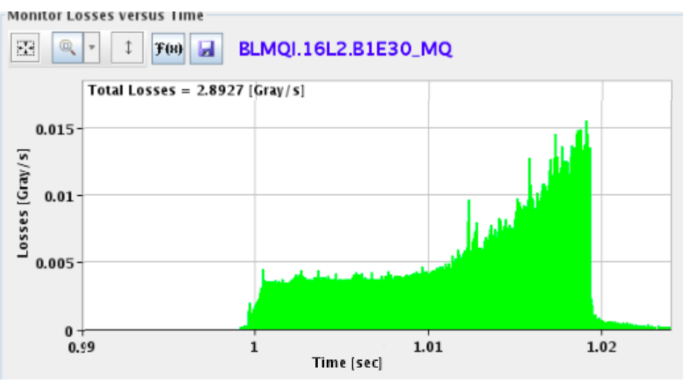
Throughout 2017 operation, abnormal losses were observed in the LHC

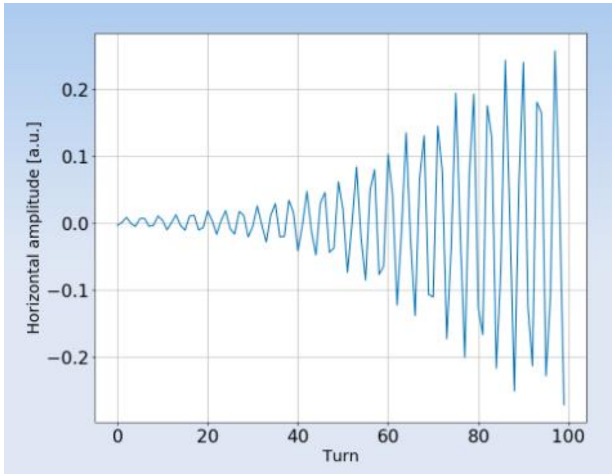
- Located in the 16th half-cell left of Point 2 ('16L2')

68 premature dumps with the following signature occurred during 2017:

- Sudden onset of high beam losses in 16L2
- Coherent beam motion with extremely fast rise times
- Beam dump either due to losses on the collimation system or directly in 16L2

To stay operational, the LHC was limited to fewer than the nominal number of bunches for most of the 2017 run. Several 16L2 events occurred also in 2018.





X. Buffat

L. Ponce *et al.*

Sequence of events in 16L2

The problems in 16L2 are thought to have been caused by air frozen inside the beam chamber, through the following sequence of events:

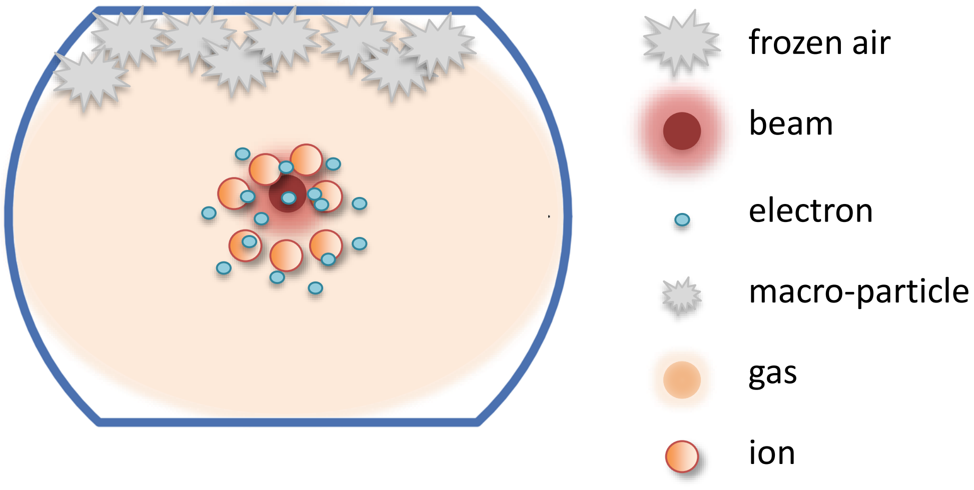
A macro-particle of frozen air (N_2, O_2) is detached, triggered by e-cloud? and enters the beam

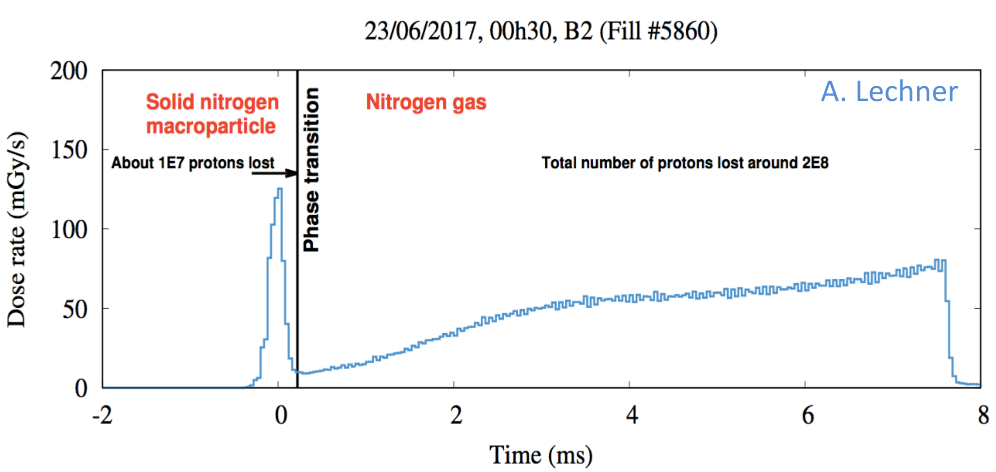
↓

The macro-particle undergoes a phase transition to a gas, leading to a a high local gas density

↓

The beam ionizes some of the gas in its path. Its interaction with the generated electrons/ions causes the fast instabilities





Sequence of events in 16L2

The problems in 16L2 are thought to have been caused by air frozen inside the beam chamber, through the following sequence of events:

A macro-particle of frozen air (N_2, O_2) is detached, triggered by e-cloud? and enters the beam

↓

The macro-particle undergoes a phase transition to a gas, leading to a a high local gas density

↓

The beam ionizes some of the gas in its path. Its interaction with the generated electrons/ions causes the fast instabilities

Our aim is to model the last part of this sequence of events:

- If we assume a high gas density in the beam chamber, can we reproduce the observations in a consistent manner?

Previous studies and development:

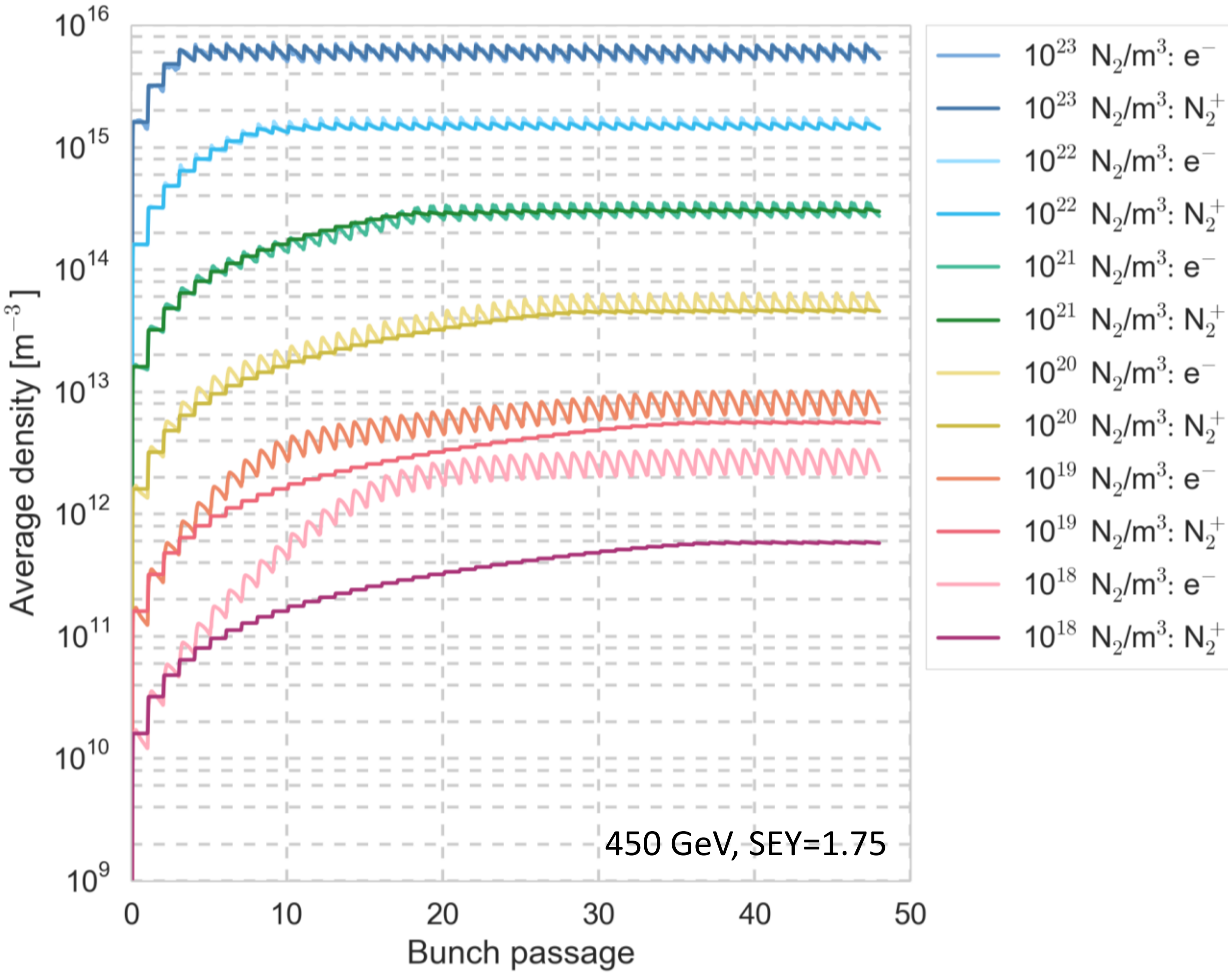
- ✓ Implementation of multi-species simulations
- ✓ Multi-species build-up and stability simulations with beam-induced ionization of N_2 gas
- See e.g. LBOC #82

New model ingredient:

- ✓ Implementation of cross-species ionization

Multi-species build-up

Multi-species simulations show that electron multipacting becomes less important than beam-induced ionization from gas densities around 10^{20} N_2/m^3 and the dynamics are qualitatively and quantitatively different compared to single-species simulations



Beam stability

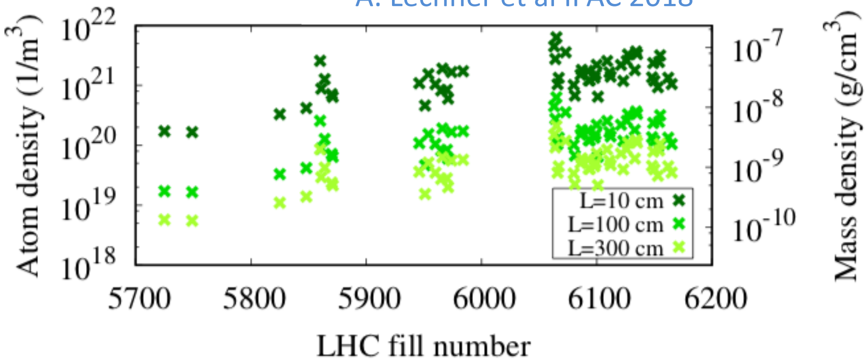
The gas density during the 16L2 events could be estimated based on the observed loss rates

