Multi-species simulations with cross-ionization: investigation of numerical runaway

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Acknowledgements: K. Poland, G. Rumolo

e-cloud meeting

29 November, 2019

Motivation

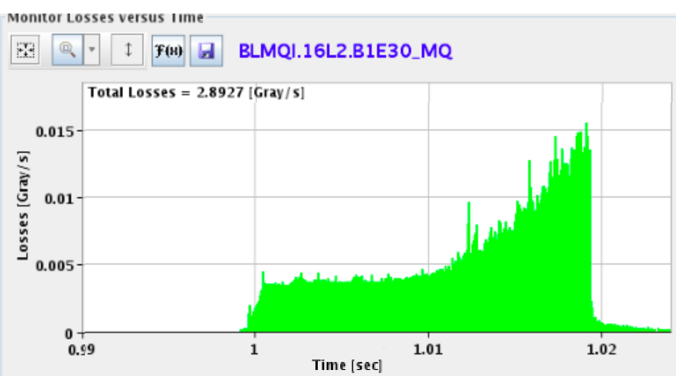
Throughout 2017 operation, abnormal losses were observed in the LHC

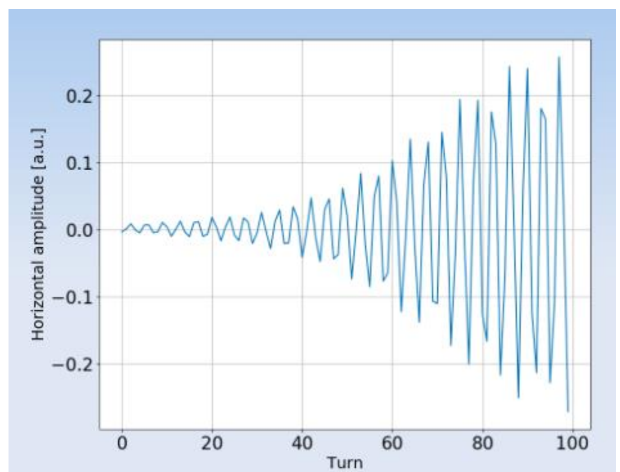
- Located in the 16th half-cell left of Point 2 (‘16L2’)

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:

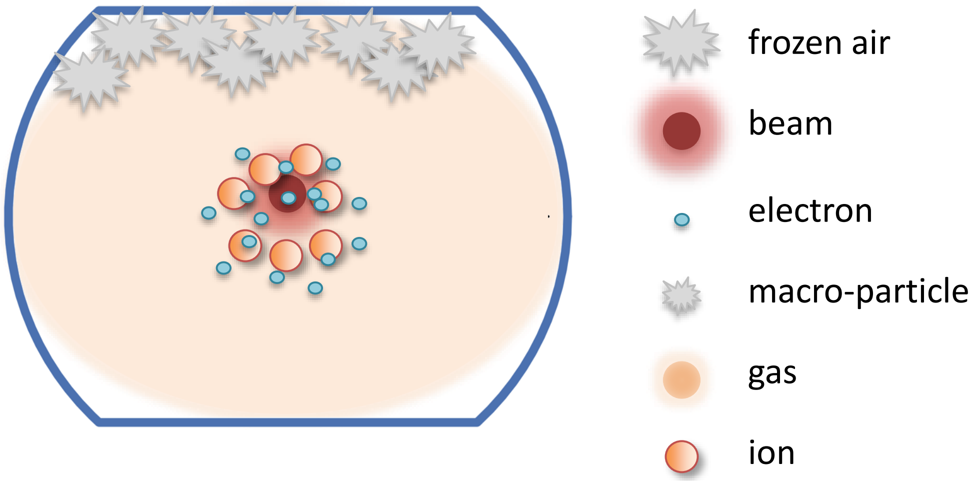
A macro-particle of frozen air (N_2, O_2) is detached, possibly triggered by e-cloud, and enters the beam

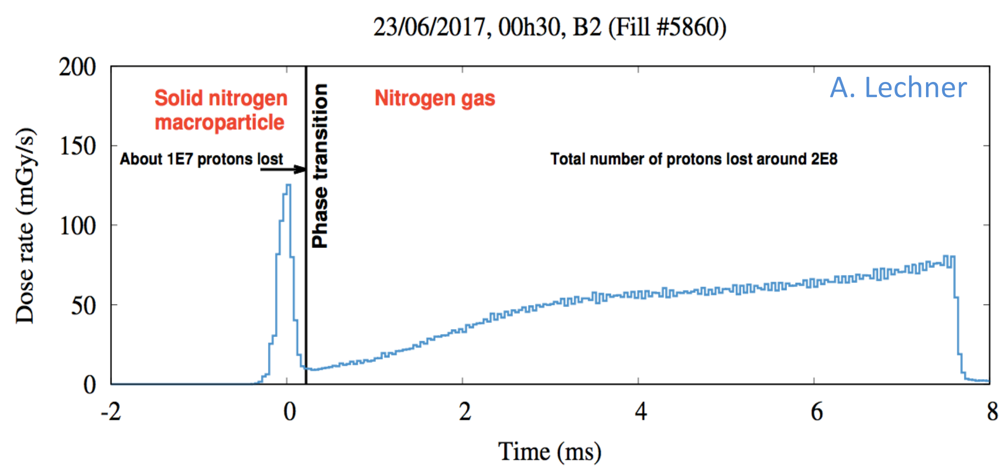
↓

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





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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 (2017-18):

- ✓ 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

Recent model ingredient (2019):

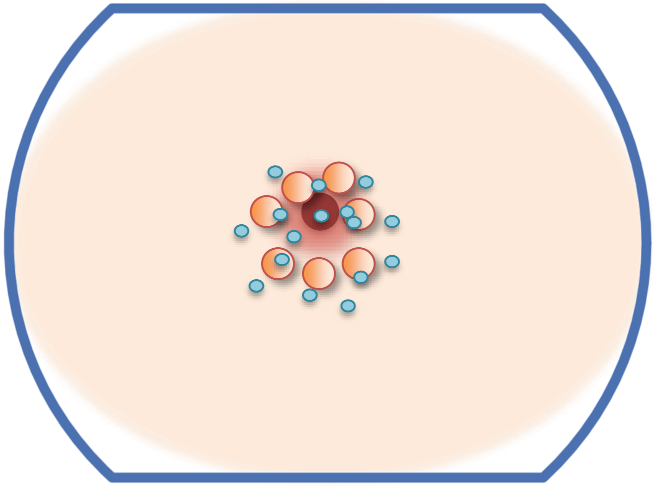
- ✓ Implementation of cross-species ionization
- ✓ First simulation study with cross-ionization
- See e-cloud meeting #69

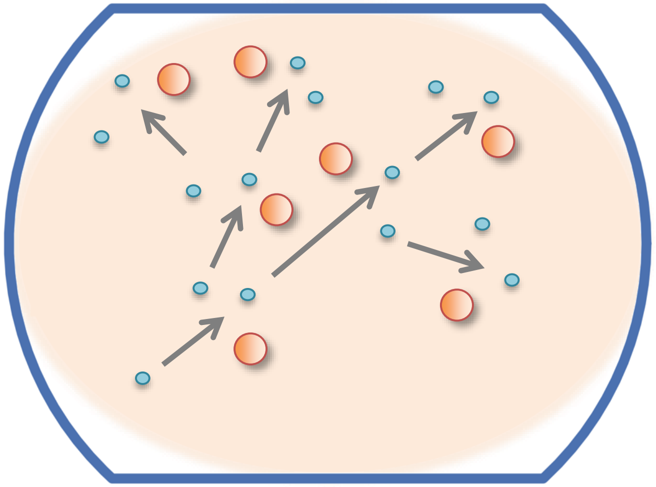
Cross-species ionization model

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

- Assume a uniform gas density in the chamber
  (no neutral macro-particles, no collisions → not full-scale plasma simulations)

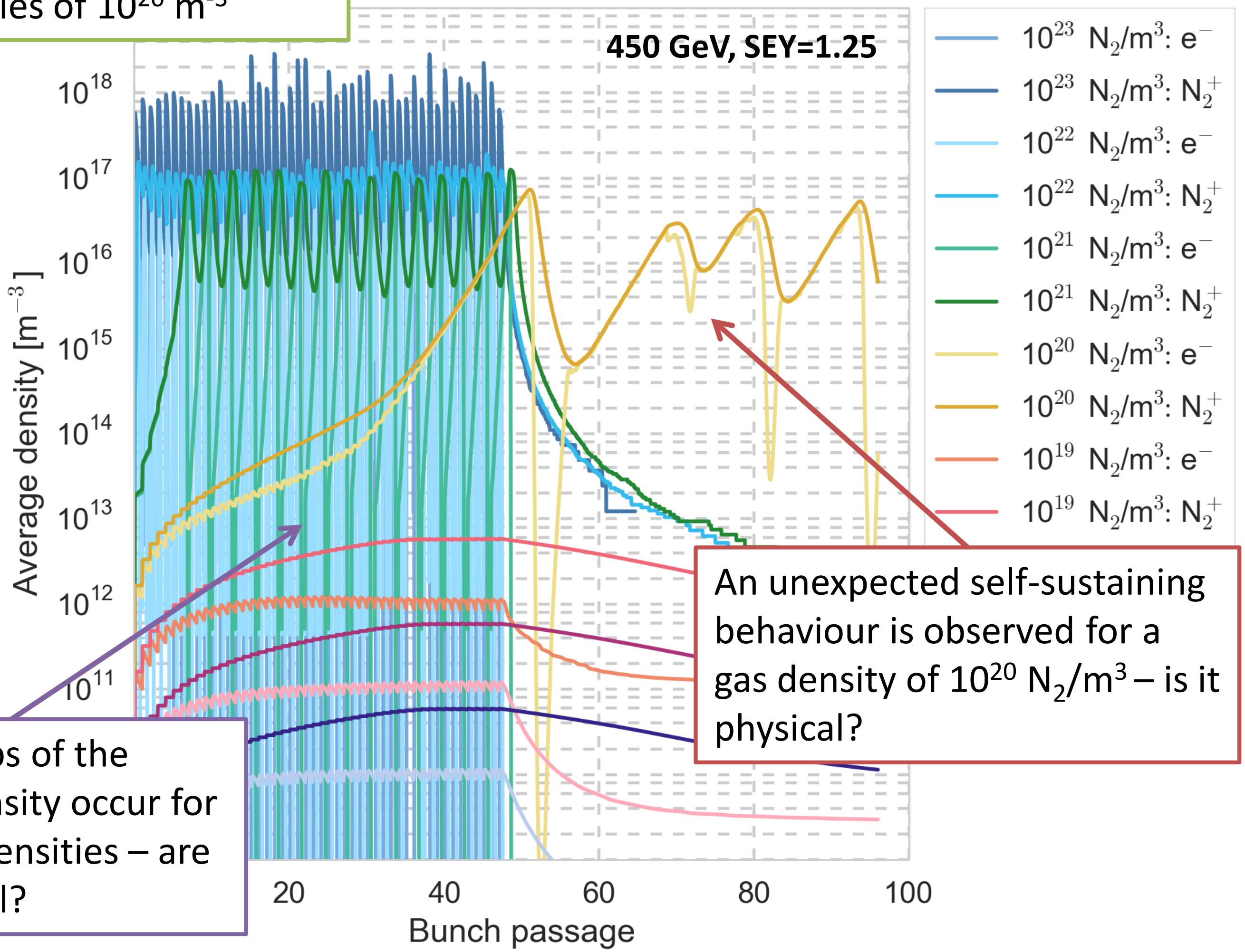
- Consider single ionization only





First cross-ionization simulations

Cross-ionization starts to have a significant impact as of gas densities of 10^{20} m^{-3}



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

Sudden drops of the electron density occur for higher gas densities – are they physical?

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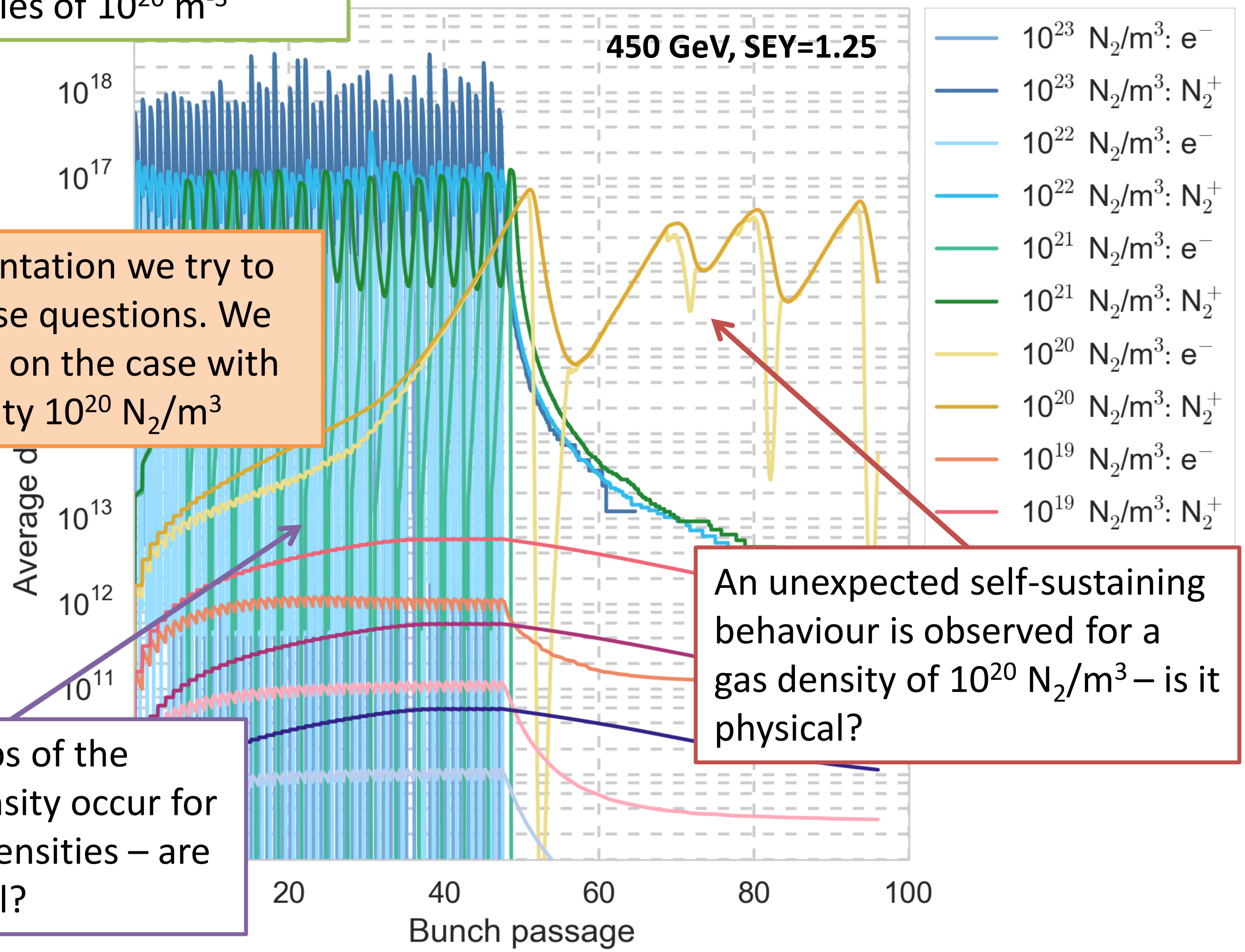

In this presentation we try to address these questions. We focus mainly on the case with gas density 10^{20} N_2/m^3

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Sudden drops of the electron density occur for higher gas densities – are they physical?

