

IONTRACE

Three-dimensional simulation of ion extraction
from a plasma through grid systems

User Manual

Part I: Plasma ion extraction

First draft, program version 2.1.1

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Chapter 1

Introduction

1.1 What the program does

IONTRACE computes how ions are extracted from a plasma and accelerated through a system of apertured grid electrodes, as in a gridded ion thruster or an ion source. For a given geometry, a set of electrode voltages and a plasma state it determines

- the electric potential in three dimensions, including the space charge of the beam and the shape of the plasma boundary in front of the first grid,
- the trajectories of the beam ions and from them the extracted current, the currents to the grids, the beam profile, the divergence and the emittance,
- optionally the neutral gas density between the grids, the charge exchange ions created in it and where they strike the grids,
- optionally the sputter erosion caused by these impacts, and, in a lifetime simulation, how the grid geometry changes over thousands of operating hours.

The calculation is stationary: the program iterates between the field and the trajectories until both fit together. It does not follow the plasma in time.

1.2 Scope of this manual

This first part covers *plasma ion extraction*, shown in the program as the kind of computation **Plasma simulation**. The program can also trace particles from an explicitly defined source through arbitrary electrode arrangements, set up beamlines and simulate time-of-flight instruments. Those parts will be described separately. Controls that belong to them are hidden in the plasma mode unless **Advanced (show all features)** is ticked.

1.3 Conventions

- Labels that appear in the program are printed like this: **Start single calculation**. A path through the menus is written File → Open setup
- The program can be used in German or English (View → Sprache / Language). The change takes effect at the next start. This manual uses the English labels.

- All lengths are in millimetres unless stated otherwise. Numbers use a decimal point everywhere, also in exported files.
- The electron temperature T_e and the ion temperature T_i are entered as energies in eV. In the formulas $k_B T_e$ and $k_B T_i$ stand for these energies, so that $k_B T_e/e$ is the number entered, read in volts. The temperatures of the neutral gas and of the walls are entered in kelvin. Current densities are entered in mA/cm²; some displays state them in A/m² (1 mA/cm² = 10 A/m²).
- All examples use the bundled setup `REX-3G-quarter.picsetup`, a freely designed three-grid system (screen, accel, decel) for xenon.
- Numbers in square brackets, such as [2], refer to the list of references at the end.

1.4 German texts in the English interface

IONTRACE is written with German labels; the English interface replaces each of them by its translation when the program starts. The labels, tooltips, status lines and diagram texts have been checked systematically on the bundled example and on a number of results. The check can only find what these cases bring onto the screen. A text that appears only in a rarely used path, or only for a particular kind of result, may therefore still be German. Such a text is a gap in the translation and not a sign of a fault: the program does the same in both languages. A note to the authors with the place where the text appeared is welcome.

Some texts are German on purpose or come from outside the interface. Table 1.1 lists them.

Table 1.1: Texts that are German also in the English interface.

Place	What is German, and why
Log at the bottom of the main window and of other windows	The lines that the computing core writes while it works. They are the record of the calculation and are kept in one language so that they can be compared and searched.
Progress windows while loading and saving	Messages that contain a number, such as “11025 Trajektorien entpackt” (11025 trajectories unpacked).
Reason for the end of a lifetime run	The status card states the reason in English. Its tooltip also quotes the reason as the run wrote it into the result file, for example “t_max_h (2500.0h) erreicht” (the operating time was reached).
Name of the gas model	BETRIEB is the internal name of the gas model from operating data (Section 9.3); it appears in the list of the active models.
Messages after an unexpected stop (Section 14.1)	The messages of the watching process.
Lifetime simulation	The protocol file is named <code>lebensdauer.json</code> (“Lebensdauer”: lifetime).

Chapter 2

Quick start

This chapter takes the bundled example from an empty program to a first result. Every step is explained in detail in the later chapters.

1. **Start the program.** After the notice on the terms of use the start area appears. Under **Examples** choose **REX-3G — quarter aperture**. Alternatively use **Open a setup** and select `setups/REX-3G-quarter.picsetup`.
2. **Look at the setup.** The main window opens on the **Setup** tab (Fig. 2.1). It shows the three grids in a section and in 3D, lists the key figures of the setup and, under **Readiness**, anything that still prevents a calculation.
3. **Start the calculation.** Press **Start single calculation** in the left column or `F5`. A live monitor shows the progress. The example allows up to 20 iteration rounds, ends after 16 because the convergence criterion is met, and takes well under a minute.
4. **Inspect the result.** When the status below the buttons reads **Finished successfully**, the tabs **Fields**, **Trajectories**, **Beam** and **Run** are filled. Start with **Run** → **Convergence** to see whether the iteration has settled (Section 6.4), and compare with the reference values of Table 2.1. Then look at the potential in **Fields** → φ xy.
5. **Save.** **File** → **Save setup** (`Ctrl+S`) stores the inputs, **File** → **Save result ...** stores the computed fields and trajectories.

Table 2.1: Reference values of the example `REX-3G-quarter.picsetup`, computed with program version 2.1 and the settings stored in the setup. The setup is a quarter of one aperture (mirror planes at $y = 0$ and $z = 0$); currents of the whole aperture are four times those of the computed cell.

Quantity	Computed cell	Whole aperture
Mesh	$113 \times 26 \times 26$ points, $h = 0.08$ mm	—
Start points (macro-particles)	625	—
Emitted current $j_i A_{\text{emit}}$	215.0 μA	859.9 μA
Reason for termination	Converged in round 16 of at most 20	
Final max $ \Delta\varphi $ (tolerance 1 V)	0.91 V	
Macro-particles through the exit face	127 of 625	—
Beam current through the exit face	43.7 μA	174.7 μA

The start positions use a fixed seed, so a repetition gives the same course of the iteration. One macro-particle carries 0.34 μA , which is the step in which the currents of this setup can change.

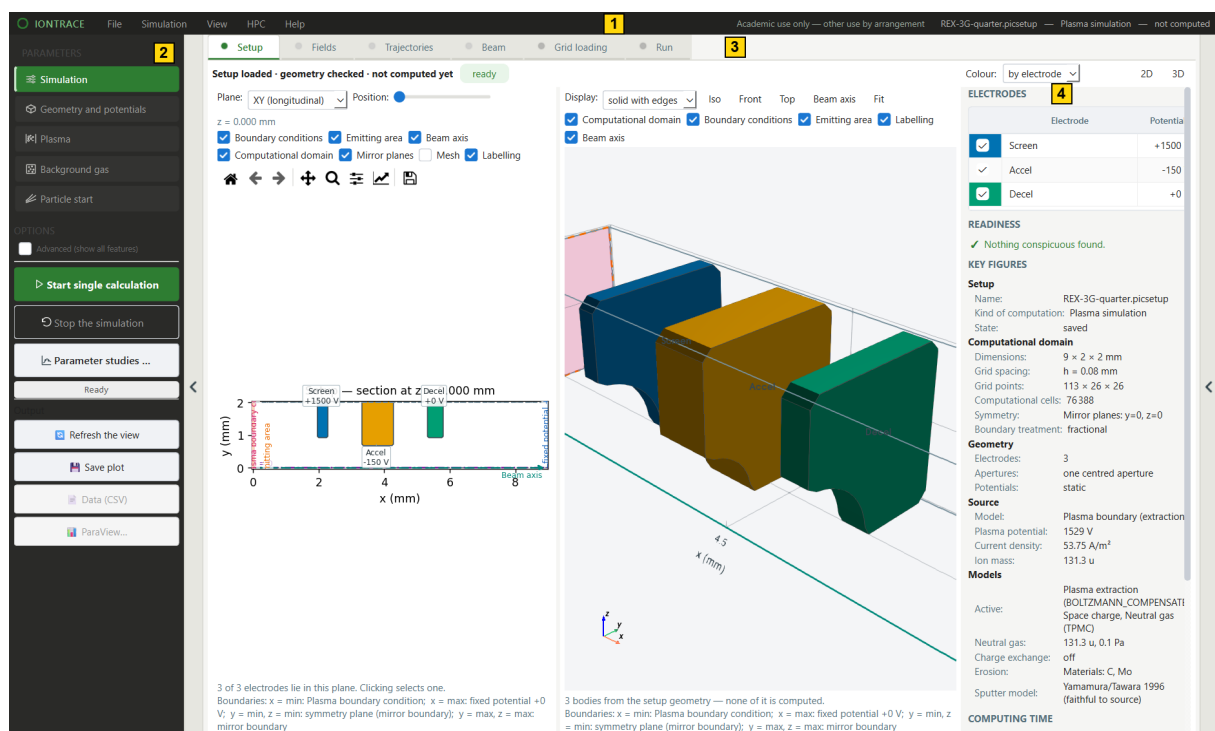


Figure 2.1: The main window with the example loaded. 1 Header with the menus, the name of the setup and the status. 2 Parameter column with the buttons that open the input dialogs and start the calculation. 3 The tabs; shown is the **Setup** tab with a section and a 3D view of the geometry. 4 Electrodes, readiness and key figures of the setup. The later figures of result tabs leave out the parameter column.

A different final round or a clearly different beam current indicates changed settings or another program version. Where the program states which of the two columns is described in Section 8.4.

Chapter 3

The main window

3.1 Layout

The window has three columns (Fig. 2.1).

Header. The dark bar at the top carries the menus and, on the right, the name of the setup, the kind of computation and a short status: **not computed**, **Results**, **Results out of date**, **Simulation running** and so on. **Results out of date** means that an input was changed after the last calculation: the pictures still show the old result.

Left column. From top to bottom:

- **Parameters:** five buttons, each opening one input dialog: **Simulation**, **Geometry and potentials**, **Plasma**, **Background gas** and **Particle start**. Each dialog has **Apply**, **OK** and **Cancel**; **Cancel** restores all values to the state before the dialog was opened.
- **Options:** the switch **Advanced (show all features)**. It reveals expert settings in the dialogs (time step, Newton parameters, relaxation and similar) and the controls of the other kinds of computation.
- **Start single calculation** and **Stop the simulation**. Stopping ends the run cleanly after the current iteration round; the partial result is shown.
- **Parameter studies ...** opens the tab for series of calculations (Chapter 12).
- A status line: **Ready**, **Computation running**, **Finished successfully** or **Computation failed**.
- **Output:** **Refresh the view**, **Save plot**, **Data (CSV)** and **ParaView ...** act on the tab that is currently shown.

Centre. The tabs with the setup and the results (Table 3.1). A coloured dot in front of each tab name shows whether its content is current.

Right column. Statistics of the last run and the log. It can be folded away with the arrow at its edge or with View → Right column (statistics / log).

3.2 Menus

File Create, open and save setups and results; export for ParaView; import and export of a background gas map; save a picture of the whole window (**F12**).

Table 3.1: The tabs of the main window in the plasma mode.

Tab	Sub-tabs	Content
Setup	—	The geometry as entered, readiness, key figures (Section 3.3)
Fields	φ xy, φ xz, φ yz, $ E $ xy, ρ xy, Debye h/λ	Sections through potential, field strength and charge density (Chapter 7)
Trajectories	Trajectories, 3D view	Ion paths in a section and in space (Chapters 7 and 11)
Beam	Beam profile, Energy	Properties of the extracted beam (Chapter 8)
Grid loading	Background gas, CEX, Erosion, Lifetime	Neutral gas, charge exchange, sputter erosion and its development in time (Chapters 9 and 10)
Run	Convergence, Parameter studies	Course of the iteration (Section 6.4); series of calculations
Simulation	Start single calculation (F5) and Cancel calculation (Shift+F5).	
View	Live view during a run, the right column, moving and resetting labels in the plots, saving the current plot, language.	
HPC	Run on the compute node . . . : sends a calculation to a cluster. The menu is only present in installations that include this function.	
Help	Introductory notes and About IONTRACE .	

3.3 The Setup tab

The **Setup** tab shows the inputs, never a result. Nothing is computed for it, so it is available immediately and always reflects the current values. Fig. 3.1 shows its right column enlarged.

- **Section (left).** **Plane** selects XY, XZ (both along the beam) or YZ (across the beam, showing the arrangement of the apertures); **Position** moves the section. The check boxes add the boundary conditions, the emitting area, the beam axis, the computational domain, the mirror planes, the mesh and the labels.
- **3D view (right).** **Display** switches between solid, transparent and sectional presentations; **Iso**, **Front**, **Top**, **Beam axis** and **Fit** set the camera.
- **Electrodes.** A click on a row highlights that electrode in both views; the tick hides it.
- **Readiness.** A list of checks. A green tick with **Nothing conspicuous found** means the calculation can start. Any other line names a problem; clicking it opens the dialog in which it can be fixed.
- **Key figures.** Domain size, grid spacing, number of grid points, symmetry, boundary treatment, plasma potential, current density, active models.
- **Computing time.** Hints on which settings make the calculation slow, with the button **What this means . . .**.

ELECTRODES

	Electrode	Potential
☒	Screen	+1500
☒	Accel	-150
☒	Decel	+0

READINESS

☒ Nothing conspicuous found.

KEY FIGURES

Setup

Name:

REX-3G-quarter.picsetup

Kind of computation:

Plasma simulation

State:

saved

Computational domain

Dimensions:

$9 \times 2 \times 2$ mm

Grid spacing:

$h = 0.08$ mm

Grid points:

$113 \times 26 \times 26$

Computational cells:

76388

Symmetry:

Mirror planes: $y=0, z=0$

Boundary treatment:

fractional

Geometry

Electrodes:

3

Apertures:

one centred aperture

Potentials:

static

Source

Model:

Plasma boundary (extraction)

Plasma potential:

1529 V

Current density:

53.75 A/m^2

Ion mass:

131.3 u

Models

Active:

Plasma extraction
(BOLTZMANN_COMPENSATION)
Space charge, Neutral gas (TPMC)

Neutral gas:

131.3 u, 0.1 Pa

Charge exchange:

off

Erosion:

Materials: C, Mo

Sputter model:

Yamamura/Tawara 1996
(faithful to source)

COMPUTING TIME

Figure 3.1: The right column of the **Setup** tab for the example: electrodes, readiness and key figures.

3.4 Files

Table 3.2: File types.

Extension	Content
<code>.picsetup</code>	A setup: all inputs, optionally with a precomputed background gas map. This is the file to keep and to share.
<code>.json</code>	The inputs only, as plain text.
<code>.picsim</code>	A result: the inputs, the fields, the trajectories, the course of the iteration and, if computed, charge exchange, erosion and lifetime data.
<code>.geo.yaml</code>	A description of bodies (solids) only.

Caution. File → Save setup as ... offers both `.json` and `.picsetup`. If no gas map has been computed, the preselected type is `.json`. Choose `.picsetup` explicitly if that is what you want.

A result file is meant for evaluation. To compute again with changed inputs, open the setup, not the result. When saving a result the program asks whether to thin out the stored trajectories. This makes the file about fifty times smaller, but the complete trajectories are needed if charge exchange or erosion are to be evaluated later from the saved file.

Chapter 4

Defining the geometry

The geometry is entered in the dialog **Geometry and potentials** (Fig. 4.1). It contains, from top to bottom, the size of the computational domain, the mesh resolution, the mirror planes, the table of grid electrodes and, folded away, additional bodies and the boundary conditions of the domain faces.

4.1 Coordinate system

- The computational domain is a rectangular box. Its corner is the origin: x runs from 0 to L_x , y from 0 to L_y , z from 0 to L_z . There are no negative coordinates.
- x is the beam axis. The plasma is at $x = 0$, the beam leaves through the face at $x = L_x$.
- y and z are the transverse directions. The four side faces of the box can act as mirror planes (Section 4.4).

4.2 Computational domain and mesh

Box length X/Y/Z set the size of the domain. Leave about one to two millimetres of plasma in front of the first grid, so that the plasma boundary can form freely, and a few millimetres of drift space behind the last grid.

Under **Mesh resolution** the fineness of the mesh is set, either by the **Cell size h** or by the **Number of points n**; the other quantity follows. With **per axis** the three directions can be given different values. The line below shows the resulting number of grid points $n_x \times n_y \times n_z$.

The mesh is the most important setting for both accuracy and computing time:

- The smallest aperture should be resolved by at least four cells across its radius. Below about three cells its round shape turns into a staircase, and the **Readiness** list says so.
- Computing time grows roughly with the third power of the refinement. Halving h costs about a factor of eight in time and memory.
- With the boundary model **Fractional (Shortley-Weller)** (Section 6.2) the wall of an aperture is placed at its true position inside a cell. This removes the error of a wall that can only lie on cell boundaries. It does not replace the resolution that the plasma boundary, the space charge and the beam need. All bundled examples use it.

Geometry

Box length X [mm]: 9.0000

Box length Y [mm]: 2.0000

Box length Z [mm]: 2.0000

Mesh resolution

Resolution via: Cell size h [mm] per axis fit

h [mm]: 0.080000

nx×ny×nz = 113×26×26 (0.08M nodes)

⚠ effective box: x 8.9600 instead of 9.0000 mm

Mirror planes (symmetry)

☒ Determine automatically from the aperture positions

Mirror at: ☐ y=0 ☐ y=max ☐ z=0 ☐ z=max

“y=0” is the box wall (plane) at y=0 – in the yz cross-section below the left edge; likewise y=max/z=0/z=max.
Active mirror planes are marked red there.