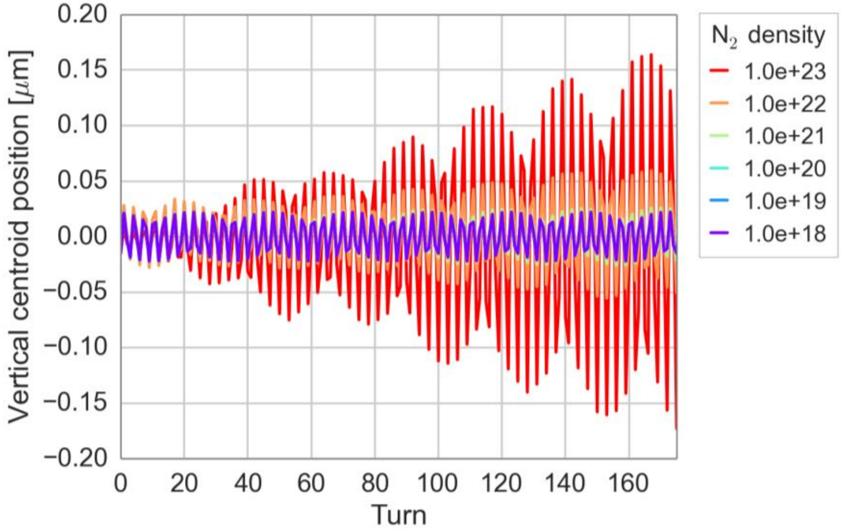
- For the 2017 events, N_2 gas densities were estimated to $10^{19} – 10^{21}$ $L^{-1}m^{-2}$, with the gas covering the length L

First multi-species beam dynamics simulations show beam instabilities for gas densities ≥ 10^{21} $L^{-1}m^{-2}$

- This covers only the upper range of the observed instabilities in the machine ($10^{19} – 10^{21}$ $L^{-1}m^{-2}$)

A. Lechner et al IPAC 2018





Electron-induced ionization, which has been neglected here, may increase the electron and ion densities for a given neutral gas density, if it is important in the studied cases

Gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma n_{\mathrm{gas}}$$

Gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma n_{\mathrm{gas}} = \left(\frac{1}{\lambda_{\mathrm{mfp}}}\right)$$

Beam-induced gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma n_{\mathrm{gas}} = \left(\frac{1}{\lambda_{\mathrm{mfp}}}\right)$$

- If the projectile is a beam particle, the path length $ds_{\mathrm{proj}} = c\ dt$ and with dN_{b} beam particles, we get

$$dN_{\mathrm{ev}} = \sigma n_{\mathrm{gas}} c\ dt\ dN_{\mathrm{b}}$$

Beam-induced gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma n_{\mathrm{gas}} = \left(\frac{1}{\lambda_{\mathrm{mfp}}}\right)$$

- If the projectile is a beam particle, the path length $ds_{\mathrm{proj}} = c\ dt$ and with dN_{b} beam particles, we get

$$dN_{\mathrm{ev}} = \sigma n_{\mathrm{gas}} c\ dt\ dN_{\mathrm{b}}$$

- In a 2D code, we deal with line densities instead of numbers

$$\frac{dN_{\mathrm{ev}}}{ds} = \sigma n_{\mathrm{gas}} c\ dt\ \frac{dN_{\mathrm{b}}}{ds}$$

Cross-species gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma n_{\mathrm{gas}}$$

- If the projectile is a cloud particle, the path length $ds_{\mathrm{proj}} = v_{\mathrm{proj}}\ dt$

Cross-species gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma(E_{\mathrm{proj}})n_{\mathrm{gas}}$$

- If the projectile is a cloud particle, the path length $ds_{\mathrm{proj}} = v_{\mathrm{proj}}\ dt$

Cross-species gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density n_{gas}

$$\frac{dN_{\mathrm{ev}}}{ds_{\mathrm{proj}}} = \sigma(E_{\mathrm{proj}})n_{\mathrm{gas}}$$

- If the projectile is a cloud particle, the path length $ds_{\mathrm{proj}} = v_{\mathrm{proj}}\ dt$ and with dN_{proj} projectiles we get

$$dN_{\mathrm{ev}} = \sigma(E_{\mathrm{proj}})n_{\mathrm{gas}}v_{\mathrm{proj}}\ dt\ dN_{\mathrm{proj}}$$

Cross-species gas ionization

The rate of gas ionization events is determined by the ionization cross-section σ and the gas density $n_{\rm gas}$

$$\frac{dN_{\rm ev}}{ds_{\rm proj}} = \sigma(E_{\rm proj})n_{\rm gas}$$

- If the projectile is a cloud particle, the path length $ds_{\rm proj} = v_{\rm proj}\ dt$ and with $dN_{\rm proj}$ projectiles we get

$$dN_{\rm ev} = \sigma(E_{\rm proj})n_{\rm gas}v_{\rm proj}\ dt\ dN_{\rm proj}$$

- In a 2D code, we deal with line densities instead of numbers

$$\frac{dN_{\rm ev}}{ds} = \sigma(E_{\rm proj})n_{\rm gas}v_{\rm proj}\ dt\ \frac{dN_{\rm proj}}{ds}$$

Electron-induced ionization

- The beam-gas ionization cross-section at injection and top energy is estimated to be around 2 Mb = 2×10^{-18} cm^2
- Electrons in the energy range of 50 – 500 eV have a 50 – 100 times larger ionization cross section than the beam particles
- The amount of ionization depends on the electron energy distribution during the simulations

BUG *et al.*, Phys. Rev E.88

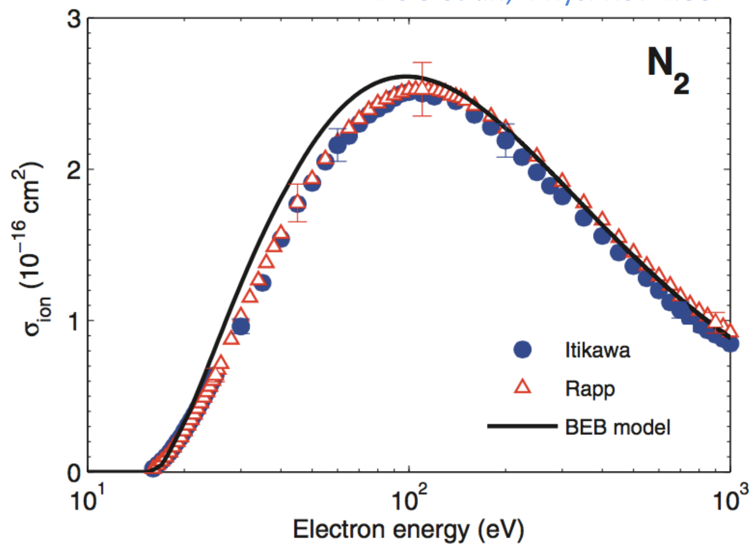
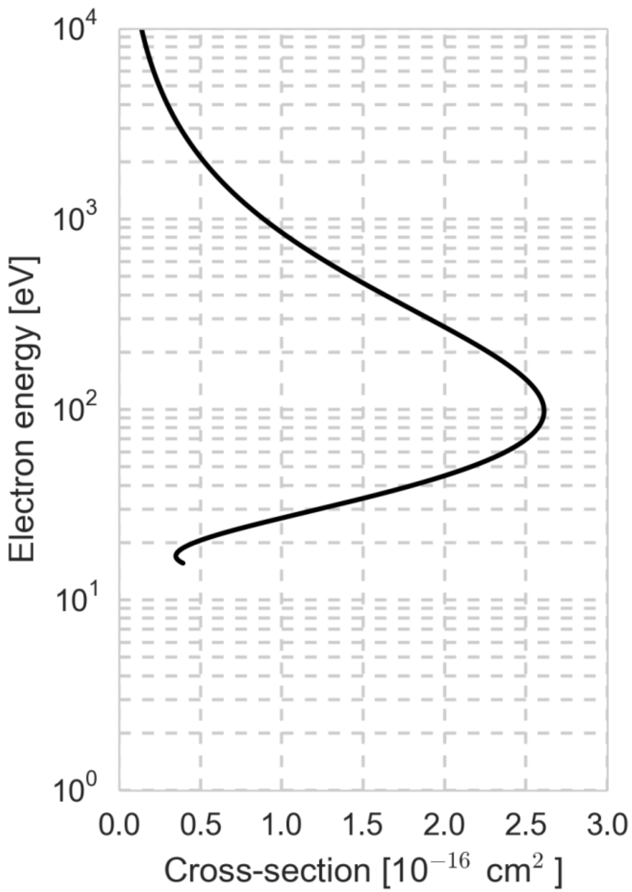


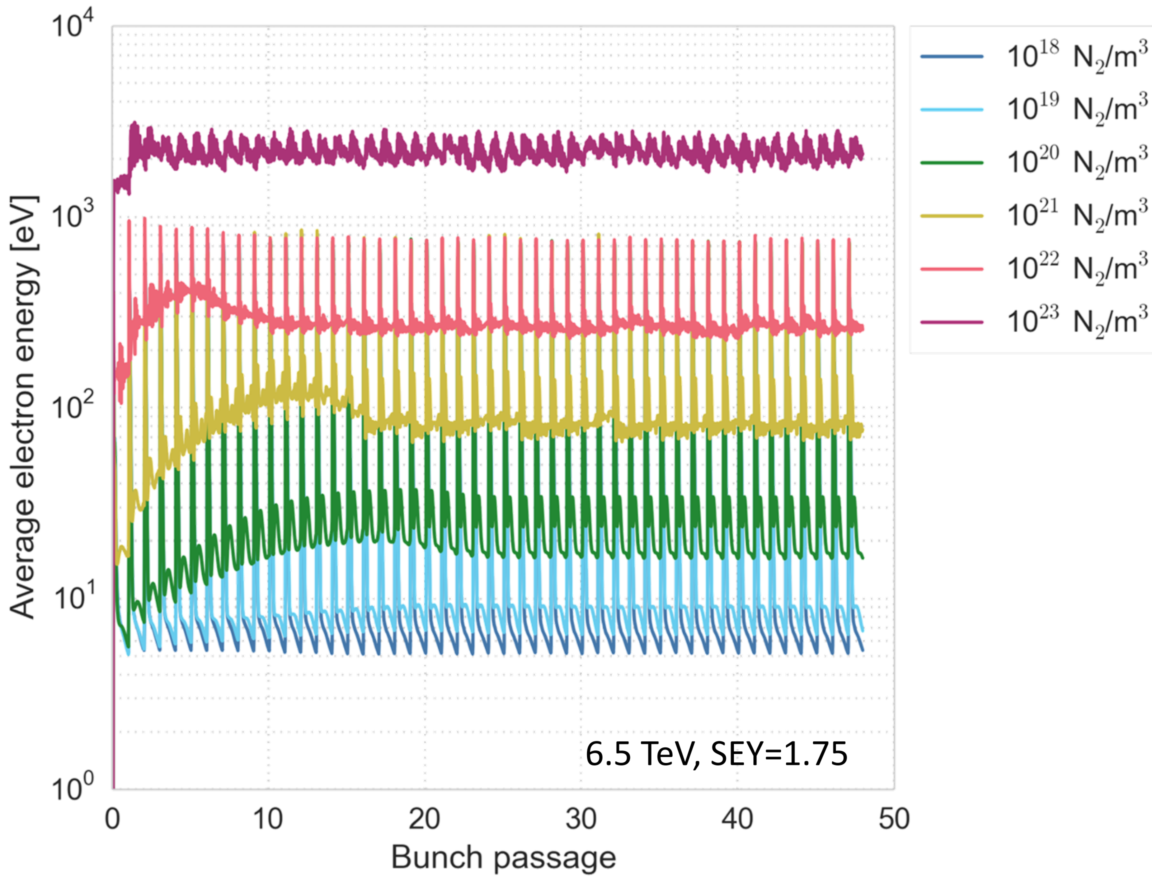
FIG. 1. (Color online) Electron-impact-ionization cross sections σ_{ion} of nitrogen recommended by Itikawa [16], measured by Rapp and Englander-Golden [17], and determined using the BEB model [18].