Energy evolution

As a first consistency check, we monitor the total energy in the system

- Previously only the kinetic energies of each cloud were saved

- Calculation and saving of the electrostatic energy was implemented as

$$U_e = \frac{1}{2}\epsilon_0 \sum_i \left(E_{x,i}^2 + E_{y,i}^2\right) \Delta h^2$$

→ energy of the total charge system, not individual clouds

Energy evolution

After the last bunch passage no external energy is injected into the system

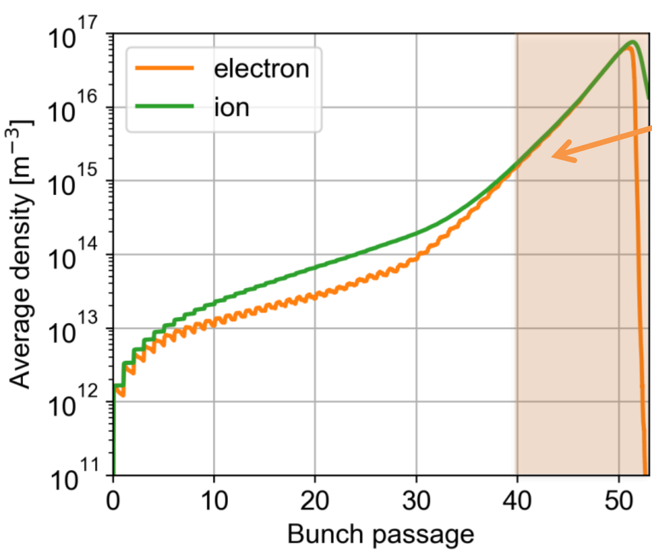
→ The total energy should stay constant or decrease

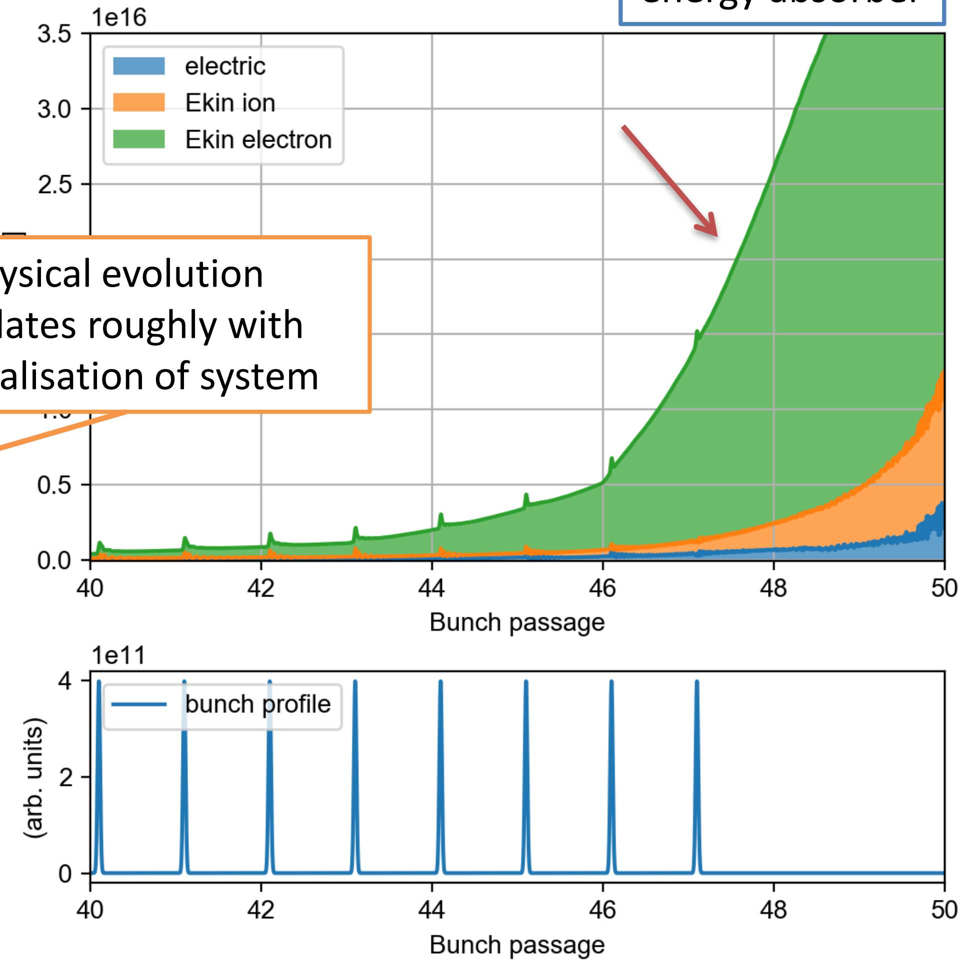
The wall is a net energy absorber

- Instead, an increase is observed in every energy component

→ The evolution after the bunch train is unphysical

Unphysical evolution correlates roughly with neutralisation of system





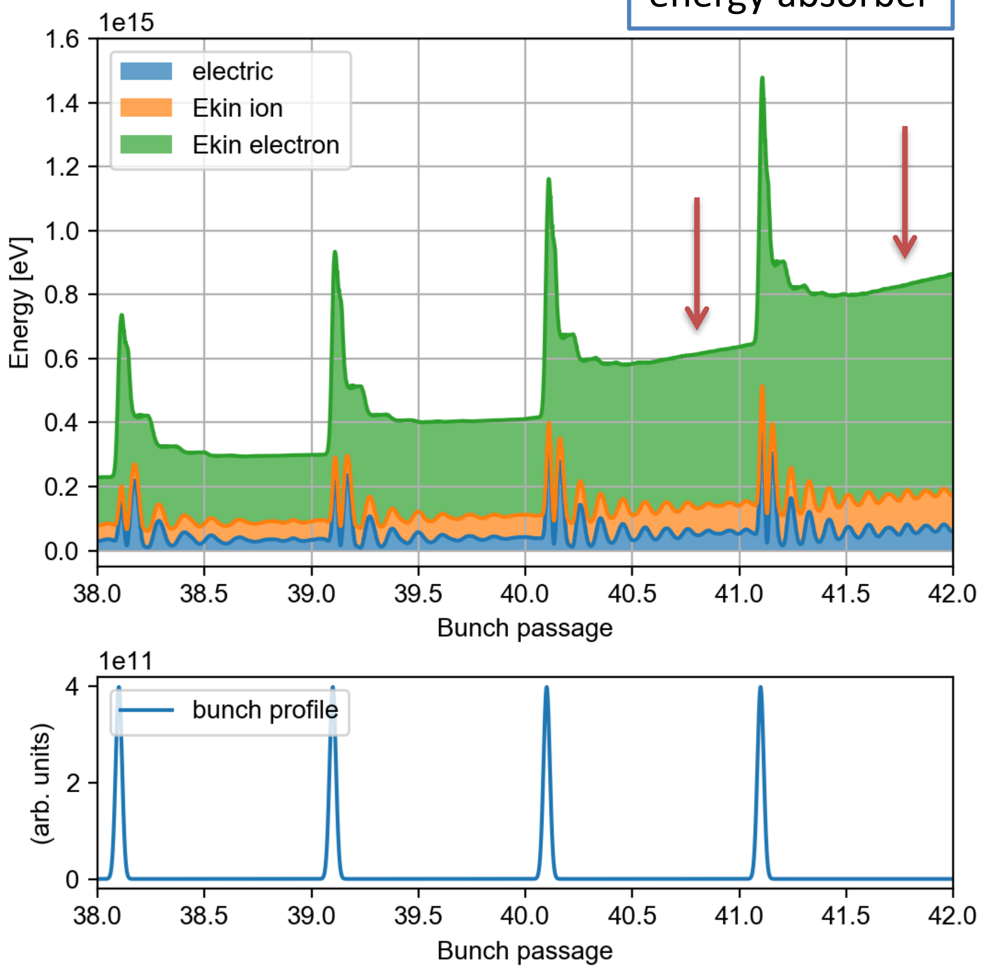
Energy evolution

During the bunch train passage, external energy is injected only during individual bunch passages

- An energy increase is observed also between bunch passages

→ The evolution becomes unphysical already during the bunch train passage

The wall is a net energy absorber



Detailed studies

To investigate the unphysical evolution, detailed studies were performed

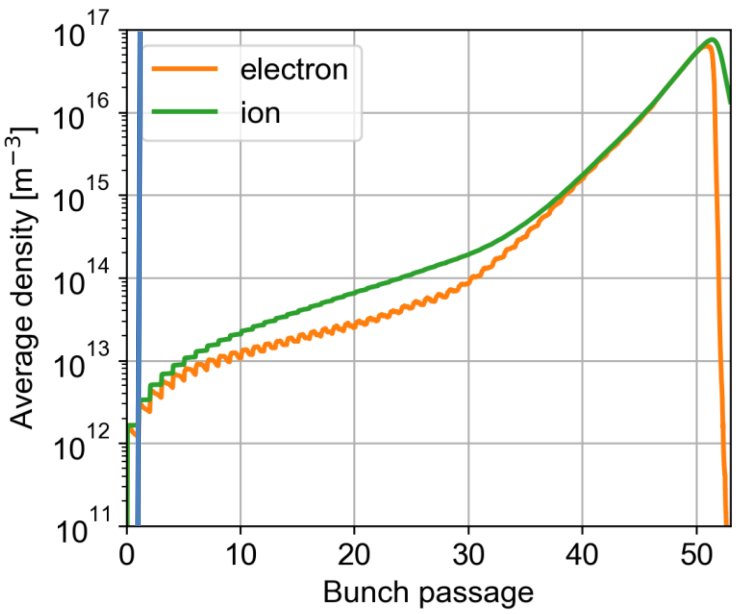
- Saved full simulation state at regular intervals along the simulation
- Restarted simulations from saved states could be run interactively in small steps, allowing the examination of different quantities along the simulation
- Both time-consuming and data-intensive

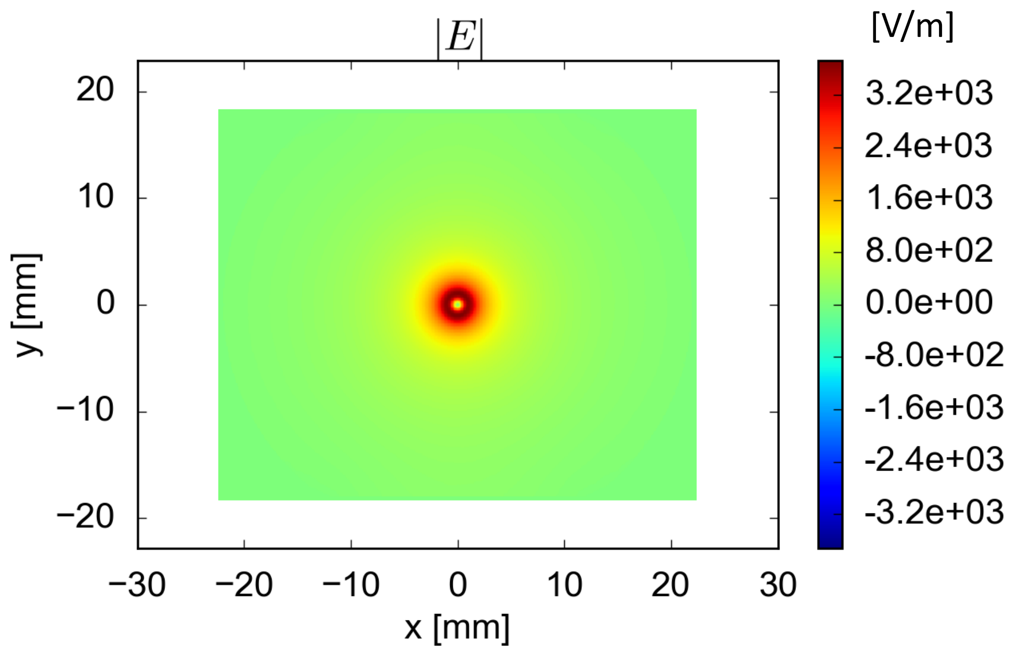
On the next slides some observations from these studies…

E-field evolution

There appears to be a correlation between the artificial energy growth, the (quasi-) neutralization of the system and increasingly noisy e-fields

Bunch passage 1





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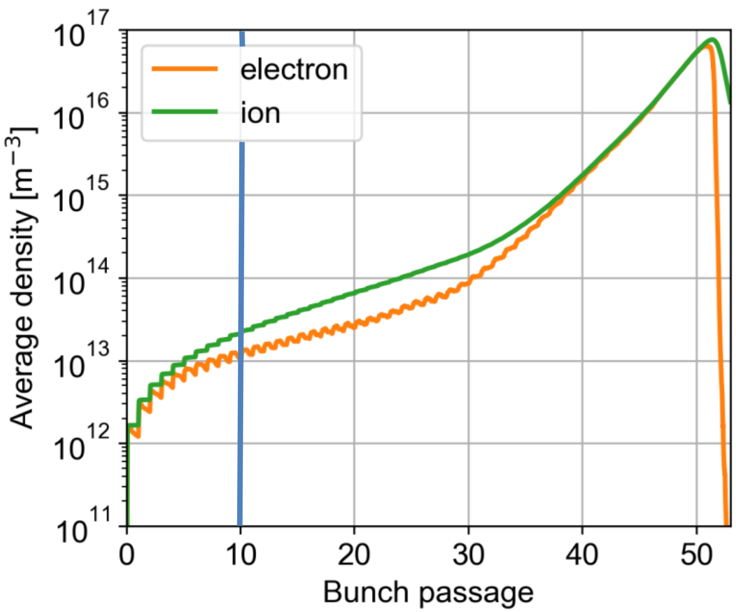
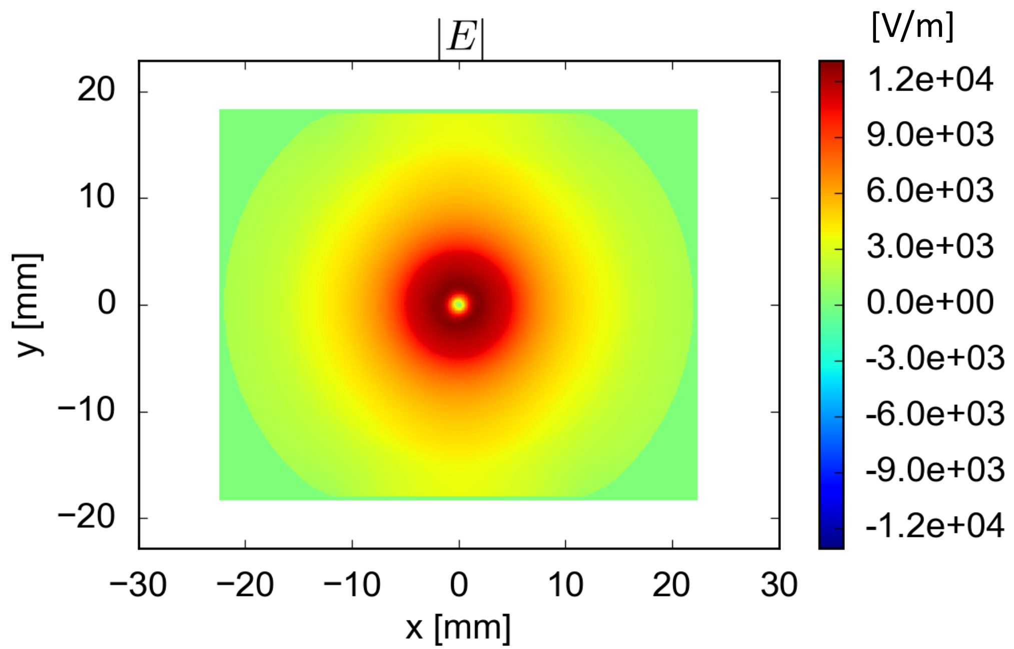
Bunch passage 10





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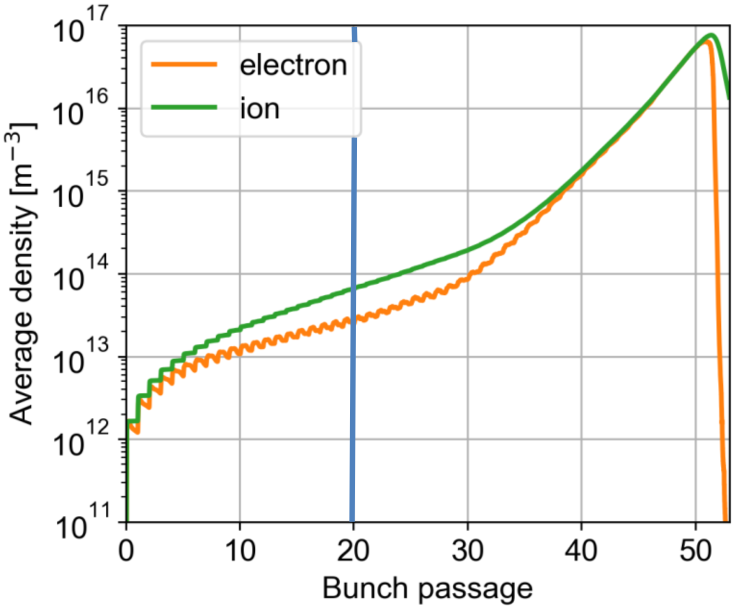
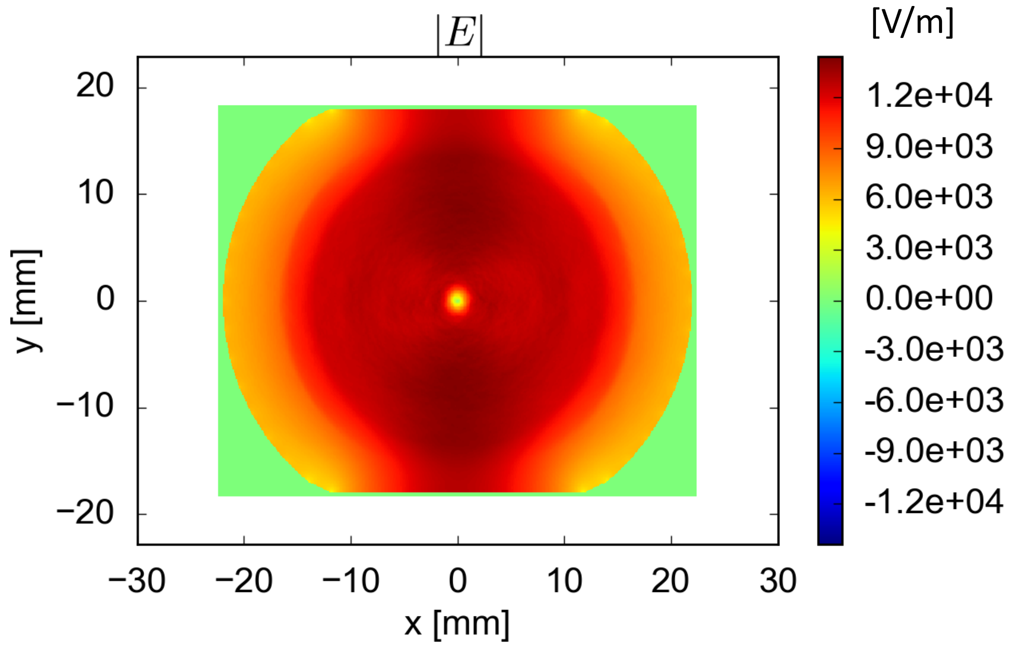
Bunch passage 20





