PyECLOUD

Reference

Manual

Giovanni Iadarola

Eleonora Belli, Lotta Mether,
Annalisa Romano, Giovanni Rumolo
CERN - Geneva, Switzerland

PyECLOUD reference manual

This document describes the main input and output parameters for the PyECLOUD code for the simulation of the electron cloud buildup in particle accelerators.

1   Input files

1.1   Simulation parameters

Other input filenames. The following variables specify the names of the other three input files which define the physical model of the simulation.	
machine_param_file	Name of the machine parameter file.
secondary_emission_parameters_file	Name of the secondary emission configuration file.
beam_parameters_file	Name of the beam parameter file (in case of a multiple beam simulation this is the master beam).

Secondary beams The code can simulate the EC buildup in the presence of more than one circulating beam. For this purpose a list of secondary beam files (one for each beam) has to be provided. In the presence of secondary beams, the master beam determines the length of the simulation, the energy used for the calculation of the bending field, and the bunch spacing used for regeneration and saving purposes.	
secondary_beam_file_list	(optional – default = []) List of names of secondary beam parameter files.

Log and progress files	
logfile_path	Path of a text file that reports some synthetic information on the ongoing simulation (Passage number, number of MPs and number of electrons in the chamber).
progress_path	Path of a text file that reports the simulation progress in percent.

Time sampling The simulated time interval is defined by the length of the beam profile (number of bunch passages) specified in the beam description.	
Dt	[s] Simulation time step. This input is not considered if beam profile is imported from file.

t_end	[s] Extra time interval after the specified beam profile. Only coasting beam present in this interval. The value of this variable can also be negative in order to stop the simulation before the end of the specified profile.

Negligible beam linear density	
lam_th	[beam part/m] When the linear density of the beam is below this value, primary electrons are not generated and beam forces on the electrons are neglected.

MP management settings	
N_mp_max	Size of the arrays allocated to store the MP sizes, positions and velocities. MP regeneration settings must be set such that this number of MPs is never exceeded.
N_mp_regen	MP regeneration threshold. When the total number of MPs exceeds N_mp_regen a regeneration of the set of MPs is applied and a new Nref is chosen in order to get a target number of MPs. The check is performed at each t=n*b_spac with n an integer.
N_mp_regen_low	Lower MP regeneration threshold. When the total number of MPs becomes smaller than N_mp_regen_low a regeneration of the set of MPs is applied and a new Nref is chosen in order to get a target number of MPs. The check is performed at each t=n*b_spac with n an integer.
t_ON_regen_low	For t< t_ON_regen_low the lower MP regeneration check is not performed.
N_mp_after_regen	Target number of MPs obtained after regeneration.
fact_split	MP split factor; when secondary emission occurs, if the size of the emitted charge is smaller than fact_split*Nref, the impacting MP is simply rescaled according to the SEY. Otherwise new MPs are generated in order to keep the MP size as close as possible to Nref.
fact_clean	MP clean factor. MPs smaller than fact_split*Nref are deleted from the MP set. This test is performed at each t=n*b_spac with n an integer.

nel_mp_ref_0	[e-/m] Initial MP size.
Nx_regen, Ny_regen, Nvx_regen, Nvy_regen, Nvz_regen	Number of mesh points in each dimension for the generation of the uniform grid for the 5-D phase space used for the MP regeneration.
regen_hist_cut	Defines a threshold value for the phase space density, below which no electrons are generated.
N_mp_soft_regen	(optional: by default soft regen is not applied, the presence of these inputs enables it) Soft regeneration threshold. The check is performed at each t=n*b_spac with n an integer. N_mp_soft_regen should be smaller than N_mp_regen.
N_mp_after_soft_regen	(optional: by default soft regen is not applied, the presence of these inputs enables it) Target number of MPs obtained after a soft regeneration.

Space charge parameters	
Dt_sc	[s] Time step for the update of the electron space charge field map.
Dh_sc	[m] Grid size for the space charge PIC solver.
t_sc_ON	[s] Electron space charge forces are neglected for t<t_sc_ON – normally t_sc_ON=0.

Multigrid parameters To be used with PyPICmode = 'ShortleyWeller_WithTelescopicGrids'	
f_telescope	Magnification factor between grids (it must be always $0 < f < 1$).
target_grid	Target grid parameters. It is a dictionary containing: 'x_min_target', 'x_max_target', 'y_min_target', 'y_max_target' and 'Dh_target'.
N_nodes_discard	Number of nodes at the edge of the internal grids which are discarded in the field interpolation (going to coarser grid).
N_min_Dh_main	Minimum size of the first internal grid in the Δh of the main grid.

Saving settings	
Dx_hist	[m] Defines the binning for the saving of the horizontal histograms.

r_center	[m] Radius of a circle around the (0, 0) point (center of the chamber) for the calculation of the local central density.
Dt_En_hist	[s] Time step used to store the energy spectrum of the electrons impacting on the chamber.
Nbin_En_hist	Number of bins used for the energy histogram.
En_hist_max	[eV] Maximum energy in energy spectrum. Larger energies are attributed to the last bin of the histogram.
flag_cos_angle_hist	Save the cosine of the incident angle of impacting electrons. (optional – default True)
cos_angle_width	Width of the histogram bins. (optional – default 0.05)
flag_movie	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Saves files with the electron density distribution at each space charge evaluation.
flag_sc_movie	(optional– default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Saves files with the electron space charge electric field distribution at each space charge evaluation.
save_mp_state_time_file	(optional – default: no MP state is saved) [s] List of instants at which MP positions and velocities are saved on file. The list can also be provided as a .mat file.
flag_detailed_MP_info	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Enables save of MP number at each time step.
flag_hist_impact_seg	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) If the chamber is a polygon, enables saving the number of electrons which impacts onto each segment of polygon.
flag_verbose_file, **flag_verbose_stdout**	(optional – default=False) True/False toggles to save detailed information of pathological impacts in output file and stdout respectively.
dec_fac_secbeam_prof	(optional – default=1) Decimation factor to decrease the number of points of the longitudinal beam profile of secondary beams.

el_density_probes		(optional – default: no probes) (List of Python dictionaries) Probes for electron density evaluation. For each of them it is necessary to indicate the position (x,y) and radius of the circle (r_obs).
save_simulation_state_time_file		(optional – default: no simulation state is saved) [s] List of instants at which the full simulation state is saved on file (pickle files). The list can also be provided as a .mat file.
x_min_hist_det, **y_min_hist_det,** **Dx_hist_det**	**x_max_hist_det,** **y_max_hist_det,**	(optional – default: no detailed histogram is saved) [m] Defines a region of the chamber where a detailed horizontal distribution histogram is saved (_det stands for detailed).

1.2 Machine Parameters

Chamber profile description	
chamb_type	(optional – default = 'ellip') Possible settings: 1. chamb_type = 'ellip' for elliptical chamber profile. 2. chamb_type = 'rect' for rectangular chamber profile. 3. chamb_type = 'polyg' or 'polyg_cython' for polygonal chamber profile.
When chamb_type = 'ellip' or 'rect' the following input variables must be provided:	
x_aper, y_aper	Horizontal and vertical semi-apertures of the transverse chamber profile.
When chamb_type = 'polyg' the following input variable must be provided:	
filename_chamb	Name of file containing horizontal and vertical vertexes of the chamber profile.

Tracking and magnetic field (the tracking algorithm has to be chosen according to the magnetic field conditions).	
track_method	(optional – default = 'StrongBdip') Possible settings: 1. track_method = 'StrongBdip' for vertical uniform magnetic field. 2. track_method = 'StrongBgen' for a generic transverse magnetic field map. 3. track_method = 'BorisMultipole' for arbitrary multipoles with Boris electron tracker.
When track_method = 'StrongBdip' the following input variables must be provided:	
B	[T] Value of the vertical uniform magnetic field. If B=-1 the magnetic field is calculated from the total length of the bending magnets (bm_totlen) and from the beam energy.
bm_totlen	[m] Total length of dipoles inside the accelerator (it must be provided when B=-1).
When track_method = 'StrongBgen' the following input variables must be provided:	

B_map_file	Name of a .mat file containing the transverse field map. The case of a quadrupole magnet with unit gradient is embedded in the code and can be used setting: B_map_file = 'analytic_quadrupole_unit_grad'.
fact_Bmap	(optional – default = 1.) Scaling factor applied to the magnetic field map.
B0x, B0y	(optional – default = 0) [T] Uniform transverse magnetic field added to the map.
B_zero_thrld	[T] Value below which the local magnetic field is approximated with 0.

When track_method = 'BorisMultipole', N_sub_steps and B_multip must be provided, while B_skew is optional:

N_sub_steps	Number of tracking sub-steps per time step.
B_multip	Magnetic momenta. Higher order multipoles and skew magnets are supported, as well as compound magnets. The formalism in PyE-CLOUD follows this formula: $B_y + iB_x = \sum_{n=0}^{\infty} \frac{1}{n!} \left(b_n + ib'_n \right) \left(x + iy \right)^n$ B_multip specifies $b_n = \frac{\partial^n B_y}{\partial x^n}$. For example: to simulate a dipole with B=8.3 T set B_multip = [8.3]; to simulate a sextupole with 100 T/m^2 set B_multip = [0., 0., 100.].
B_skew	The skew parameters can be included through B_skew. For a skew quadrupole with a gradient of 12 T/m, set B_multip to [0.,0.] and B_skew to [0.,12.]. B_skew specifies $b'_n = \frac{\partial^n B_x}{\partial x^n}$ and defaults to *None*.

Optics parameters (can be provided also in the beam parameter file(s) independently for the different beams) — not needed if transverse beam size is directly defined in the beam parameter files.	
betafx, betafy	[m] Horizontal and vertical beta functions at the simulation section.
Dx, Dy	(optional – default = 0) [m] Horizontal and vertical dispersion functions at the simulation section.