Electron energies

Electron energies during the multi-species build-up were previously analysed

- See e-cloud meeting #67



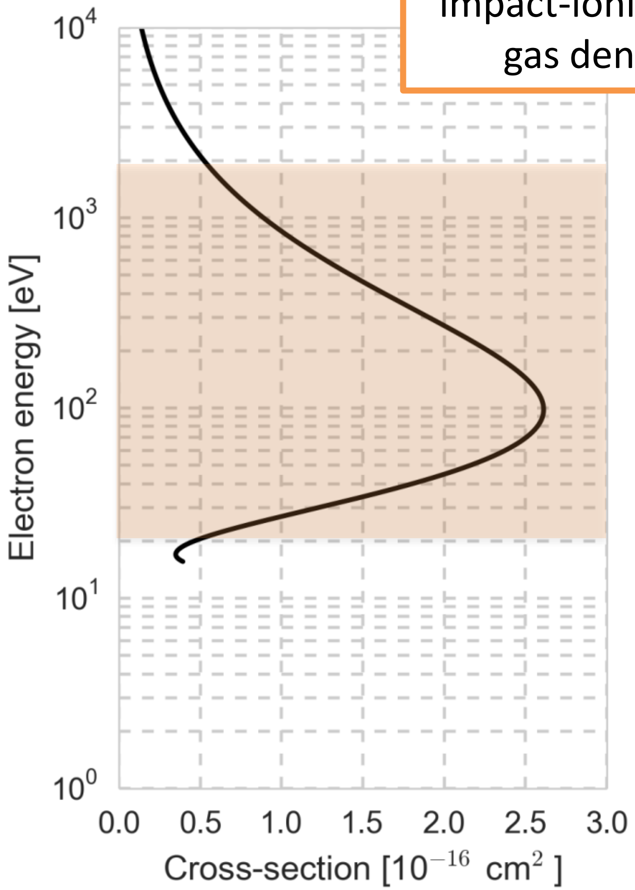


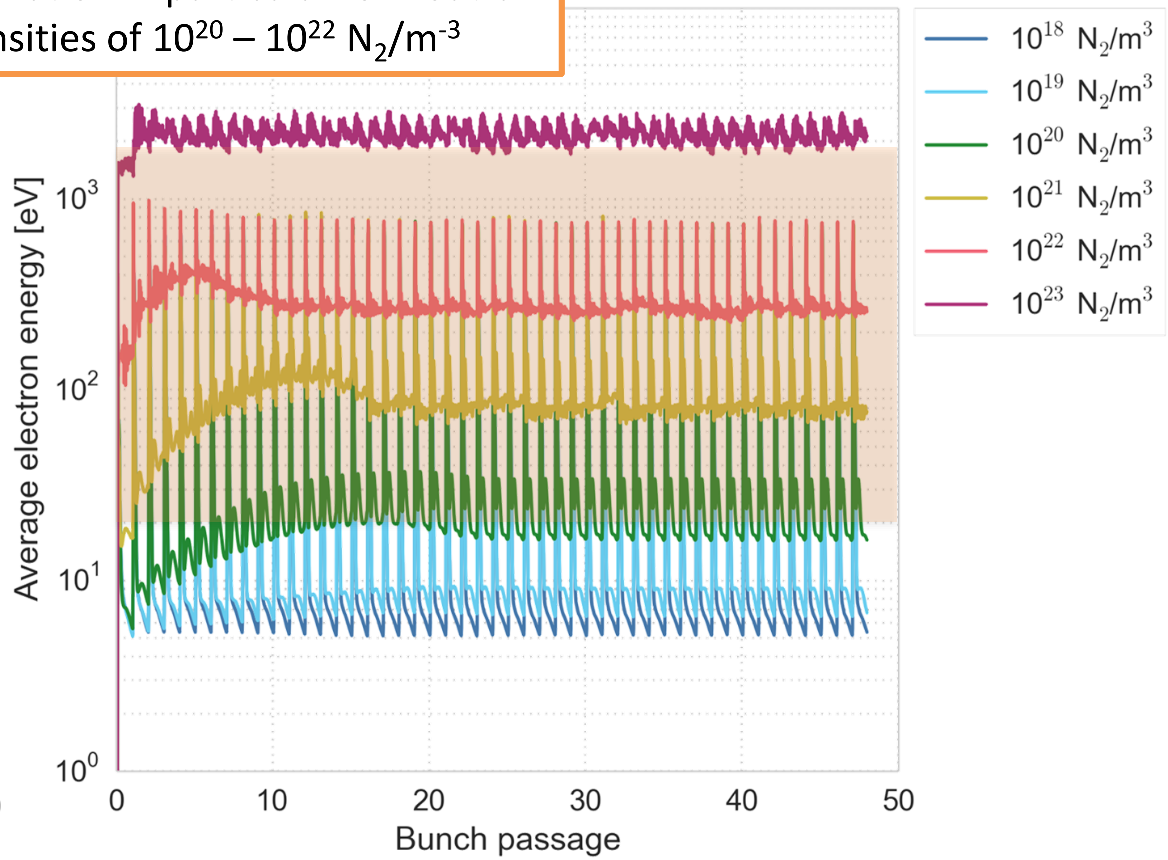
Electron energies

Electron energies during the multi-species build-up were previously analysed

- See e-cloud meeting #67

Energies are favourable for electron impact-ionization in particular for neutral gas densities of $10^{20} – 10^{22}$ N_2/m^{-3}



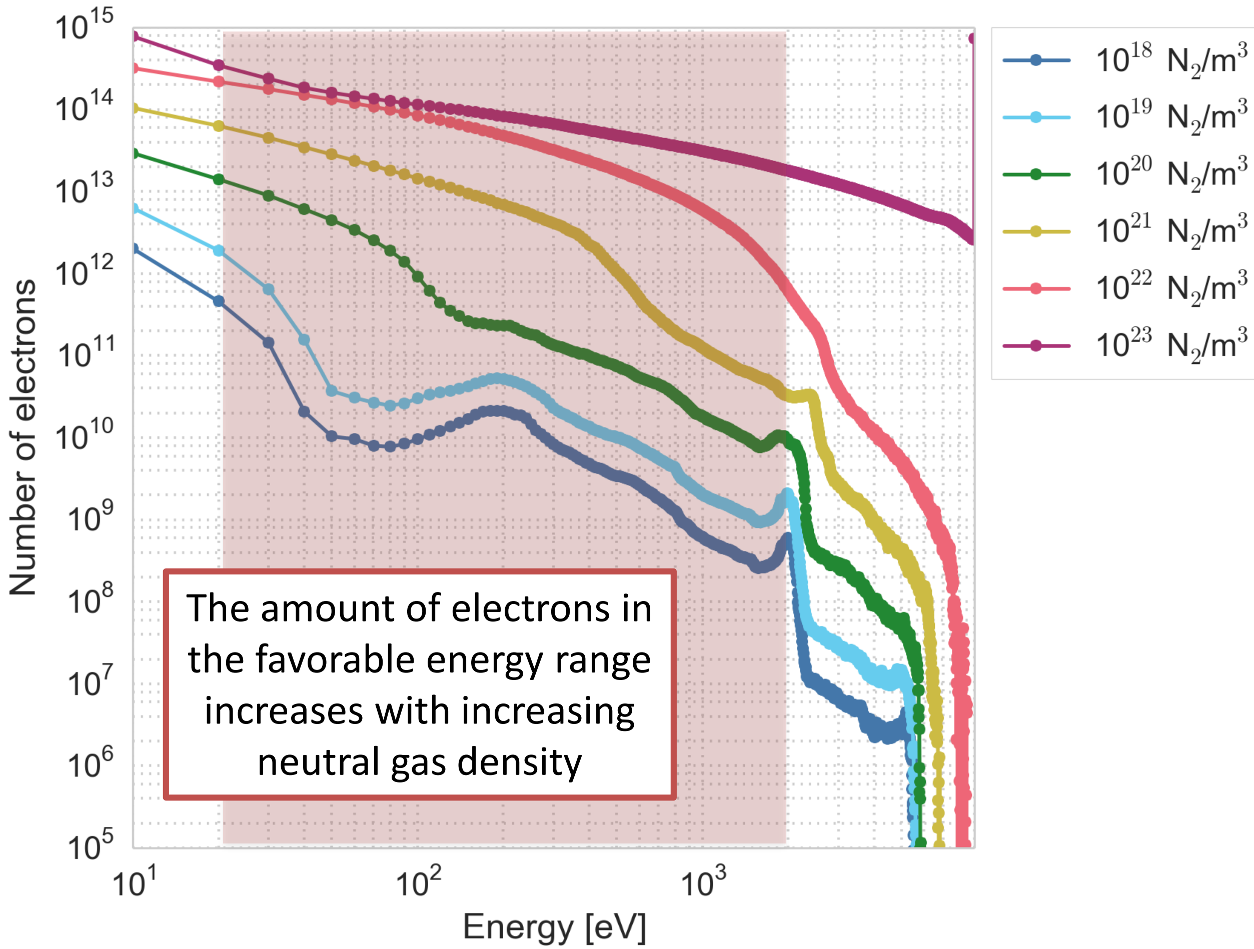


Electron energy spectrum

Electron energies during the multi-species build-up were previously analysed

- See e-cloud meeting #67

Energies are favourable for electron impact-ionization in particular for neutral gas densities of $10^{20} – 10^{22}$ N_2/m^{-3}