Reduce: Quarter (×4) Half (×2)

Grid electrodes (ion optics)

Thin apertured plates in the beam path. Not needed for pure trajectory computations -- there you build the electrodes as bodies (below).

	Label	x from [mm]	x to [mm]	Voltage [V]	Form	Aperture r/y [mm]	Aperture z [mm]	Material
1	Scre...	2.0	2.3	1500.0	RC	0.95		Mo
2	Accel	3.3	4.3	-150.0	RC	0.7		C
3	Decel	5.3	5.8	0.0	RC	0.95		C

+ row

- row

Material...

Aperture position: Absolute (y, z)

Apertures of this electrode...

Polygon...

Centre the array

Hexagonal pattern...

> Cross-section yz (view along x)

> Bodies (solids) and box faces

Free voltages: none — each electrode carries its own value

Free voltages ...

Check the computational domain ...

Apply

OK

Cancel

Figure 4.1: The dialog **Geometry and potentials** with the three grids of the example.

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Whether a mesh is fine enough for the quantity you are interested in is shown only by a comparison with a finer mesh (Chapter 13).

Caution. The number of points is a whole number, so the box that is actually computed, $(n - 1)h$, can differ from the entered length by up to half a cell. The dialog then shows a warning with the effective size. For a symmetry cell this matters, because the current per aperture and the gas density depend on its area. The button **fit** adjusts h so that it divides the box exactly.

4.3 Grid electrodes

Each row of the table **Grid electrodes (ion optics)** is one plate with apertures. Rows are added and removed with **+ row** and **– row**.

Table 4.1: Columns of the grid table.

Column	Meaning
Label	Name of the electrode. A row without a label is ignored.
x from, x to	Upstream and downstream face of the plate. Their difference is the thickness.
Voltage [V]	Potential of the electrode.
Form	Shape of the aperture: round, rectangular, elliptical or a polygon.
Aperture r/y	For a round aperture the <i>radius</i> . For a rectangle or an ellipse the <i>full</i> width in <i>y</i> .
Aperture z	Full width in <i>z</i> for a rectangle or an ellipse; not used for a round aperture.
Material	Material of the electrode. It determines the sputter yield in the erosion calculation.
Hole position	Summary of the aperture positions. A double click opens the list of apertures of this electrode.

The order of the rows is the order along the beam. The first row is the electrode that faces the plasma (the screen grid): the plasma potential is referred to its voltage (Section 5.2).

Aperture positions. An electrode without explicit positions has one aperture in the middle of the box, at $(L_y/2, L_z/2)$. **Apertures of this electrode ...** opens a list in which any number of aperture centres can be entered. This is also the way to displace the aperture of one grid against another, for example to study a misalignment between screen and accel grid. **Aperture position** chooses whether the values are absolute coordinates or offsets from the box centre.

Further tools.

- **Hexagonal pattern ...** writes the two aperture centres of a hexagonal unit cell into every electrode and sets the matching box size from the pitch (Section 4.4).
- **Centre the array** moves all apertures of all electrodes together so that the pattern sits in the middle of the box.
- **Polygon ...** defines the corners of a polygonal aperture.

- **Material ...** defines an additional sputter material.
- **Cross-section yz (view along x)** unfolds a live picture of the apertures of all electrodes with the active mirror planes marked in red. Below it, the dialog reports geometry errors: an electrode outside the box, overlapping electrodes, an aperture larger than the box.

Note. The grid table has no entry for chamfers or countersinks. A profiled aperture edge is built as a body of the type **Surface of revolution (meridian profile)** (Section 4.5).

4.4 Symmetry and unit cells

A single aperture of a large grid behaves as if it were surrounded by identical neighbours. It is therefore enough to compute a small symmetry cell whose side faces mirror the particles and the field. This reduces the computing time by the same factor by which the domain shrinks.

With **Determine automatically from the aperture positions** (the default) the program derives the mirror planes from the geometry:

- An aperture in the middle of the box: no mirror planes. The whole aperture is computed.
- One aperture whose centre lies on a box face or in a corner: the faces through the centre become mirror planes. An aperture centred on the corner (0, 0) gives a quarter model with mirrors at $y = 0$ and $z = 0$.
- Two or more aperture centres: all four side faces mirror. This describes a periodic unit cell.

The buttons **Quarter ($\times 4$)** and **Half ($\times 2$)** convert a full, centred setup into the reduced one: they halve the box, move the apertures to the corner or the edge and set the mirror planes. Currents and other totals are multiplied by the symmetry factor where the program states values for the whole aperture.

For a hexagonal grid pattern the smallest unit is a rectangle with a quarter aperture in two opposite corners. **Hexagonal pattern ...** creates it from the pitch p : the box becomes $p/2$ by $p\sqrt{3}/2$.

Caution. The automatic rule cannot tell a periodic cell from a real arrangement of several apertures. If you model several complete apertures that are *not* meant to continue periodically, untick the automatic setting and leave all four mirror boxes empty.

4.5 Bodies and domain faces

The folded section **Bodies (solids) and box faces** adds electrodes of other shapes. For plasma extraction through plane grids the grid table is normally sufficient; bodies are needed for profiled aperture edges, shields, housings and similar parts. Bodies take part in every calculation in the same way as the grid electrodes: in the field, as walls for the particles and in the erosion. Where bodies overlap they are joined.

A body is created by choosing its **Type** and pressing **+ Add**; **Edit ...** changes it and **– Remove** deletes it. **Preview** shows the bodies without starting a calculation.

Table 4.2: Types of bodies. All lengths in mm.

Type	Entries
Sphere	Centre and radius.
Spherical section	A sphere cut off by two planes: centre, radius, lower and upper cut relative to the centre.
Box	Centre, the three edge lengths and an edge radius for rounded edges.
Cone or frustum	Axis, centre, length and the radius at each end; a radius of 0 gives a point.
Torus or ring	Axis through the hole, centre, ring radius and tube radius.
Ellipsoid	Centre and the three semi-axes.
Plate with holes	Normal axis, centre, thickness and the two extents, and a list of apertures with position and radius, one per line.
Cylinder or tube	Axis, centre, length, outer radius and inner radius; an inner radius of 0 gives a solid cylinder.
Cylinder segment	As the tube, with a starting angle and an opening angle.
Extruded polygon	Extrusion axis, centre, the corners of the polygon, one per line, and the length.
Surface of revolution (meridian profile)	Axis, reference point and the profile as pairs of axial position and radius, one per line. A list of aperture centres repeats the same profile at several places. This is the type for chamfered or countersunk apertures.

Every body has in addition a **Label**, a **Potential [V]** and a **Material** (typed as text, for example Mo or C), a displacement **Position: displacement [mm]** and a rotation **Rotation about [degrees]** (Fig. 4.2). The three angles are applied in the order x , y , z . The selector **Rotation about** below them chooses the pivot: the body's own centre (local) or the origin of the domain (global). The displacement is applied after the rotation.

With **Emitting area (plasma/screen side)** a body takes the role of the first grid: the plasma potential is referred to it and the beam starts in front of it. The grid table may then be empty. The remaining properties of a body (transparent mesh electrode, detector face, voltage formula) belong to the other kinds of computation.

Geometry files. **Save as a geometry file ...** writes the bodies into a text file `.geo.yaml`; **Load a geometry file ...** replaces the current bodies by those of a file, after a confirmation. The file contains bodies only, optionally with the box size and the cell size. Grid electrodes and boundary conditions are not part of it. Geometry files can also describe unions, intersections and differences of bodies; such a combined body is shown in the list, and its potential and material can be edited, but not its shape.

Domain faces. **Box boundary conditions (explicit)** sets the condition on each of the six faces of the domain: **Dirichlet** (a fixed potential, entered in the table), **Neumann** (no field component normal to the face) or **Plasma** (the plasma potential of the **Plasma** dialog). Without it the defaults apply: the face at $x = 0$ is the plasma, the side faces are open or mirrors as set above, and the face at $x = L_x$ is controlled by **Right box face: Dirichlet** in the **Simulation** dialog.

Geometry

Axis: x

Centre [mm]: x 0.000 y 0.000 z 0.000

Length [mm]: 10.000

Outer radius [mm]: 5.000

Inner radius [mm] (0 = solid): 0.000

Material and electrical properties

Label:

Potential [V]: 0.000

Voltage formula (empty = a fixed value):

Material: Mo

☐ Emitting area (plasma/screen side)
 ☐ transparent to particles (mesh electrode)

Transmission [0...1]: 1.000

Driven by: empty = static

☐ Detection surface — ions arriving here count as detected

Position: displacement [mm]: x 0.000 y 0.000 z 0.000

Rotation about [degrees]: x 0.000 y 0.000 z 0.000

Rotation about: local (about the body)

OK

Cancel

Figure 4.2: The dialog of a body, here a **Cylinder or tube**. Above, the entries of the shape; below, the entries that all bodies share.

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4.6 Additional materials

Material ... below the grid table opens the dialog **Custom material (sputter parameters)**. It defines a material that is not among the predefined ones (Mo, C, C-C, Ti, W). The dialog opens with the values of molybdenum (Fig. 4.3).

U_s, Q, W and s belong to the target material, not to the projectile.
The starting values are those of Mo. For a material without values in the table the source gives $Q = 1.0$, $W = 0.35 \cdot U_s$ and $s = 2.5$.

Name	
Z (atomic number)	42
Mass [amu]	95.950
Density [kg/m ³]	10280.0
U _s [eV] (binding energy)	6.820
Q (target factor)	0.8500
W (electronic denominator)	2.3900
s (threshold exponent)	2.800
E _{th} [eV] (the compatibility model only)	0.00
f (angular exponent)	1.500
θ _{opt} [deg]	60.0

OK Cancel

Figure 4.3: The dialog **Custom material (sputter parameters)**.

Table 4.3: Entries of a custom material.

Entry	Meaning
Name	Name under which the material appears in the Material column. A predefined name cannot be used; an existing custom name replaces that material.
Z (atomic number), Mass [amu]	Atomic number and mass of the target atoms.
Density [kg/m³]	Density of the solid. It converts the number of sputtered atoms into a removed thickness.
U_s [eV] (binding energy)	Surface binding energy.
Q (target factor), W (electronic denominator), s (threshold exponent)	Material parameters of the formula of Yamamura and Tawara [8]. For a material without tabulated values the source gives $Q = 1.0$, $W = 0.35 U_s$ and $s = 2.5$; entering 0 for W uses $0.35 U_s$.
f (angular exponent), θ_{opt} [deg]	Dependence of the yield on the angle of incidence (Section 10.1): the exponent and the angle of the largest yield.
E_{th} [eV]	A fixed threshold energy. It is used by the compatibility model only; Yamamura/Tawara computes the threshold from U_s and the two masses.

All of these belong to the target material, not to the ion. Custom materials are saved with the setup.

4.7 Checking the geometry

Check the computational domain ... opens a window that shows how the program has actually divided the domain into cells: vacuum, solid, fixed potential and plasma source. It changes nothing and starts no calculation. Use it when a result looks implausible; a body that is thinner than a cell, for instance, may not appear in the mesh at all.

Chapter 5

Plasma and particle start

5.1 The model in brief

The plasma is not simulated particle by particle. It enters through three quantities: the electron temperature T_e , the ion density n_i of the plasma and the plasma potential U_{plasma} .

- **Ions** start on the face $x = 0$ with the Bohm velocity

$$v_B = \sqrt{\frac{z k_B T_e}{m_i}}$$

and are followed through the field as macro-particles. Together they carry the emitted current density

$$j_i = 0.5 n_i z e v_B.$$

The ion temperature T_i adds a thermal spread to the start velocity (Section 5.2).

- **Electrons** are treated as a fluid in thermal equilibrium. Their density follows the local potential (Boltzmann relation) and is tied to the local ion charge density ρ_{ion} , so the equation that is solved for the potential φ is

$$-\varepsilon_0 \nabla^2 \varphi = \rho_{\text{ion}} \left[1 - \exp\left(\frac{e(\varphi - U_{\text{plasma}})}{k_B T_e}\right) \right].$$

Where φ is close to U_{plasma} the two charges cancel: that is the plasma. Where φ falls well below it the electrons are gone and the full ion charge remains: that is the beam. The electron term is applied upstream of the front face of the first grid only; the face $x = 0$ is held at U_{plasma} .

- **The plasma boundary** (the meniscus) is therefore not an input. It forms where the solution places it, and it moves when voltages or density change.

What n_i refers to. The entry n_i is the reference density from which the emitted current density is computed. It is *not* the ion density on the emitting face: ions that leave the face with v_B and carry j_i have the density $j_i/(z e v_B) = 0.5 n_i$ there. The relation has the form of the usual estimate of the Bohm current, in which n_i is the density of the undisturbed plasma and the factor accounts for the fall of the density towards the edge of the sheath; for Boltzmann electrons this fall is $\exp(-1/2) \approx 0.61$, commonly rounded to 0.5 (see, for example, [1]). In keeping with this, the derived plasma potential contains the potential drop $k_B T_e/2e$ of the presheath (Table 5.1), and the Debye length shown in the program is computed from n_i itself. If the density of your

plasma is known at another place, or if the ion current density is known from a measurement, enter the current density directly (input mode A below); the ions are started with j_i , and n_i then follows from it.

Not included are magnetic fields and collisions during the iteration. Charge exchange with the neutral gas is evaluated after the iteration has finished (Chapter 9).

5.2 The Plasma dialog

Figure 5.1: The dialog **Plasma**. Grey fields are derived values.

Input mode decides which of two coupled quantities is entered; the other is computed and shown in grey:

- **A: $j_i + T_e \rightarrow n_i$:** you enter the ion current density.
- **B: $n_i + T_e \rightarrow j_i$:** you enter the ion density.

Both are linked by $j_i = 0.5 n_i z e v_B$ (Section 5.1).

Table 5.1: Entries of the **Plasma** dialog.

Entry	Meaning
$n_{\text{ion}} (1/m^3)$	Ion density n_i of the plasma, the reference density of the emitted current (Section 5.1).
$T_e (eV)$	Electron temperature. It sets the Bohm velocity, the Debye length and the potential drop in the sheath.
$T_i (eV)$	Ion temperature. It sets the thermal spread of the start velocity (see below).
Thermal spread of the ions	Switches the spread from T_i on or off. Default: on.

Entry	Meaning
U_plasma (V)	Plasma potential. Normally derived from the voltage of the first grid and T_e : $U_{\text{plasma}} = U_{\text{screen}} + \frac{k_B T_e}{2e} \ln\left(\frac{m_i}{2\pi m_e}\right) + \frac{k_B T_e}{2e}$. The first term after U_{screen} is the potential drop in front of a floating wall, the second that of the presheath. With manual a measured or assumed value can be typed in.
j_i (mA/cm²)	Ion current density emitted from the plasma.
Start energy (eV, total)	Empty: the ions start with the Bohm velocity. A number fixes the start energy instead.

For the example ($n_i = 3.5 \cdot 10^{17} \text{ m}^{-3}$, $T_e = 5 \text{ eV}$, xenon, screen grid at 1500 V) the dialog derives $v_B = 1917 \text{ m/s}$, $U_{\text{plasma}} = 1528.9 \text{ V}$ and $j_i = 5.37 \text{ mA/cm}^2$ (53.7 A/m²).

The total emitted current is the current density times the emitting area, $I = j_i A_{\text{emit}}$. How much of it leaves the grid system as beam, and how much ends on the screen grid, is a result of the calculation.

The ion temperature spreads the start velocity of the ions. Transverse to the beam direction both components are drawn from a normal distribution of width $\sqrt{k_B T_i / m_i}$; along the beam direction the same width is added around the Bohm velocity (or around the fixed start energy). Because every start point carries a fixed current, the longitudinal velocity is drawn from the distribution of the ions that cross the emitting surface, that is the velocity distribution weighted with the velocity itself. The emitted current is not changed. After acceleration through the voltage U the transverse spread leaves an angle of about $\sqrt{k_B T_i / (e U)}$ in the beam: for $T_i = 0.1 \text{ eV}$ and 1500 V this is 8 mrad. The draw uses a fixed seed, so every PIC round and every repetition of a run starts the same ions.

With **Thermal spread of the ions** switched off, all ions start exactly parallel with the Bohm velocity and **T_i** has no effect. This was the behaviour of program versions before October 2026; the switch exists to continue such a result unchanged.

With **Advanced (show all features)** a second group **Numerics — how it is computed** appears in this dialog. Its entries are described in Section 6.3.

5.3 Ion species and doubly charged ions

Species, charge number and mass of the beam ions are set in the **Simulation** dialog (**Ion species**, **Charge number z**, **Mass (u)**). Predefined are Xe, Kr, Ar, He, N, N₂, O and O₂; any other mass can be typed in.

Doubly charged fraction (%) adds a share of doubly charged ions to a singly charged beam. It can be given as a particle fraction or as a current fraction. Both charge states follow the same paths; the doubly charged ions are faster by $\sqrt{2}$ and arrive with twice the energy, which matters for the space charge and for the erosion.