Residual gas ionization parameters (if the following input parameters are omitted primary electron generation by residual gas ionization is not enabled).	

gas_ion_flag	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Enables primary electron generation by residual gas ionization.
P_nTorr	[nTorr] Pressure in the vacuum chamber.
sigma_ion_MBarn	[MBarn] Ionization cross section of the residual gas.
Temp_K [K]	Temperature of the residual gas.
unif_frac	Fraction of primary electrons uniformly distributed inside the chamber. The remaining part is generated according to the transverse distribution of the beam.
E_init_ion	[eV] Initial energy of the generated electrons.

Photoemission parameters (if the following input parameters are omitted primary electron generation by photoemission is not enabled).	
photoem_flag	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Enables primary electron generation by photoemission.
inv_CDF_refl_photoem_file	Name of a .mat file providing the inverse of the Cumulative Distribution Function (CDF) for the angular distribution of the reflected photons. If inv_CDF_refl_photoem_file = 'unif_no_file' the reflected photons have uniform angular distribution and no file needs to be provided.
k_pe_st	[m^{-1}] Number of photoelectrons to be generated per proton and per unit length.
refl_frac	Fraction of photoelectrons generated by reflected photons.
alimit	[rad] Extent (1σ) of the Gaussian angular distribution of photoelectrons generated by non-reflected photons.

energy_distribution	Can be one of:
	'gaussian': $p(E) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(\frac{(E-\mu)^2}{2\sigma^2}\right)$ 'log-normal': $p(E) = \frac{1}{E\sigma\sqrt{2\pi}}e^{\frac{(\log(E)-\mu)^2}{2\sigma^2}}$ 'rect': $p(E)$ uniform for $\mu - \sigma < E < \mu + \sigma$ 'mono': $E = \mu$ 'lorentz': $p(E) = \frac{1}{\pi}\frac{\sigma}{\sigma^2+(E-\mu)^2}$ The Lorentz and normal distributions are cut at 0 to prevent negative energies of photoemitted electrons.
e_pe_sigma	[eV] σ from above.
e_pe_max	[eV] μ from above.
x0_refl, y0_refl	[m] Impact of non-reflected photons.
out_radius	[m] Radius of a circle external to the chamber.
phem_resc_fact	Rescaling factor on the position vector of the generated photoelectrons.
photoelectron_angle_distribution	See secondary_angle_distribution in the secondary emission parameters.

Uniform initial distribution Simulation starts with electrons uniformly distributed in the chamber (if the following input parameters are omitted this feature is not enabled).	
init_unif_flag	(optional – default=0) (1 $\Rightarrow$ On, 0 $\Rightarrow$ Off) Enables uniform electron distribution at the beginning of the simulation.
Nel_init_unif	Initial number of electrons.
E_init_unif	[eV] Initial energy of the generated electrons.
x_max_init_unif, x_min_init_unif, y_max_init_unif, y_min_init_unif	[m] Edges of the region where the electrons are generated.

1.3 Beam parameters

Basic definitions	
m0_part	(optional – default=proton mass) [Kg] Mass of beam particles.
energy_eV	[eV] Total energy of the beam particles.
Dp_p	(optional – default=0) Momentum spread (r.m.s.) of the beam. This parameter is not used if the transverse beam size is directly provided (vars. sigmax, sigmay).
nemittx, nemitty	[m] Normalized transverse emittance of the beam. These parameters are not used if the transverse beam size is directly provided (vars. sigmax, sigmay).
x_beam_pos, y_beam_pos	(optional – default=0) [m] Transverse position of the beam within the vacuum chamber.
sigmax, sigmay	(optional – default=-1) [m] Transverse geometrical beam size. If sigmax, sigmay=-1 the beam size is calculated through the energy, the normalized emittance, the dispersion and the momentum spread of the beam.

Transverse electric field of the beam	
beam_field_file	Name of a .mat file containing the map of the transverse beam electric field. If beam_field_file = -1 or beam_field_file = 'computeFD' the beam field map is computed using the embedded Finite Difference (FD) Poisson solver. If beam_field_file='computeBE' the electric field is computed using the Bassetti-Erskine formula and the image terms for the elliptical boundary conditions (this option is available only when the chamber profile is elliptical). If beam_field_file='compute_FDSW_multigrid' the beam field map is computed using the embedded Finite Difference (FD) Poisson solver in the multigrid case.
save_beam_field_file_as	(optional – default: the beam field map is not saved) Name of the file where the employed field map is saved.

When beam_field_file = -1 or beam_field_file = 'computeFD' the following parameter must be provided:

Dh_beam_field	Grid size for the FD solver and for the saved field map.

When beam_field_file = 'computeBE' the following parameters must be provided:	
Nx, Ny	Number of points of the employed field map.
nimag	Number of image terms.

When beam_field_file = 'compute_FDSW_multigrid' the following parameters must be provided:	
Dh_beam_field	Grid size for the FD solver and for the saved field map.
f_telescope_beam	Magnification factor between grids (it must be always $0 < f < 1$)
target_grid_beam	Target grid parameters. It is a dictionary containing: 'x_min_target', 'x_max_target', 'y_min_target', 'y_max_target' and 'Dh_target'.
N_nodes_discard_beam	Number of nodes at the edge of the internal grids which are discarded in the field interpolation (going to coarser grid).
N_min_Dh_main_beam	Minimum size of the first internal grid in the Δh of the main grid.

Beam longitudinal profile	
b_spac	Bunch spacing. It is used to generate the beam profile when it is defined in the form of a bunched beam. It is also the time interval for cleaning and regeneration of the MP set, as well as for saving.
fact_beam	Rescaling factor applied to the beam profile.
coast_dens	[p/m] Coasting beam density added to the beam profile.
flag_bunched_beam	Two possible settings: 1. flag_bunched_beam = 0 the beam profile is loaded from file. 2. flag_bunched_beam = 1 the beam profile is generated from a filling pattern.

When flag_bunched_beam = 1 the following parameters must be provided:	
sigmaz	[m] Bunch length (1σ).
t_offs	[s] Delay in the longitudinal profile (n.b. if t_offs=0 only half of the first bunch is simulated).

filling_pattern_file	Name of a file providing the intensities of the different bunches (zeros for empty slots). The data can be provided also in form of a python list with no need to provide an input file, e.g. filling_pattern_file=4*(72*[1.]+8*[0.]).

When flag_bunched_beam = 0 the following parameter must be provided:

beam_long_prof_file	Name of a .mat file providing the longitudinal beam profile. This file will also define the time step used for the simulation.

1.4 Secondary emission parameters

Choice of the model	
switch_model	(optional – default=0) Different secondary emission models: 1. switch_model = 0 or 'ECLOUD' for the model used in ECLOUD. 2. switch_model = 'ACC_LOW' for a more accurate treatment of low energy impacts. 3. switch_model = 'ECLOUD_nunif' for the model used in ECLOUD, with sey info in the chamber shape file. 4. switch_model = 'cos_low_ene' for cosine low energy dependence. 5. switch_model = 'flat_low_ene' for flat low energy dependence.

Secondary Electron Yield (parametrized as described in G. Iadarola's thesis).	
Emax	Energy corresponding to the maximum SEY.
del_max	Maximum of the SEY curve.
R0	Weight of the reflected electron component.
E_th	Maximum energy for true secondary electrons.
sigmafit	Sigma parameter of the lognormal distribution.
mufit	Mu parameter of the lognormal distribution.

Other parameters	
switch_no_increase_energy	switch_no_increase_energy = 1 checks that the true secondaries do not have more energy than the corresponding impacting electrons. Typically this feature is NOT enabled.
thresh_low_energy	Maximum energy for which the energy check is performed.
scrub_en_th	Minimum energy of scrubbing electrons (for scrubbing current estimations).

secondary_angle_distribution	Can be 'cosine_2D' or 'cosine_3D'. For new electrons, θ describes the angle between the surface normal and their initial velocity vector. $\mathrm{d}n/\mathrm{d}\theta = \cos\theta$ or $\mathrm{d}n/\mathrm{d}\theta = \cos\theta\sin\theta$ in the 2D or 3D cases, respectively. More info here. The more accurate is the 3D cosine distribution which takes into account the surface element $\sin\theta$ in spherical coordinates. Still 'cosine_2D' is kept as default for backwards compatibility.

2 Output

The main PyECLOUD output is in a single .mat file (by default called 'Pyecltest.mat'). It can be opened in python, for example using the myloadmat_to_obj module in the main PyECLOUD folder.

The file contains arrays of different shape. Defining N_steps the number of time steps in the simulation, N_pass the number of bunch passages and N_bins the number of bins in the horizontal plane used to produce histograms, the main output variables have the following shapes:

Variables saved at each time step:

- t(N_steps)

- En_emit_eV_time(N_steps)

- En_imp_eV_time(N_steps)

- En_kin_eV_time(N_steps)

- Nel_emit_time(N_steps)

- Nel_imp_time(N_steps)

- Nel_timep(N_steps)

- cen_density(N_steps)

- lam_t_array(N_steps)

Variables saved at each bunch passage (and related axes):

- t_hist(N_pass)

- xg_hist(N_bins)

- N_mp_corrected_pass(N_pass)

- N_mp_impact_pass(N_pass)

- N_mp_pass(N_pass)

- N_mp_ref_pass(N_pass)

- energ_eV_impact_hist(N_pass, N_bins)

- nel_hist(N_pass, N_bins)

- nel_impact_hist_scrub(N_pass, N_bins)

- nel_impact_hist_tot(N_pass, N_bins)

Example plots, for one of the simulations in the PyECLOUD test suite, are produced by the script:

      doc/example/000_plot_main_output.py

and reported in the following pages (with some description).