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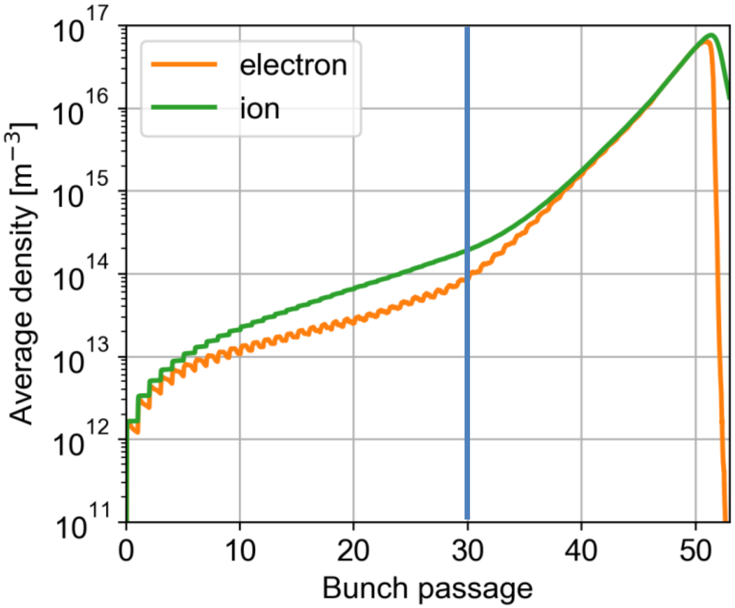
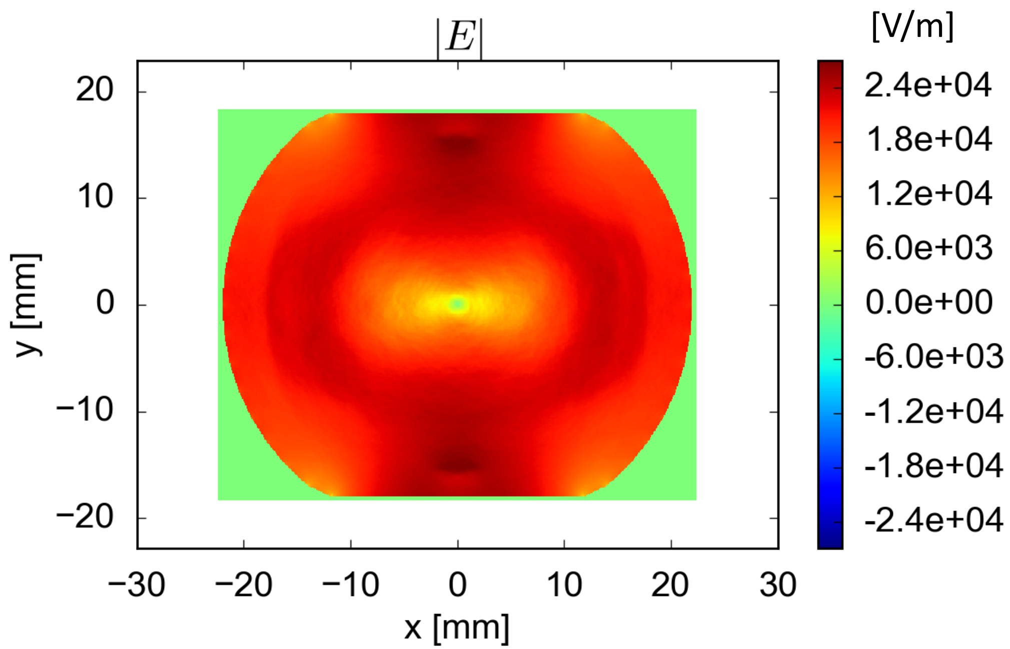
Bunch passage 30





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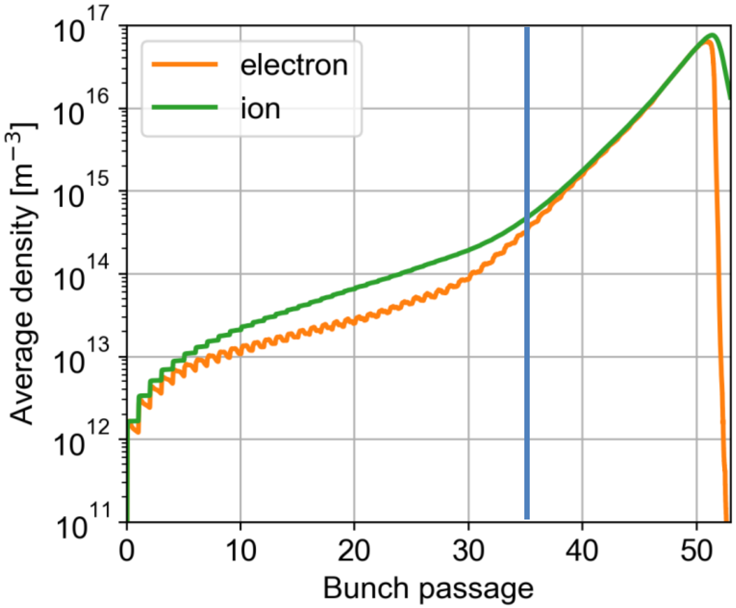
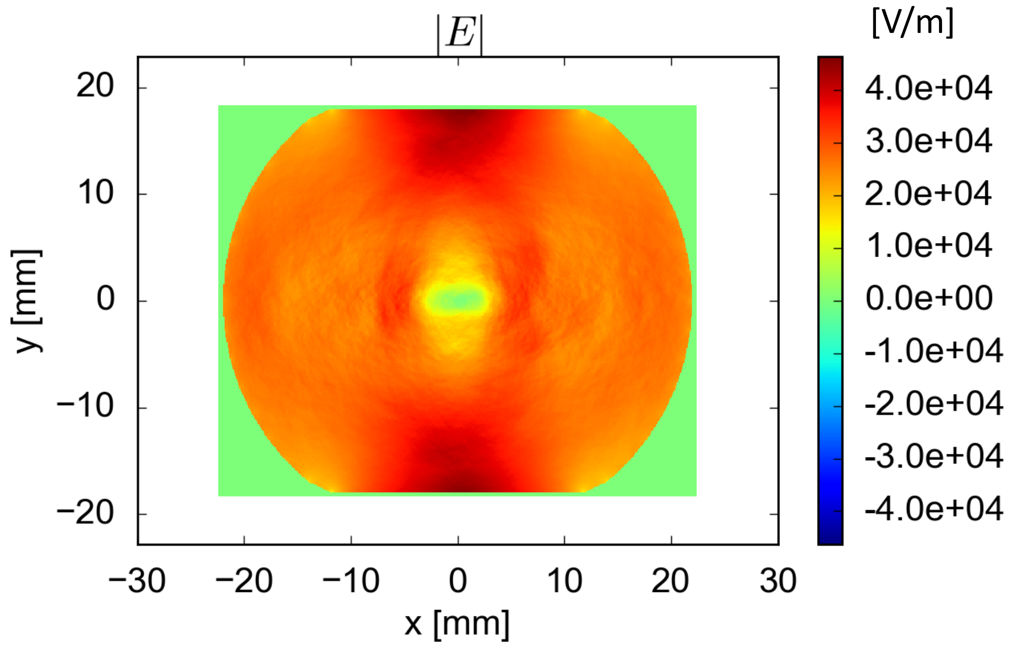
Bunch passage 35





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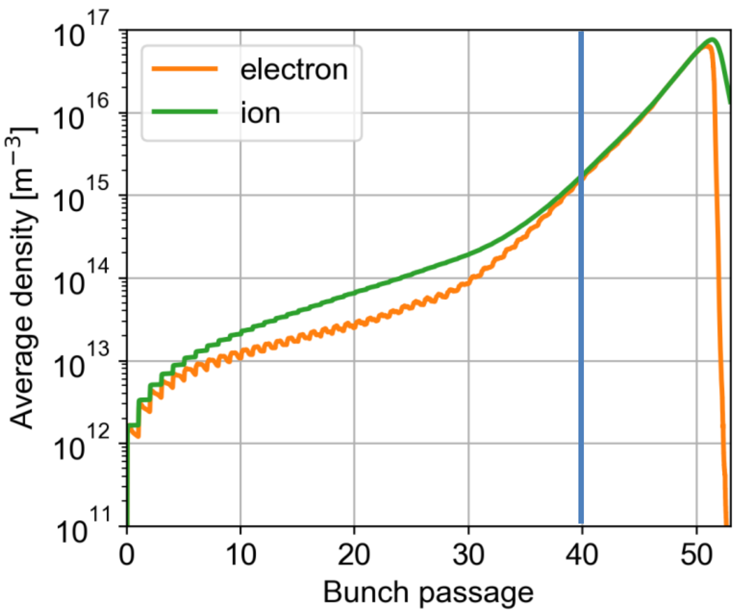
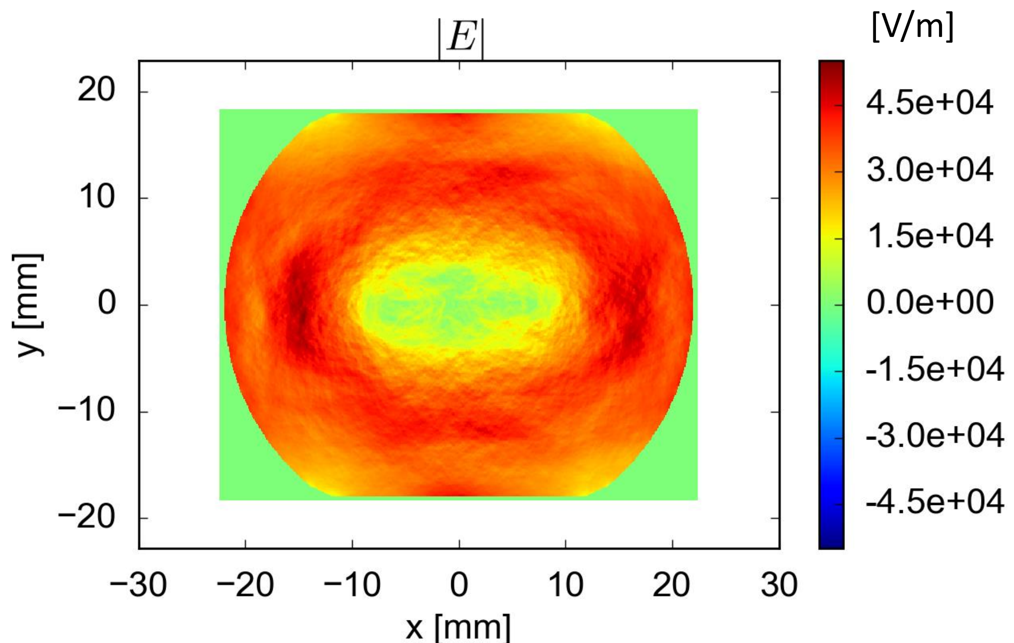
Bunch passage 40





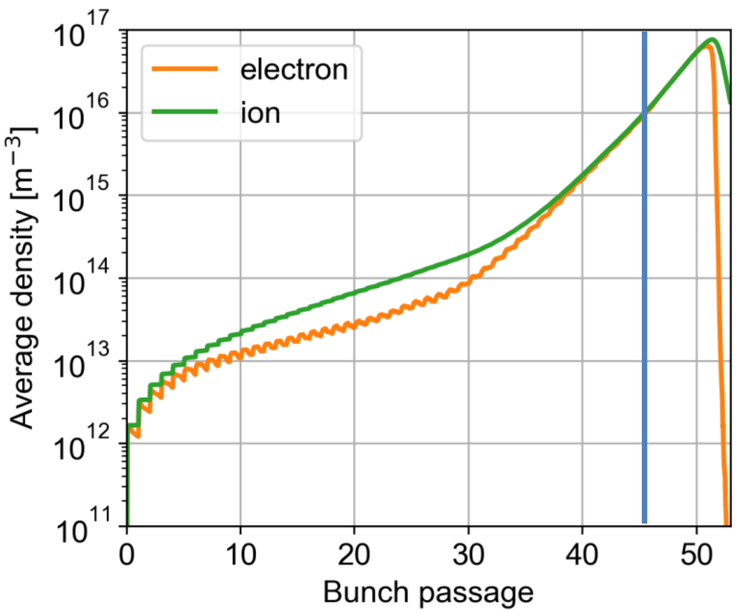
Here the energy evolution is already unphysical

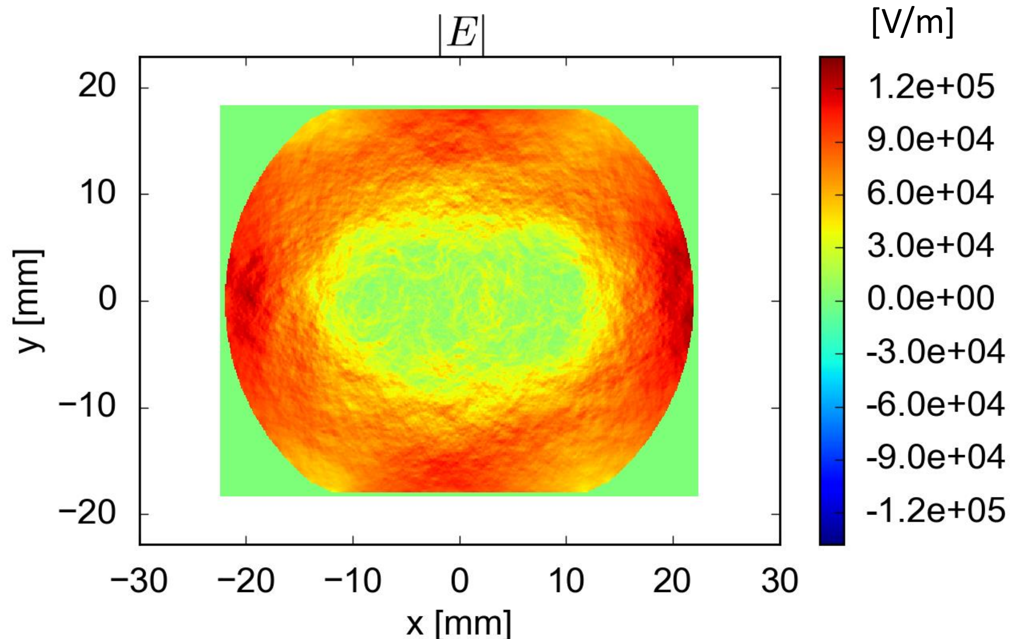
E-field evolution

There appears to be a correlation between the artificial energy growth, the (quasi-) neutralization of the system and increasingly noisy e-fields