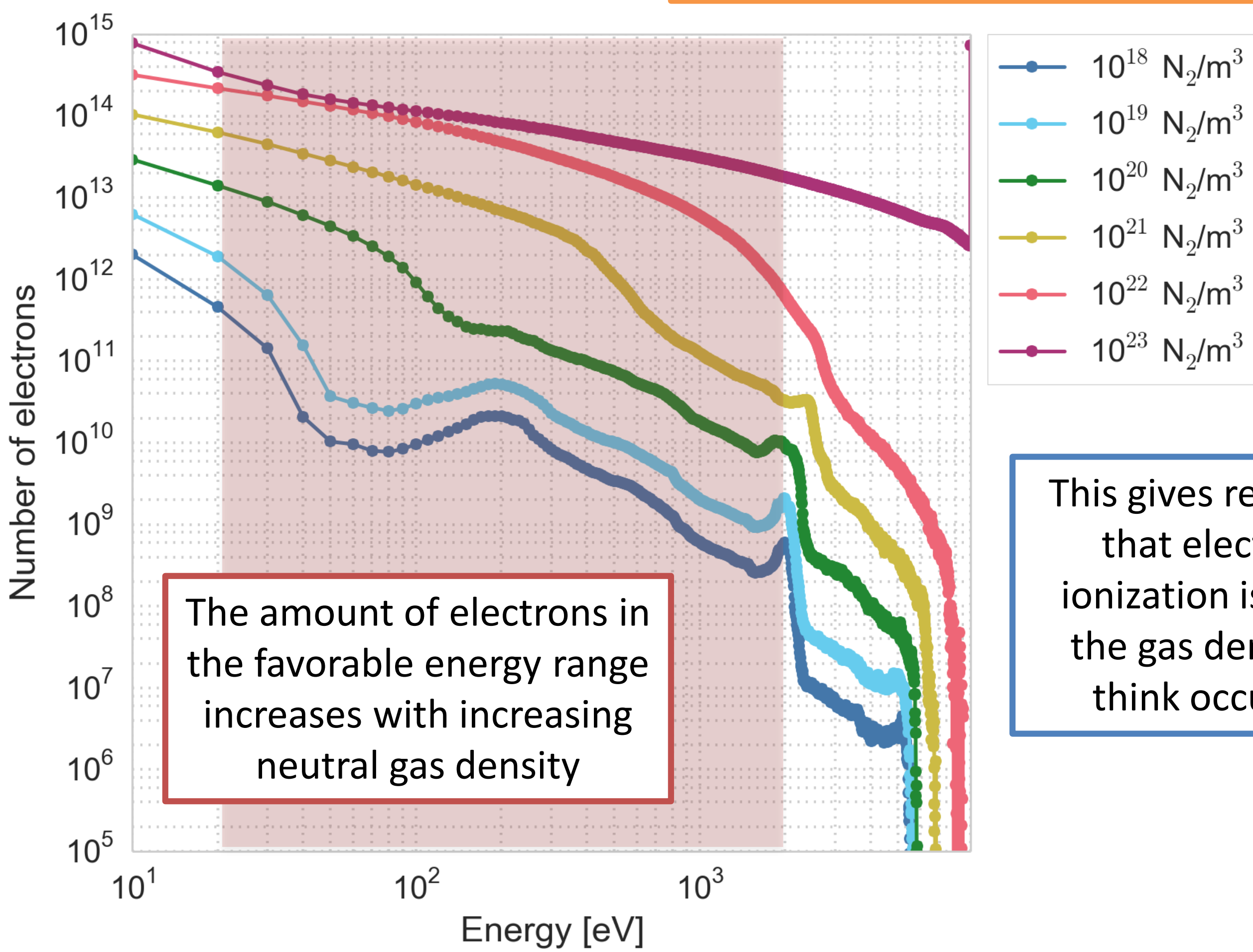
The amount of electrons in the favorable energy range increases with increasing neutral gas density

Electron energy spectrum

Electron energies during the multi-species build-up were previously analysed

- See e-cloud meeting #67

Energies are favourable for electron impact-ionization in particular for neutral gas densities of $10^{20} – 10^{22}$ N_2/m^{-3}



The amount of electrons in the favorable energy range increases with increasing neutral gas density

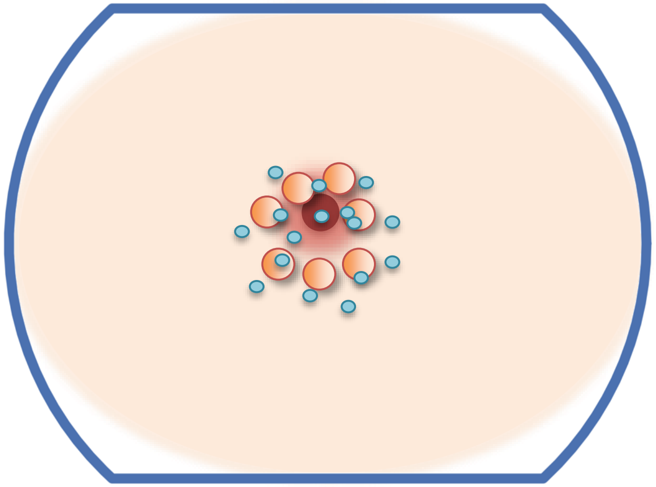
This gives reason to believe that electron impact-ionization is important for the gas densities that we think occurred in 16L2

Cross-species ionization model

For the implementation of the cross-species ionization, we want to keep the same simplifying assumptions as are made for the beam-induced ionization

- Assume a uniform gas density in the chamber
  (no neutral macroparticles – we don't want to go to full-scale plasma simulations)

- Consider single ionization only



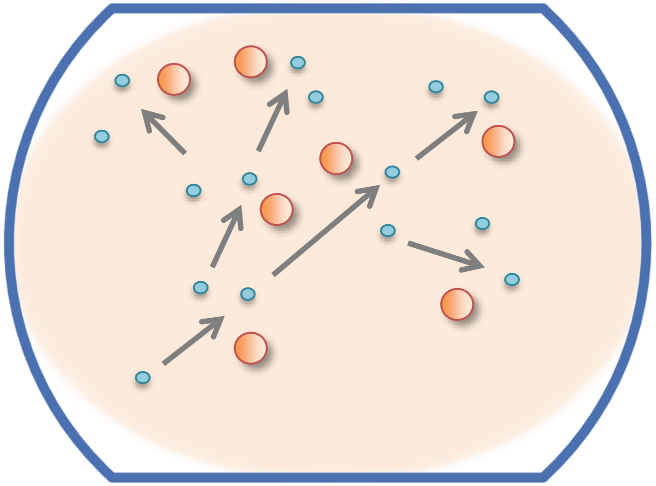
Cross-species ionization in PyECLOUD

A new cross-species ionization module has been implemented in PyECLOUD

- Holds the necessary information on the user defined cross-species ionization processes
- Handles the generation of particles through cross-species ionization
- Can handle multiple projectiles and any number of ionization processes per projectile

Other generation processes (secondary emission, photoemission, beam-induced ionization) are performed separately for each cloud

- Since the cross-species ionization includes interactions between clouds, all clouds must be handled together
- The generating function is called once per time step during build-up simulations



Generation of ionization products

`Cross_Ionization.generate()` Called from buildup simulation

- Loop over projectiles
  - Determine the energies of each macroparticle (MP) in the projectile cloud
  - Loop over processes for current projectile
    - Call process generation function

Projectile MP info →

`Ionization_Process.generate()`

Generation of ionization products

Projectile MP info →

`Cross_Ionization.generate()`

`Ionization_Process.generate()`

- Interpolate the user input cross-section to the projectile MP energies
- Determine the number of product particles to be generated by each projectile MP, using their weight

$$\frac{dN_{\mathrm{ev}}}{ds} = \sigma(E_{\mathrm{proj}}) n_{\mathrm{gas}} v_{\mathrm{proj}} \; dt \; \frac{dN_{\mathrm{proj}}}{ds}$$

Generation of ionization products

Projectile MP info →

```
Cross_Ionization.
generate()
```

```
Ionization_Process.generate()
```

- Interpolate the user input cross-section to the projectile MP energies
- Determine the number of product particles to be generated by each projectile MP, using their weight

$$\frac{dN_{\mathrm{ev}}}{ds} = \sigma(E_{\mathrm{proj}})n_{\mathrm{gas}}v_{\mathrm{proj}}\ dt\ \frac{dN_{\mathrm{proj}}}{ds}$$

- Loop over products of process
  - For each product calculate the number of new MPs to produce, based on the current default weight of the product cloud
    - Non-integer parts define probability to generate 1 MP

Generation of ionization products

Projectile MP info

`Ionization_Process.generate()`

`Cross_Ionization.generate()`

- Interpolate the user input cross-section to the projectile MP energies
- Determine the number of product particles to be generated by each projectile MP, using their weight

$$\frac{dN_{\mathrm{ev}}}{ds} = \sigma(E_{\mathrm{proj}}) n_{\mathrm{gas}} v_{\mathrm{proj}} \; dt \; \frac{dN_{\mathrm{proj}}}{ds}$$

- Loop over products of process
  - For each product calculate the number of new MPs to produce, based on the current default weight of the product cloud
    - Non-integer parts define probability to generate 1 MP
  - Define coordinates of new MPs:
    - Initial position corresponding to position of projectile
    - Initial velocities according to initial energy defined by user input
- Return information on new MPs for product clouds

`Cross_Ionization.generate()`

New product MP info

Generation of ionization products

`Cross_Ionization.generate()`

- Loop over projectiles
  - Determine the energies of each macroparticle (MP) in the projectile cloud
  - Loop over processes for current projectile
    - Call process generation function
    - Add info on new MPs from process to list of new MPs for each cloud
- After looping over all projectiles and processes, generate new MPs in each cloud
- Keep record of number of particles and number of MPs generated per cloud every time step
  - Saved to output by pyecloud_saver

Projectile MP info →

New product MP info ←

`Ionization_Process.generate()`

Defining the ionization processes

Cross-species ionization is activated by adding in the `simulation_parameters` input file a dictionary that describes the desired ionization processes:

```
cross_ion_definitions = {projectile 1: {process 11: process_definitions,
                                        process 12: process_definitions},
                         projectile 2: {process 21: process_definitions,
                                        process 22: process_definitions}}
```

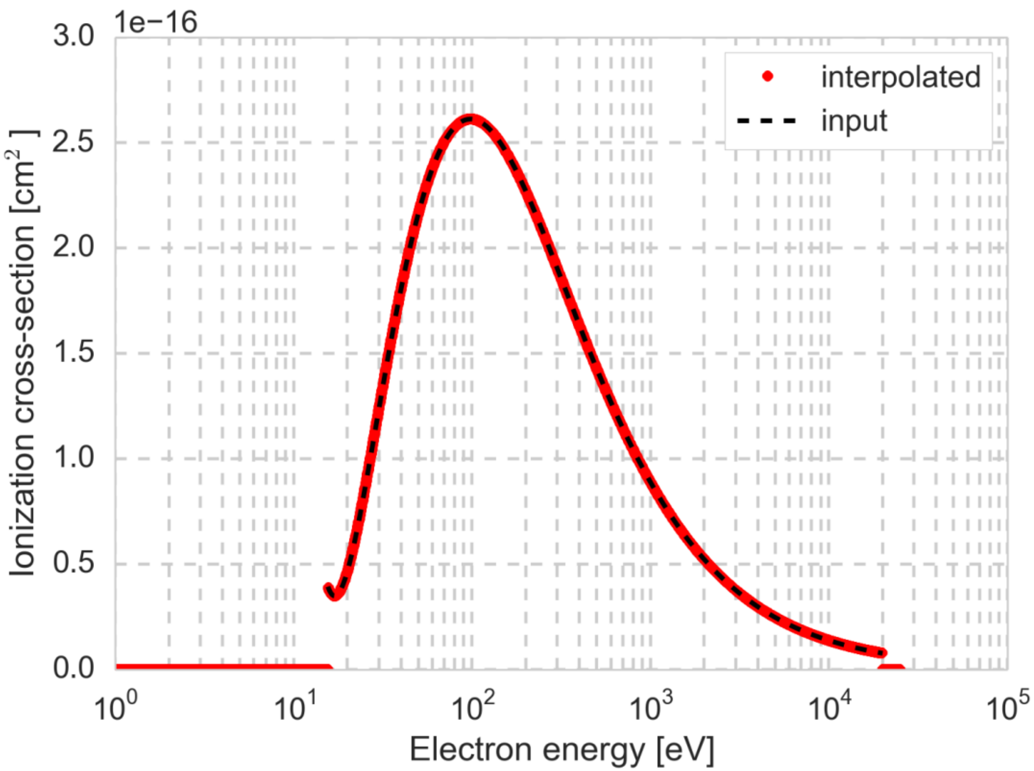
```
process definitions = {target_density, products, cross_section_file,
                       initial_product_energy, flag_extract_sigma}
```

- projectiles and products must of course correspond to existing clouds

Test routine

The cross-species ionization module also contains a self-test routine, which runs by default at the beginning of a simulation, and saves a file for every process