Var. name: lam_t_array
Beam density at each time step

1e12

Beam profile [p/m]

Var. name: Nel_timep
Number of electrons in the chamber at each time step

1e9

Number of e^- per unit length [m^{-1}]

Var. name: Nel_imp_time
Number of electrons that impact the walls in each time-st

Var. name: Nel_emit_time
Number of electrons emitted by walls in each time-step
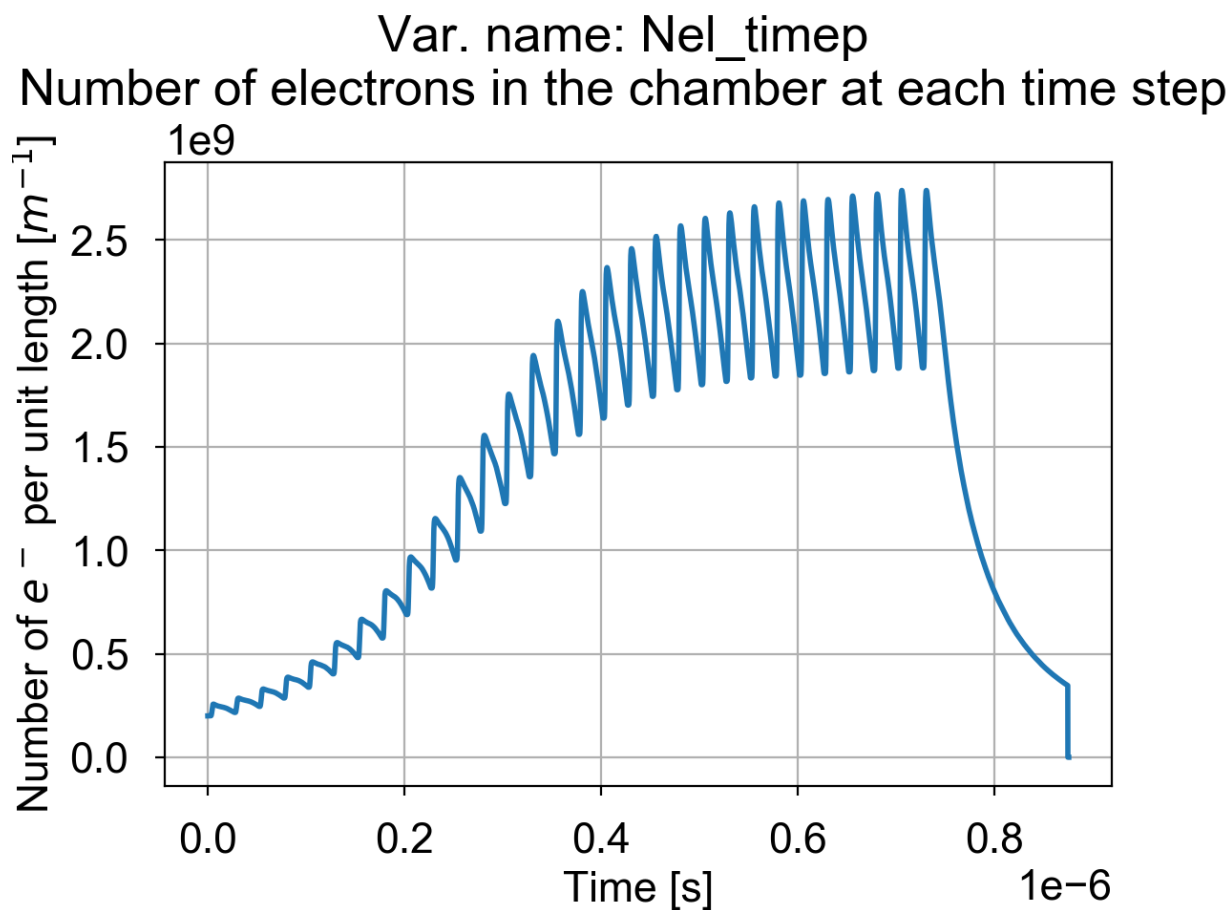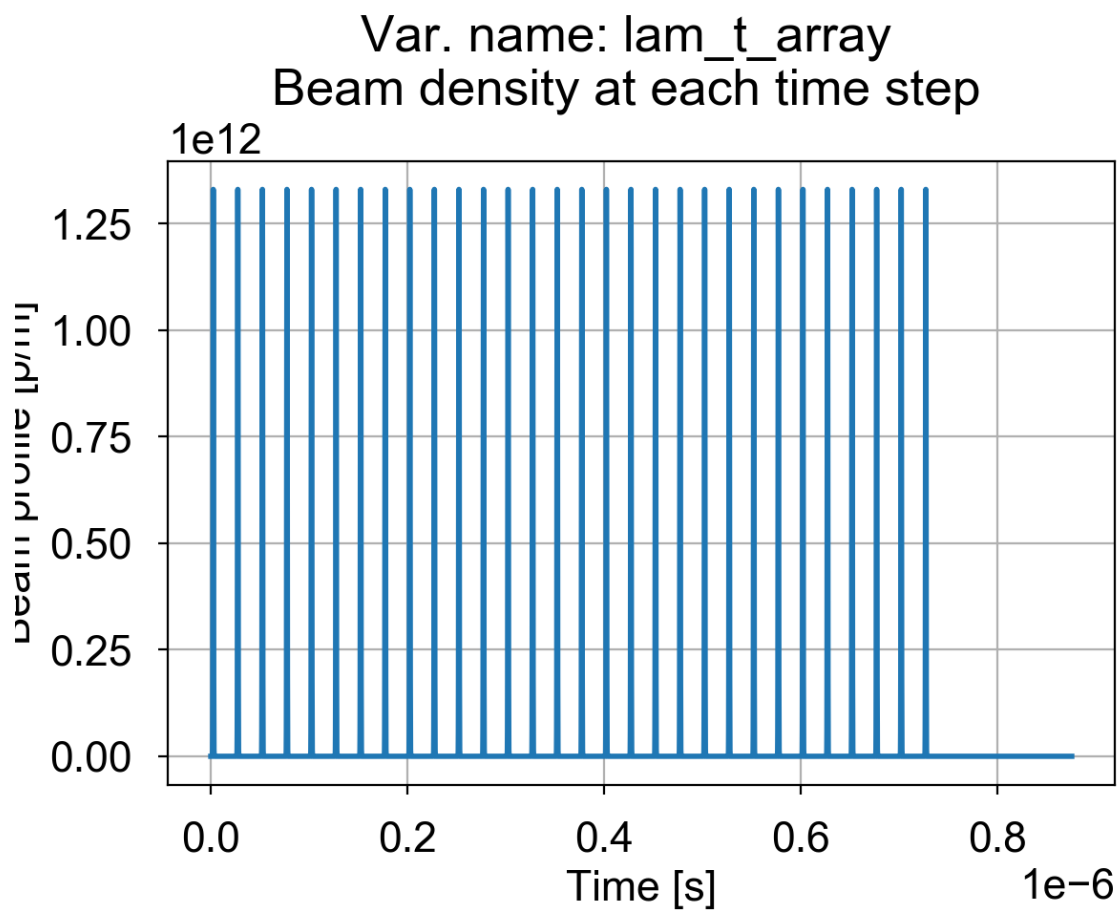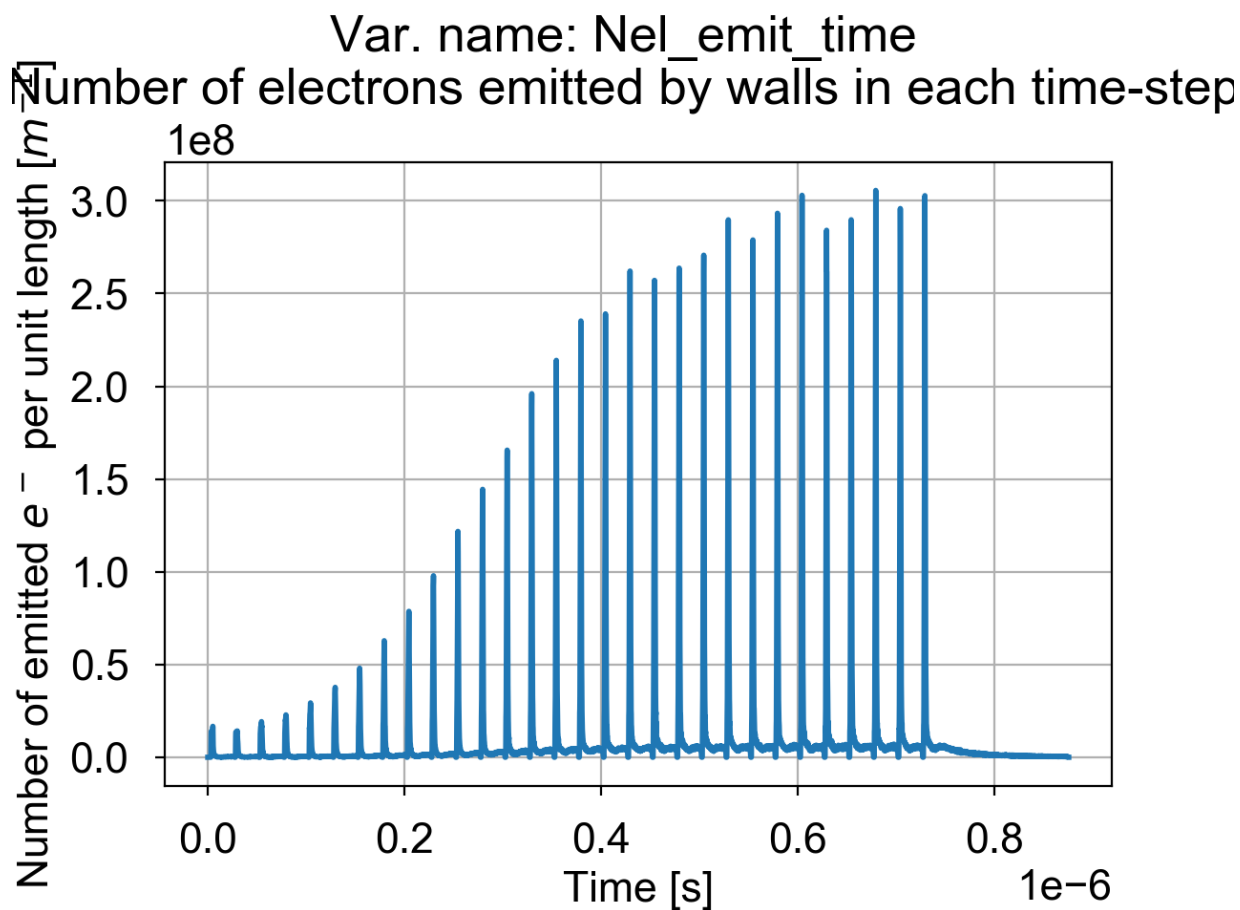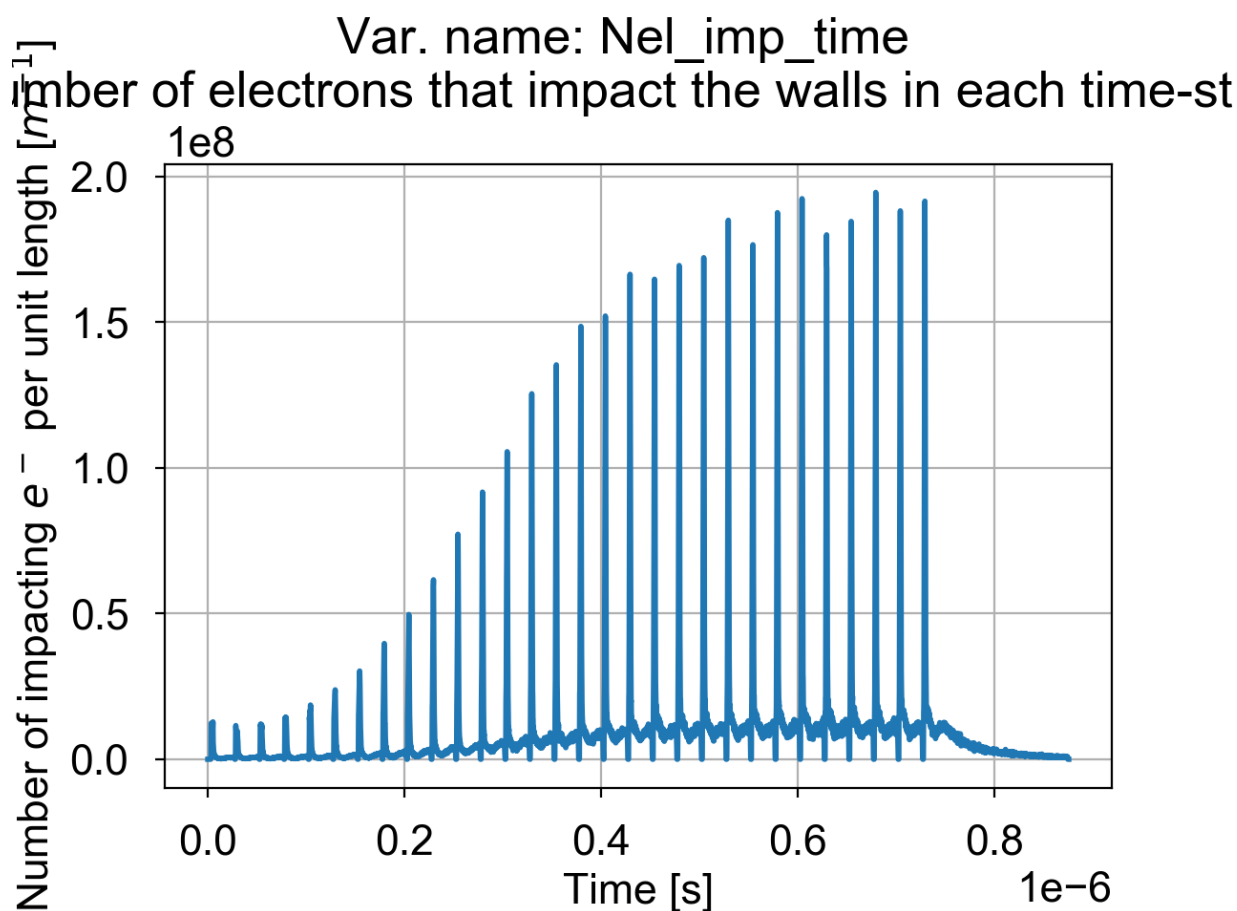
Var. name: En_imp_eV_time
Electron energy deposited on the walls in each time-ste
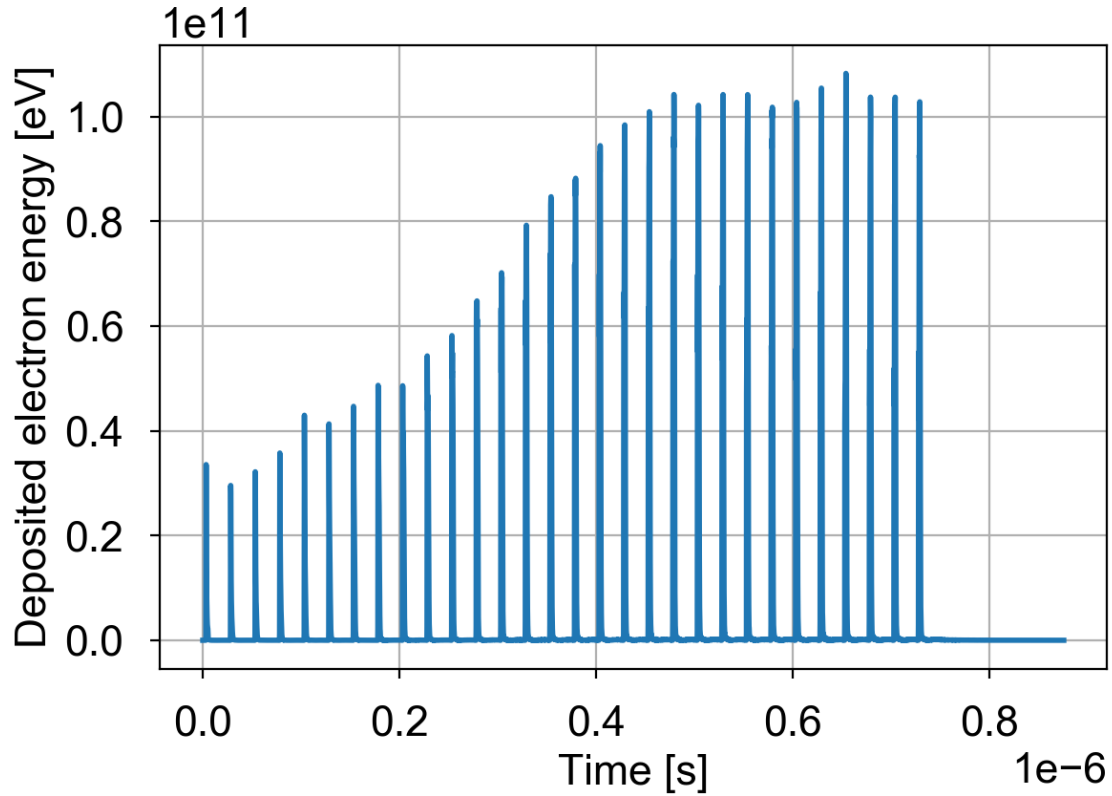
Var. name: En_emit_eV_time
Electron energy emitted by the walls in each time-step