Also the e-field magnitude becomes suspiciously large

Bunch passage 45





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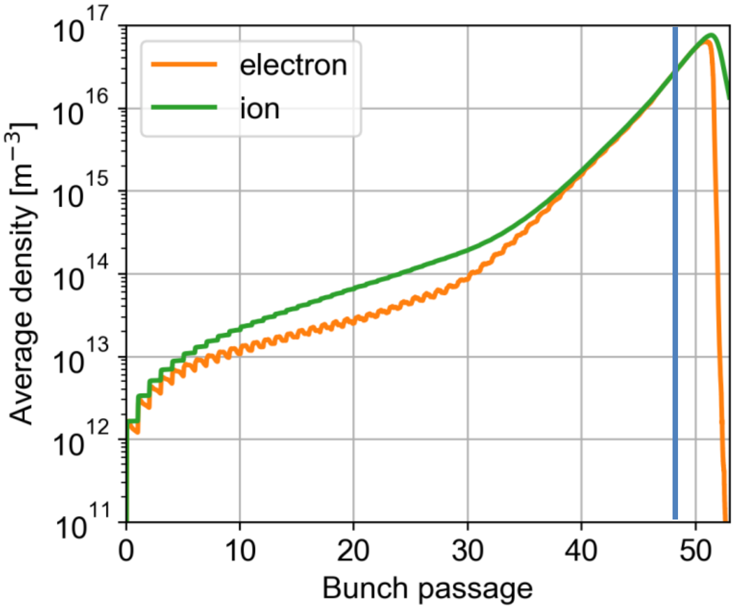

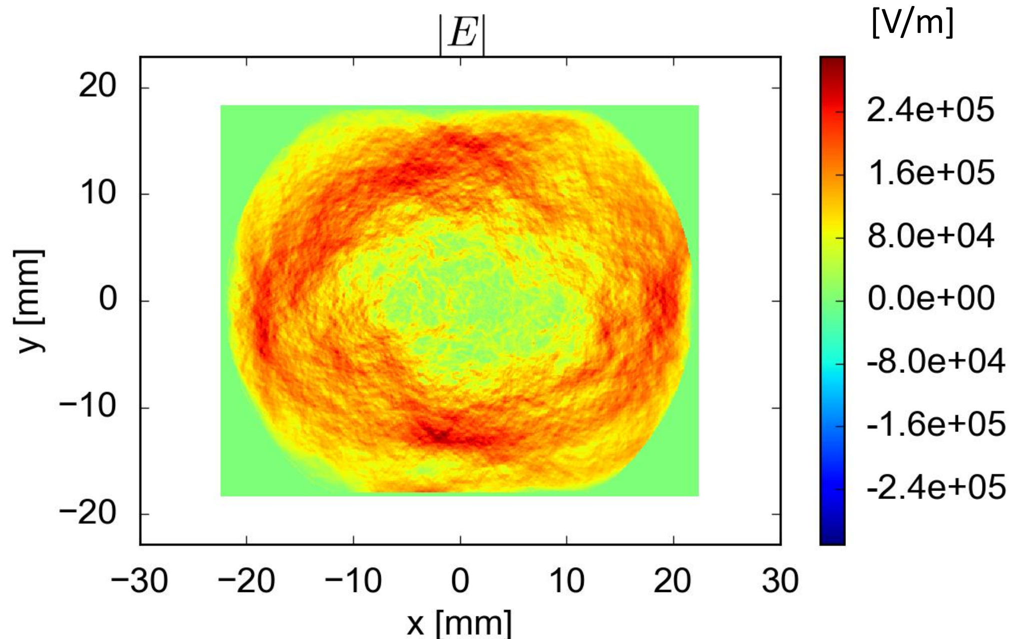

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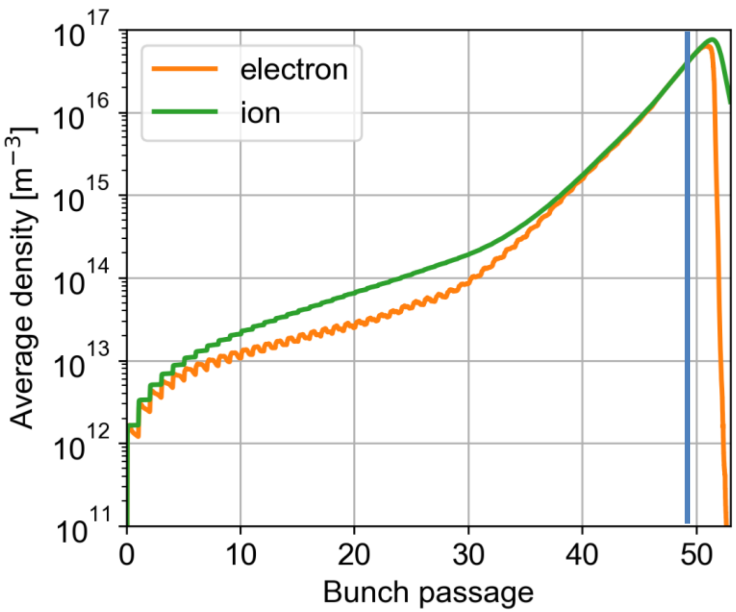

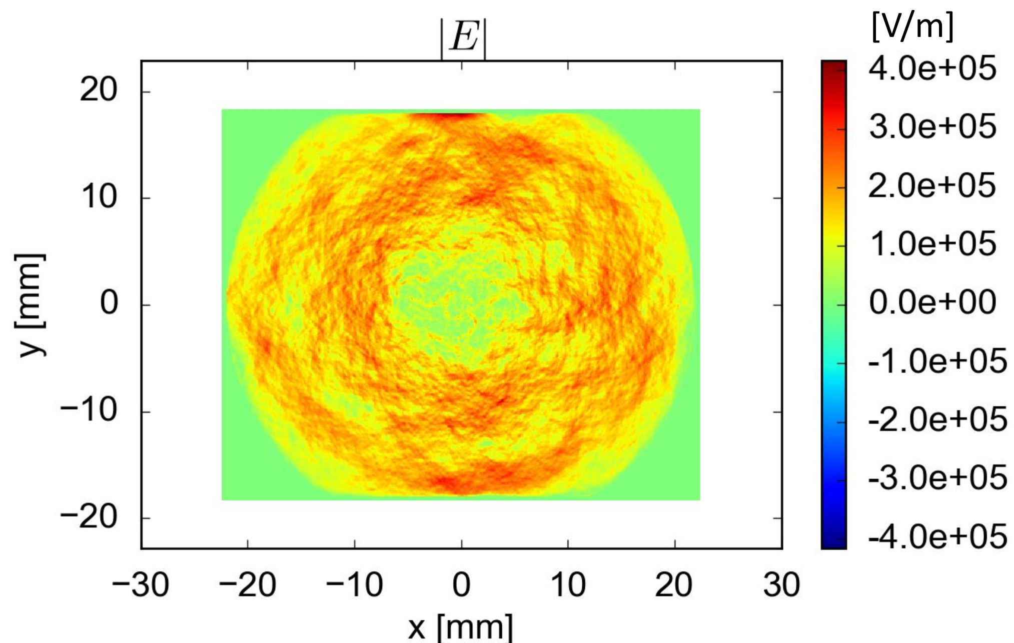

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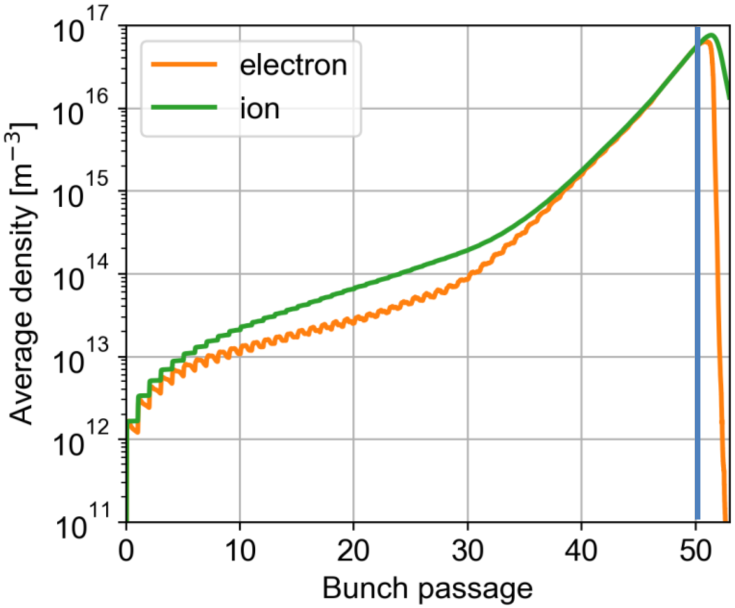
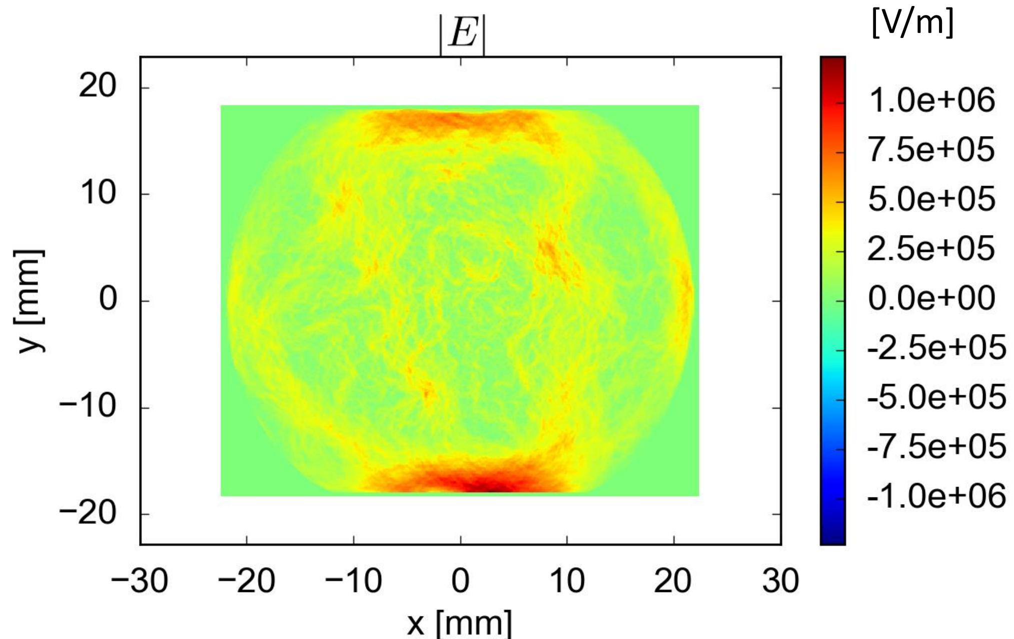
Bunch passage 50





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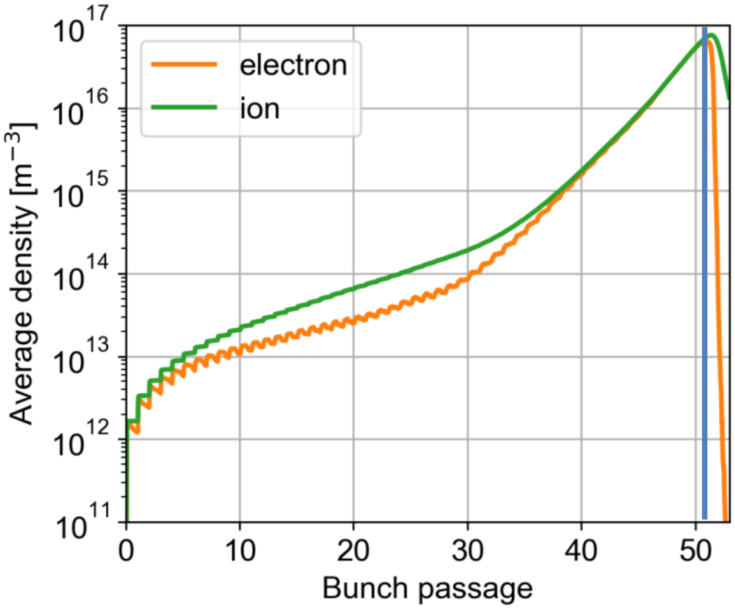
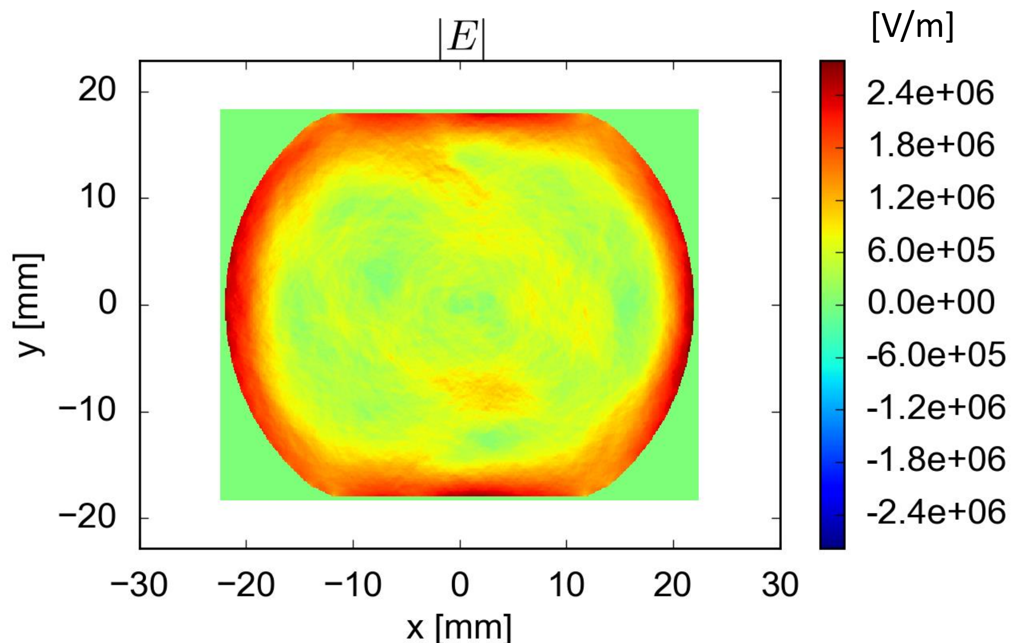
Bunch passage 51





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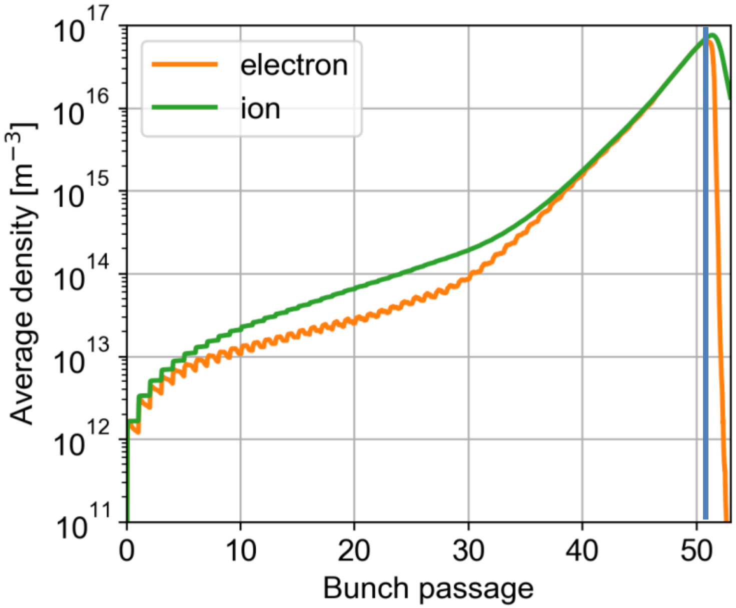

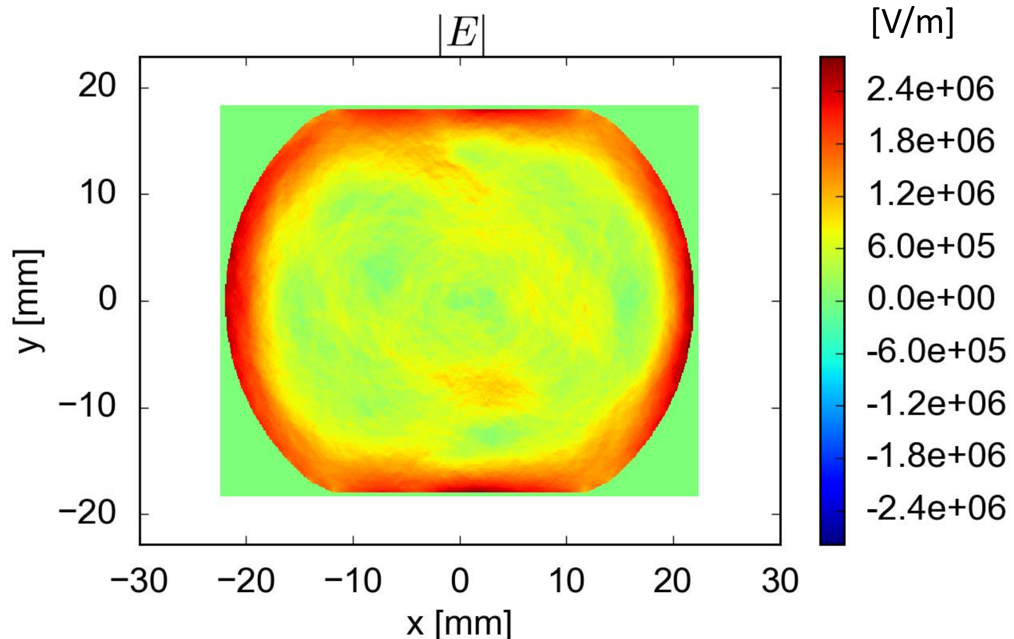

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It looks like the simulation suffers from **numerical heating**, where local noise in the electric field artificially accelerates the electrons → unphysical energy growth