Estimate ... suggests a value for xenon from a simple balance of the discharge. It needs the electron temperature, the plasma density and the neutral gas density in the discharge chamber and takes into account direct double ionisation and stepwise ionisation via Xe⁺. The value is only entered when you press **Apply**. Treat it as a lower limit; a measured value takes precedence.

5.4 Particle start

Emitting area

☒ The whole left wall

y_min (mm): 0.000

y_max (mm): 2.000

z_min (mm): 0.000

z_max (mm): 2.000

Trajectory range

x_start (mm): the plane of emission in x 0.000

Distribution

Mode: A uniform grid

n_beamlets: 625

n_min (suggestion): ≥ 625 (25 × 25 grid, whole wall)

Use the suggestion

☐ Mesh grid (uniform, sub-mesh from n_beamlets)

Pattern: Grid with jitter (recommended)

Jitter/random seed: 12345

Grid basis: 676 (= 26 × 26). Higher values lead to sub-grid sampling (s=ceil(sqrt(n))). The number of trajectories drawn is now in the tab 'Trajectories (2D)'.

Info

Aperture: r = 0.95 mm (ROUND), A = 2.835 mm²
 Cell size: h = 0.080 mm
 Cells across the aperture: ~443
 Emitting surface: 4.000 mm², ~625 cells

Check start positions...

Apply

Figure 5.2: The window **Particle start at the plasma boundary**.

The window **Particle start** determines where on the plasma face the macro-particles start and how many there are.

- **Emitting area.** With **The whole left wall** ions start over the full face $x = 0$. Those that do not find an aperture strike the screen grid; this is the physically correct picture and the default. Unticked, a rectangle can be entered.
- **n_beamlets.** The number of start points. They are arranged on a square pattern, so 100 means 10×10 .
- **n_min (suggestion).** One start point per mesh cell of the emitting face. Fewer points leave streaks in the charge density; the window warns about this. **Use the suggestion** adopts the value.
- **Pattern.** **Grid with jitter (recommended)** displaces each point randomly within its cell. A strictly regular grid can imprint a cross on the beam footprint. **Random (Monte Carlo)** places the points freely.
- **Jitter/random seed.** With a fixed seed the start positions are identical in every round and in every run, so results are reproducible.
- **Check start positions ...** shows the start points without running a calculation.

More start points give smoother densities, at proportionally higher cost for the trajectory part of the calculation. How to check whether their number is sufficient is described in Chapter 13.

Chapter 6

Simulation settings

6.1 How a calculation proceeds

A single calculation is an iteration between field and particles. One pass is called a *PIC round*.

1. **Preparation.** The geometry is turned into a mesh and a first estimate of the field without beam is computed.
2. **Field.** The potential is solved for the current ion charge density. Because the electron term depends on the potential itself, this is a nonlinear problem; it is solved by Newton's method, and each Newton step solves a large linear system.
3. **Trajectories.** All macro-particles are started and followed through the field until they leave the domain or strike an electrode.
4. **Charge.** Along its path every particle deposits charge on the mesh. This gives a new charge density, which is mixed with the previous one.
5. **Check.** The largest change of the potential against the previous round, $\max|\Delta\varphi|$, is determined. If it is below the tolerance, the calculation ends; otherwise it continues with step 2.

6.2 The Simulation dialog

Table 6.1: Entries of the **Simulation** dialog.

Entry	Meaning
Solver	Method for the linear systems. AMG (algebraic multigrid) is the recommended choice. GS (Gauss–Seidel) is only useful for very small meshes or for comparison.
Multigrid	Implementation of the multigrid solver. AMGCL (parallel, recommended) uses all processor cores and is several times faster than PyAMG (fallback) , which is used automatically when AMGCL is not available.

Entry	Meaning
Boundary model	Staircase: walls follow the cell boundaries, so a round aperture becomes a stepped one and its radius changes in steps of one cell. Fractional (Shortley-Weller): next to the wall of an aperture the field equation uses the true distance to the wall [5], and the particles strike the wall at its true position. The radius of the aperture is then represented within a fraction of a cell. The plane faces of the grid electrodes lie on mesh planes in both models. Recommended; it removes the staircase error, not the need to check the mesh (Chapter 13).
Plasma model	Boltzmann compensated (beam-coupled) is the plasma model of Section 5.1. Laplace (ion optics, no plasma) switches the plasma off and computes the vacuum field only.
Ion species, Charge number z, Mass (u), Doubly charged fraction	See Chapter 5.
Maximum number of PIC rounds	Upper limit for the iteration.
Stop early once the potential has converged with Largest change of potential max. $\Delta\varphi$	The convergence criterion: the calculation ends as soon as the potential changes by less than this value from one round to the next at every point of the mesh. It is tested from the second round on.
Also stop when max. $\Delta\varphi$ no longer falls	A second way to finish: the change has stopped falling and the particle balance is steady. The exact conditions and what they do and do not show are given in Section 6.4.
Store trajectories	How many trajectories are kept in the result: Complete trajectories (default), Selected trajectories (a reproducible sample, limited by a Fraction (%) and a largest number) or End points only . All particles are computed in every case; the field, the space charge and the currents to the electrodes do not depend on this setting. It saves memory for large numbers of start points. See the note in Section 7.4.
Switch off space charge (test trajectories)	The ions do not act back on the field. One round is then enough.
Drift compensation	Neutralisation of the beam behind the last grid. off: the beam keeps its full space charge. Cutoff (hard): no space charge beyond a given x . Boltzmann: electrons from the neutraliser reduce the space charge depending on the local potential.
Right box face: Dirichlet	Fixes the potential on the exit face of the domain, usually at 0 V. Without it that face is left free and the potential downstream can drift. The examples fix it.
Save diagnostic plots for every round	Writes pictures of trajectories, charge density and potential for each round into a folder. Useful for analysing a run that does not converge.

With **Advanced (show all features)** the time step of the particle integration (**dt**, normally **auto**) and the parameters of the Gauss–Seidel solver appear in addition.

Simulation

Solver: AMG

Ion species: free (mass entered by hand)

Charge number z: 1

Mass (u): 131.2930

free · 131.2930 u · q/m = 7.3489e+05 C/kg

Doubly charged fraction (%): 0.00

particle fraction

Estimate ...

Multigrid: AMGCL (parallel, recommended)

Store trajectories: Complete trajectories

Boundary model: Fractional (Shortley-Weller)

Plasma model: Boltzmann compensated (beam-coupled)

PIC convergence

Maximum number of PIC rounds: 20

☒ Stop early once the potential has converged

Largest change of potential max. $|\Delta\phi|$: 1.000 V

☒ Also stop when max. $|\Delta\phi|$ no longer falls

▪ Fine tuning: when does the curve count as flat?

The simulation ends as soon as the max. $|\Delta\phi|$ of a round falls below 1.000 V, at the latest after 20 rounds. It also ends as soon as max. $|\Delta\phi|$, averaged over 5 rounds, falls by less than 5.0 % per round while the result quantities stand still (at the earliest after 8 rounds).

☐ Save diagnostic plots for every round

Select...

☐ Switch off space charge (test trajectories)

Drift compensation: off

x_neutral: 6.000 mm

f_comp: 0.900

U_comp: ☒ auto 0.00 V

T_comp: 1.00 eV

Right box face: ☒ Dirichlet

0.00 V

dt_eff (ns): —

Charge-exchange reactions

☐ Charge exchange during the run

sigma model: pullins_xenon (Xe-SCX, A=87.3 B=13.6)

Collision partner: free (mass entered by hand) (amu): 131.2930

← from the beam

A (A^2): 87.30

B (A^2): 13.600

sigma_const (m^2): 5.000e-19

applies to: —

z: 1

+

—

← from setup

Table: Load $\sigma(E)$...

no table loaded

☒ Xe²⁺; also compute single exchange (estimate)

☒ Track secondary ions (otherwise statistics only)

Max. secondary trajectories: 500

Apply

OK

Cancel

Figure 6.1: The dialog **Simulation**.

6.3 Numerical parameters

The following entries are found in the **Plasma** dialog under **Numerics — how it is computed** when **Advanced (show all features)** is ticked. The defaults are suitable for most cases.

Table 6.2: Numerical parameters.

Entry	Meaning
sc_relax_omega	Mixing factor ω for the charge density: $\rho = \omega \rho_{\text{new}} + (1 - \omega) \rho_{\text{old}}$. A value of 1 takes the new density completely. Smaller values (0.3 to 0.5) damp oscillations of the iteration at the price of more rounds. This is the first parameter to change when a calculation does not converge.
adaptive	Lets the program halve ω by itself when the beam collapses into backflow.
ρ mixing	Picard is the simple mixing above. Anderson uses the history of several rounds.
Newton tol (V), Newton max-iter	Accuracy and maximum number of steps of the nonlinear field solution within one round.
Newton damping	Fraction of each Newton step that is applied. Reduce to 0.3 to 0.7 only if the field solution itself fails to converge.
Adaptive Newton damping	Lets the program adjust that fraction. On by default.
Inexact Newton (Eisenstat-Walker)	Solves the linear systems only as accurately as each Newton step needs. Faster, but it can shift results slightly; off by default.

For high emission currents the dialog shows a recommendation for ω in red. As a rule of thumb, an emitted current per aperture of up to about 20 μA needs no damping, up to 100 μA $\omega \approx 0.7$, up to 500 μA $\omega \approx 0.5$, and above that $\omega \approx 0.3$.

Note. In setups with mirror planes the program replaces an ω of 1 by 0.3 on its own and writes a line into the log.

6.4 Running a calculation and judging convergence

The live monitor. A few seconds after the start of a run the window **Live monitor** opens (Fig. 6.2). It shows, round by round:

- **Self-consistency (per PIC round):** the change of the potential from round to round, the quantity the convergence criterion tests;
- **Newton convergence (inner iteration):** the course of the nonlinear field solution within the current round;
- **Number of trajectories** by result, and the **Currents**;
- **Emittances at the right boundary face**;
- **Charge exchange (CEX)**, if it is switched on;

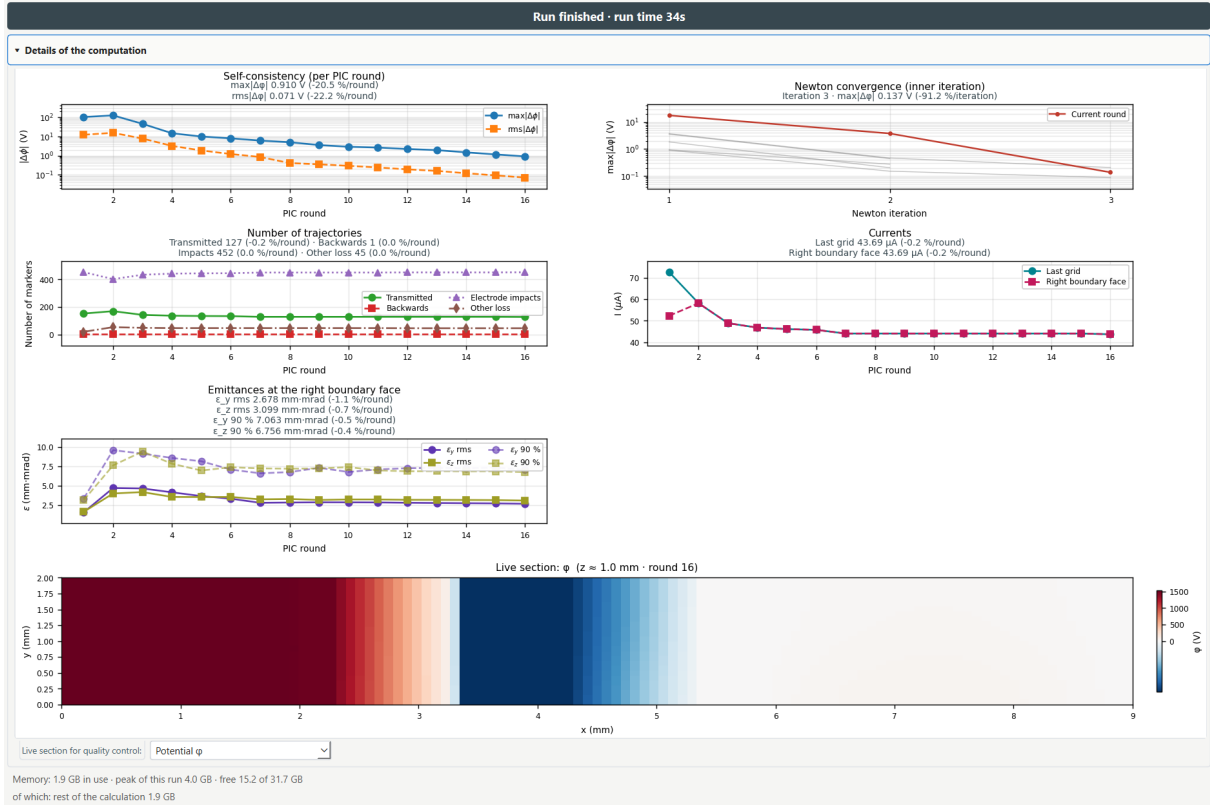


Figure 6.2: The **Live monitor** at the end of the example run.

- a section through the domain in the middle plane. The selector **Live section for quality control** chooses what it shows: potential, field strength, charge density, the kind of each cell, or nothing.

A line at the bottom reports the memory in use. The monitor can be switched off with **View** → **Show live view**; the change takes effect at the next run. During a lifetime simulation the monitor starts anew with every step.

After the run the same information is in **Run** → **Convergence** (Fig. 6.3). **View** switches the plot of that tab between **Convergence of the potential**, **Beam and current**, **Particle balance** and **Course of the computation**. The line **Field solver** names the solver that was actually used. The folded sections **Further key figures** and **Values per PIC round** contain the current at the last grid, the emittances, the loss current to each electrode and the particle counts for every round; a click on a row marks that round in the plot. **Log (CSV)** writes the table to a file.

The cards at the top (Fig. 6.4) state the last round, the final max $|\Delta\varphi|$, the reason for termination, the extracted ion current and the transmission. There are three reasons for termination. The card names the criterion that ended the run (**max. $|\Delta\varphi| \leq \dots$** , **noise floor reached at $\dots$** or **maximum number of rounds $\dots$ reached**); the status line above reads **Converged**, **Noise floor reached** or **Not converged**.

Converged. In the last round the potential changed by less than the tolerance at every point of the mesh. This is a statement about the last *step* of the iteration, not about the distance to the final solution. With a mixing factor $\omega < 1$ (Section 6.3) only the fraction ω of each new charge density is adopted, and the steps are correspondingly shorter: a step of 1 V with $\omega = 0.3$ corresponds to about 3 V of an undamped iteration. Converged therefore means that the iteration has come to rest within the tolerance. Whether the quantities you need have come to rest as well is checked separately (Chapter 13).

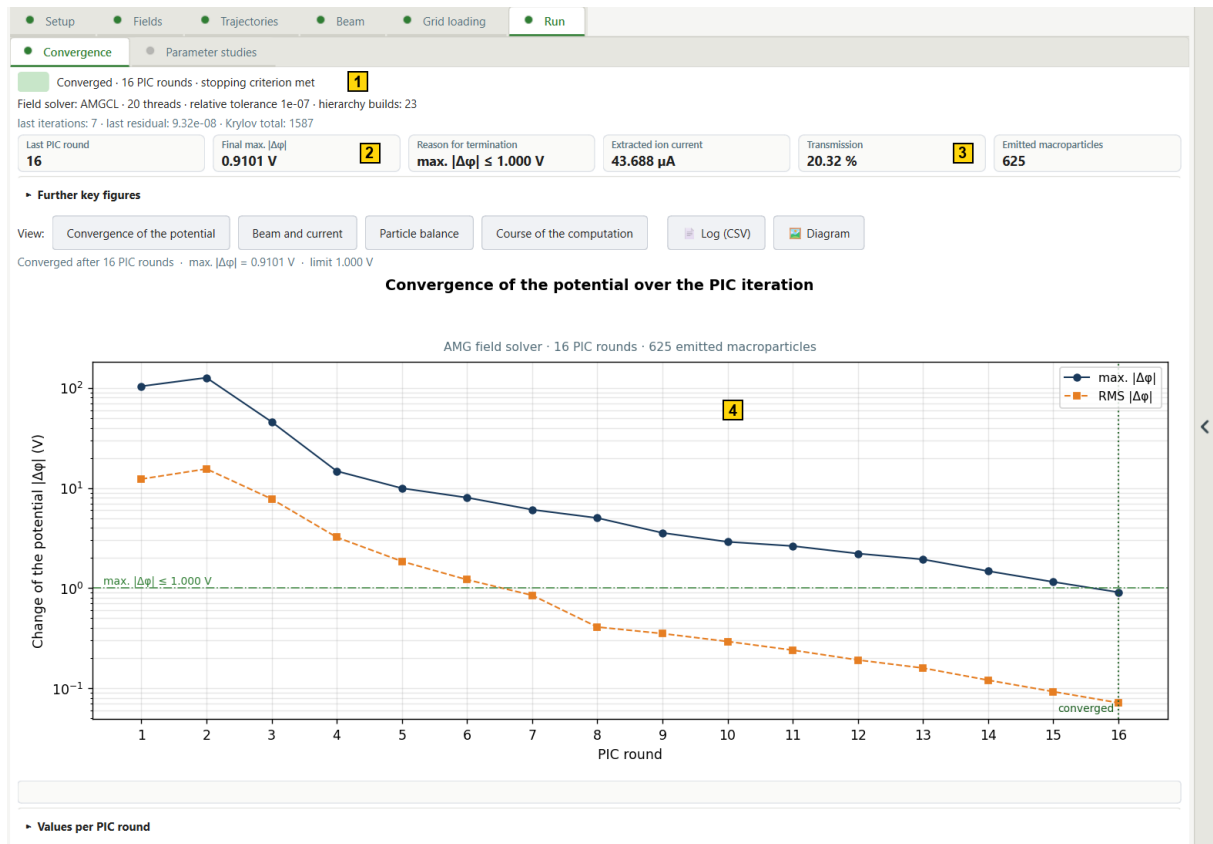


Figure 6.3: The tab Run → Convergence after the example run. 1 Status line. 2 Cards with the last round, the final max $|\Delta\varphi|$ and the reason for termination. 3 Cards with the extracted ion current, the transmission and the number of macro-particles. 4 The largest change of the potential per round; the green line is the tolerance.