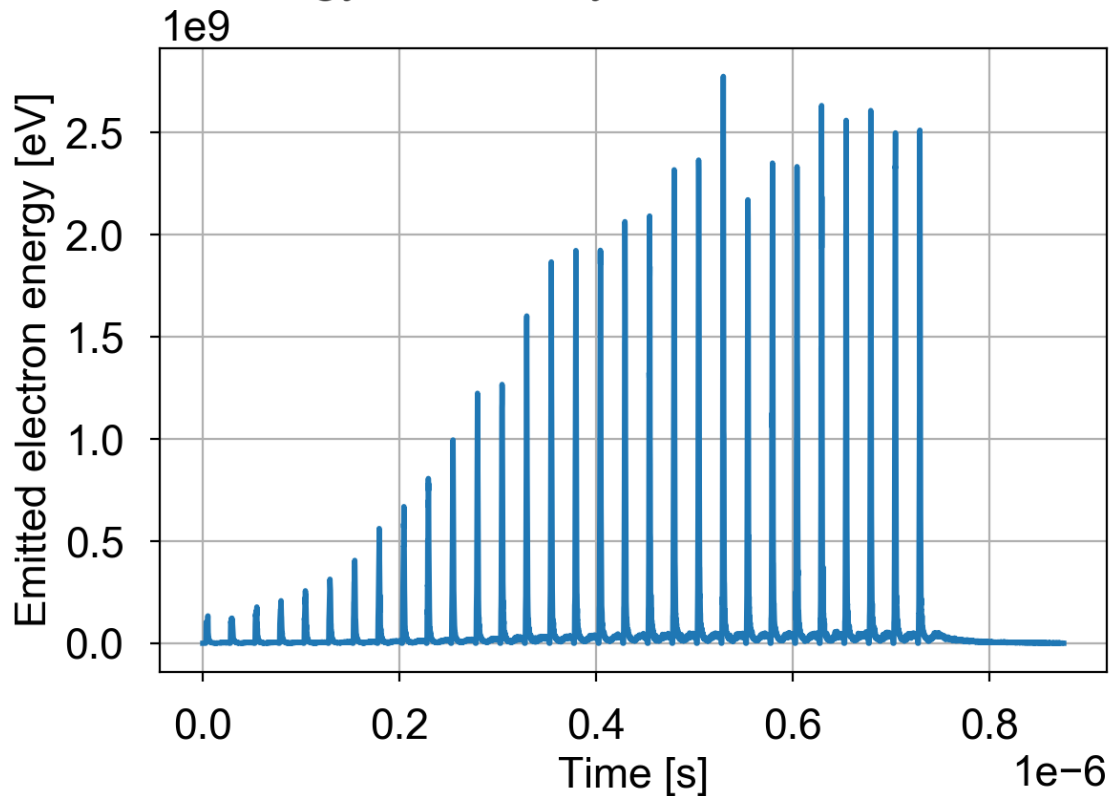
Var. name: En_kin_eV_time
Total kinetic energy of the electrons at each time-step
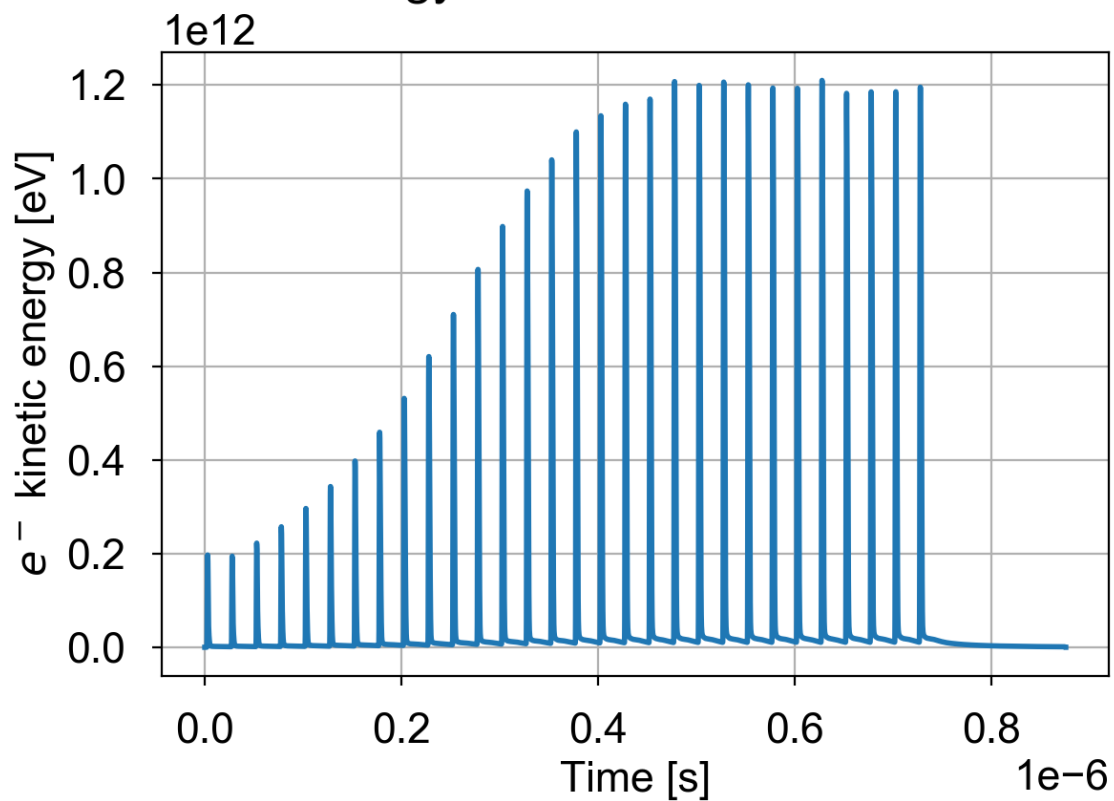
Var. name: cen_density
electron density at the beam position
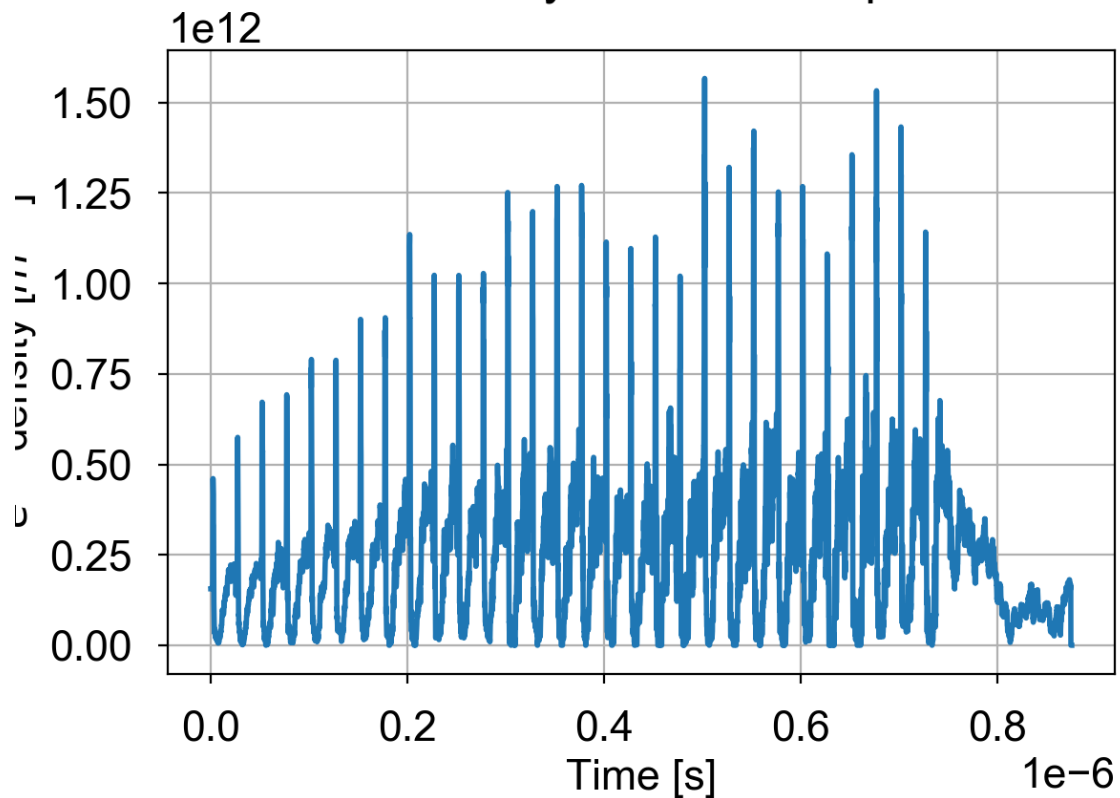
Var. name: N_mp_pass
Number of MP at each passage
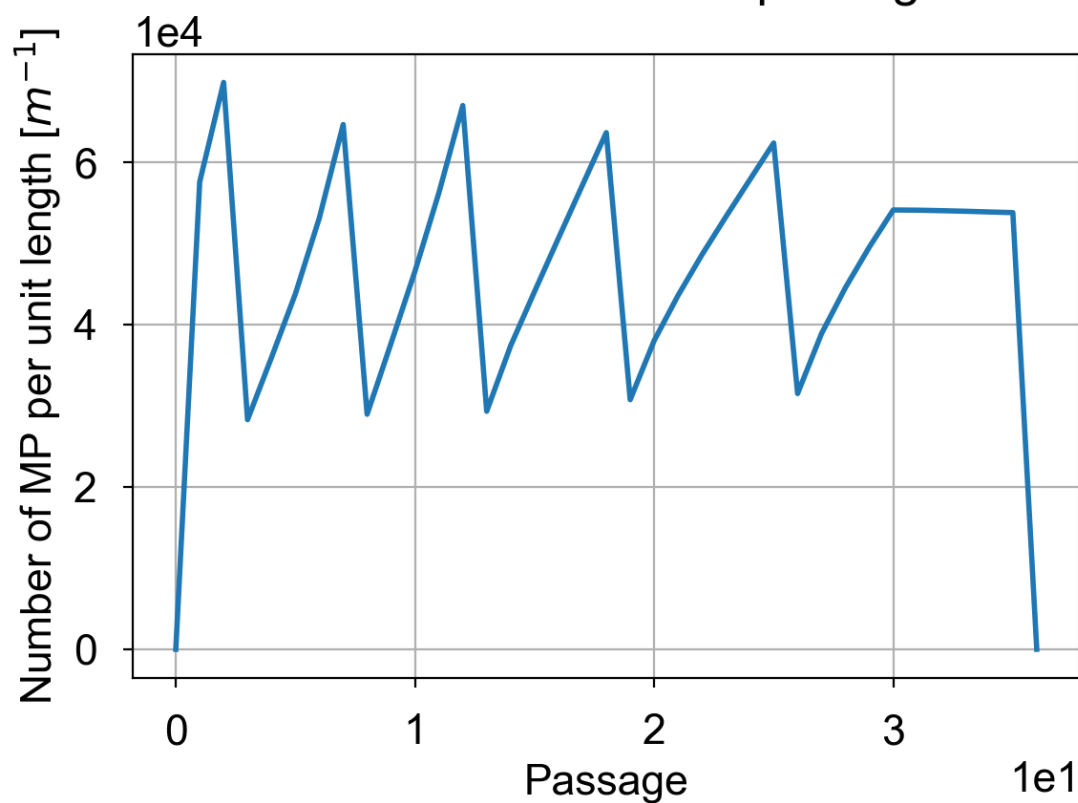