Numerical heating

Well known phenomenon in PIC plasma codes

- Can typically be avoided by ensuring the stability conditions:

$$\Delta x < 3.4\lambda_D \qquad \lambda_D = \sqrt{\frac{\epsilon_0 k_B T_e}{n_i e^2}}$$

$$\Delta t \lesssim \omega_p^{-1} \qquad \omega_p^{-1} = \sqrt{\frac{\epsilon_0 m_e}{n_e e^2}}$$

  - Based on saved average quantities, these conditions are satisfied in our simulation

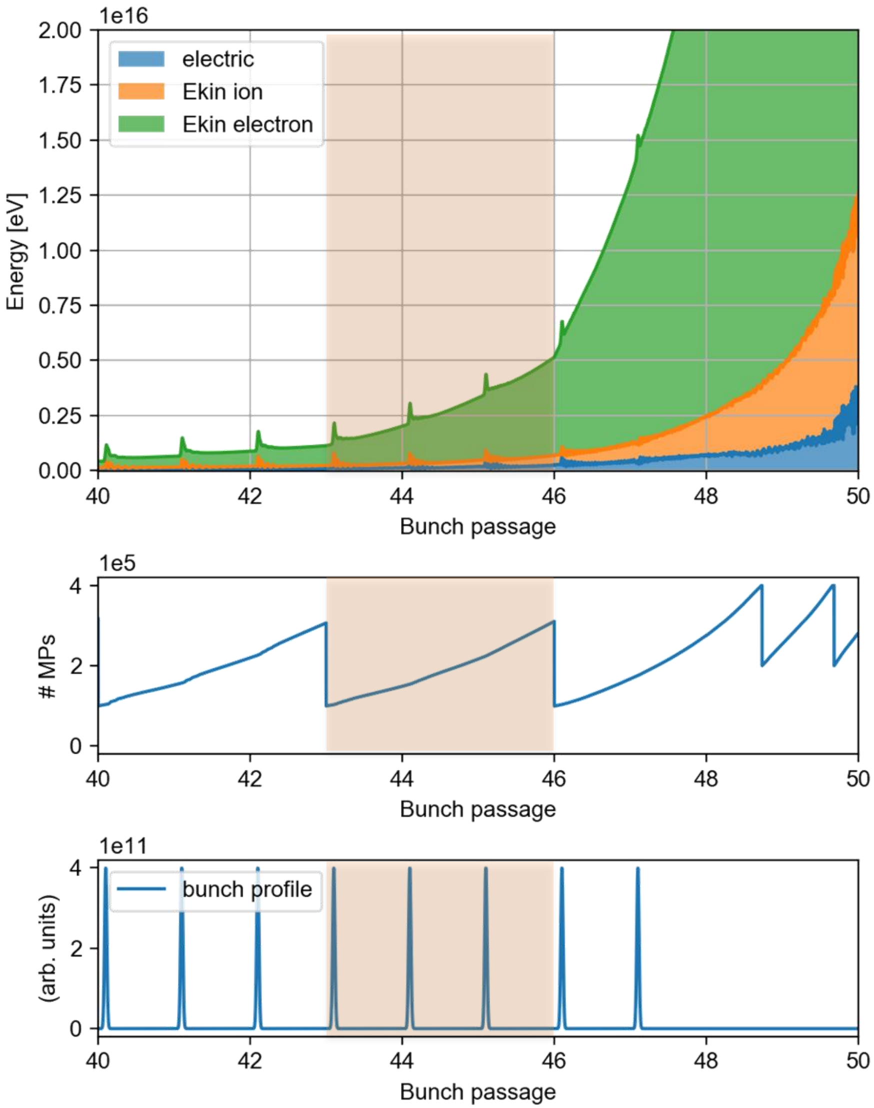
- However, it is based on assumption of thermal Maxwell-Boltzmann distribution

- Generally a problem for “cold” plasmas, with no spread in velocities
  - e.g. astrophysical plasmas

Regeneration

To keep the number of macro-particles manageable during simulations (with exponentially increasing number of particles), macro-particles are merged throughout the simulation, to keep their number within requested limits

- When merged in large steps, a correlation is observed between the merging events (regenerations) and the slope of the (unphysical) energy growth



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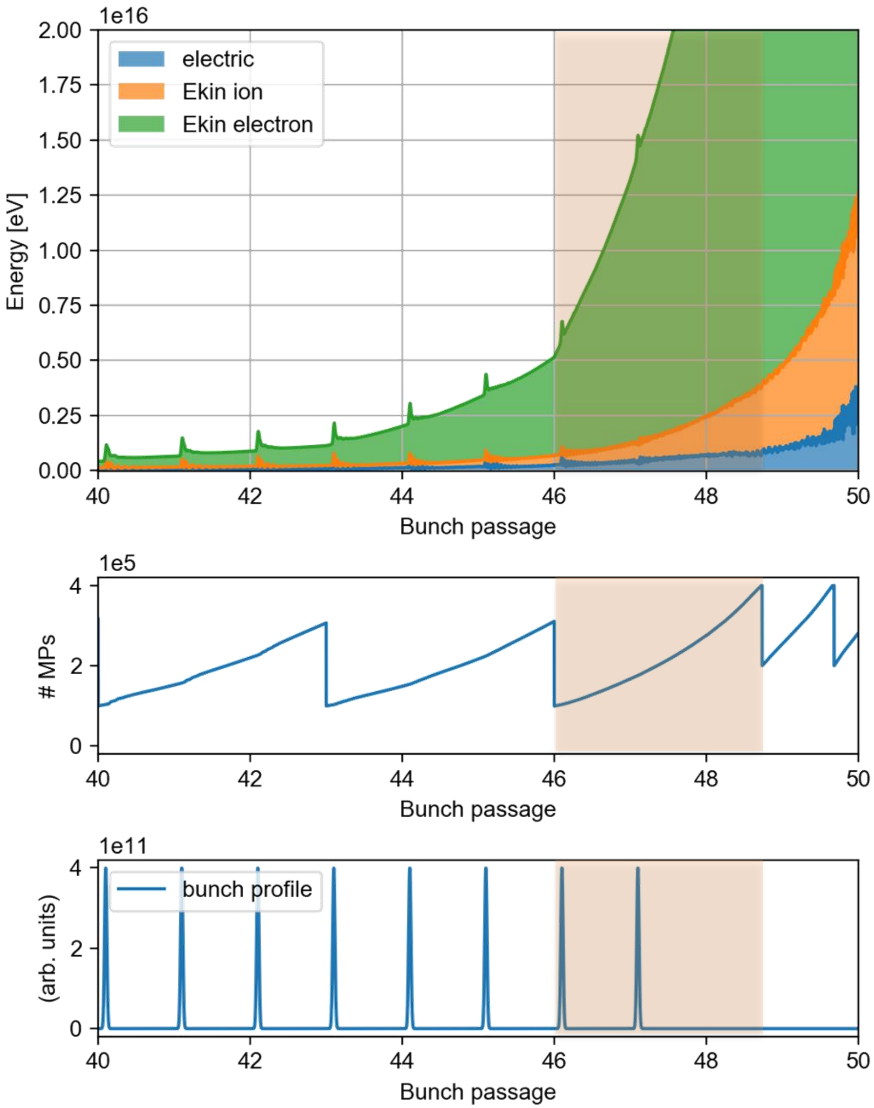
→ The regenerations inject more noise into the system



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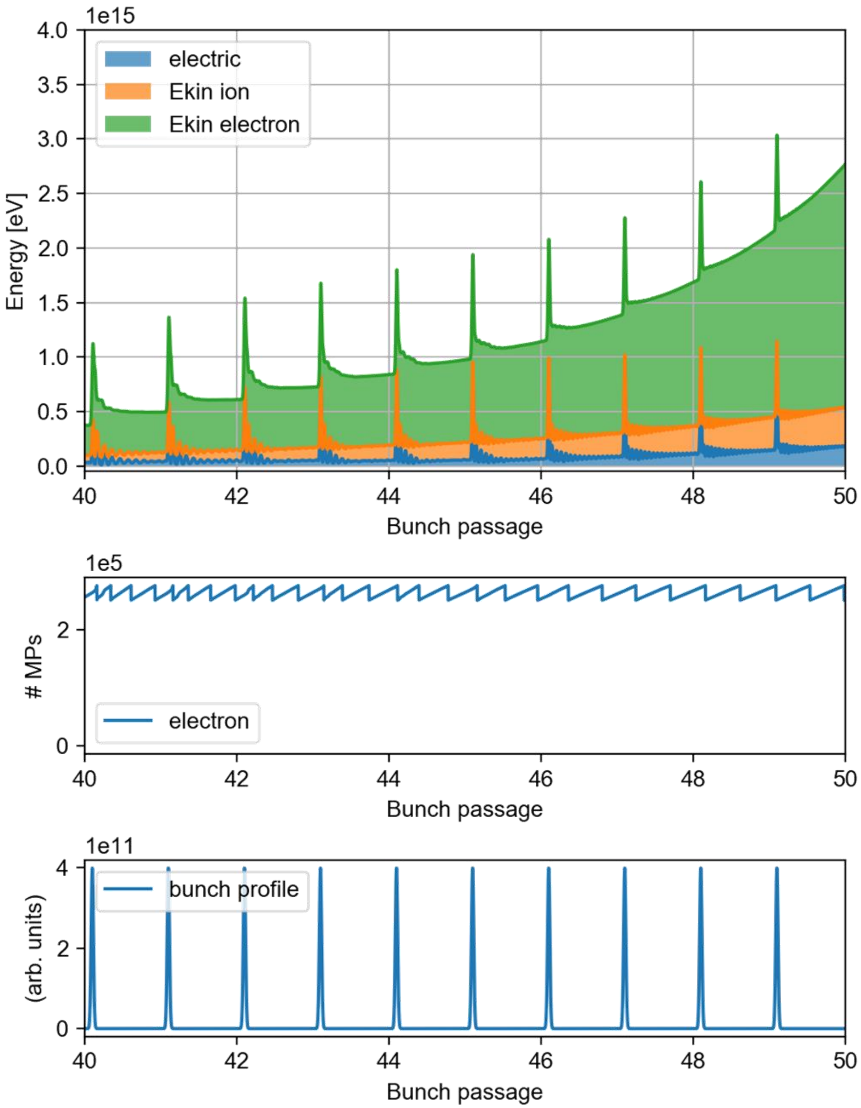
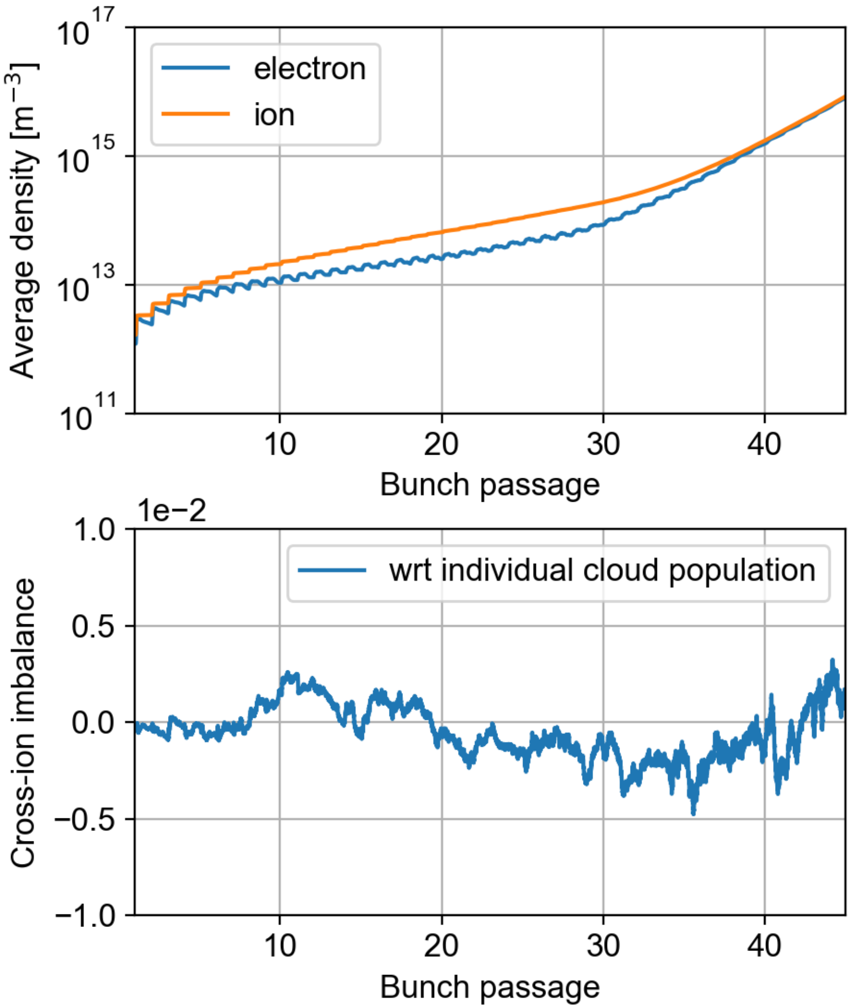
With smaller regenerations, no evident correlation occurs. The unphysical evolution is slightly damped and postponed, but not mitigated



Cross-ionization imbalance

Another source of artificial imbalance is introduced in the system by the cross-ionization

- In principle the same amount of electrons and ions should be generated
- Since a probabilistic algorithm is used, which depends on the macro-particle weight of each cloud, small fluctuations in the numbers occur
- The introduced imbalance is small compared to the number of particles in the clouds



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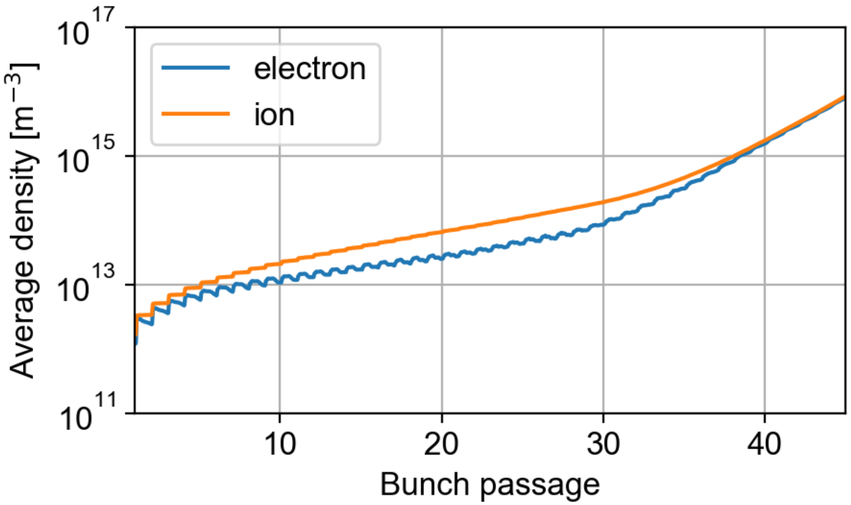
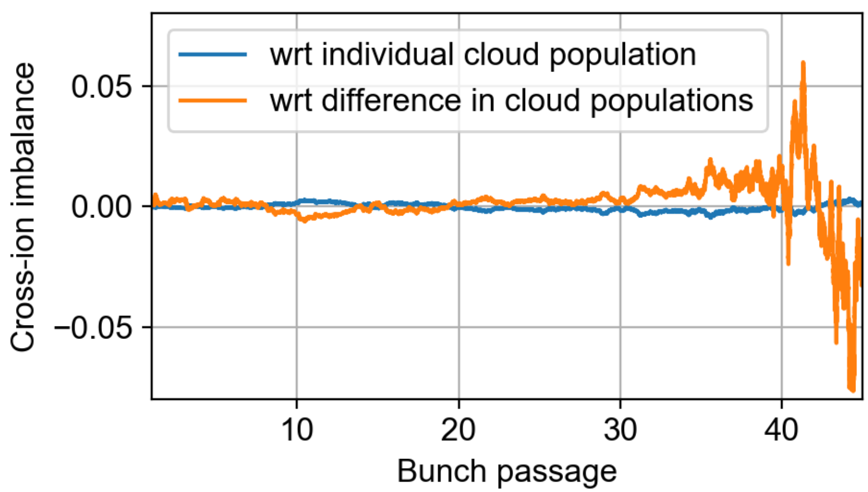
- Since a probabilistic algorithm is used, which depends on the macro-particle weight of each cloud, small fluctuations in the numbers occur
- The introduced imbalance is small compared to the number of particles in the clouds
- But not so small with respect to the net charge (electrons - ions), which essentially determines the fields