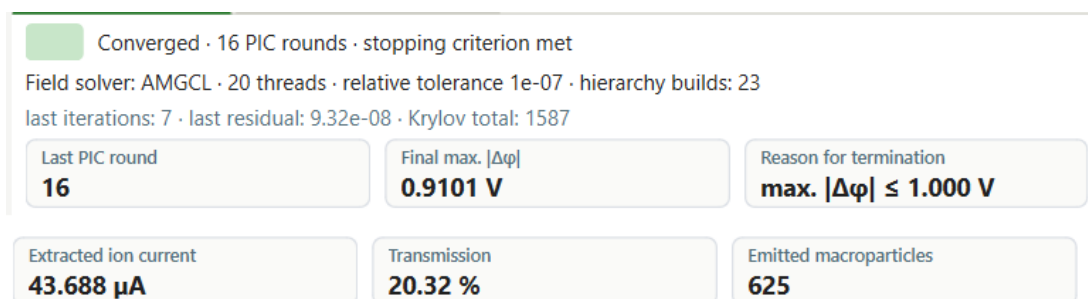


Figure 6.4: The status line and the cards of Fig. 6.3, enlarged. The currents are those of the computed cell (Table 2.1).

Noise floor reached. This exit is taken when all of the following hold (the numbers are the defaults stored in a setup):

- over the last five rounds $\max |\Delta\varphi|$ fell on average by less than 5 % per round;
- the numbers of macro-particles that were transmitted, struck an electrode, returned to the plasma or were lost each changed by less than 1 % from round to round, three rounds in a row;
- the damping of the iteration did not change within these rounds;
- and all of this still held after three further rounds.

The exit therefore establishes that the iteration no longer makes progress and that the particle balance is steady. It does not establish why. The name expresses the usual cause, a level set by the finite number of macro-particles, below which the potential cannot settle; but a slow oscillation that leaves the particle counts unchanged, or a limit of the field solution, looks the same to the test. The level at which the curve came to rest is shown as **noise floor reached at** Before such a result is used, check two things: that the quantities you need are steady over the last rounds (**View** → **Beam and current**), and that the level falls when the number of start points is increased (Section 5.4). If it does not fall, the cause is not the number of particles; continue with Table 6.3. A tolerance that lies below the level is not reached by allowing more rounds.

Maximum number of rounds reached. Neither of the above happened. The result is the state after the last round. Look at the curve: if it is still falling, allow more rounds; if it jumps, see Table 6.3. The status line then reads **Not converged**.

In the example of Fig. 6.3 the change falls from about 100 V to 0.91 V and the run ends as **Converged** in round 16 of at most 20. The particle counts no longer change after round 7 apart from single macro-particles, and the beam current stays at 43.7 to 44.0 μA for the computed quarter cell (Table 2.1).

Table 6.3: Typical patterns of a run that does not converge.

Observation	Remedy
The change stays at 100 V or more and jumps up and down; the transmitted current alternates between high and almost zero.	The space charge iteration oscillates. Lower sc_relax_omega to 0.3 to 0.5 (halve again if necessary), allow more rounds, or tick adaptive . Newton damping does not help here.
The curve is flat at a few volts but above the tolerance, and currents and trajectory counts are steady.	The iteration has come to rest above the tolerance. Repeat with more start points (n_beamlets): if the level falls, it is set by the number of macro-particles, and the tolerance can only be reached with more of them. A larger tolerance is justified only if the quantities you need do not depend on it (Chapter 13).
The curve is flat but currents and trajectory counts keep changing.	A slow oscillation; the log notes that the run is stuck. Reduce ω .
The field solution reports the maximum number of Newton steps in every round.	Leave Adaptive Newton damping on; otherwise set Newton damping to 0.3 to 0.7.

The example, with the mixing factor $\omega = 0.3$, reaches the tolerance of 1 V in 16 rounds. If the

change of a comparable setup is still far above the tolerance after that many rounds, the cause is usually an instability, not too few rounds.

6.5 Computing time

- The field solution takes most of the time, typically more than 80 %. Its cost is set by the number of grid points.
- Use a symmetry cell wherever the geometry allows it. A quarter aperture has a quarter of the unknowns.
- Use the fractional boundary model. A staircase wall needs a much finer mesh to place an aperture radius equally well.
- The **Computing time** section of the **Setup** tab lists the settings of the current setup that cost most.

Chapter 7

Fields and trajectories

7.1 The common toolbar

Above the field sections, the trajectory view and the 3D view there is one shared toolbar labelled **View**.

Table 7.1: The toolbar **View**.

Control	Meaning
Show trajectories	Draws the ion paths over the field maps, in the trajectory view and in the 3D view. One switch for all of them.
through the right face only	Shows only the ions that reach the exit face of the domain, that is, the extracted beam.
eroded wall	Uses the wall of a lifetime simulation instead of the original geometry wherever a wall is drawn. Which point in time is shown is chosen in the Lifetime tab. Without a lifetime simulation the switch has no effect.
Averaging $\pm$	Averages the field over several layers on both sides of the section. 0 shows the single layer.
Body labels	Where the name and potential of each electrode are written, or Off .

The time behind **View updated** is the time of the last redraw. It says nothing about whether the data are current; that is the job of the field status described below.

7.2 Potential sections

The tabs φ xy, φ xz and φ yz show the potential in volts on a plane through the domain. The control groups on the right are:

Field status. A coloured badge states how the shown field relates to the shown geometry (Table 7.2). The button next to it offers the appropriate action, for example **Recompute the potential field . . .**

Section. The slider and the arrow buttons move the plane; the line below gives its position.

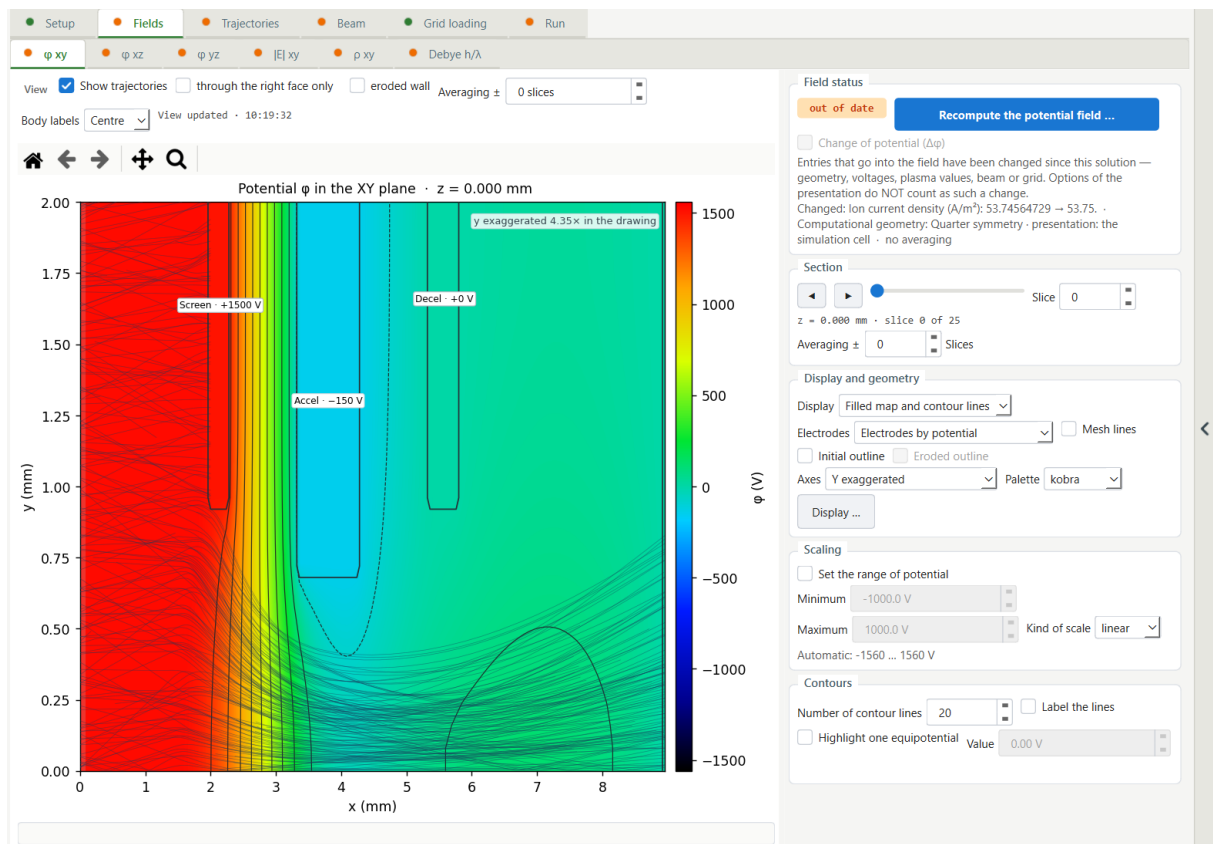


Figure 7.1: Fields $\rightarrow \varphi xy$: the potential in the plane through the beam axis with the ion trajectories. The plasma (red) bulges into the screen aperture; the equipotential lines show the lens formed between screen and accel grid. The drawing is stretched in y ; the factor is written in the picture.

Table 7.2: Field status.

Badge	Meaning
up to date	Field and geometry belong together.
out of date	An input that enters the field has been changed since the calculation: geometry, voltages, plasma values, beam or mesh. The text below the badge names what changed. Display options never make a field out of date.
overlay only	An eroded wall is drawn on top of the field of the original geometry. The field has <i>not</i> been recomputed for the eroded shape (Section 10.7).
approximate field	The potential was recomputed for the shown wall with the charge distribution of the original run. It is not self-consistent.

Display and geometry.

- **Display:** filled map, contour lines, or both.
- **Electrodes: Electrodes by potential** colours the bodies with their own potential. **Highlight the electrodes neutrally** draws them grey with the potential written beside them. **Highlight the material removed** additionally hatches the region that was material originally and is not any more.
- **Mesh lines** shows the computational mesh.
- **Initial outline** and **Eroded outline** draw the original and the eroded wall as lines; **Wall from fill level** decides how the eroded wall is determined (Section 10.7).
- **Axes: True to scale, Y exaggerated** (the default, uses the available area), or true to scale and rotated by 90°.
- **Palette:** the colour scale.
- **Display ...** opens a dialog with all presentation settings of the view.

Scaling. With **Set the range of potential** the colour limits are fixed by hand; otherwise they are chosen automatically and the range used is shown.

Contours. Number of contour lines, their labels, and **Highlight one equipotential** for a single line at a chosen value, for example 0 V.

Moving the mouse over the plot shows the position and the potential at that point below the picture, read from the mesh values.

7.3 Field strength, charge density and Debye resolution

|E| xy shows the electric field in V/mm, derived from the potential that is currently shown. **Quantity** selects the magnitude, one component, vector arrows or field lines. **Highlight E_crit** marks the contour $E = k_B T_e / (e \lambda_D)$, an indicator of where the plasma sheath lies.

ρ xy shows the charge density of the ions in C/m³. With **ρ_{net}** the electron contribution is subtracted, so the plasma appears neutral and only the sheath and the beam carry net charge.

Debye h/λ compares the cell size h with the local Debye length λ_D in the plasma region. Green means $h/\lambda_D \leq 5$, yellow up to 10, red above. The plasma model used here tolerates cells larger than the Debye length, so the colours are a guide and not a hard limit: if large parts of the plasma region are red, check the result against a finer mesh.

Field lines. In the **|E|** tab, **Quantity** → **Field lines** draws lines that follow the direction of the field (Fig. 7.2); their density is set with **Line density**. **Equipotential lines** (on by default) lays grey lines of constant potential underneath, so that the two families, which cross at right angles, can be read together. In the potential tabs the same lines are switched on under **Display ...**, section **Field lines and vector arrows**, with **Draw field lines**.

Field lines show the direction of the field; how close they lie is only a rough indication of its strength. No line is drawn inside electrodes or where the field is weaker than one thousandth of the largest value in the plane. Field-free regions, for example inside the plasma or behind a shield, therefore stay empty. Without this limit the numerical residue of the solver would appear there as smooth but meaningless curves.

The 3D view draws field lines as tubes coloured by the field strength (**Field lines: show**). **Seed** selects where they start: on a mesh across the domain (the default), along a line, or in a cloud of

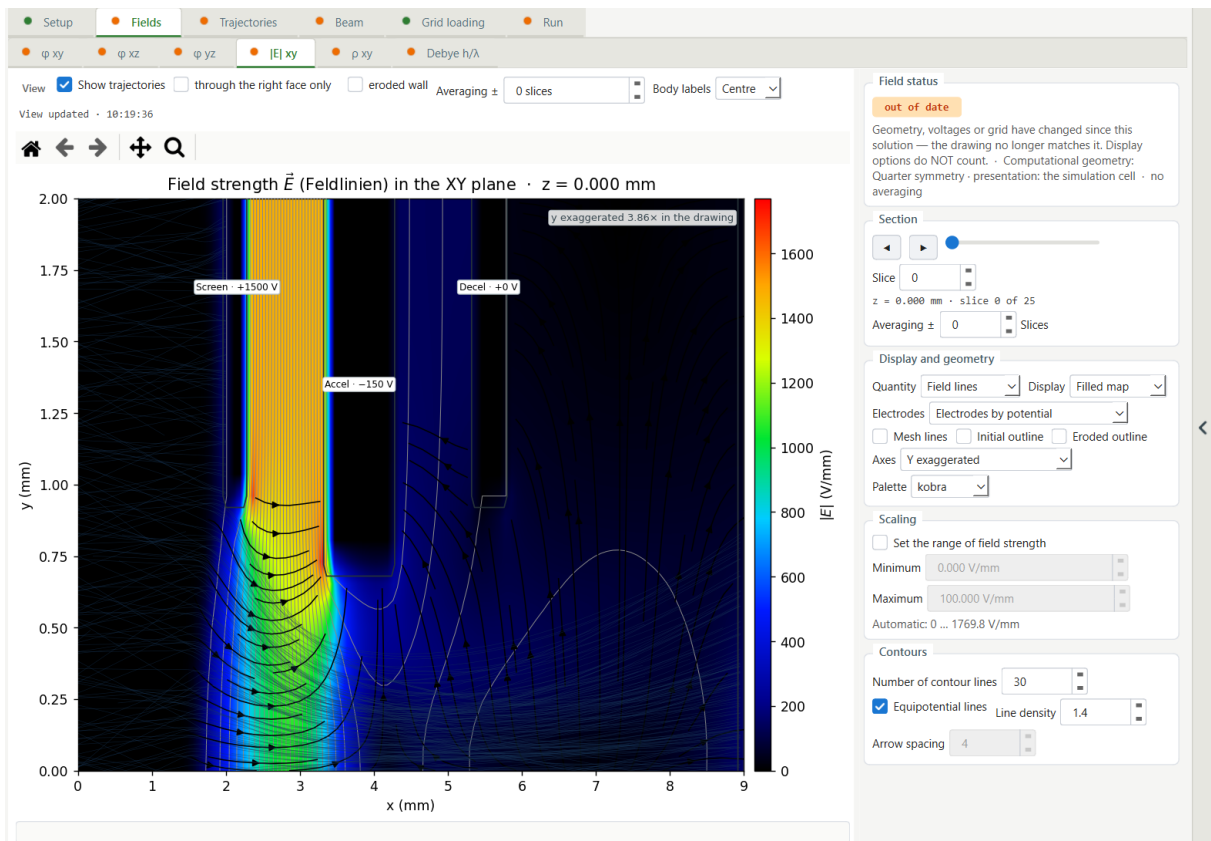


Figure 7.2: Fields $\rightarrow |E|_{xy}$ with **Quantity** set to **Field lines**: black field lines with arrows over the map of the field strength, grey equipotential lines underneath. The thin lines in the background are the ion trajectories.

points around a centre. **Number**, **Direction** and **Tube** set their count, whether they are followed along or against the field, and their thickness.