Var. name: N_mp_impact_pass
Number of macroparticles that impact for each passage
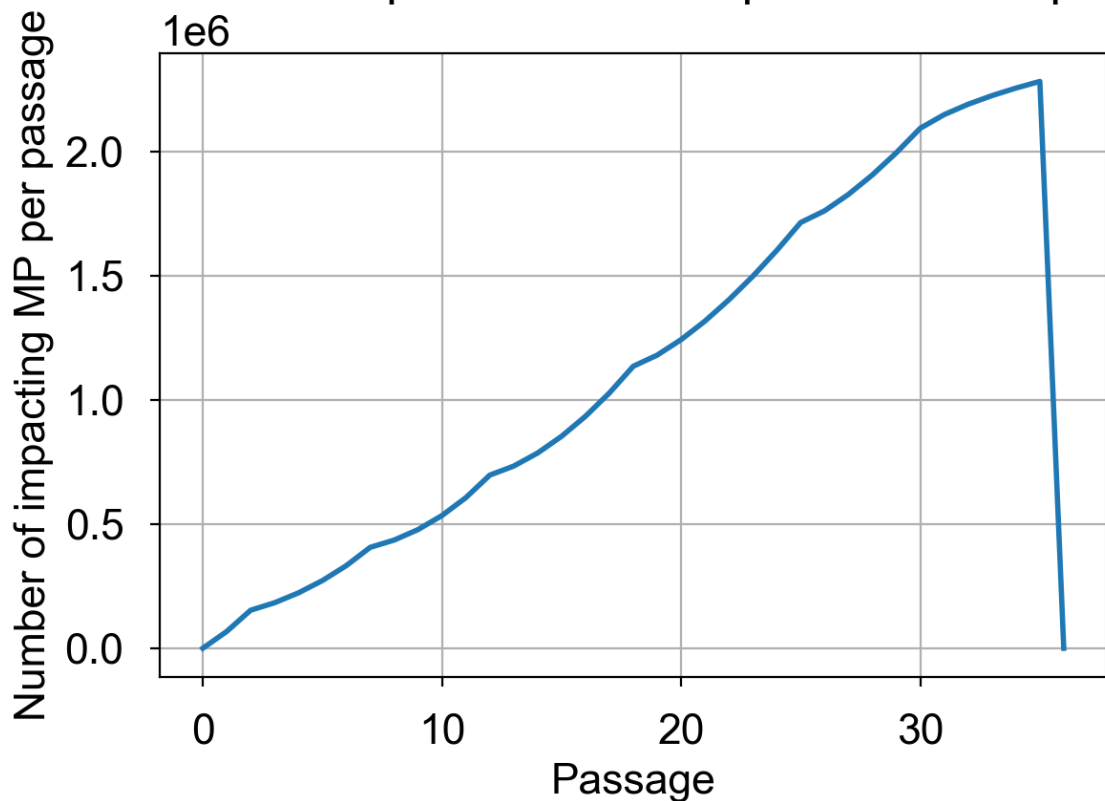
Var. name: N_mp_corrected_pass
Number of macroparticles for which fallback algorithm is used
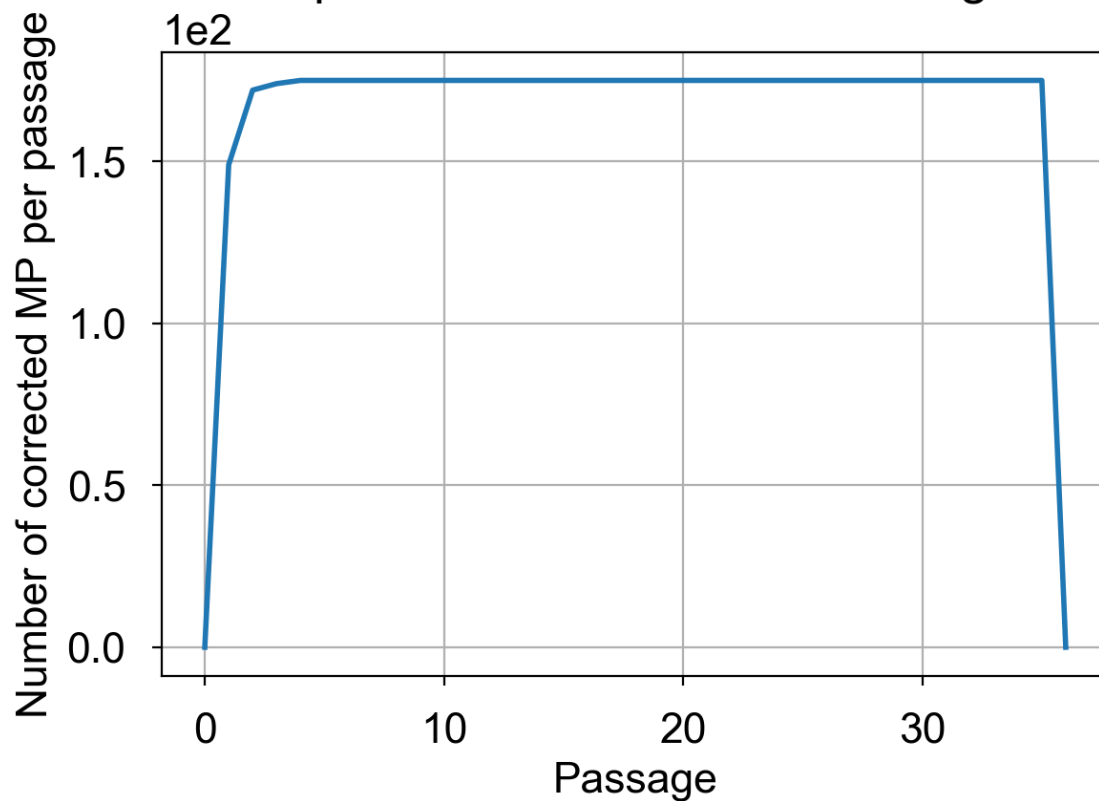
Var. name: N_mp_ref_pass
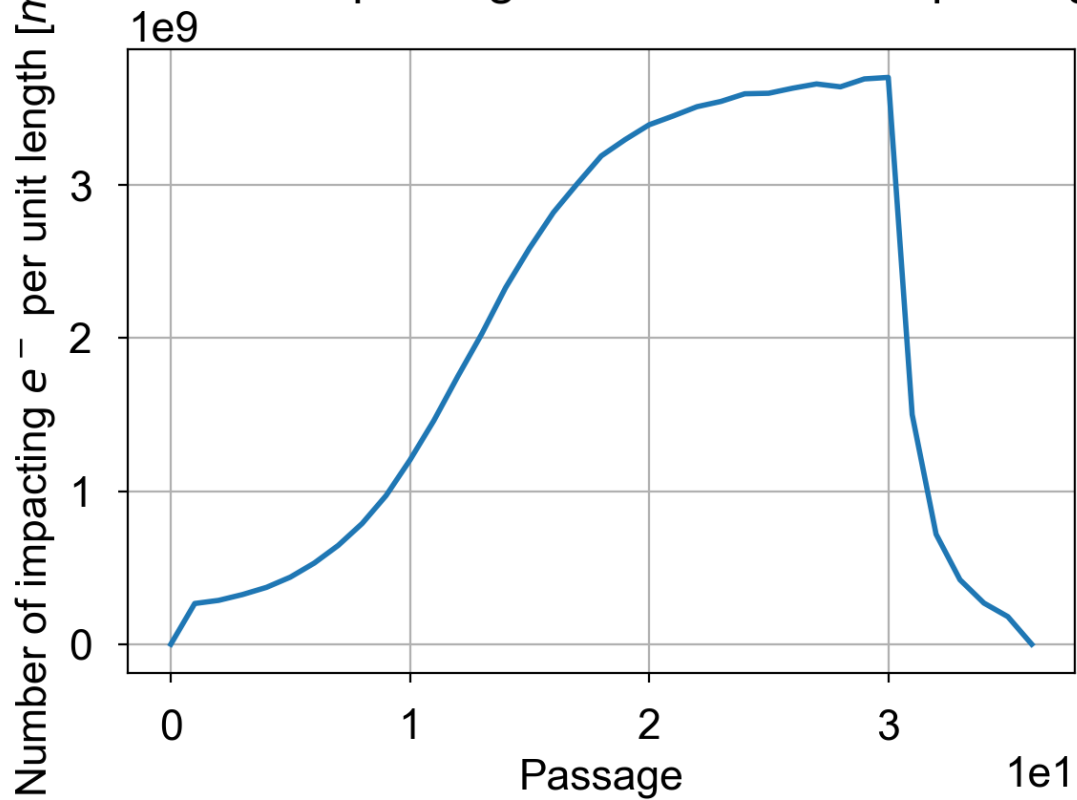Reference macroparticle size at each passage