An option was implemented to enforce the algorithm to use the same probabilities for all clouds, removing the imbalance, but this didn't cure the simulation

Noise reduction

To decrease numerical noise, the number of macro-particles needs to be increased

- A clean e-cloud build-up simulation typically requires around 250 000 macro-particles
- For these studies the number was pushed up to 8 million per cloud

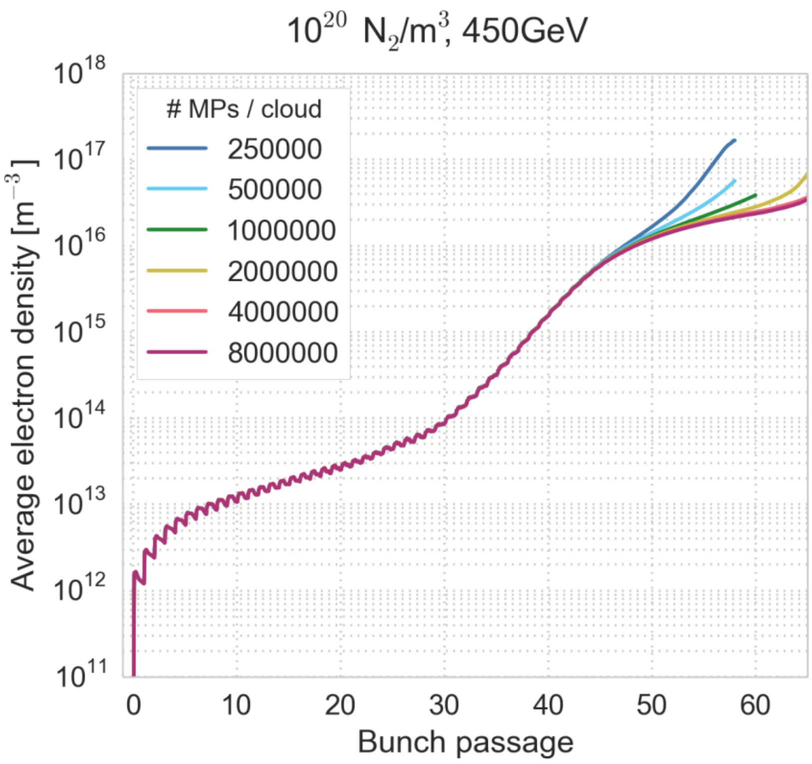
In order to keep the computational time within reasonable limits a parallelization scheme had to be introduced in the build-up simulation (not available up to now)

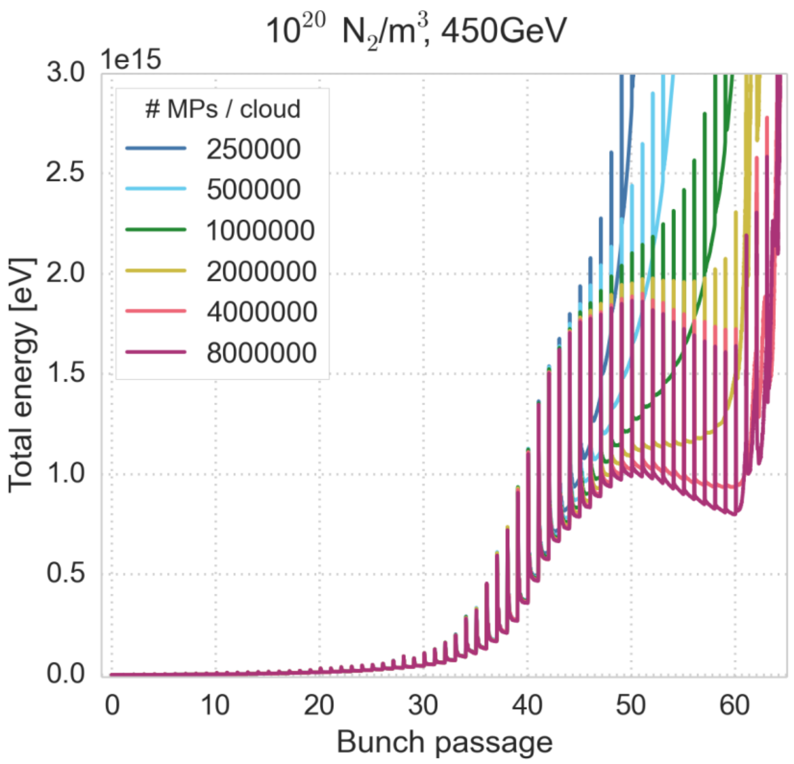
- The parallelization is done on the particle-by-particle operation and is effective only for a very large number of particles

Macro-particle number scan

We scan the number of macro-particles per cloud

- The numerical breakdown can be pushed to later in the bunch train with increasing macro-particle numbers
- Before the breakdown, the simulation is converged wrt the macro-particle number





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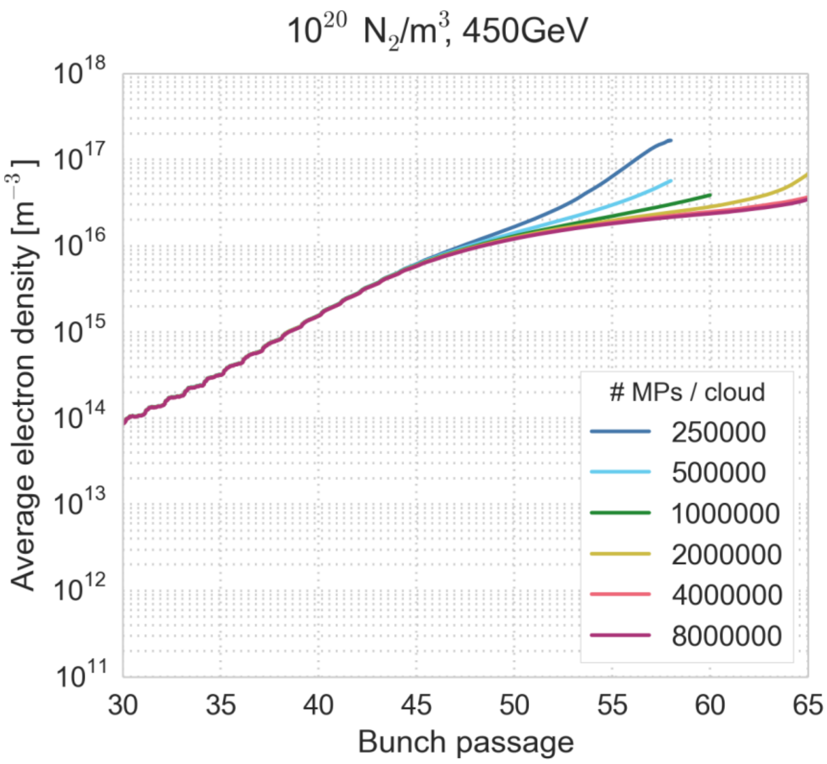

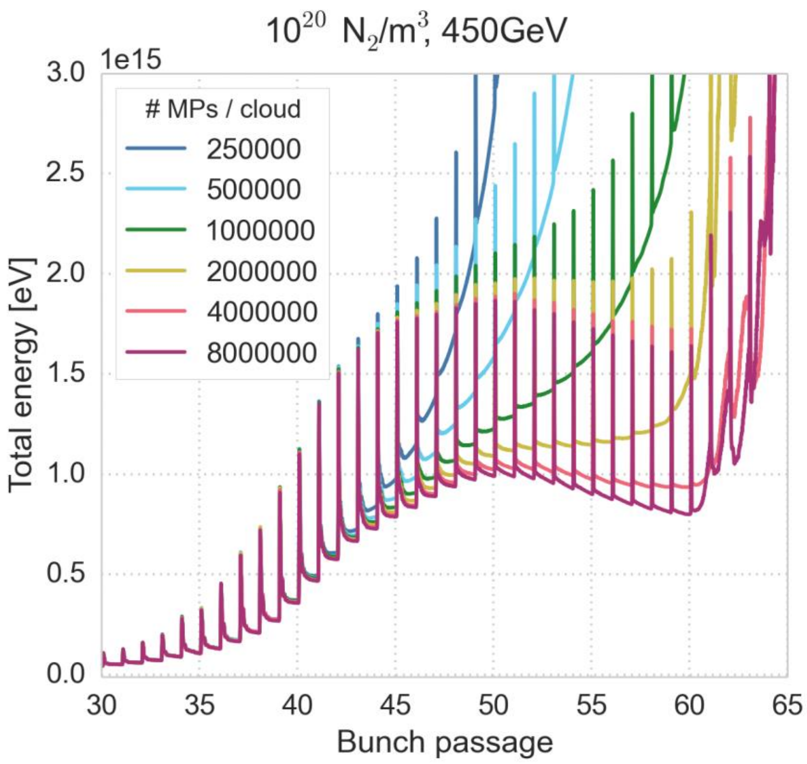

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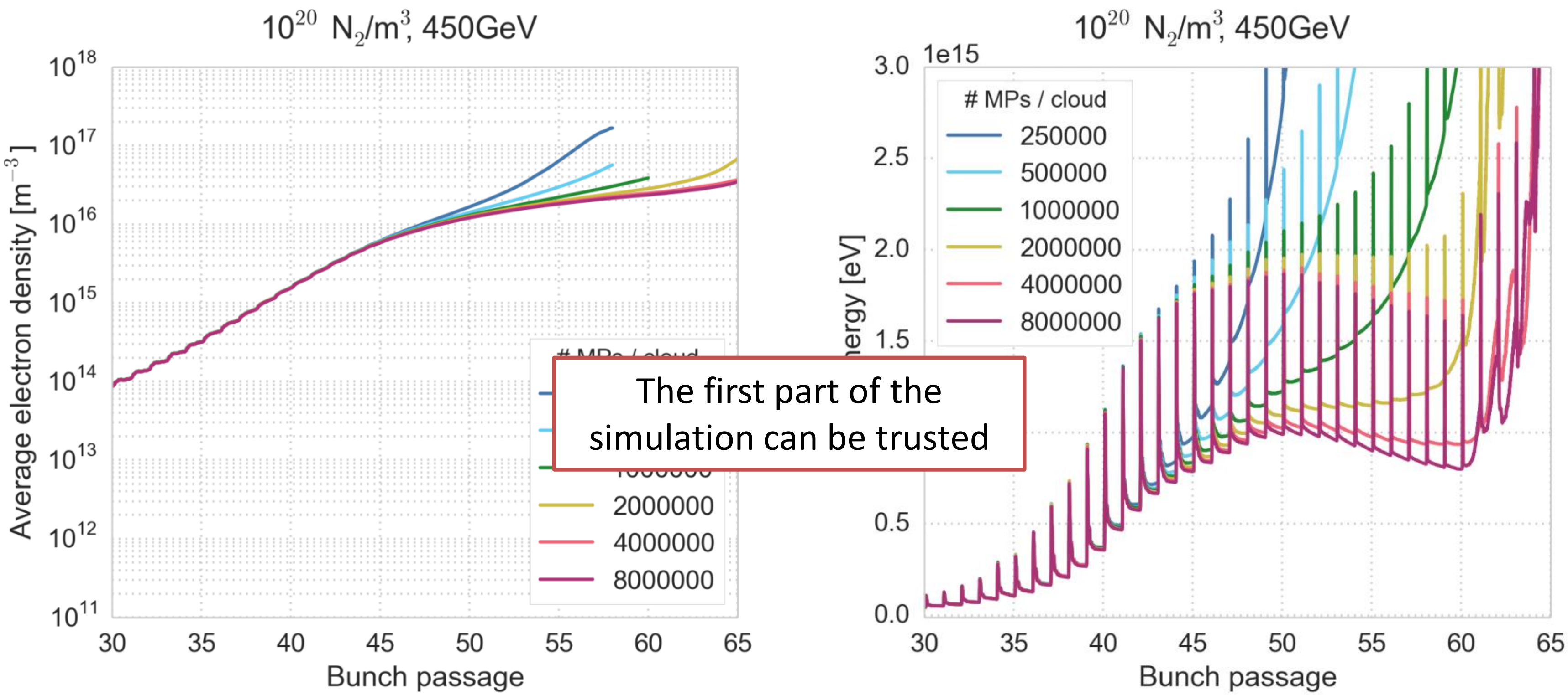
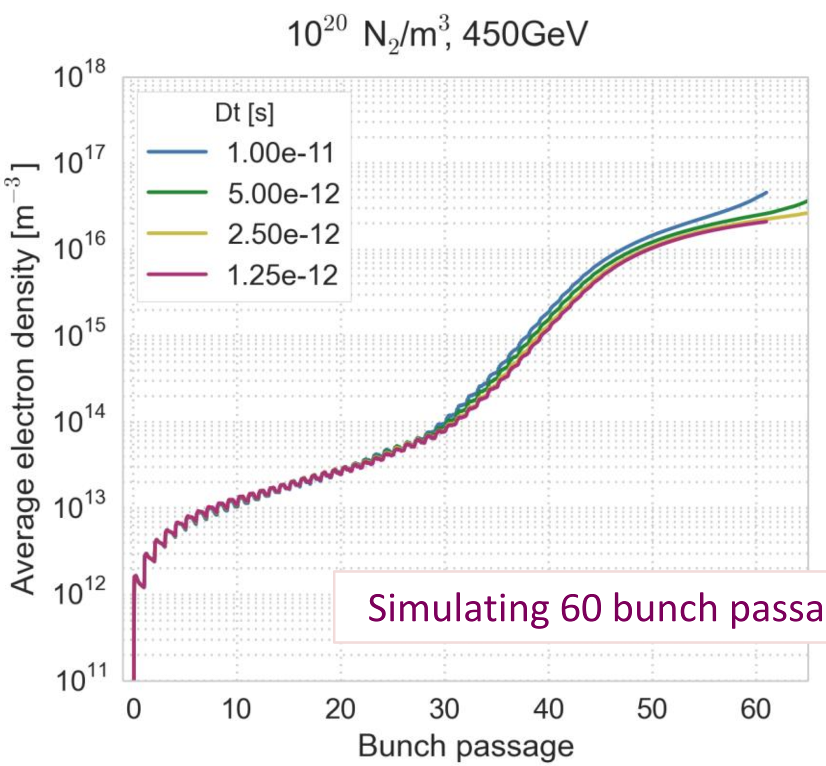
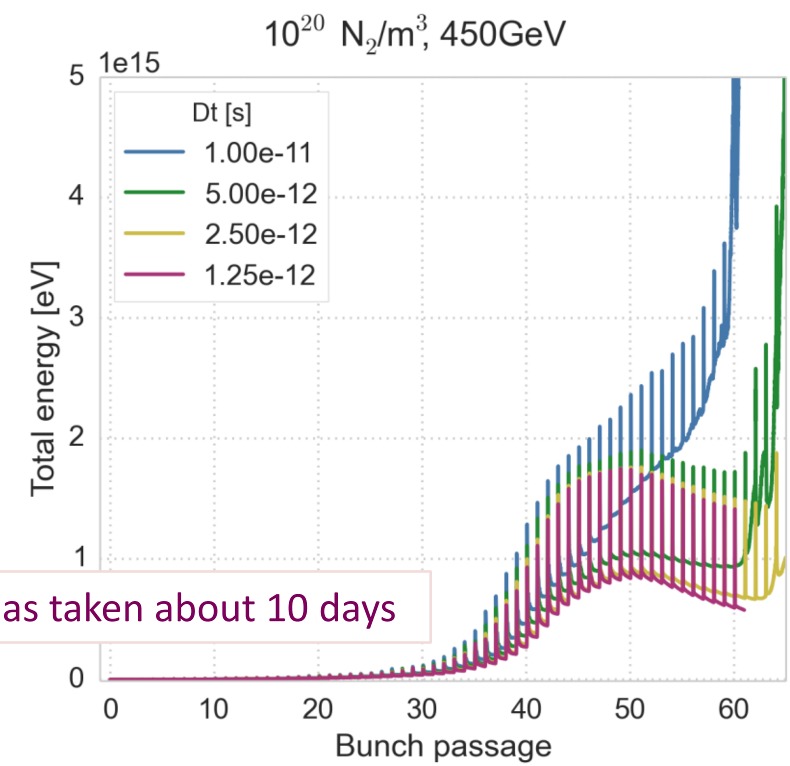