7.4 The trajectory view

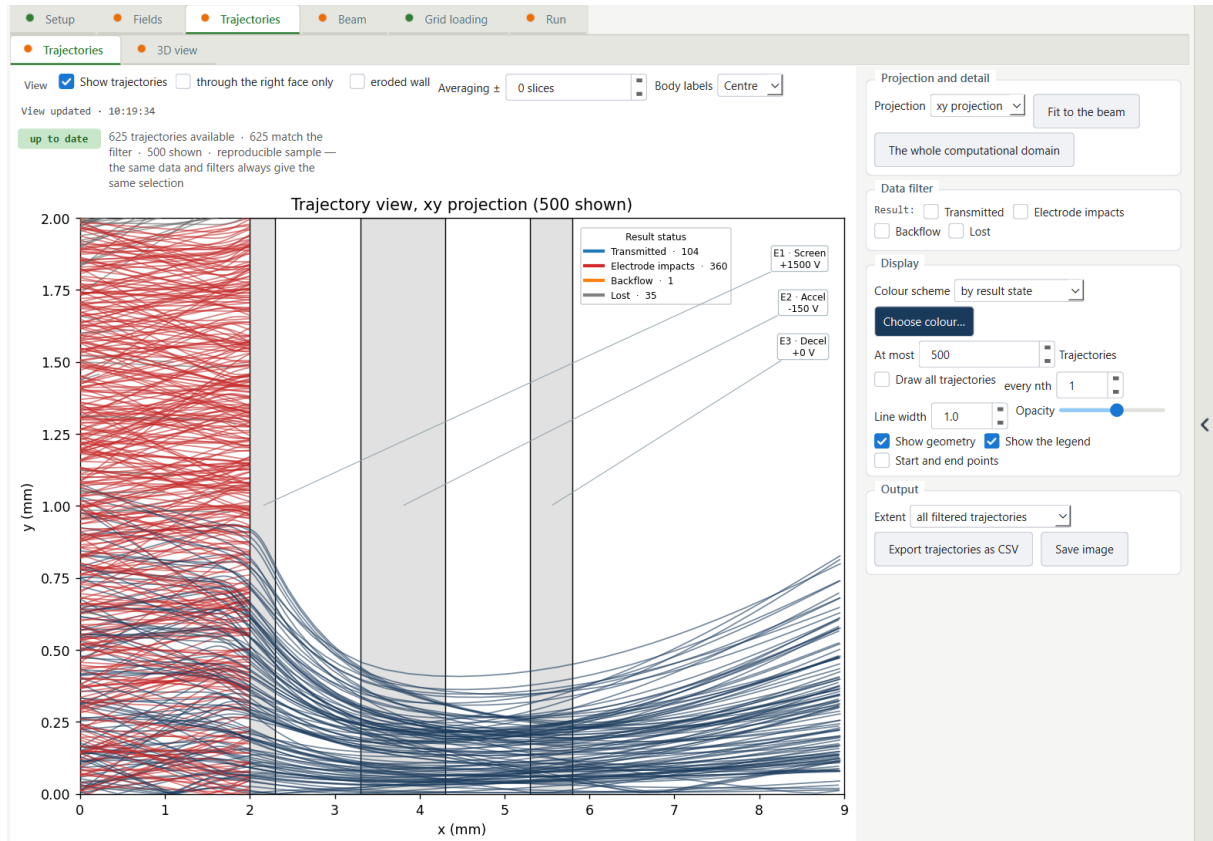


Figure 7.3: Trajectories → Trajectories: ion paths projected onto the xy plane, coloured by what became of each ion.

Trajectories → Trajectories draws the stored ion paths projected onto a plane. Each ion ends in one of four ways, and the colours follow this result: **Transmitted** (left through the exit face), **Electrode impacts**, **Backflow** (returned to the plasma side) and **Lost** (left through a side face).

- **Projection and detail:** the plane, and whether the picture is fitted to the beam or shows the whole domain.
- **Data filter:** which results and which aperture channels are shown.
- **Display:** colour scheme, line width, opacity, and how many trajectories are drawn.

Note. By default at most 500 trajectories are drawn. If more match the filter, a reproducible sample is shown, and the status line above the plot says so. This limit concerns the picture only. The evaluations (beam profile, energy, charge exchange, erosion) use every *stored* trajectory.

Caution. With **Store trajectories** set to **Selected trajectories** (Section 6.2) only a sample of the trajectories is stored. The currents in the **Statistics** column and in the **Convergence** tab are counted during the run from all particles and remain correct. The **Beam profile** tab, however, evaluates the stored trajectories: its **Total current** then covers the stored sample only and is too low. Use **Complete trajectories** when the beam profile is to be evaluated quantitatively.

Chapter 8

Beam properties

8.1 Beam profile

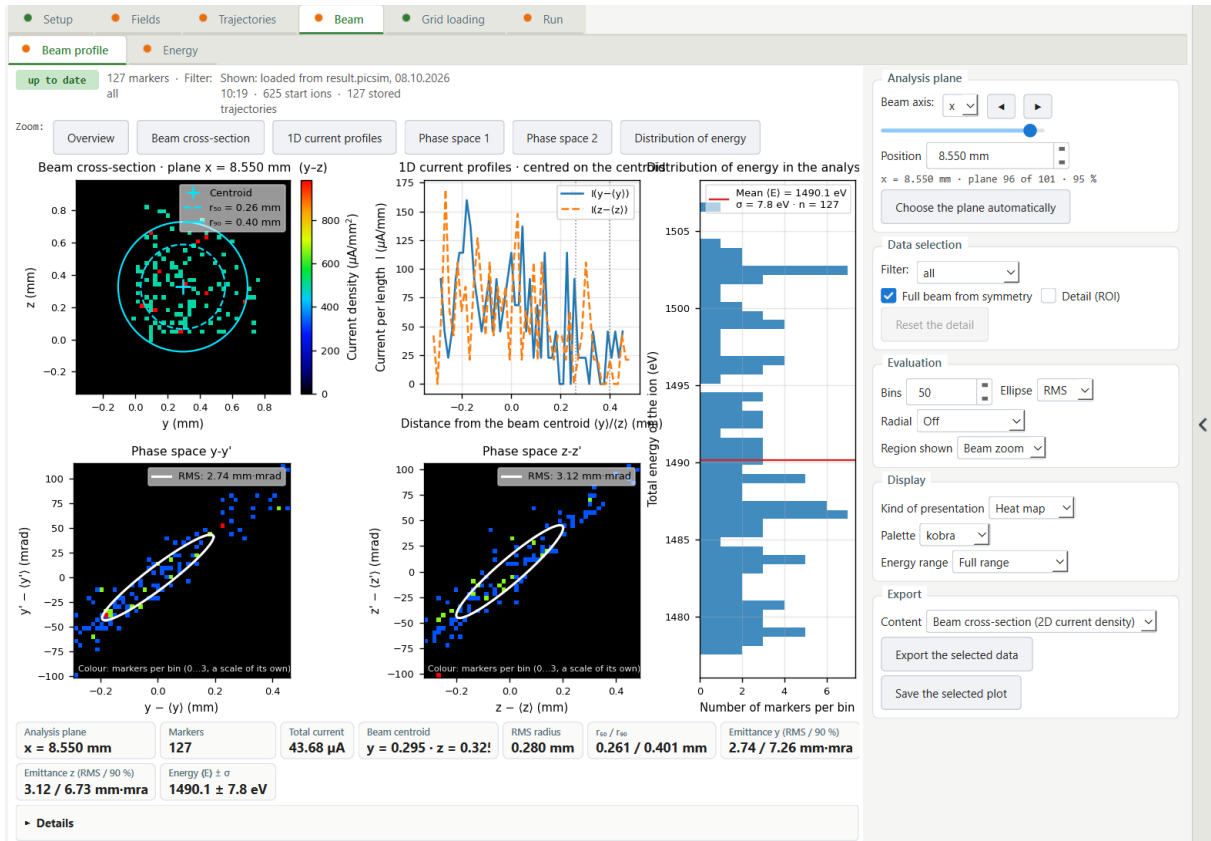


Figure 8.1: Beam → Beam profile: cross-section of the beam, current profiles, the two phase spaces and the energy distribution in the analysis plane, with the key figures below. The figures are those of the computed quarter cell (see the caution in the text).

The tab evaluates the beam in an *analysis plane* perpendicular to the beam axis. Every trajectory counts once, at the place where it first reaches the plane.

Analysis plane. The slider moves the plane in steps of one per cent of the domain length, by default to 95 %; the arrow buttons step to the neighbouring plane, and the position can be typed in millimetres. **Choose the plane automatically** selects the plane that is crossed by the most trajectories. **Beam axis** is x for plasma extraction.

Data selection. The filter restricts the evaluation to one result of the trajectories, for example the transmitted ions, and **Channel** to one aperture (Section 8.3). With **Full beam from symmetry** (on by default) a quarter or half model is completed to the full beam by mirroring, and the current is scaled accordingly; the status line then reads **Full beam reconstructed from symmetry**. **Detail (ROI)** restricts the evaluation to a rectangle drawn with the mouse in the cross-section: profiles, phase spaces, energy distribution and key figures then use only the trajectories inside it, and the status line gives their share of the current. **Reset the detail** removes the rectangle.

Caution. The completion to the full beam is applied only if the mirror planes are ticked by hand in the geometry dialog. With **Determine automatically from the aperture positions** (Section 4.4), which the bundled example uses, the tab evaluates the computed cell even though **Full beam from symmetry** is ticked, and the status line carries no remark on the symmetry. Total current, centroid, radii and emittances are then those of the quarter or half beam: in the example the total current is that of the quarter cell (Table 2.1) and the centroid lies off the axis, as in Fig. 8.1. To evaluate the full beam, untick the automatic setting, tick the mirror planes $y = 0$ and $z = 0$ and compute again.

Evaluation and Display. The number of classes of the histograms; which phase-space ellipse is drawn (RMS, 90 %, both or none); and a radial profile, either **Ring current $I(r)$** , the current per millimetre of radius, or **Density $j(r)$** , the current density over the radius. **Region shown** switches between the surroundings of the beam and the whole cross-section of the domain. The cross-section can be drawn as a density map or as a **Point cloud**. **Energy range $\rightarrow$ Main distribution** limits the energy axis to the range that contains 98 % of the trajectories. These settings change the pictures only, not the key figures.

Enlarging one plot. The row **Zoom** shows one of the plots alone: **Beam cross-section, 1D current profiles**, the two phase spaces or **Distribution of energy**; **Overview** returns to all of them. A double click into a plot does the same, **[Esc]** returns.

Export the selected data writes the data of the chosen plot as a table.

Table 8.1: Key figures of the beam profile.

Key figure	Definition
Total current	Number of macro-particles crossing the plane times the current each represents.
Beam centroid	Mean position in the two transverse directions.
RMS radius	$\sqrt{\langle r^2 \rangle}$ about the centroid.
r_{50} , r_{90}	Radii that enclose 50 % and 90 % of the current.
Emittance (RMS)	$\varepsilon_{\text{rms}} = \sqrt{\langle q^2 \rangle \langle q'^2 \rangle - \langle qq' \rangle^2}$ for each transverse direction q , with $q' = v_q/ v_x $. Geometric, not normalised, in mm mrad.
Emittance (90 %)	The phase-space ellipse that contains 90 % of the particles, on the same scale as ε_{rms} .
Energy	Mean kinetic energy and its standard deviation in eV.

The phase-space plots show the transverse position against the angle q' in mrad. A narrow, tilted distribution means an orderly diverging or converging beam; its width across the tilt is what the emittance measures.

Note. The tab states no single number for the beam divergence, such as a half-angle that contains 90 % of the current. The divergence is read from the phase-space plots, or computed from the exported data (**Export the selected data**).

8.2 Energy

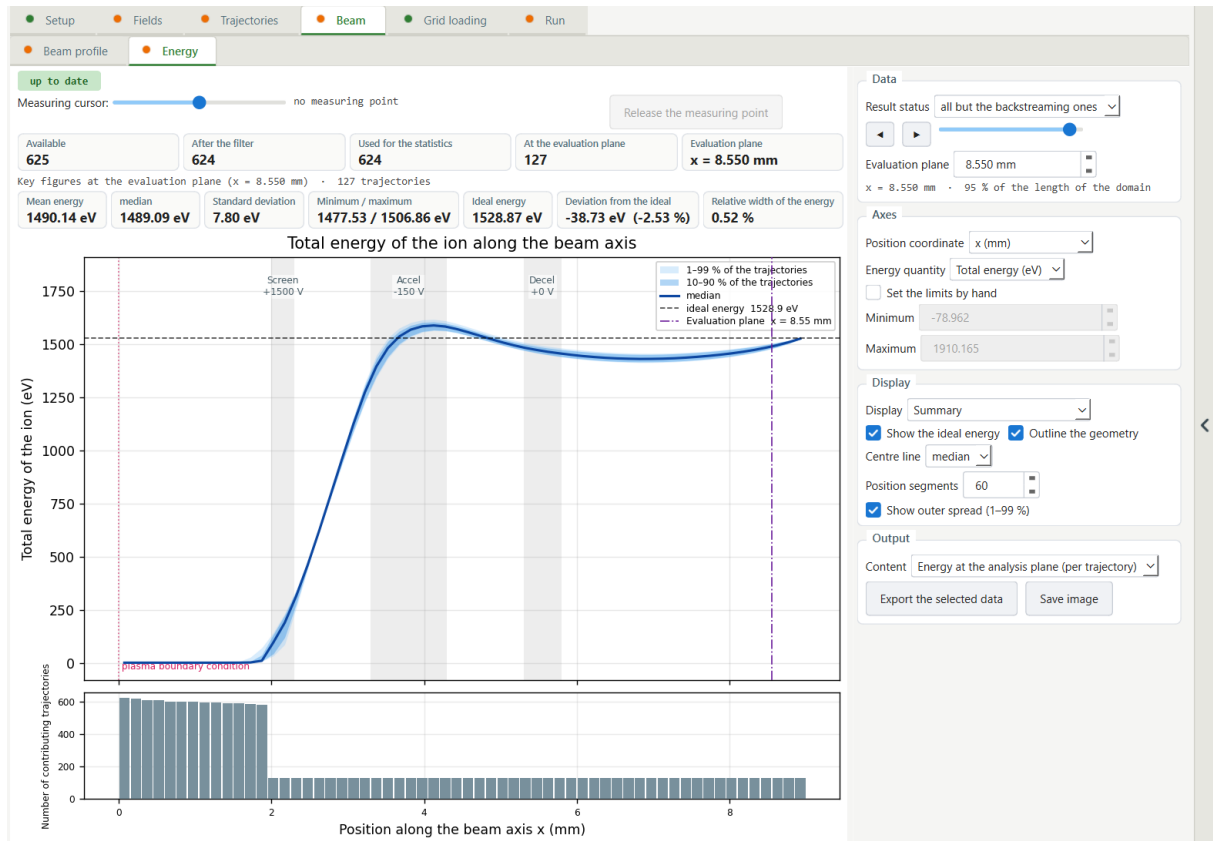


Figure 8.2: Beam → Energy, presentation **Summary**: the energy of the ions along the beam axis with the bands of spread, the positions of the electrodes and, below, the number of trajectories in each segment. Behind the screen grid only the extracted ions remain.

Beam → Energy shows the kinetic energy of the ions (Figs. 8.2 and 8.3). **Display** selects one of three presentations:

Summary

The energy along the beam axis, condensed over all trajectories: a centre line (**Centre line**: median or mean), the band that contains 10 to 90 % of the trajectories and, with **Show outer spread (1–99 %)**, a second, wider band. The axis is divided into **Position segments**; the bar chart **Number of contributing trajectories** below shows how many trajectories pass each segment. A segment drawn in red is passed by none, pale bars mark segments with few trajectories, where the statistics are weak.

Individual trajectories

One line per trajectory, at most **Max. individual trajectories** (a reproducible sample; 0 draws all). The lines can be coloured by the result of the trajectory or by aperture.