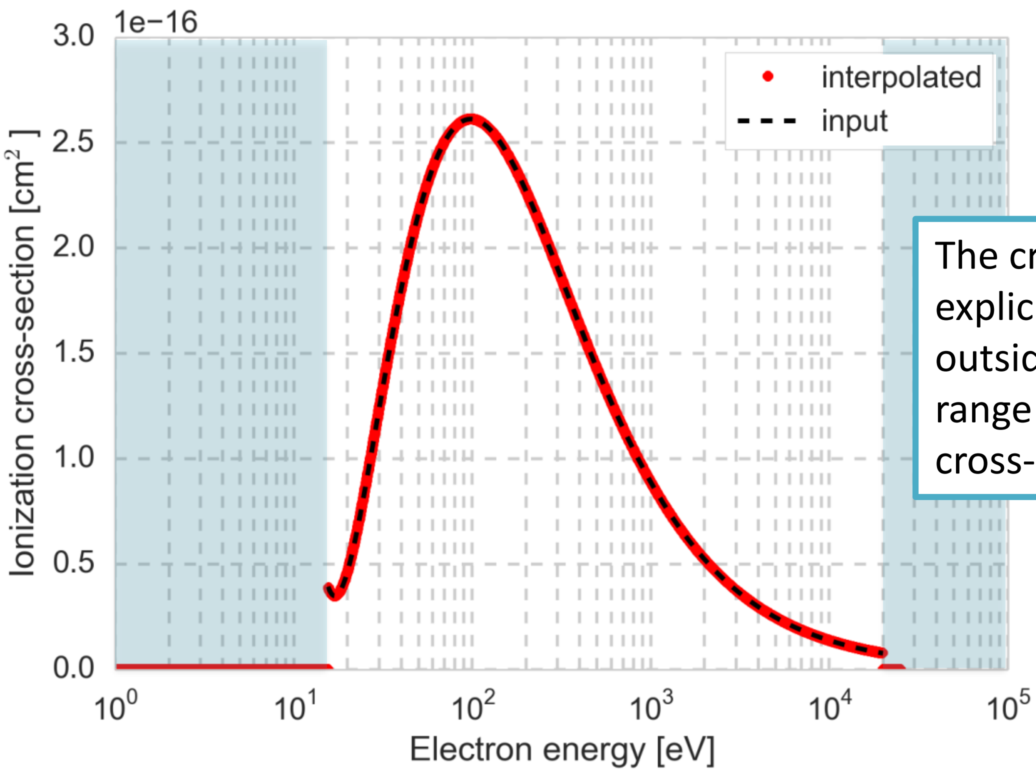
- The interpolation of the cross-section for an array of energies



Test routine

The cross-species ionization module also contains a self-test routine, which runs by default at the beginning of a simulation, and saves a file for every process

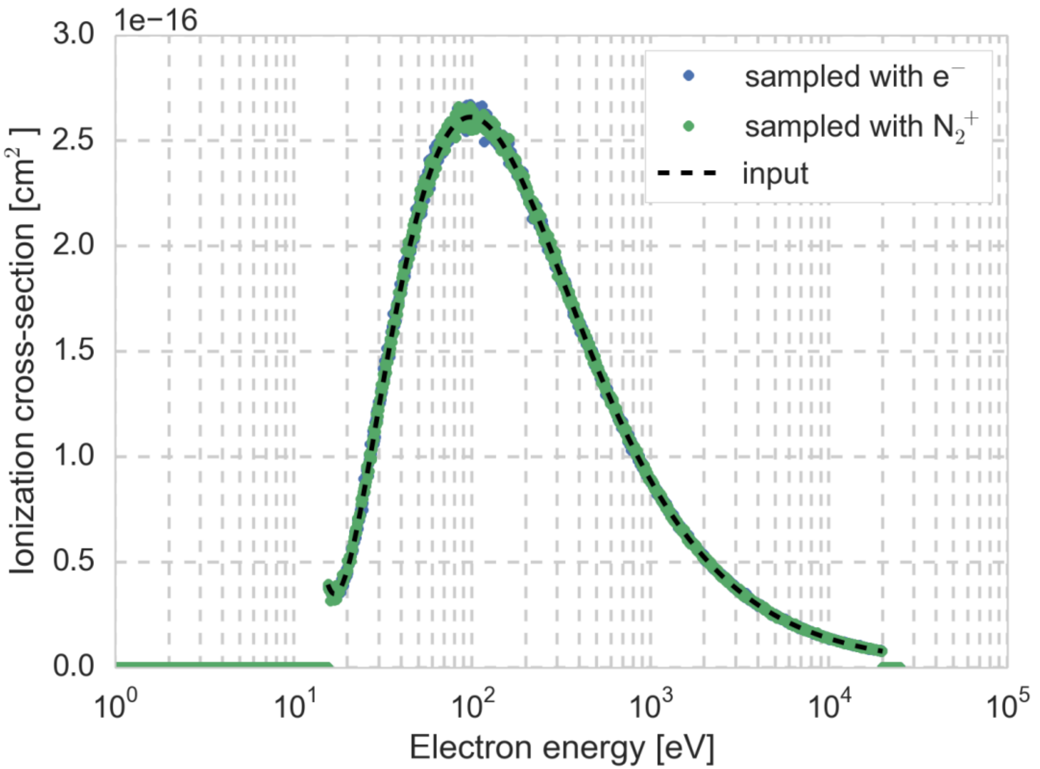
- The interpolation of the cross-section for an array of energies



The cross-section is explicitly set to zero outside the energy range given in the cross-section input file

Test routine

- Reconstructed cross-sections based on the generation algorithm
  - For each energy in an array of energies, a mono-energetic projectile macroparticle distribution is passed to the `generate()` function
  - The cross-section at the corresponding energy is estimated based on the ratio between the total number of new particles to be generated and the total number of projectile particles initially passed to the function



First simulation study

Considered the same simulation set-up as previously studied with multi-species build-up without cross-species ionization

- Added electron-induced ionization

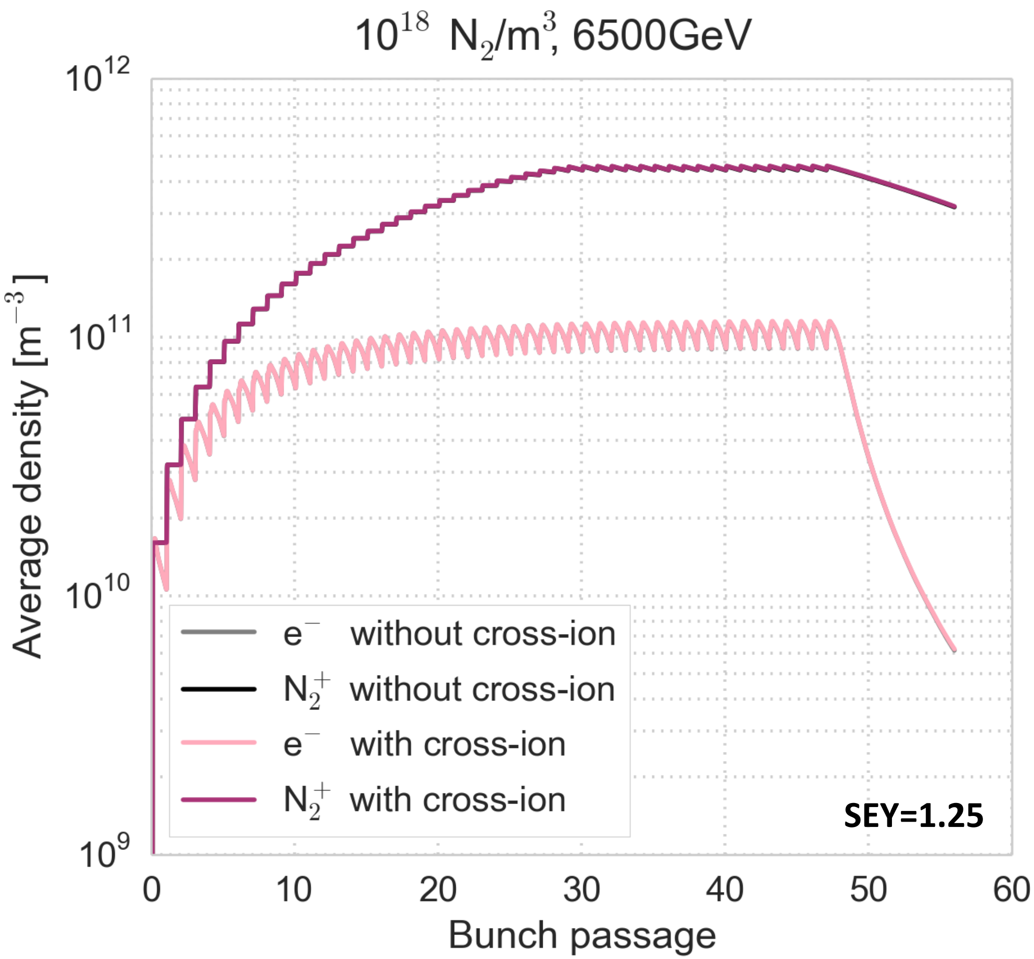
```
cross_ion_definitions =
{'electron':
  {'electron-n2':
    {'target_density': 1.00e+20,
     'products': ['n2', 'electron'],
     'cross_section':'cross_section_n2_15.59_20000.00_N1000_log.mat’,
     'E_eV_init': 0.,
     'extract_sigma': True}}}
```

- Scan over gas densities

10^{18} N_2/m^3

Comparing the densities against the equivalent simulation without cross-species ionization

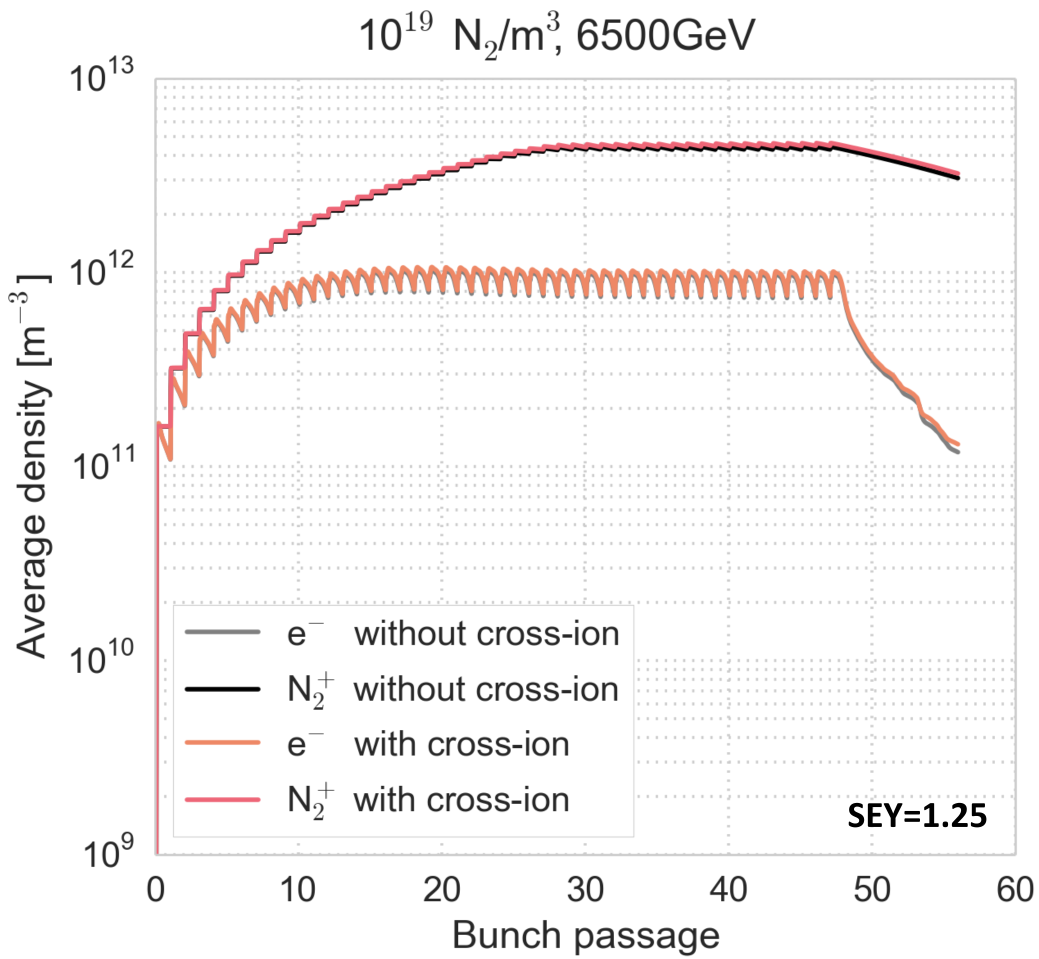
- There is no impact of the electron-induced ionization