Time step scan

We scan the time step, keeping a large number of macro-particles

- Here electric fields are updated at each step (in typical build-up simulations updates can be done every 5-10 time steps)
- The numerical breakdown can be pushed to later in the bunch train also with decreasing simulation time step
- Before the breakdown convergence wrt the time step is decent





Simulating 60 bunch passages has taken about 10 days

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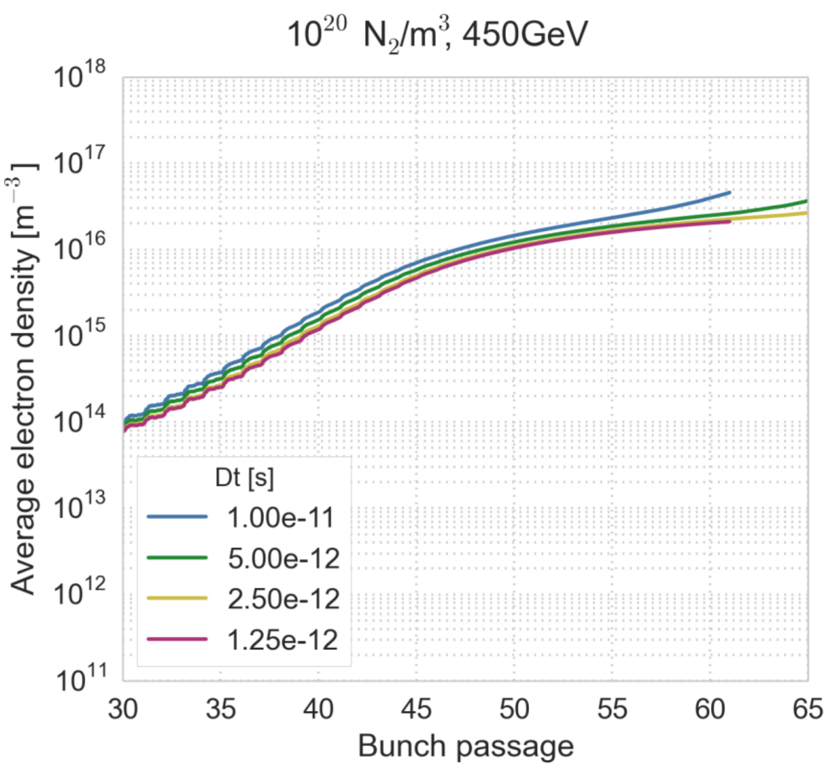
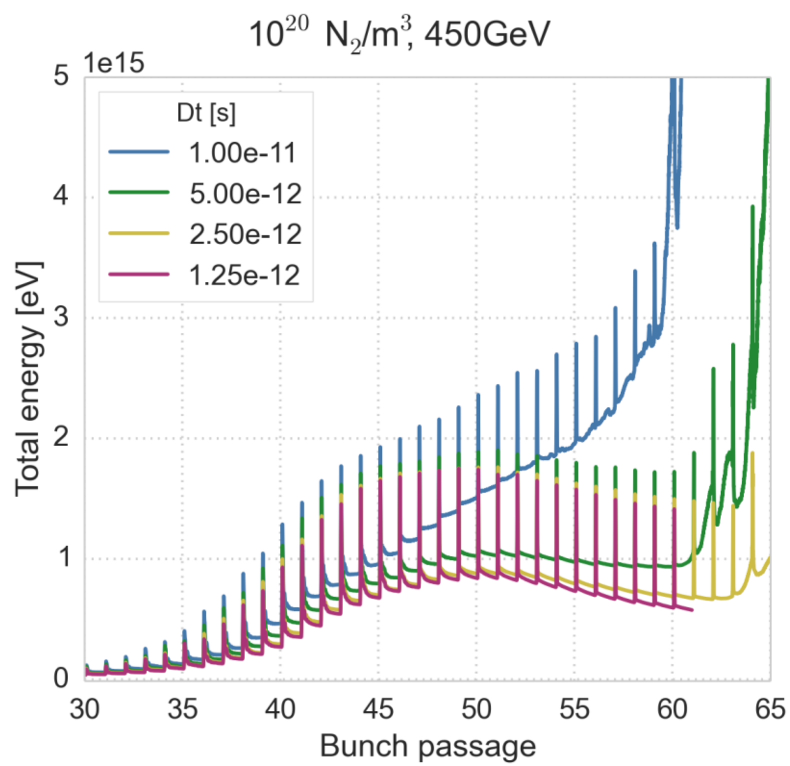
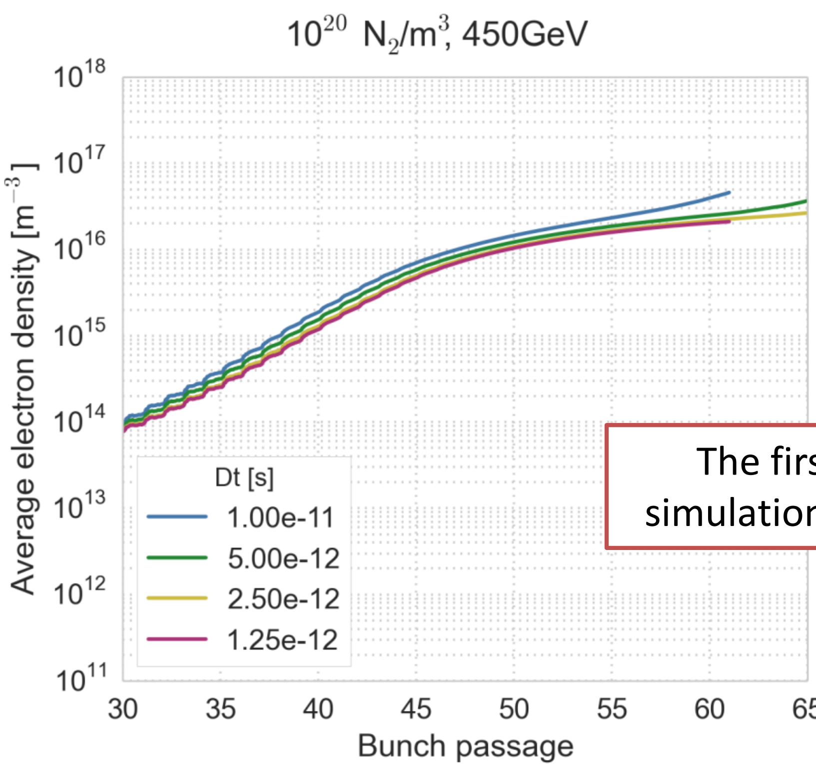


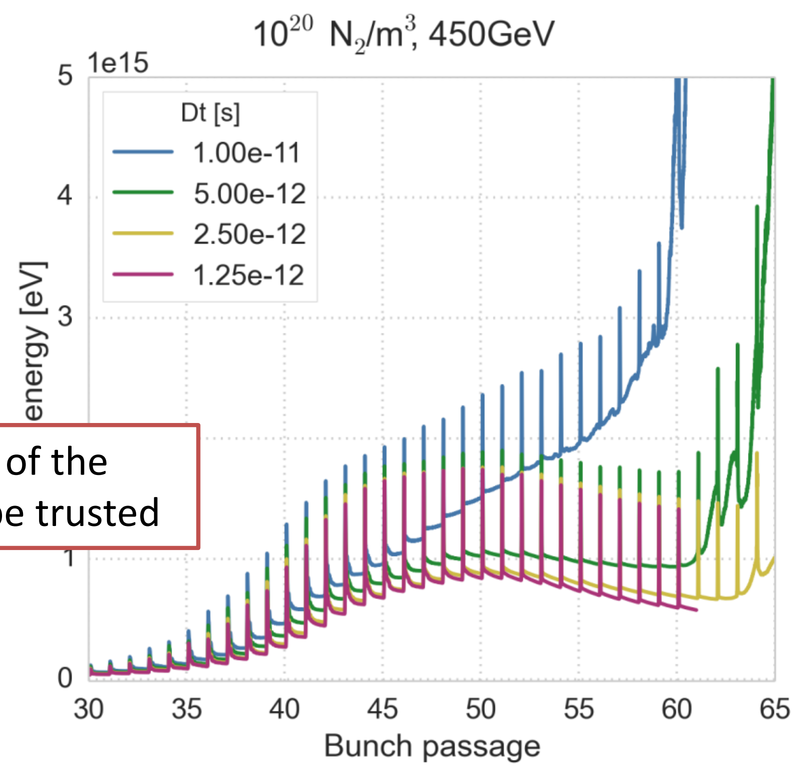


Time step scan

We scan the time step, keeping a large number of macro-particles

- Here electric fields are updated at each step (in typical build-up simulations updates can be done every 5-10 time steps)
- The numerical breakdown can be pushed to later in the bunch train also with decreasing simulation time step
- Before the breakdown convergence wrt the time step is decent



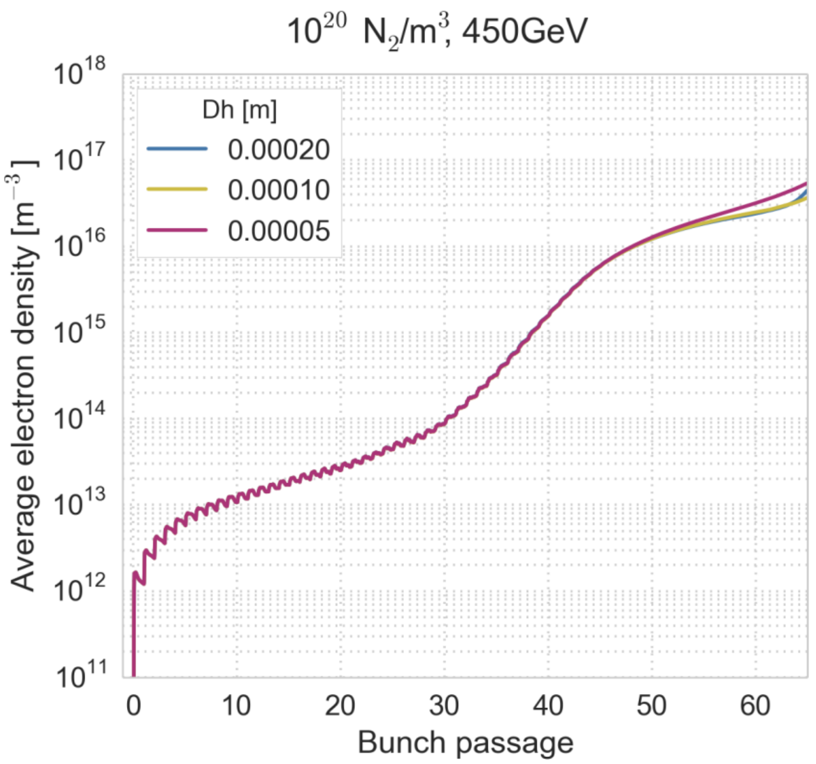


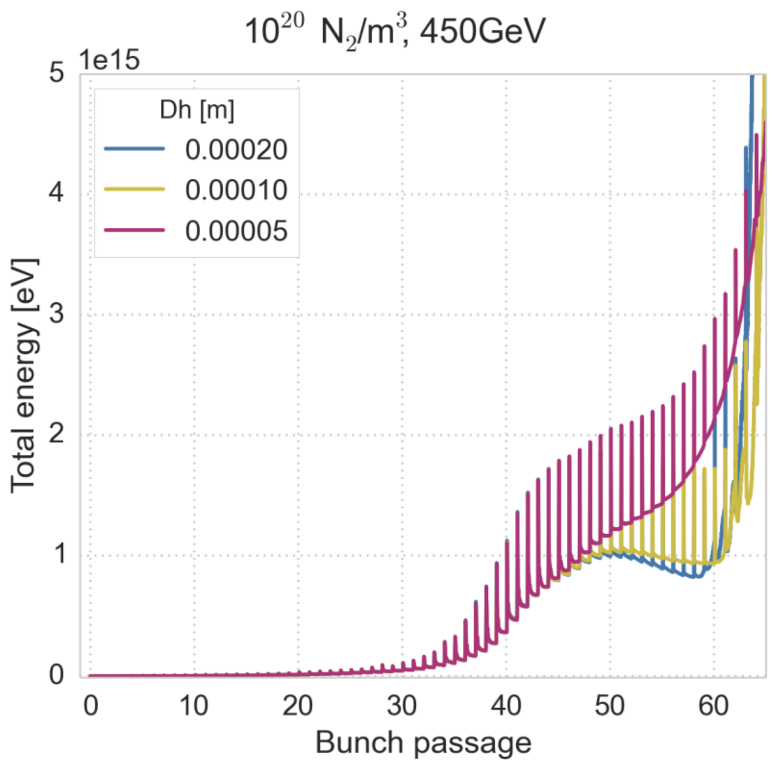
The first part of the simulation can be trusted

Grid cell size scan

We keep a large number of macro-particles and a time step of 5 ps and scan the grid size

- The dependence on the grid cell size is non-linear
  - For a fixed number of macro-particles, going to a smaller cell size makes the fields more noisy and the numerical instability set in earlier, but a larger cell size is also prone to numerical instability
- Before the breakdown, the simulation is converged also wrt to the grid cell size





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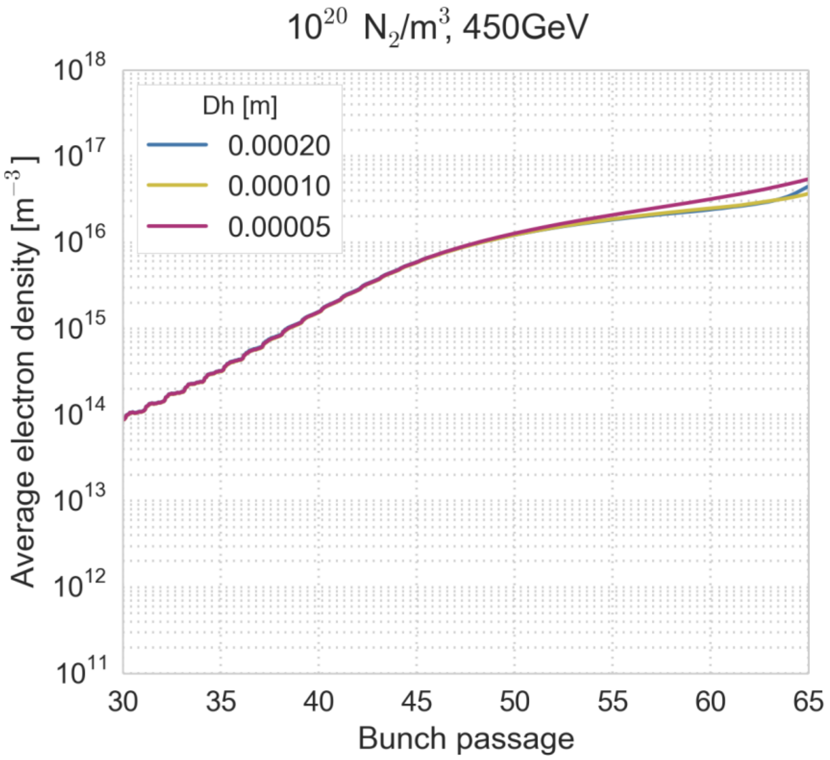