Energy at the evaluation plane

The distribution of the energy in one plane as a histogram, with lines for the mean, the median,

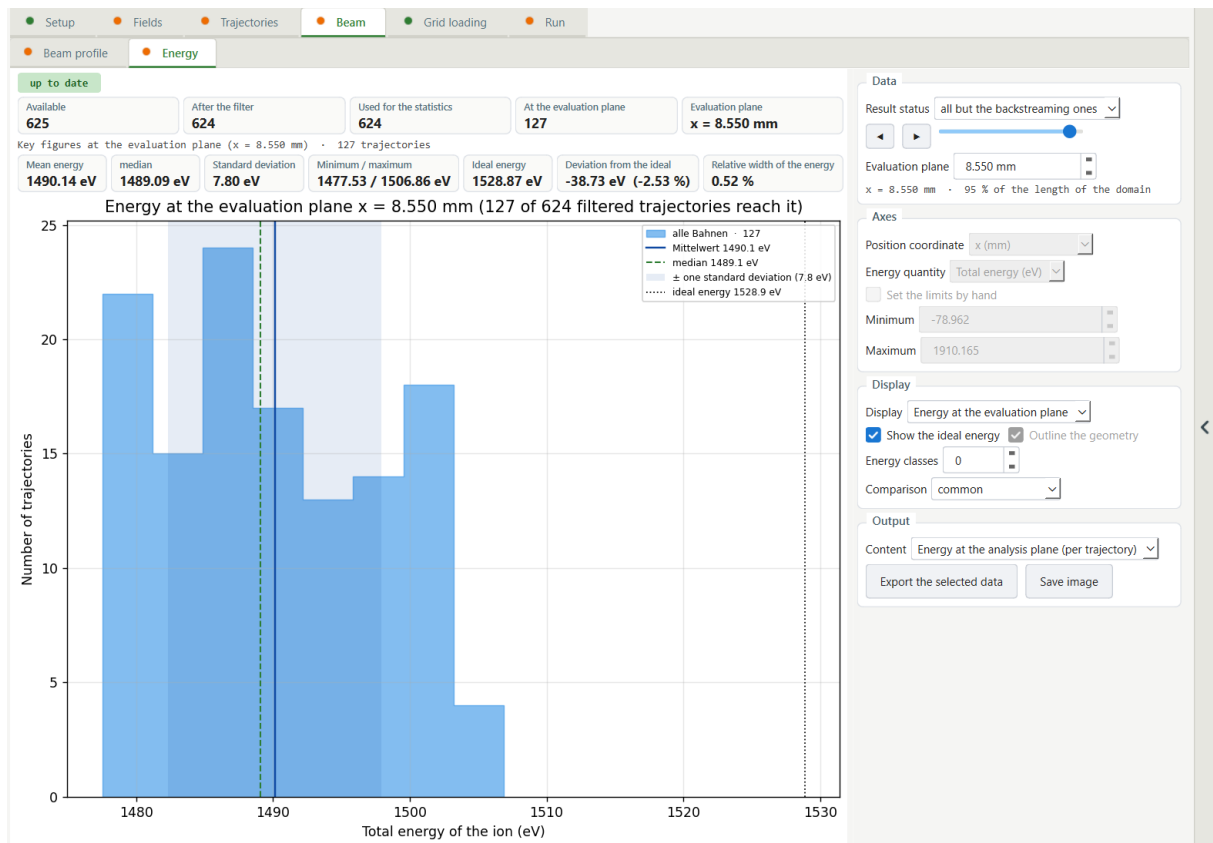


Figure 8.3: Presentation **Energy at the evaluation plane**: the distribution of the energy at 95 % of the domain length. The dotted line is the ideal energy.

the standard deviation and the ideal energy. **Comparison** splits it by the result of the trajectories or by aperture.

Under **Data**, **Result status** selects which trajectories enter; the default is all except those that return to the plasma. **Evaluation plane** sets the plane, by default at 95 % of the domain length, to which all key figures of the tab refer: the mean energy, the median, the standard deviation, the smallest and largest value, the **Relative width of the energy** (standard deviation divided by the mean) and the **Deviation from the ideal**. As in the beam profile every trajectory counts once, where it first reaches the plane; the badge **Plane not reached** appears if none gets there. The cards **Available**, **After the filter** and **Used for the statistics** state how many trajectories remain at each stage.

Under **Axes** the horizontal axis can be the position x or the **Path length s** , and the vertical axis the energy, the speed or the speed in units of the speed of light.

Show the ideal energy adds the energy an ion would have from the potential difference between the plasma and the exit face alone. The gap between this line and the computed energy at the exit is the potential hill of the beam's own space charge. **Outline the geometry** marks the positions of the electrodes along the axis.

Note. If a result was saved with thinned-out trajectories (Section 3.4), each trajectory consists of about 100 points. The summary interpolates between them, so it shows no false gaps, and the values at the evaluation plane are unchanged.

8.3 Several apertures

In a setup with more than one aperture centre in the first grid every trajectory is assigned to an *aperture channel*: the aperture whose centre is nearest to it in the yz plane. The channels are named A1, A2 and so on, with the position of the centre. Selectors for them then appear in several tabs:

- **Beam profile:** **Channel** restricts all plots and key figures to one aperture; **all** evaluates the whole beam.
- **Energy:** **Aperture channel**, and the colouring and comparison **by aperture channel**.
- **Trajectories** and the 3D view: one tick box per channel under **Aperture channels**, and the colour scheme **by aperture channel**.
- **Erosion:** **Aperture** selects the aperture whose surfaces are shown, or **all (together)**.

Choosing a channel changes the evaluation only. The trajectories were computed in the field of all apertures together, including the space charge of the neighbouring beamlets.

Note. In a mirrored unit cell with two aperture centres (Section 4.4) the two channels are fragments of equivalent apertures and should give the same figures within the statistical noise.

8.4 Where the currents are stated

Currents appear in three places, and they are not counted in the same way.

- The **Statistics** column on the right gives the extracted current, the beam current through the exit face and, under **CURRENTS**, the current at the screen grid, behind the last grid and in a freely chosen plane; the table below lists the current to each electrode and its share of the extracted and of the beam current. These currents are counted during the run from all particles. They are the currents of the *computed cell*: for a quarter aperture a quarter of the current of the aperture.
- The **Convergence** tab gives the same quantities for every round, also for the computed cell; its card **Extracted ion current** is the current through the exit face. Its planes lie slightly differently (at the front face of the last grid instead of its back face), so the values can differ a little from those of the **Statistics** column.
- The **Beam profile** tab counts the stored trajectories that cross the analysis plane. With **Full beam from symmetry** it states the beam current of the whole aperture, provided the mirror planes are set by hand; with automatically determined mirror planes it states the current of the computed cell (see the caution in Section 8.1).

Chapter 9

Background gas and charge exchange

9.1 Why the gas matters

Not all propellant leaves the discharge chamber as ions. The neutral atoms flow through the same apertures. A fast beam ion that passes close to a slow neutral atom can take over its electron: the result is a fast neutral and a slow ion. This slow *charge exchange ion* (CEX ion) is created in the middle of the grid system, does not have the energy to leave it, and is pulled onto the negative accel grid. These impacts are the main cause of grid erosion in normal operation.

To compute them, the program needs the density of the neutral gas in the whole domain: the *background gas map*.

9.2 The Background gas dialog

Background gas

Mode: TPMC (Knudsen flow, pressures entered by hand) [v] [Operating data ...]

Background gas: free (mass entered by hand) [v] (amu): 131.2930 [] T_{gas} (K): 300.0 [] T_{wall} (K): as gas []

Linear-model parameters

p_{plasma} (Pa): 1.000e-01 [] p_{vacuum} (Pa): 1.000e-04 []

TPMC parameters

Inlet pressure (Pa): 1.000e-01 []

Facility background (Pa): 0.000e+00 []

Pumping boundaries (capture per face)

x_{min} (inlet): 100 % []

x_{max} (outlet): 100 % []

y_{min} (side): 0 % []

y_{max} (side): 0 % []

z_{min} (side): 0 % []

z_{max} (side): 0 % []

Reflection: diffuse [v]

blue = reflecting · red = pump

3D plot showing a rectangular domain with axes x (0.0 to 1.0), y (0.0 to 1.0), and z (0.0 to 1.0). The x=0 face is blue (reflecting), and the x=1, y=0, y=1, z=0, and z=1 faces are red (pump). The x=1 face is also labeled 'x (beam)'.

Apply [OK] [Cancel]

Figure 9.1: The dialog **Background gas**.

Mode selects how the gas map is obtained:

TPMC (Knudsen flow, pressures entered by hand)

Test particles are started at the plasma side and followed through the grid system, bouncing off the walls, until they leave. Their dwell time in each cell gives the density. You enter the **Inlet pressure** of the neutral gas on the plasma side.

Linear ($p_{\text{plasma}} \rightarrow p_{\text{vacuum}}$, quick look)

A straight-line pressure drop from one end of the domain to the other. Instant, and only suitable for a first plausibility check.

Compute neutral gas state from operating data

The pressure on the plasma side is not entered but derived from quantities known from operation: beam current, mass flow or mass utilisation efficiency, number of apertures and the background pressure of the vacuum facility. This is the mode to use for a real thruster. The inputs are entered in a separate window opened with **Operating data ...** (Section 9.3).

Table 9.1: Entries for the TPMC mode.

Entry	Meaning
Background gas	Gas species and mass. It also determines which slow ions are created by charge exchange.
T_{gas} (K)	Temperature of the inflowing gas.
T_{wall} (K)	Temperature of the electrode surfaces. It changes the density near the walls, not the transmission.
Inlet pressure (Pa)	Neutral gas pressure on the plasma side, for <i>one</i> aperture. Typical values lie between 0.01 and 1 Pa.
Facility background (Pa)	A uniform pressure added everywhere, as in a vacuum chamber. 0 corresponds to operation in space.
Capture fractions of the faces	How much of the gas reaching a domain face is pumped away. 100 % at inlet and outlet is a perfect pump.
n_{markers}	Number of test particles. More gives a smoother map.
max_{bounces}	Safety limit for wall collisions per particle. Not an accuracy setting; do not reduce it.
Seed	Start value of the random numbers, for reproducibility.

The same dialog contains the settings for the charge exchange itself:

- **Charge exchange during the run** switches the evaluation on.
- **sigma model** selects the cross section σ (Table 9.2).
- **Collision partner** is the gas species the ions collide with.
- **Track secondary ions** follows the slow ions to where they end. This is required for erosion.

The formulas are used at the energy the beam ions have, also where this lies above the range of the measurements; for a xenon beam of 1 to 2 keV the xenon fit is an extrapolation. In addition to the predefined models the dialog accepts a constant cross section, own coefficients of the same formula, and a table of values.

Table 9.2: Predefined charge exchange cross sections. E is the kinetic energy of the ion in eV, σ is in $\text{\AA}^2 = 10^{-20} \text{ m}^2$.

Reaction	σ	Source
$\text{Xe}^+ + \text{Xe}$	$87.3 - 13.6 \log_{10} E$	Fit of Miller et al. [2] to their measurements between 1 and 300 eV.
$\text{Xe}^{2+} + \text{Xe}$ (both electrons)	$45.7 - 8.9 \log_{10} E$	The same work, measured at ion energies of 2 to 600 eV. Used for the doubly charged fraction of the beam.
$\text{Xe}^{2+} + \text{Xe}$ (one electron)	2.8 above 10 eV, 0 below	An estimate: [2] gives the onset and the value at 600 eV, but no formula. Can be switched off.
$\text{N}_2^+ + \text{N}_2$	$40.9 - 5.14 \log_{10} E$	Fitted to the table of Phelps [4] between 30 eV and 5 keV.
$\text{N}^+ + \text{N}_2$	4.76	Mean of the table of [4] between 30 and 1000 eV.
$\text{Kr}^+ + \text{Kr}$	$68.0 - 11.0 \log_{10} E$	An estimate between argon and xenon, not a measurement.
$\text{Ar}^+ + \text{Ar}$	$52.0 - 8.0 \log_{10} E$	Approximate values, not fitted to a specific measurement.

Caution. The cross section models are valid for one combination of beam ion and gas only. The ion species (**Simulation** dialog) and the collision partner must both be set to a predefined species, for example Xe. With a freely typed ion mass and no species the charge exchange cannot be evaluated, and the run says so.

9.3 Gas state from operating data

In operation the neutral gas pressure in the discharge chamber is rarely known, but the beam current and the propellant flow are. The mode **Compute neutral gas state from operating data** derives the pressure from these. **Operating data ...** opens the window **Background gas — neutral-gas state from operating data**. It has three pages, listed on the left; a page that still needs an input is marked in red. The window works on a copy of the settings: **Apply** adopts them, **Cancel** restores the last confirmed state.

The model. The window computes one *representative inner channel* of a large hexagonal grid: a hexagonal cell around one aperture whose side faces reflect the gas atoms like mirrors. From the operating data follows the flow of neutral atoms that must pass through each channel:

$$\dot{m}_{\text{ion}} = \frac{I_{\text{beam}}}{z e} m, \quad \dot{m}_{\text{feed}} = \frac{\dot{m}_{\text{ion}}}{\eta_m}, \quad \dot{m}_{\text{neutral}} = \dot{m}_{\text{feed}} - \dot{m}_{\text{ion}},$$

divided by the number of apertures. Two test-particle calculations in the cell, one starting on the discharge side and one on the facility side, give the probabilities W_{fwd} and W_{back} that an atom entering the cell passes the grid system. With the transport coefficient $G = A_{\text{cell}} W / \sqrt{2\pi m k_B T}$ of each direction the net flow through the channel is

$$\dot{N}_{\text{channel}} = G_{\text{fwd}} p_{\text{RIT}} - G_{\text{back}} p_{\text{facility}},$$

which is solved for the pressure p_{RIT} on the discharge side. The transmission is computed for the actual geometry; no tube formula and no optical transparency is used. The button ? on the card **Representative inner grid channel** shows the full description.

Page 1: Operating data.

Representative inner grid channel

- IONTRACE computes one channel in the interior of the grid.
- The neutral gas flow follows from the ion current and the gas balance.
- A TPMC computation gives the transmission, the backflow, the pressure in the thruster and the distribution of the neutral gas.
- Radial differences at the edge of the complete grid are not taken into account.

1. Operating data

2. Channel model

3. Computation and results

Gas and reservoirs

Gas species: Xe 131.2930 u

Gas temperature RIT side: 450.0 K

Gas temperature facility: 300.0 K

Facility background pressure: 0.001000000 Pa $= 1 \times 10^{-3}$ mbar

Grid arrangement

Number of apertures: 121 Apertures

Grid type: hexagonal

Centre spacing (pitch): 2.4000 mm

Wigner-Seitz cell
inradius 1.2 mm,
circumradius 1.386 mm,
area 4.988 mm²

Ion current

Prescribed is: per aperture

Ion current per aperture: 134.1000 μA

Total beam current: 16.226100 mA
computed from the current per aperture

Gas balance

Prescribed is: Mass utilisation efficiency

Mass efficiency η_m : 52.200 %

Computed from the operating data

Total beam current: **16.23 mA**
134.1 μA per aperture

Ion mass flow: **0.02208 mg/s**

mass flow fed: **0.0423 mg/s**
0.4333 sccm

residual neutral mass flow: **0.02022 mg/s**
Mass efficiency 52.2 %

neutral particle flow per channel: **$7.664 \times 10^{14} \text{ s}^{-1}$**
total $9.274 \times 10^{16} \text{ s}^{-1}$

Show computation details ...

done — RIT pressure 0.1036 Pa, forward transmission 0.1385

Apply Cancel

Figure 9.2: The window for the operating data, page **Operating data**. On the right the quantities that follow from the entries.

Table 9.3: Entries of the page **Operating data**.

Entry	Meaning
Gas species	The propellant.
Gas temperature RIT side	Temperature of the neutral gas in the discharge chamber (default 450 K).
Gas temperature facility	Temperature of the gas that flows back from the vacuum chamber (default 300 K).
Facility background pressure	Pressure in the vacuum chamber, in Pa or mbar. It is the pressure of the reservoir behind the grids, not the local density between them.
Number of apertures	Only converts between the values of one channel and those of the whole grid.
Centre spacing (pitch)	Distance between neighbouring aperture centres. The line Wigner-Seitz cell shows the resulting hexagonal cell and its area.
Ion current per aperture, Total beam current	One of the two is entered, chosen with Prescribed is ; the other follows from the number of apertures.

Entry	Meaning
Mass efficiency η_m , mass flow fed	One of the two is entered, again chosen with Prescribed is . The mass flow can be given in mg/s or in sccm (referred to 273.15 K and 101325 Pa).
active grid diameter	For documentation only; not used in the calculation.

On the right, **Computed from the operating data** shows the total beam current, the ion mass flow, the mass flow fed, the residual neutral mass flow and the neutral particle flow per channel. An impossible balance, for example a feed below the ion mass flow, is reported there.

Page 2: Channel model. A sketch drawn from the loaded geometry shows the discharge side, the grids at their true position, the facility side and the hexagonal cell (Fig. 9.3). The program assigns the roles **Screen grid**, **Accel grid** and **Decel grid** to the electrodes and determines the **Direction of extraction**. A traffic light states the outcome: green means recognised without doubt; yellow means ambiguous, and the calculation stays blocked until **Roles and direction confirmed** is ticked; red names an obstacle, for example a cell that does not fit into the computational domain.

The table **Grid surfaces** sets, for each grid, the wall temperature and how gas atoms leave the surface: **diffuse (cosine distribution)**, the default and the usual assumption for technical surfaces, **specular (mirror)**, or **mixed (Maxwell)** with a **Diffuse fraction**. A **Sticking fraction** above zero removes that share of the atoms at the wall.