10^{19} N_2/m^3

Comparing the densities against the equivalent simulation without cross-species ionization

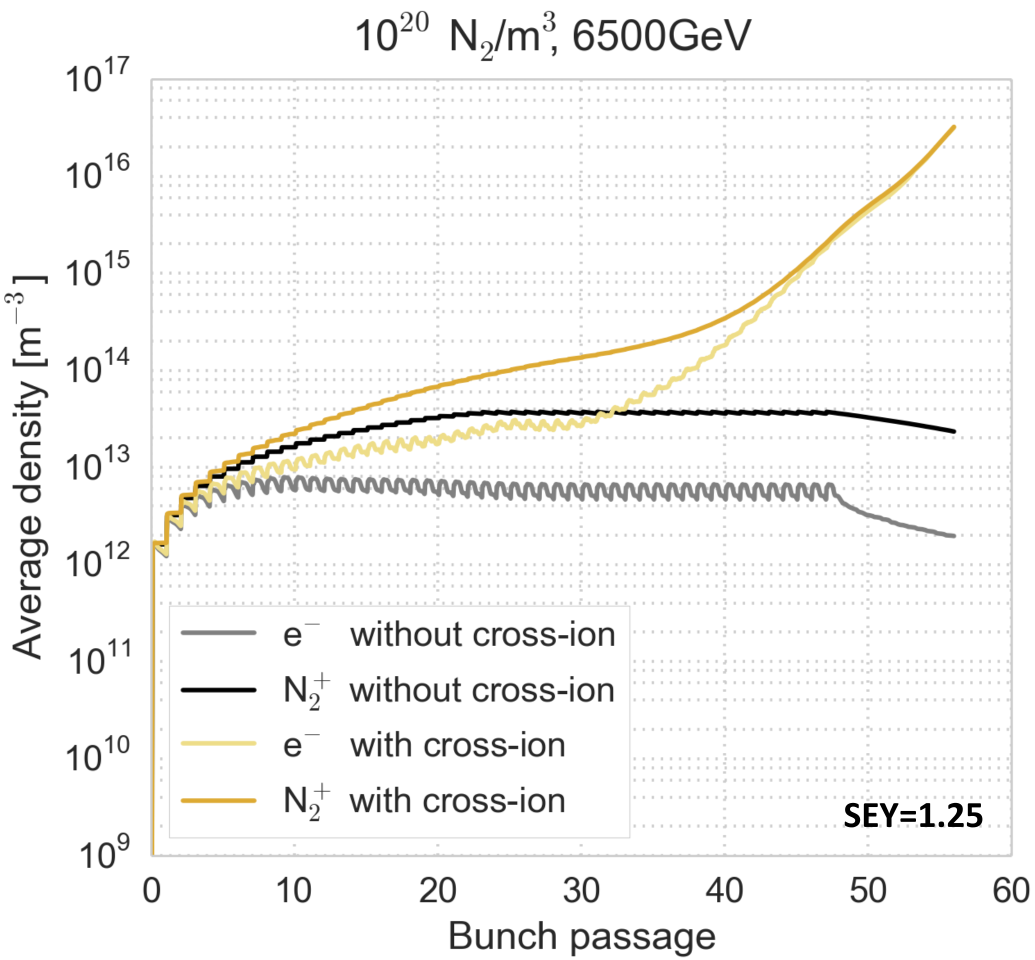
- There is hardly any impact of the electron-induced ionization



10^{20} N_2/m^3

Comparing the densities against the equivalent simulation without cross-species ionization

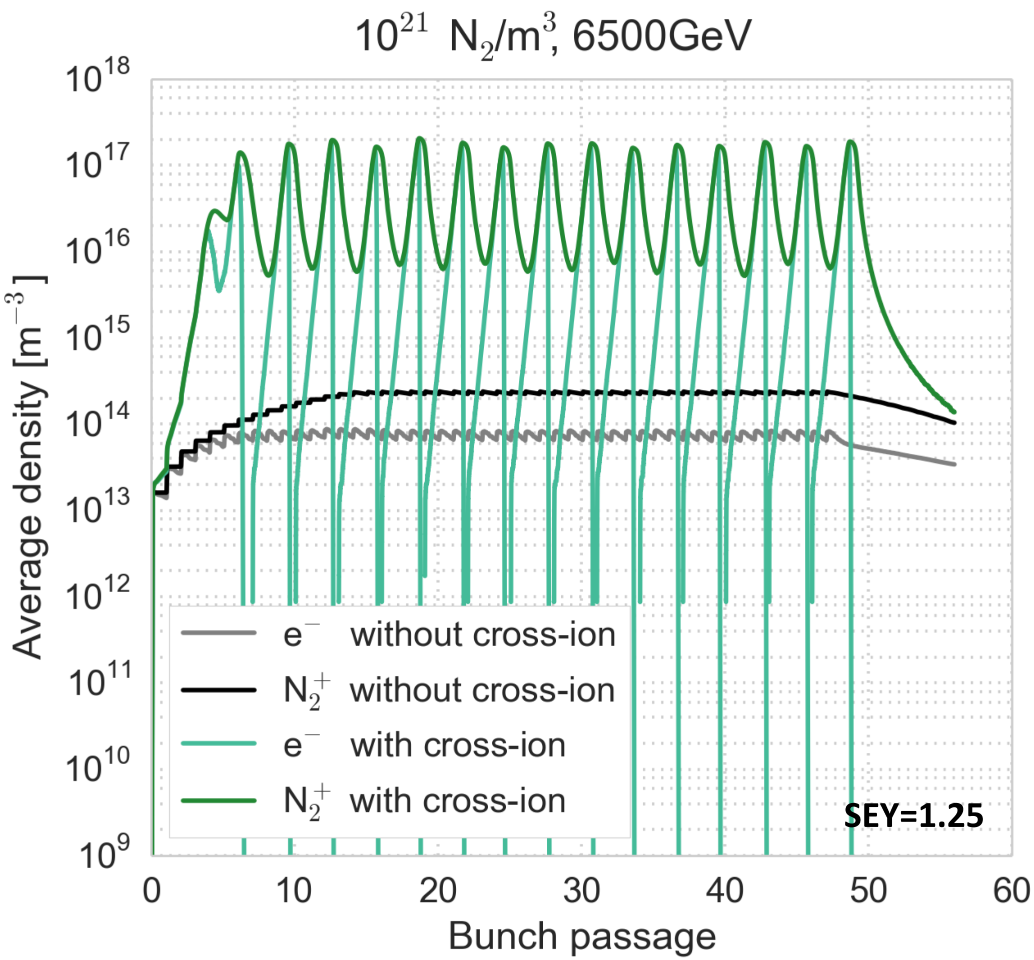
- The densities grow significantly over the bunch train – in agreement with predictions
- Densities continue growing after the end of the bunch train (?)



10^{21} N_2/m^3

Comparing the densities against the equivalent simulation without cross-species ionization

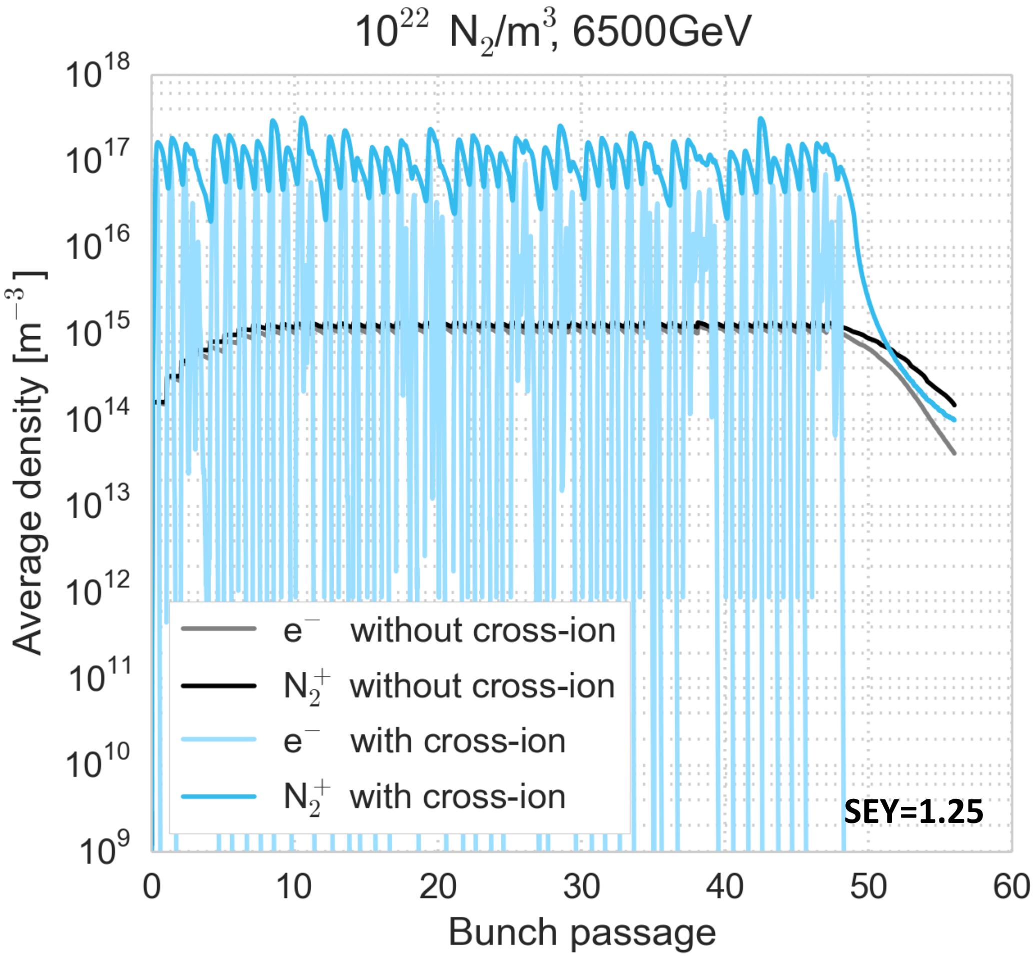
- The densities grow significantly within a few bunch passages
- Electrons very noisy



10^{22} N_2/m^3

Comparing the densities against the equivalent simulation without cross-species ionization