Var. name: sum(nel_hist, axis=1)
Number of electrons at each passage

Var. name: sum(nel_hist, axis=0)
number of electrons in each slice
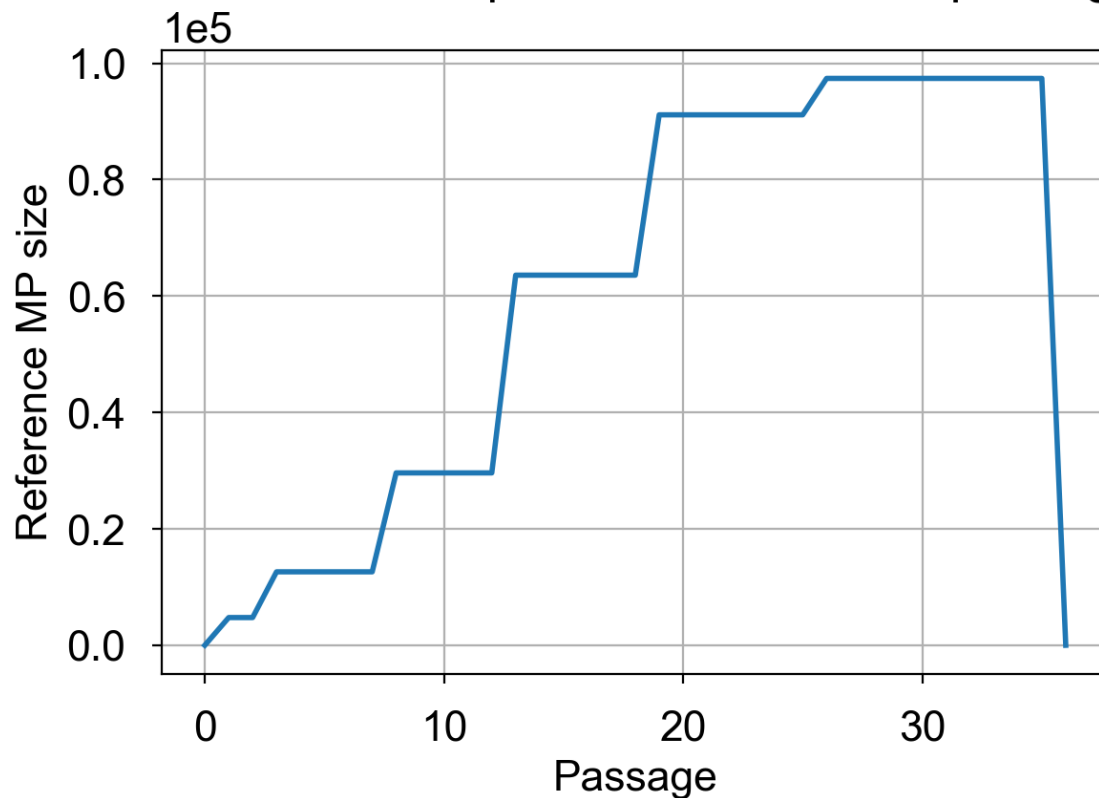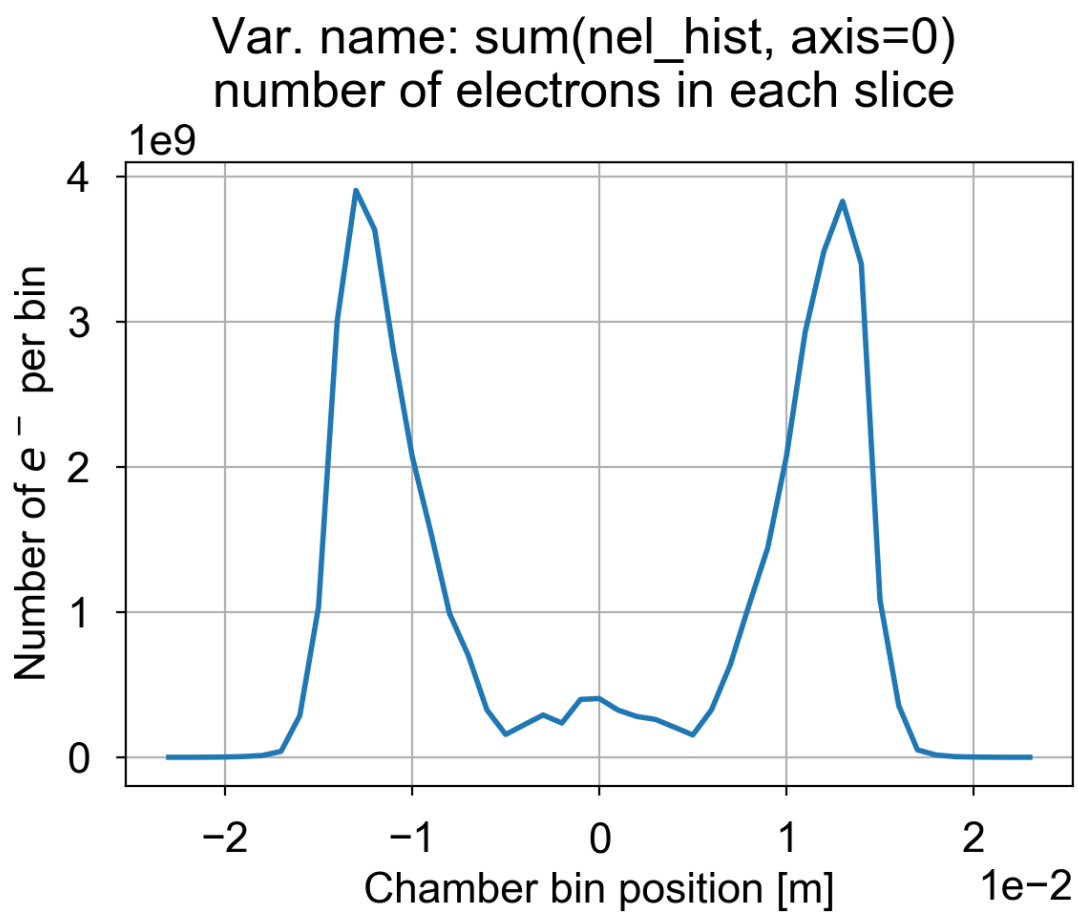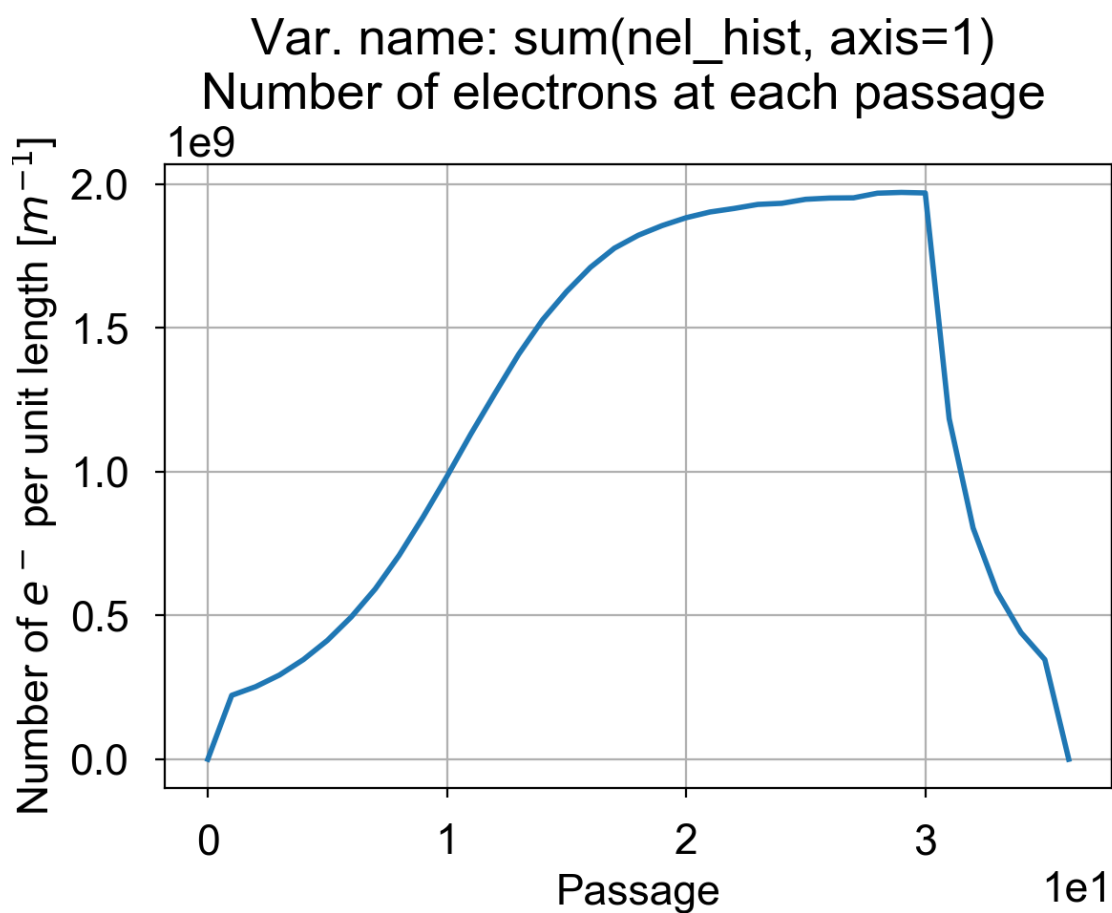
Var. name: np.sum(ob.nel_impact_hist_scrub, axis=1)
Number of impacting scrubbing electrons [E>E_scrub]
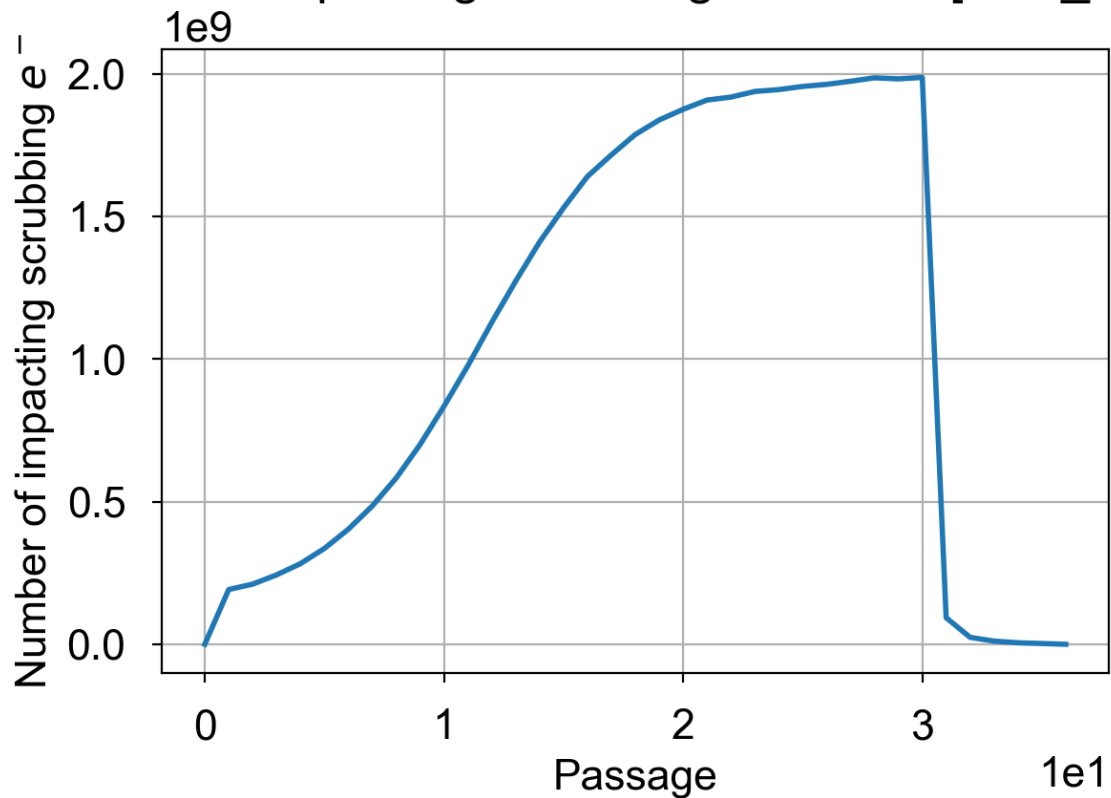
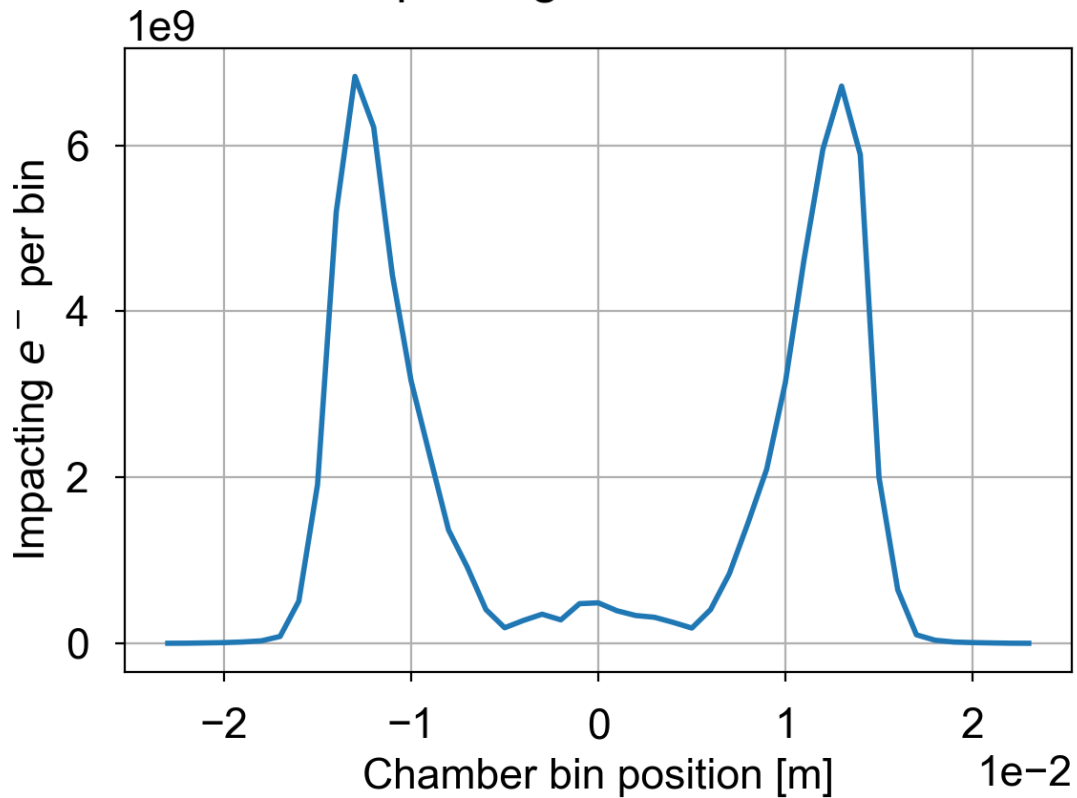Var. name: sum(nel_impact_hist_scrub, axis=0)