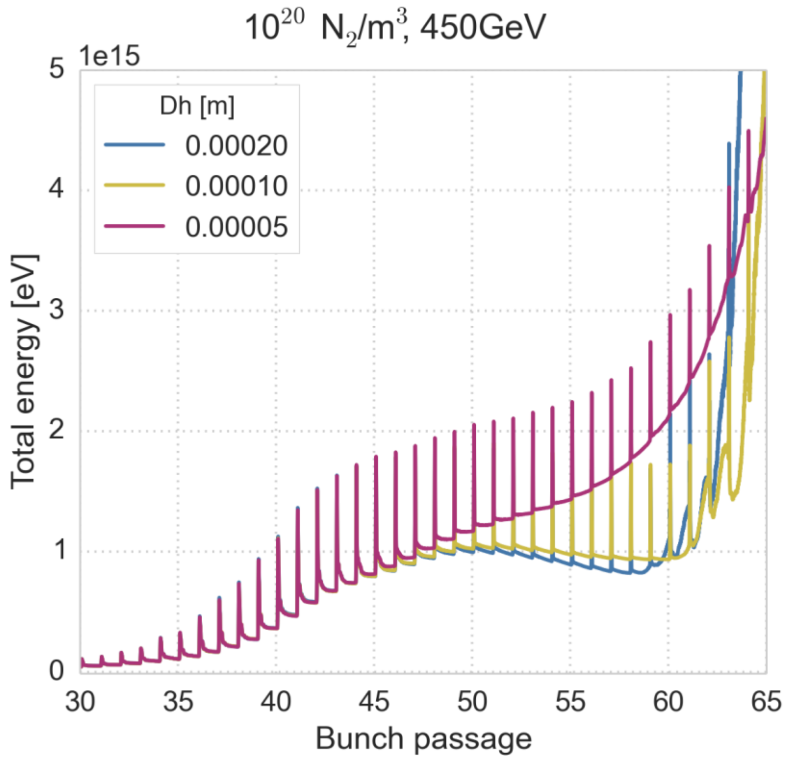

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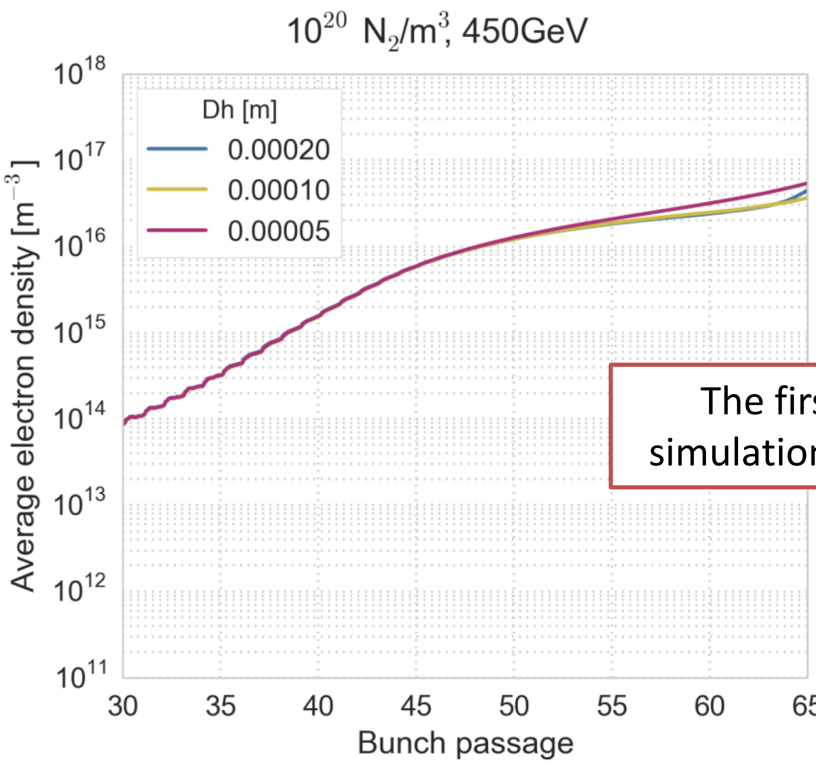
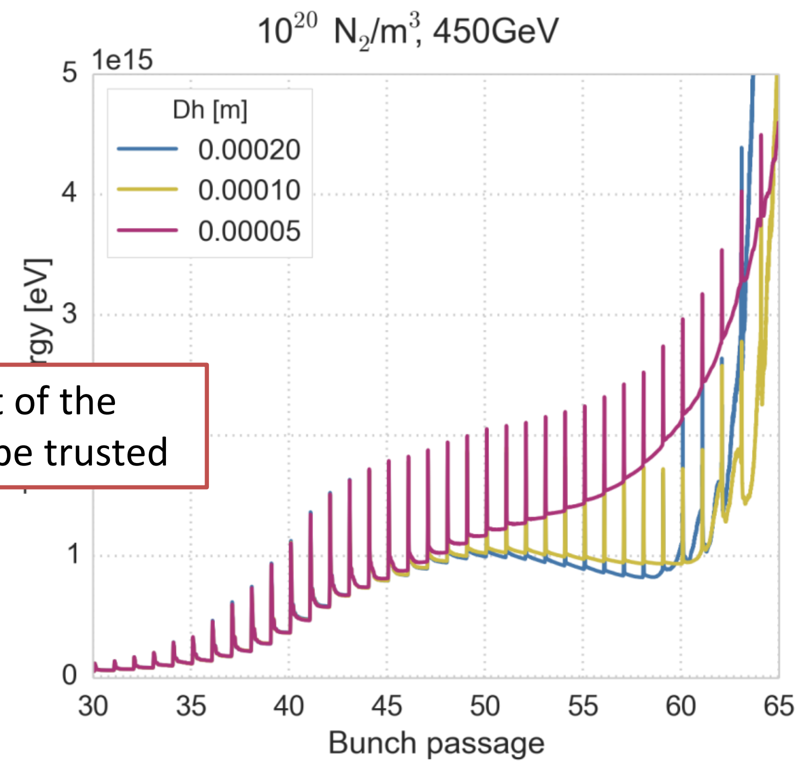
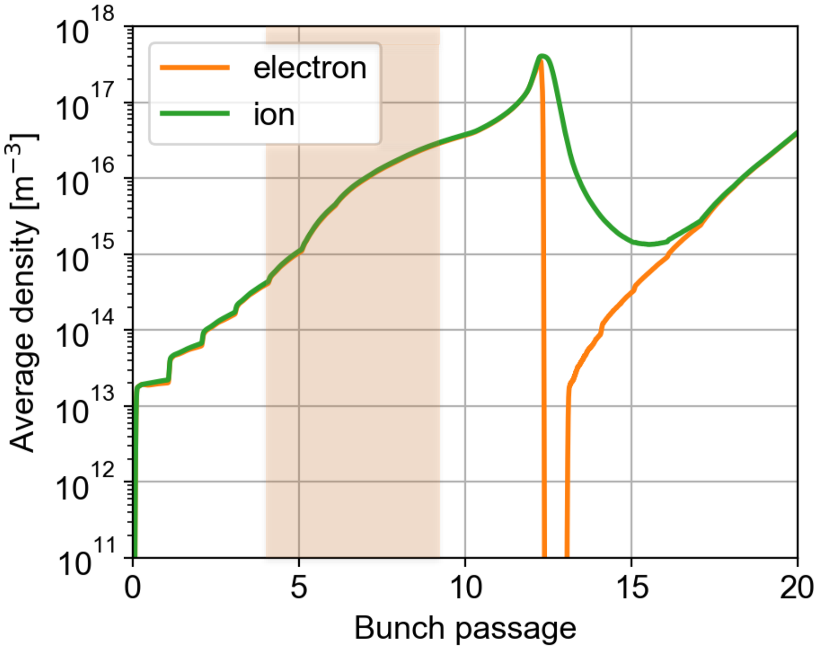


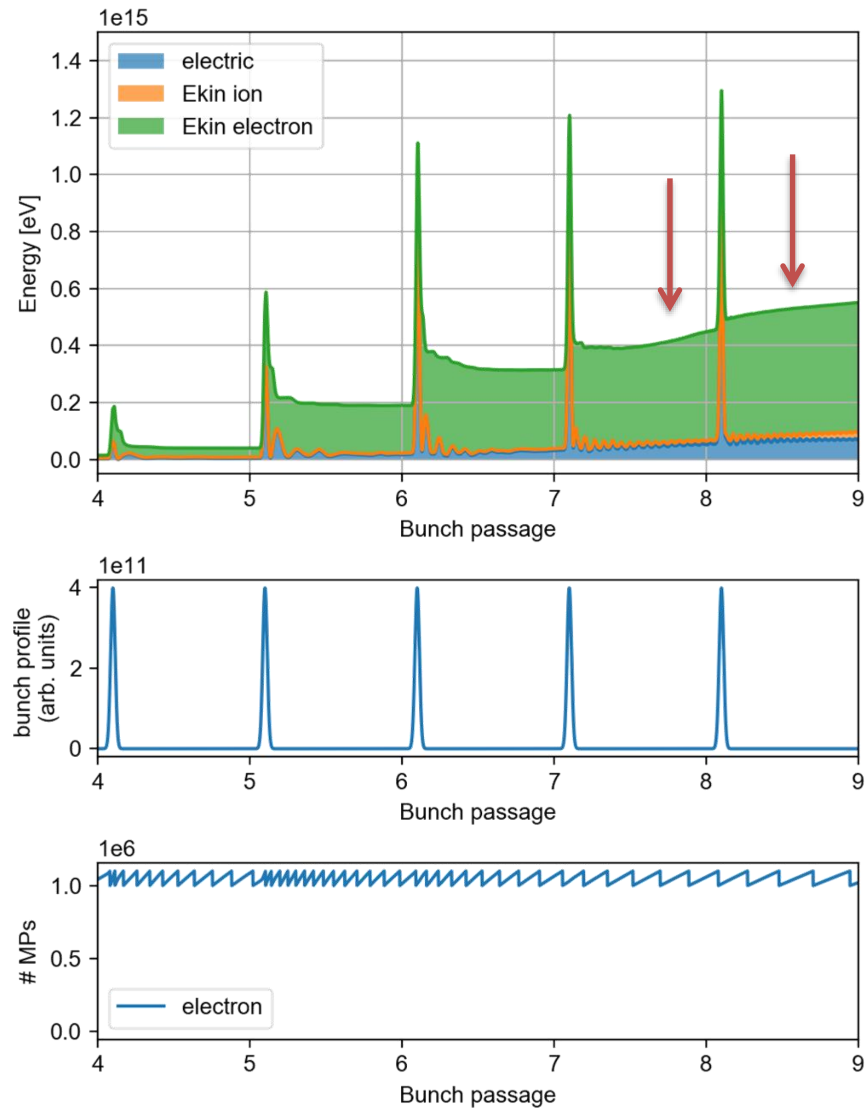


The first part of the simulation can be trusted

Higher gas densities

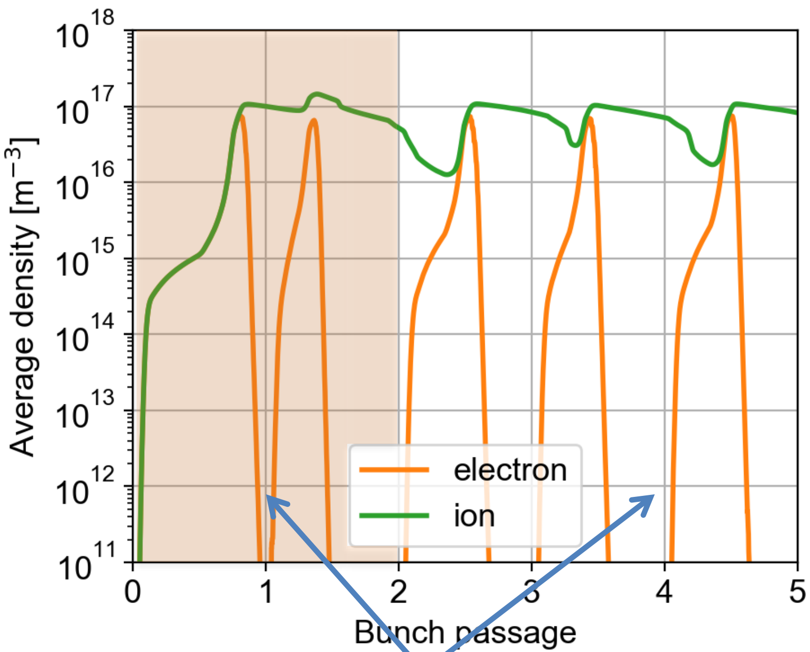
Increasing the gas density by a factor of 10 to 10^{21} m^{-3}, the numerical breakdown occurs already at the beginning of the simulation



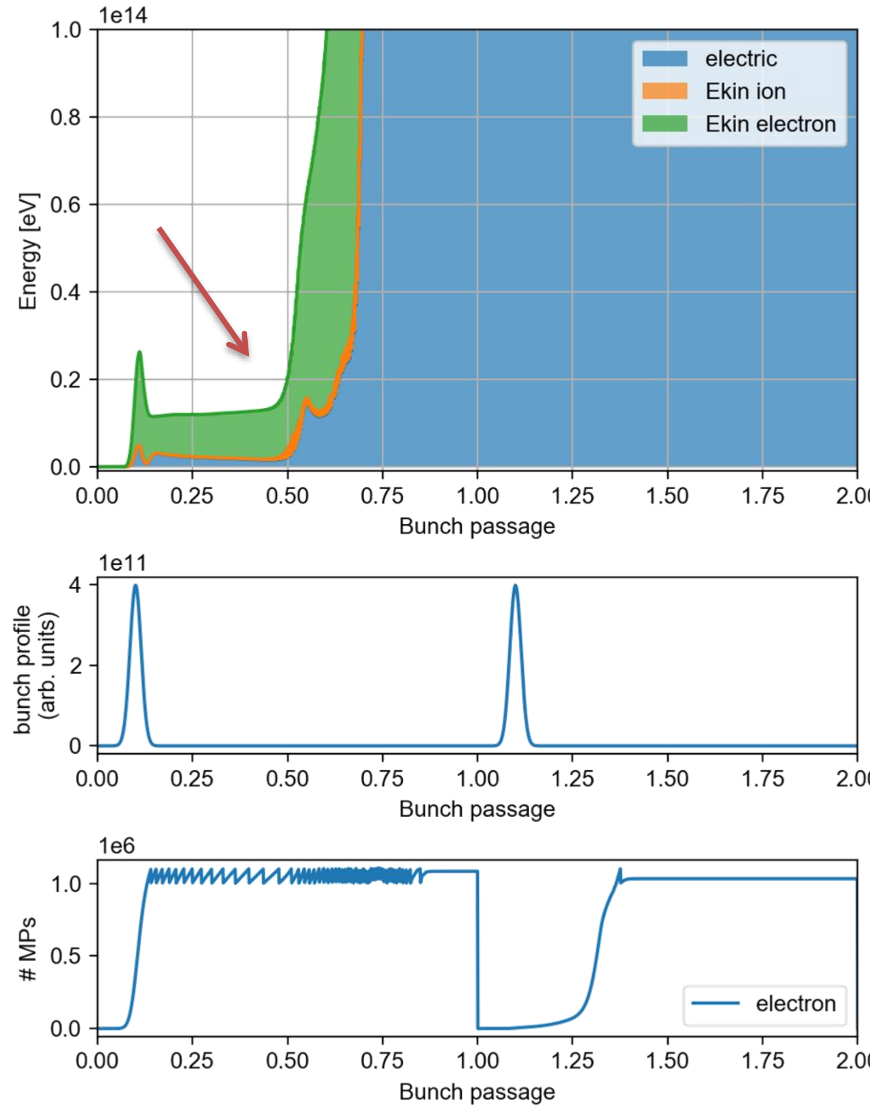


Higher gas densities

Increasing the gas density by another factor of 10 to 10^{22} m^{-3}, the numerical breakdown occurs during the first bunch passage



Sudden drops of the electron density occur when the simulation is already compromised



Conclusions

We have identified the limit of our simulation model due to numerical heating

- For a gas density of 10^{20} m^{-3} the simulation is converged for about 50 bunch passages
- We cannot currently simulate gas densities above 10^{20} m^{-3}, as the breakdown occurs after only a few bunch passages

The simulation is converged wrt numerical parameters until the runaway starts

- This indicates that this model is sufficient to cover the evolution until that point
- To improve the simulation further neutrals would need to be tracked and collisions modelled → full-scale plasma simulations (would require huge development efforts)

Conclusions

Based on what we have so far, we can conclude that

- Cross-ionization increases the electron and ion densities up to at least 10^{17} m^{-3}
- Based on previous instability simulation studies (with a different initial state without cross-ionization, but similar average electron and ion densities), this could be compatible with the observed instabilities
- Refined instability simulations could be done starting from the results of build-up simulations with cross-ionization with a reasonable effort (a few more weeks of work)

Further ingredients

- Neutrals
- Collisions respecting momentum conservation laws
  - Impact ionization (could we take into account the ionization energy)
    $e^- + N_2$
  - Coulomb collisions between charged particles (compensate for underestimation within individual cells in PIC)
    $e^- + e^-$, $N_2^+ + N_2^+$, $e^- + N_2^+$
  - Elastic collisions
    $e^- + N_2$, $N_2 + N_2$
  - Charge exchange and momentum transfer
    $N_2^+ + N_2$

Time steps

A PyECLOUD build-up simulation has 2 different time steps

- The main time step that determines the propagation of the beam etc typically set to Δt ≈ 25 ps
- A time step for updating the electric fields from the charge distribution typically set to Δt_sc = 5 * Δt ≈ 125 ps

In the cross-ionization simulations the time steps were set much smaller than for a standard build-up simulation

- Δt = 5 ps
- Δt_sc = 5 * Δt = 25 ps

Still, it was found that even more frequent updates of the electric fields are required

- A convergence scan wrt the time step with Δt_sc = Δt was performed