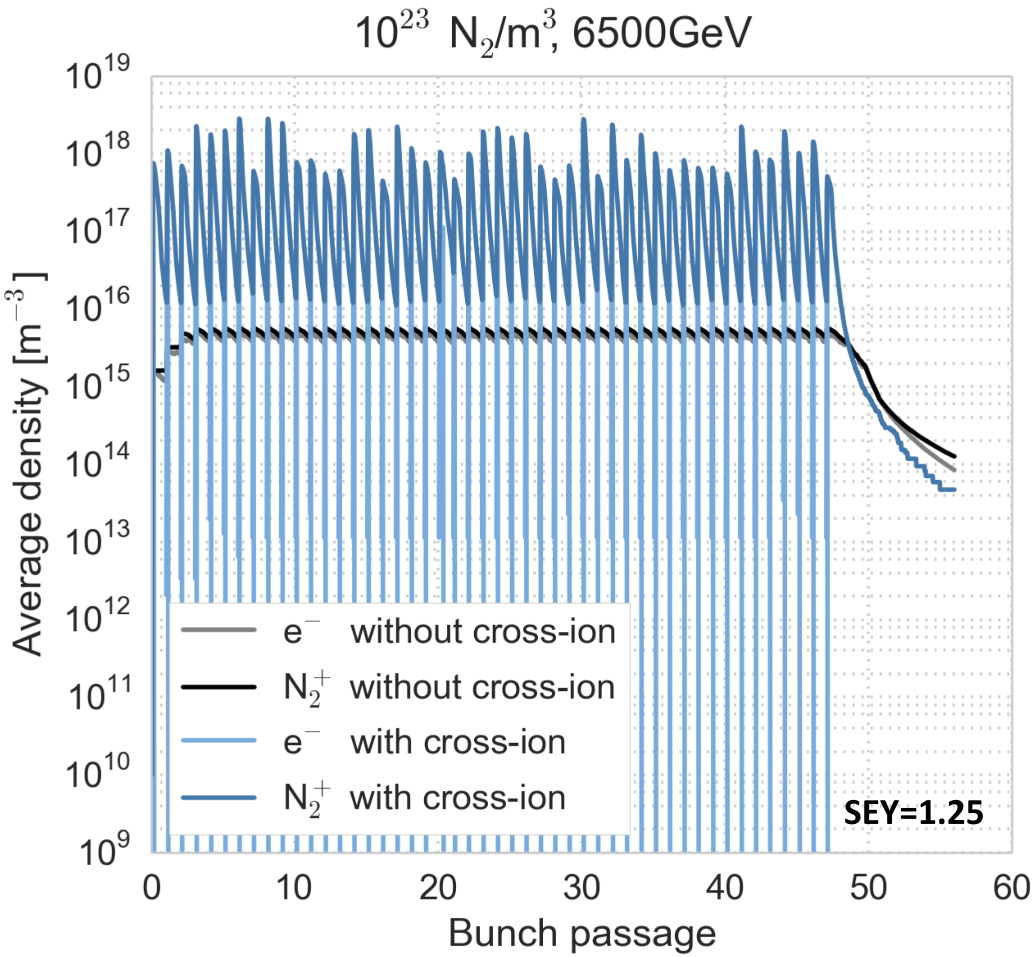
- The densities reach a saturation value within a single bunch passage
- Electrons very noisy



10^{23} N_2/m^3

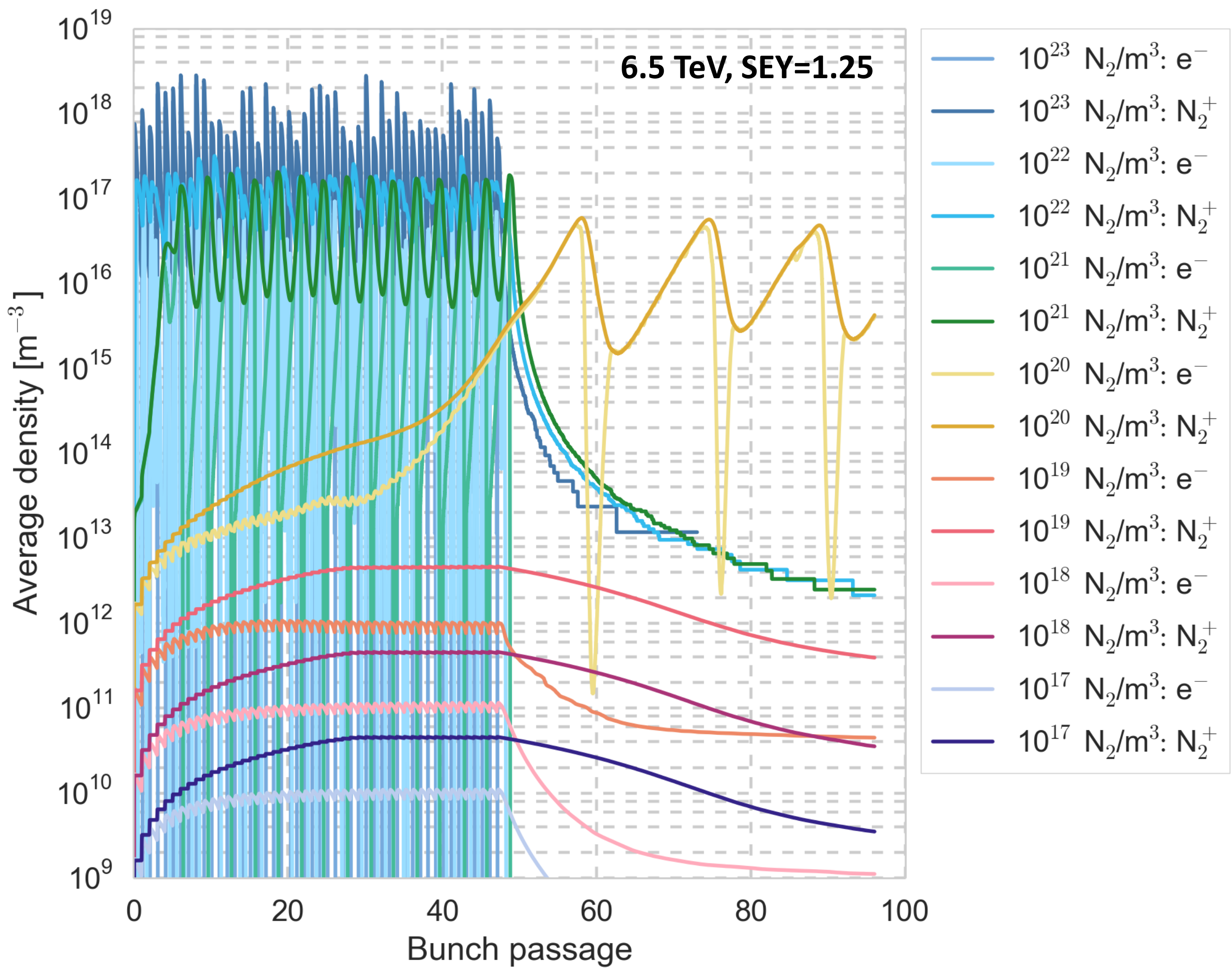
Comparing the densities against the equivalent simulation without cross-species ionization

- The densities reach a saturation value within a single bunch passage
- Electrons very noisy, ions also somewhat noisy



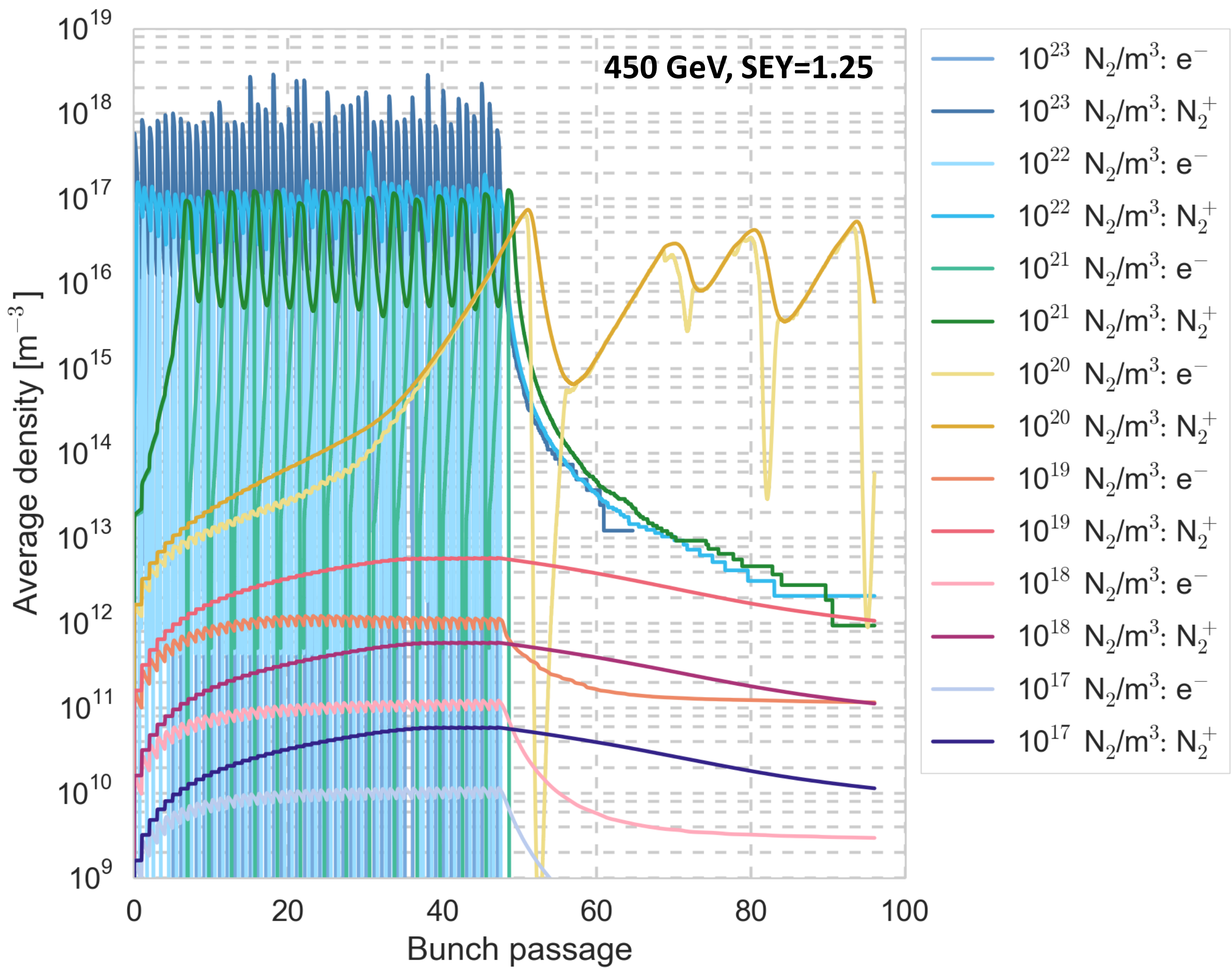
Density dependence

For gas densities from 10^{20} N_2/m^3, electron and ion densities in the range $10^{16} – 10^{17}$ m^{-3} are reached. For higher gas densities, electron and ion densities are similar, but reached faster