Note. If the computational domain is a mirrored unit cell with two aperture centres (Section 4.4), the window computes exactly one of the equivalent channels and takes the centre spacing from the aperture pattern. If the pitch entered on page 1 differs from it by more than 0.5 %, a note states both values. The entered pitch is then used for the gas balance only.

Page 3: Computation and results. **Profile** sets the statistical accuracy of the transmission: **Preview** (3 %), **Default** (1 %), **Precise** (0.3 %) or **Set by hand**. The **Readiness** list must be complete before **Start the calculation** is enabled. The result cards give the **RIT pressure**, the **RIT neutral gas density**, the **Forward transmission** and **Back transmission** with their statistical uncertainty, the **Backflow fraction** and the residual neutral mass flow. If an input is changed afterwards, the page says that the result belongs to older inputs.

For the bundled example the roles are not stored in the setup, so the traffic light on page 2 first shows **Confirmation needed**; after ticking **Roles and direction confirmed** the calculation can be started.

The calculation also produces the gas map. **Apply** hands it to the tab Grid loading → Background gas; **Show the results in the background-gas tab** does the same and switches to that tab. In this mode **Compute the map** in the tab uses the same operating data.

Caution. The model describes an inner channel of a large hexagonal grid in free molecular flow. It does not describe the edge of the grid, radial differences across the grid, or the expansion of the gas far downstream. Round, rectangular and elliptical apertures are supported. The aperture centres must lie on mesh nodes, and the hexagonal cell must lie completely inside the computational domain; otherwise the window refuses to start and names the reason.

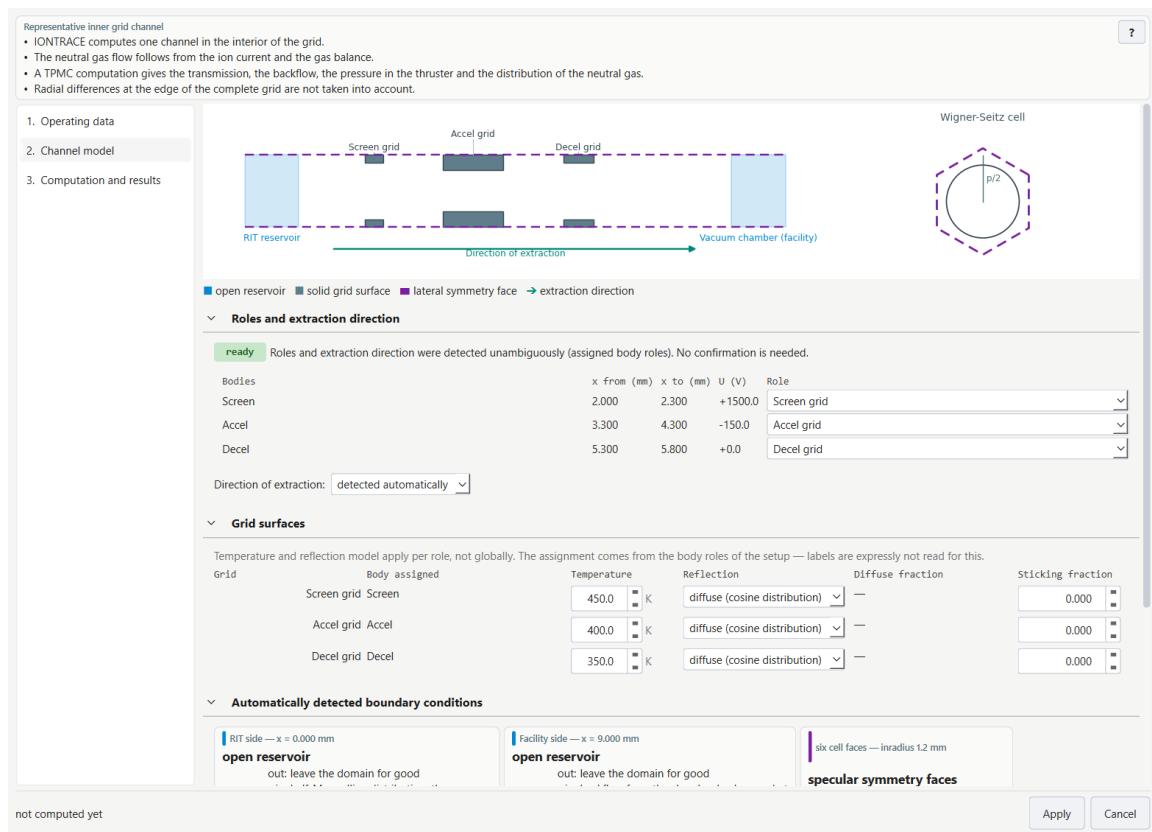


Figure 9.3: Page **Channel model**: the sketch of the channel drawn from the geometry of the example, the roles of the electrodes and the properties of the grid surfaces.

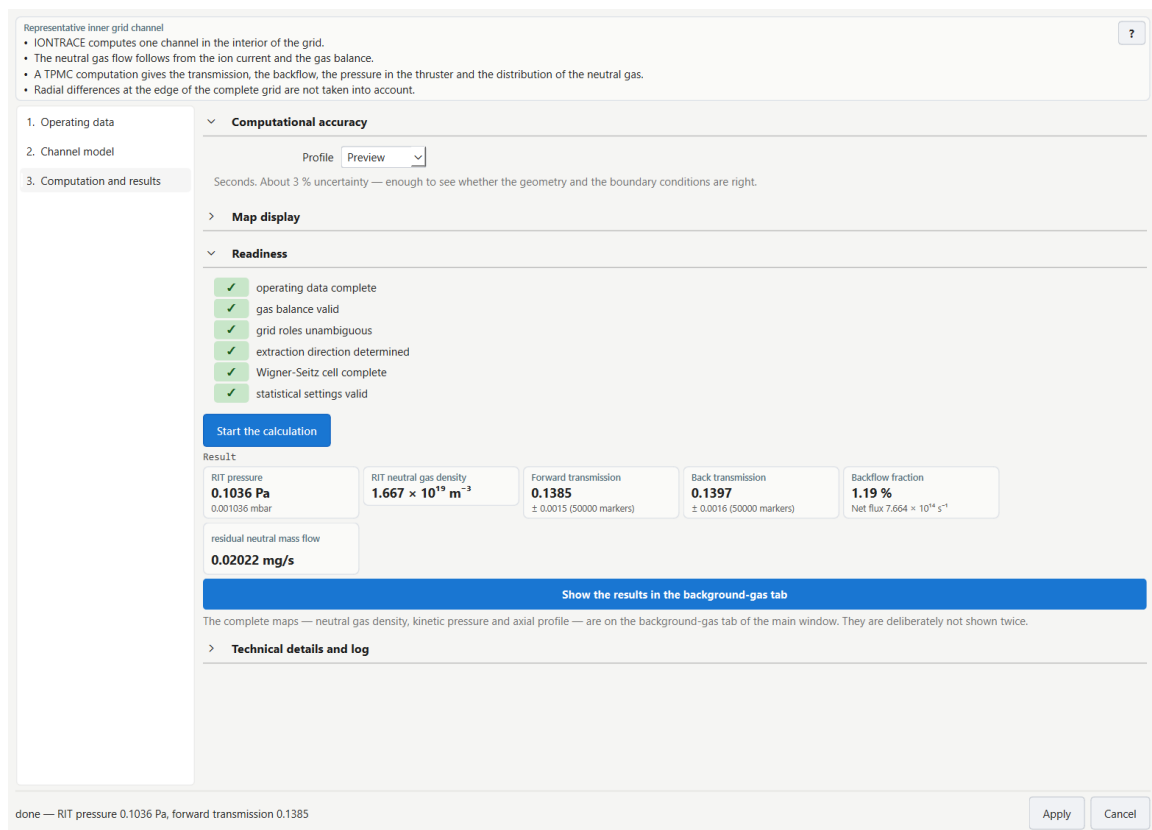


Figure 9.4: Page **Computation and results** after a calculation with the profile **Preview** for the example: the pressure and density on the discharge side and the two transmission probabilities.

9.4 The gas map

Grid loading → Background gas shows the map and its state. **Compute the map** is the only action in this tab that costs computing time. The map can be shown as density, as an equivalent pressure, or as an axial profile.

A gas map belongs to the geometry and gas settings it was computed for. When one of them changes, the card **State of the map** turns to **out of date**. Voltages, materials and display options do not affect it. When a calculation is started with an outdated map, the program asks whether to recompute it, to run without charge exchange, or to cancel.

The map can be stored inside the `.picsetup` file, so that it does not have to be recomputed after loading.

9.5 The CEX tab

Grid loading → CEX shows where the slow ions are born (**Birth map**), the paths they take (**Secondary trajectories over birth map**) and where they strike (**Impacts on electrodes**). The cards state the total rate at which they are created and the current they represent.

Compute charge exchange repeats this evaluation on the existing result, for example after the gas map has changed. It does not solve the field again and takes seconds.

Note. Key figures in this tab are stated for the whole aperture, also when only a symmetry cell was computed. The value for the computed cell is shown beneath.

Chapter 10

Erosion and lifetime

10.1 From impacts to erosion

Each ion that strikes an electrode removes atoms from it. How many is given by the *sputter yield* $Y(E, \theta)$, which depends on the ion species, its energy E , the angle of incidence θ against the surface normal and the material of the electrode.

Table 10.1: Sputter models.

Model	Use
Yamamura/Tawara 1996	The empirical formula of Yamamura and Tawara [8] for the yield at normal incidence, for any atomic ion on any single-element target, with the material parameters tabulated there. Inaccurate close to the sputter threshold, in particular for xenon on carbon below about 250 eV.
Tartz/Neumann 2007	The description of Tartz and Neumann [6], fitted to their measurements of xenon on carbon materials, including its own dependence on the angle. Valid for this combination only; with any other the calculation refuses to start.
Tartz/Neumann 2007 for carbon, otherwise Yamamura/Tawara 1996	Chooses per electrode. The recommended setting for xenon thrusters with a carbon accel grid and a molybdenum screen grid.

A fourth entry, **Compatibility: earlier hybrid form**, reproduces results of earlier program versions and should not be used for new work.

The work of Yamamura and Tawara treats normal incidence only. For oblique incidence the program multiplies their yield by a factor of the form introduced by Yamamura et al. [7],

$$\frac{Y(E, \theta)}{Y(E, 0)} = \cos^{-f} \theta \exp \left[f \cos \theta_{\text{opt}} \left(1 - \frac{1}{\cos \theta} \right) \right],$$

with the two material parameters f and θ_{opt} (Table 4.3), which do not depend on the energy. Angles above 85° are treated as 85° .

Predefined materials are molybdenum (Mo), graphite (C), carbon–carbon composite (C-C), titanium (Ti) and tungsten (W). Further materials can be defined with **Material ...** in the geometry dialog (Section 4.6). The carbon–carbon composite uses the sputter parameters of

graphite and differs from it only in its density; the lower yield at oblique incidence that was measured for this material [3] is not reproduced.

The projectile of the erosion is the slow ion created by charge exchange, that is, the species set as **Collision partner** in the **Background gas** dialog. Its sputter yield can only be computed for a predefined species; with a freely typed mass the trajectories are computed, but the erosion calculation refuses to start.

Molecular ions. For nitrogen and oxygen the program offers atomic and molecular ions (N, N₂, O, O₂), and charge exchange cross sections for N⁺ and N₂⁺ in nitrogen. A molecular ion is followed as one particle with its full mass. Only when it strikes a wall is it treated as its atoms: each atom receives the share of the energy that corresponds to its mass, and the yields are added. For N₂⁺ of energy E this gives

$$Y_{N_2}(E, \theta) = 2 Y_N(E/2, \theta).$$

The log notes this for every combination of ion and material.

Caution. The sputter formula is fitted mainly to noble gas ions. For nitrogen on tungsten it gives yields about 1.5 times the measured ones. Chemical effects, such as the formation of nitrides or chemical erosion of carbon by oxygen, are not included. Erosion results for molecular gases are estimates to be calibrated with **Scale factor of the sputter yield**.

Scale factor of the sputter yield multiplies all yields by a constant. It is meant for calibrating the model against a measured erosion and is reported separately from the model name.

Caution. Most charge exchange ions strike the accel grid with an energy close to the accel voltage, typically 150 to 400 eV. This is the range in which sputter yields are small, steep in energy and least certain. A change of the sputter model can change the computed erosion by a large factor. State the model with every result.

As an indication of the accuracy of the general formula: compared with 127 published measurements of xenon on Mo, W, Ti and C, the formula of [8] as implemented gives in the median 0.77 times the measured yield, with a mean deviation of 33 %, and is furthest off for tungsten and near the threshold. This uncertainty of the model is independent of how well a calculation has converged (Chapter 13).

10.2 The Erosion tab

Grid loading → Erosion shows the impacts on one electrode as maps of three surfaces: the **Front face** towards the plasma, the **Aperture wall** (unrolled), and the **Back face** towards the beam.

Compute the erosion distribution creates the impacts: a chosen number of slow ions is started according to the birth map and followed to the wall. The map can be shown as erosion rate in nm/h, as current density or as atom flux. The table lists impacts, current and sputter rate per surface.

10.3 Redeposition

Sputtered atoms do not disappear. They fly in straight lines until they meet a surface, and part of them settles there. The folded group **Redeposition** in the **Erosion** tab balances where the

sputtered material goes. It needs an erosion distribution; then **Compute redeposition** follows, from every impact, a number of sputtered atoms through the geometry.

- **Rays per hit:** how many directions are followed from each impact. More gives smoother maps.
- **Emission:** the angular distribution of the sputtered atoms about the surface normal, **Cosine (Lambert)** or a power of the cosine with the **Exponent n**.
- **Sticking:** probability that an atom stays where it lands. With a value below 1 the remaining atoms leave the surface again diffusely and are followed further.

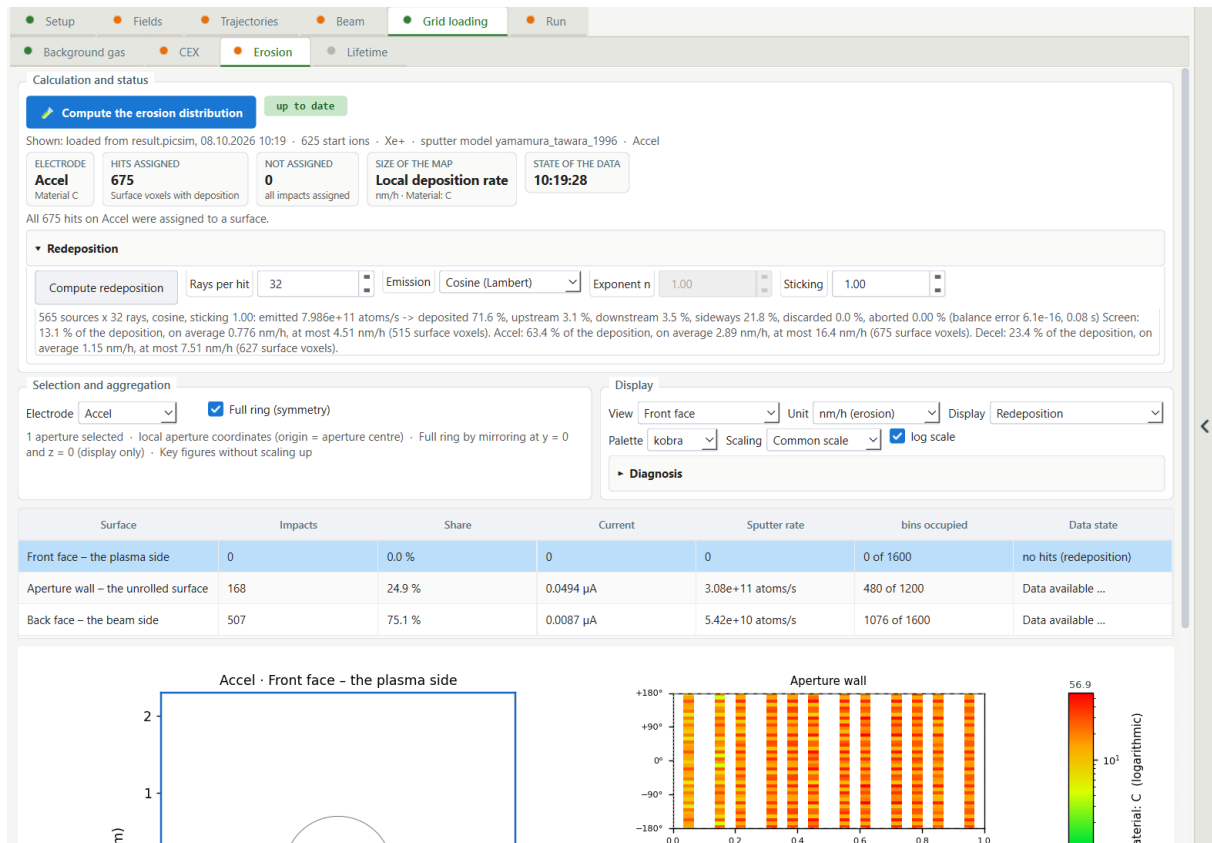


Figure 10.1: Grid loading → Erosion for the accel grid of the example with the group **Redeposition** unfolded and the map switched to **Redeposition**. The text below the settings is the balance.