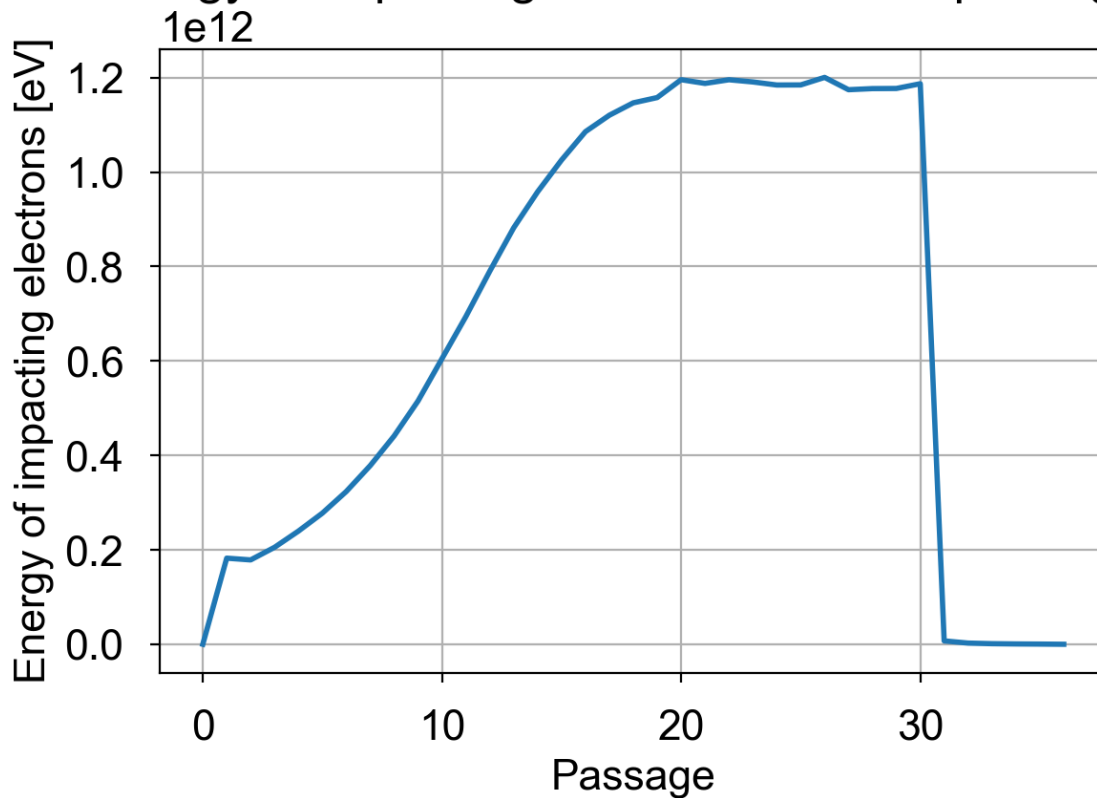Impacting scrubbing electrons in each slice
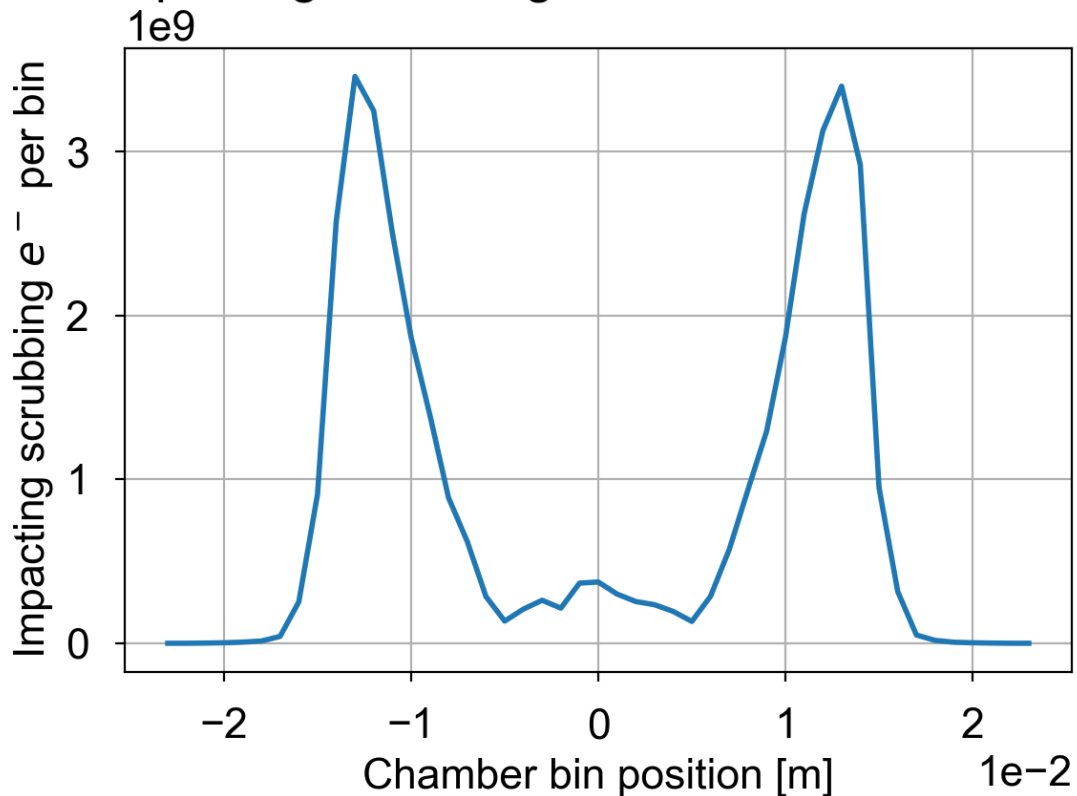
Var. name: sum(nel_impact_hist_tot, axis=1)
Number of impacting electrons at each passage

Var. name: sum(nel_impact_hist_tot, axis=0)
Number of impacting electrons in each slice

Var. name: sum(energ_eV_impact_hist, axis=1)
Energy of impacting electrons at each passage

Var. name: sum(energ_eV_impact_hist, axis=0)
Total energy of impacting electrons per passage [eV]