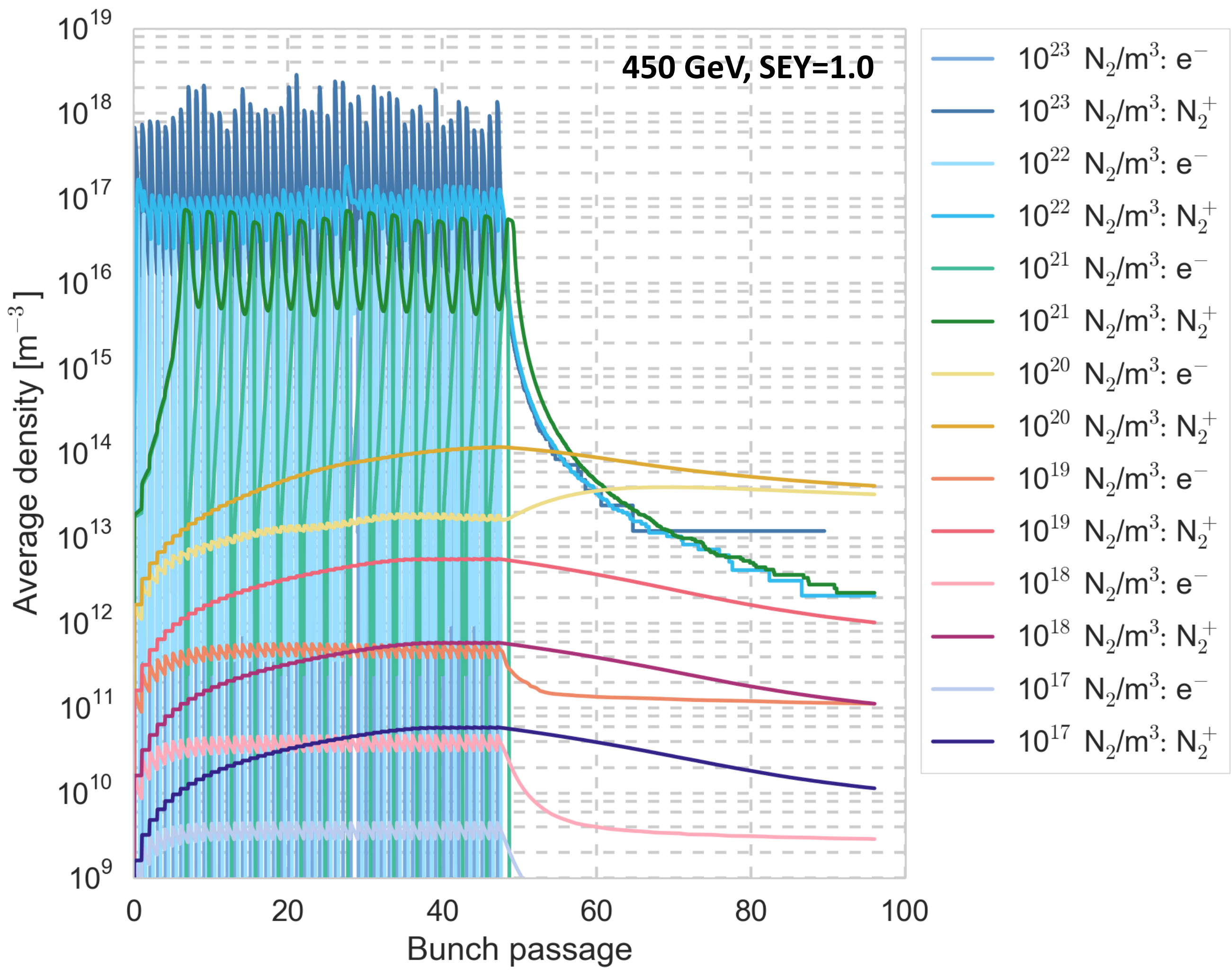
450 GeV, SEY 1.25

For gas densities from 10^{20} N_2/m^3, electron and ion densities in the range $10^{16} – 10^{17}$ m^{-3} are reached. For higher gas densities, electron and ion densities are similar, but reached faster



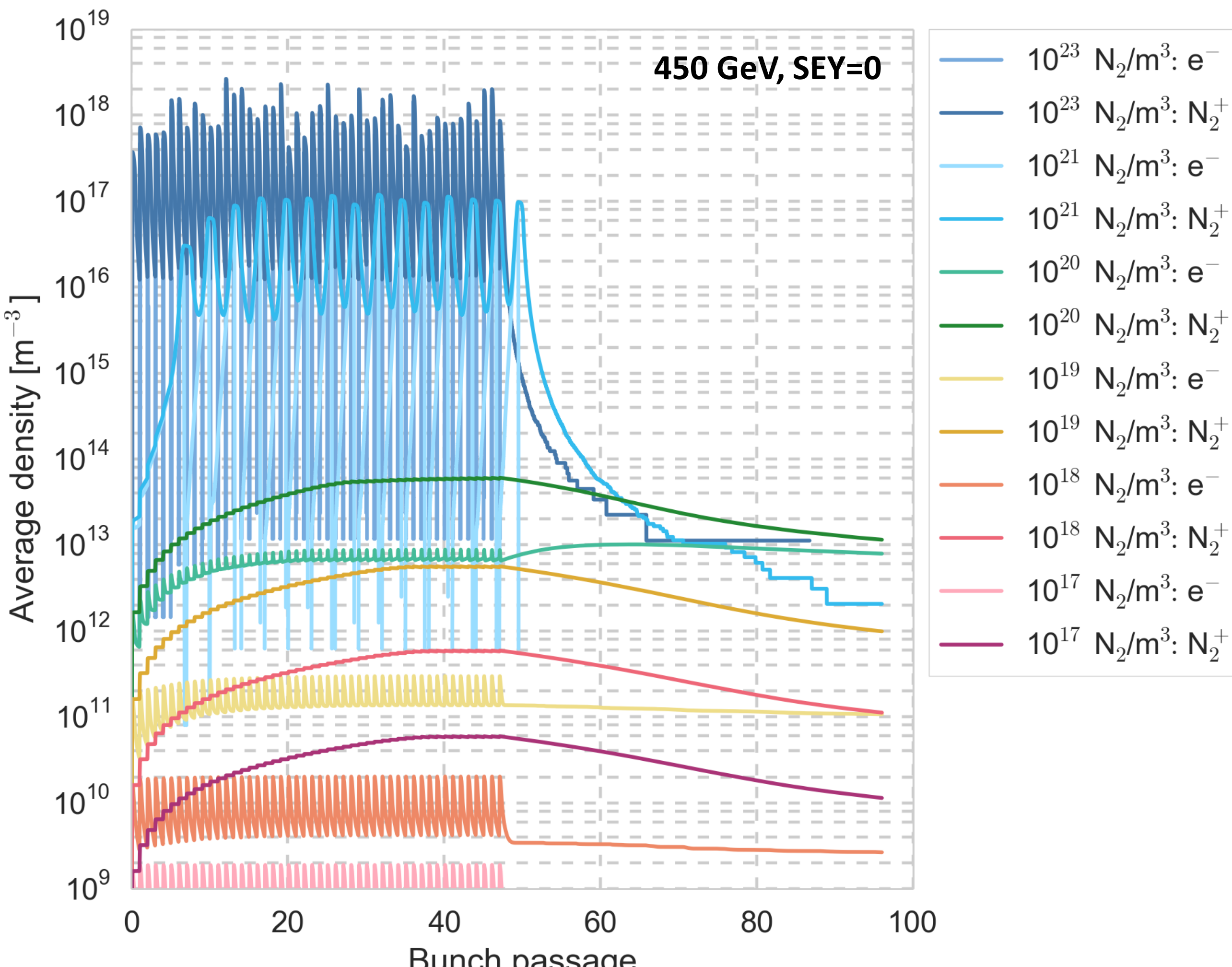
450 GeV, SEY 1.0

With SEY = 1.0, the results are very similar to the previous case, mainly the behaviour of the 10^{20} N_2/m^3 gas density is modified



450 GeV, perfect absorber

Wit perfect absorber boundary conditions, the results are very similar to the case with SEY = 1.0



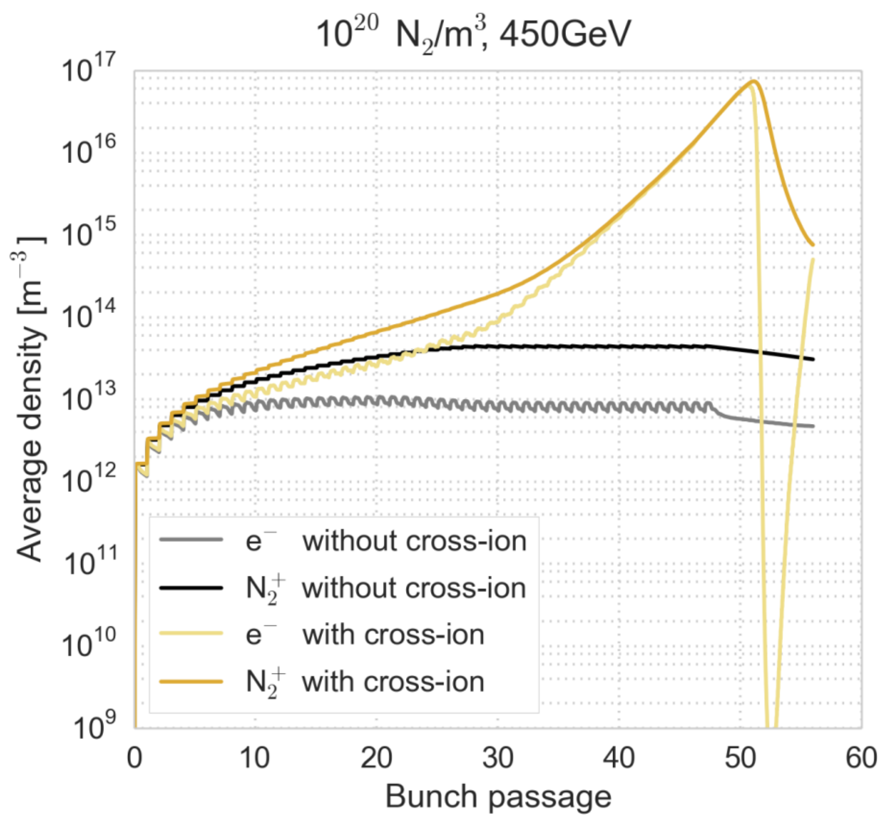
Observations

An unexpected self-sustaining behaviour is observed for a gas density of 10^{20} N_2/m^3 – is it physical?

- Appears to be a combined effect of secondary emission and cross-species ionization – it is suppressed for low or no SEY

- From a first look at the available output no clear physical inconsistency could be identified

- Further checks, e.g. the evolution of the total energy in the system, will be performed



More observations

With the cross-species ionization, the cloud densities can increase by several orders of magnitude over a single or just a few bunch passages

- Although PyECLOUD has good macroparticle size management for electron multipacting, the routines are not perfectly adapted to this case
  - Normally the macroparticle number is checked for, and adjusted if needed, at the end of each bunch passage
  - Asynchronous macroparticle regeneration has already been implemented, where their number is checked and adjusted if needed, at every time step
  - Plan to implement more suitable handling of decreasing macroparticle numbers – hope to reduce the noisiness of electron numbers

Currently cross-species ionization is performed at every simulation time step

- If generation over this time step is small → poor sampling of the cross-section
  - To be investigated if there is a need for a separate ionization time step

Conclusion & Outlook

- Electron-induced ionization was estimated to be important in the 16L2 events
- A module for cross-species ionization has been implemented in PyECLOUD to allow for simulations including electron-induced ionization
- First simulation studies have been performed and show that the ionization has a significant effect for gas densities from 10^{20} N_2/m^{-3}, as was predicted
- In some cases, a self-sustaining behaviour is seen, where generation occurs in the absence of beam – still unclear if the behaviour is physical and real
- Further checks and small code improvements e.g. on macroparticle management are required to confirm validity and improve results
- Convergence scans to be performed before full-blown simulation studies