The result is a balance (Fig. 10.1): which share of the sputtered atoms is deposited on an electrode, which leaves the domain upstream towards the plasma, downstream with the beam, or sideways; and for every electrode its share of the deposit and the mean and largest deposition rate in nm/h. In the group **Display** of the tab the map can then be switched between **Erosion**, **Redeposition** and **Net (erosion – redeposition)**. The 3D view offers erosion and redeposition under **Quantity**.

In a lifetime simulation **Balance the redeposition** repeats this balance in every step, with the settings of the **Erosion** tab, and the **Lifetime** tab states the shares of the last balanced step.

Caution. The redeposition is a balance only. The deposited material does not change the geometry, the field or the erosion rate: an aperture that would in reality partly close again by deposition keeps widening in the lifetime simulation. Material sputtered from the walls of the vacuum facility is not included.

10.4 The lifetime simulation

A single calculation gives the erosion *rate* of the new grid. As the apertures widen, the field, the beam and the gas flow change, and with them the rate. The lifetime simulation follows this development by repeating the whole chain in steps of operating time:

1. Compute the field and the beam on the current geometry.
2. Compute the charge exchange ions and their impacts.
3. Convert the impacts into a removal rate for every wall cell.
4. Advance the operating time by one step and remove the material.
5. From time to time, recompute the gas map on the eroded geometry.
6. Store a snapshot and continue with step 1.

It is started in Grid loading → Lifetime with **Start lifetime simulation**. Requirements are a finished single calculation with charge exchange and a current gas map.

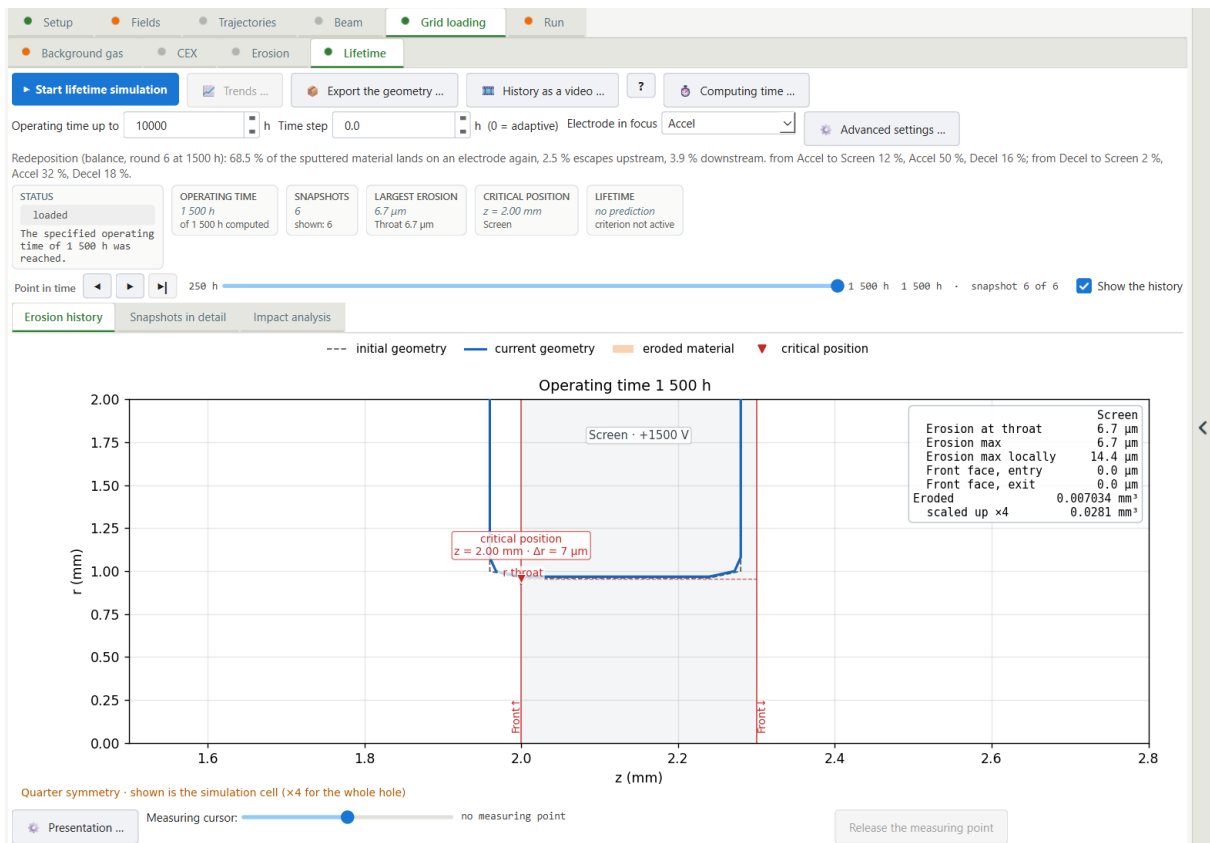


Figure 10.2: Grid loading → Lifetime after a short run of the example. The plot shows the wall radius over the axial position: the original geometry dashed, the current one in blue, the removed material shaded. Earlier points in time appear as coloured lines.

Table 10.2: Settings of the lifetime simulation. The first three are in the tab, the others under **Advanced settings**

Entry	Meaning
Operating time up to	Total operating time to simulate, in hours.
Time step	Length of one step in hours. With 0 the program chooses the step itself so that a given number of cells is emptied per step.
Electrode in focus	The electrode whose erosion is evaluated in the plot and the table. It can be changed after the run.
Voxel threshold per step	For the automatic time step: how many wall cells may be emptied in one step.
Max. steps	Upper limit for the number of steps.
N_target erosion	Number of slow ions followed per step. More gives smoother erosion.
PIC rounds per step	Iteration rounds of the field and beam calculation in each step.
Warm start from the previous step	Each step starts from the field of the previous one, which saves most of the rounds.
Current control	Lag control adjusts the plasma density after each step so that the beam current stays at the target value, as a thruster controller would.
Calibrate j_i at $t=0$	Adjusts the plasma density before the first step until the target beam current is met.
Sputter model, Scale factor	See Table 10.1.
Erosion $\rightarrow$ field	The eroded shape is fed back into the field calculation. On by default; without it the erosion would not change the beam.
Sub-voxel	The wall recedes continuously within a cell instead of in steps of whole cells (Section 10.7).
Wall direction from the eroded shape	The angle of incidence is taken from the eroded surface, not from the original straight bore.
Primary-beam impacts	Also counts erosion by beam ions that strike a grid directly. In normal operation this is zero.
Recompute the gas map every ...	When the gas map is renewed on the eroded geometry: after a number of removed cells or after a number of hours.
Measure the neutral-gas transparency, Transparency every ...	Determines at intervals how much neutral gas the eroded grid system lets through (Section 10.6). Off by default.

10.5 Reading the Lifetime tab

The cards above the plot give the operating time reached, the number of snapshots, the **Largest erosion** and the **Critical position**.

Point in time. The slider selects the snapshot. This choice also determines which wall the

field tabs and the 3D view show when **eroded wall** is ticked.

Erosion history. The wall radius over the axial position, averaged around the aperture.

Snapshots in detail. One row per step (Table 10.3).

Impact analysis. Energy and angle distributions of the stored impacts, per step or for the whole run (Section 10.8).

Table 10.3: Columns of **Snapshots in detail**. All erosion values are increases of the *radius*, not of the diameter.

Column	Meaning
Erosion at the throat	Widening of the narrowest point of the aperture. This is what changes the ion optics.
Erosion max	Largest widening along the aperture, averaged around the circumference.
Erosion max locally	Largest widening in any direction around the circumference. Larger than the previous value when the erosion is not rotationally symmetric, as in a hexagonal pattern.
Front face, entry / exit	Recession of the upstream and downstream face of the electrode.
I_beam	Extracted beam current in this step.
I_focus	Beam current striking the electrode in focus directly. Zero means erosion by charge exchange ions only.

Caution. The program does not predict a lifetime. It detects one event only: the onset of direct beam impact on a grid, and only if **Primary-beam impacts** is switched on. Whether a given widening of the accel aperture is acceptable (electron backstreaming, structural failure) must be judged from the computed geometry.

Continuing a run. If a lifetime result for the same geometry and mesh is present, the start button reads **Continue from ... h**, and the operating time entered counts as additional hours. Voltages, current and gas settings may be changed between the segments.

10.6 Trends and neutral-gas transparency

Trends ... in the **Lifetime** tab opens the window **Lifetime trends** (Fig. 10.3) with four plots over the operating time: the currents, the transmission, the widening of the aperture together with the recession of the faces, and the number of removed cells together with the time step.

As the apertures widen, more neutral gas escapes through the grids. At the same propellant flow the pressure in the discharge chamber then falls. The *neutral-gas transparency* quantifies this: it is the probability that a gas atom entering the first aperture from the discharge side leaves the grid system downstream (**Neutrals outward**), and the same for an atom entering the last aperture from the facility side (**Neutrals inward**). Both are computed with the channel model of Section 9.3 on the eroded wall and are drawn in the transmission plot of the trends window, the outward value with its statistical uncertainty.

A value is obtained on two occasions:

- Whenever the gas map is recomputed during the run, provided the gas mode is **Compute**

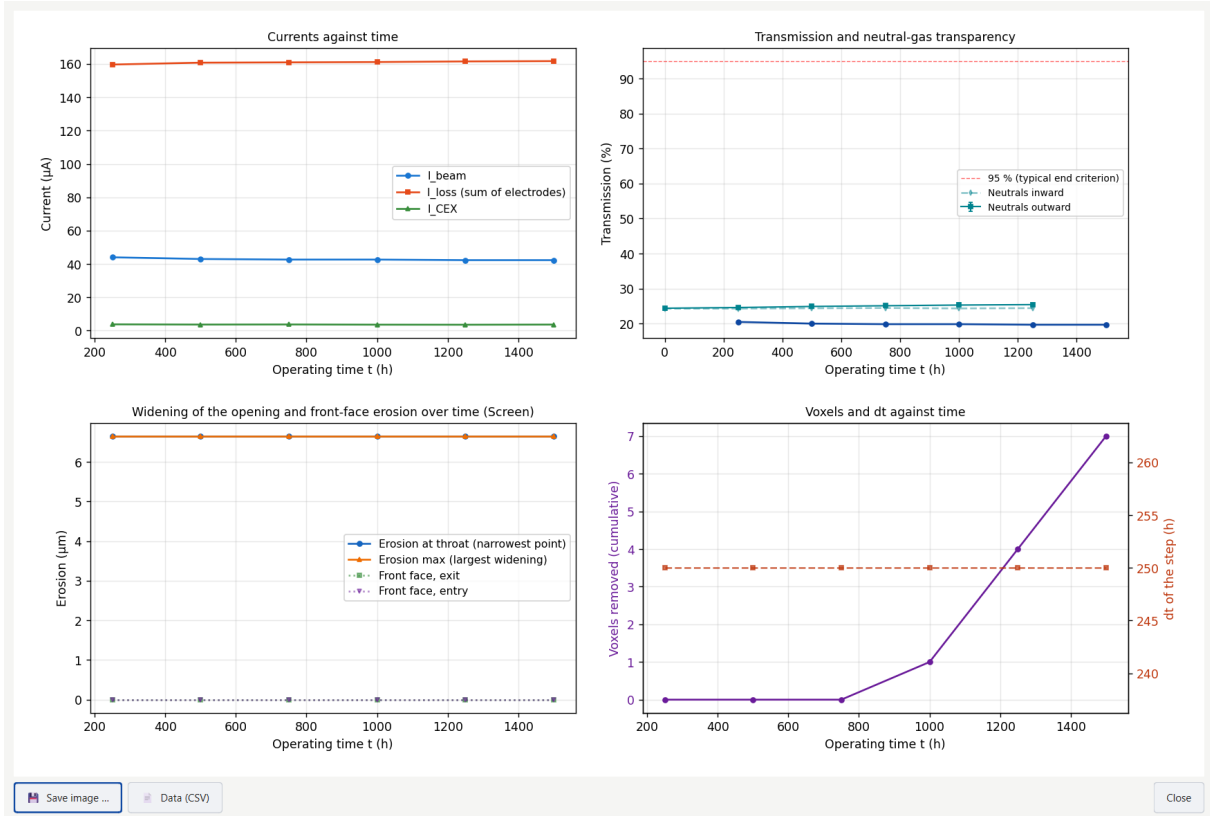


Figure 10.3: The window **Lifetime trends** after a short lifetime simulation of the example with the measurement of the neutral-gas transparency switched on.

neutral gas state from operating data. This costs nothing extra.

- With **Measure the neutral-gas transparency** ticked (window **Lifetime — advanced settings**, section **Background gas and transparency**): at the start of the run as a reference, and then after the number of removed cells or the number of hours entered under **Transparency every . . .**. This measurement works with any gas mode and does not change the gas map the run uses.

In both cases the roles of the electrodes must have been assigned in the window for the operating data (Section 9.3). The values are saved with the result and written, step by step, into the protocol file `lebensdauer.json` of the run.

10.7 The eroded wall in the other tabs

With **eroded wall** ticked, the field tabs draw the wall of the selected lifetime snapshot (Fig. 10.4). Two points need care.

The field is not the field of the eroded wall. A snapshot stores the geometry, not the fields. The eroded outline is laid over the field of the original calculation, and the field status reads **overlay only**. To see the field that belongs to the eroded shape, press **Compute the field for this state of the wall . . .**

Two ways to draw the eroded wall. During the lifetime simulation every wall cell has a *fill level* between 1 (untouched) and 0 (empty). The field calculation places the wall where the fill level is one half. In the stored cell occupancy, however, a cell counts as material until it is

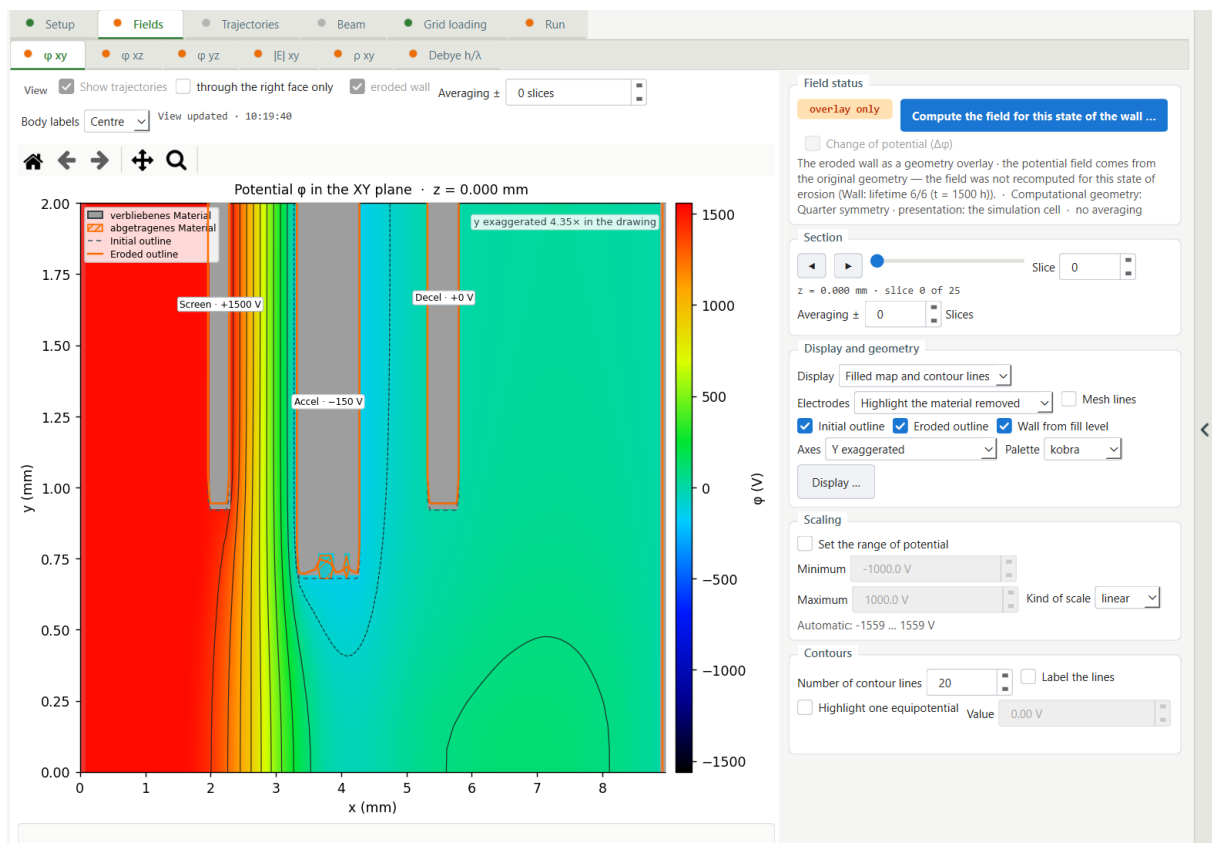


Figure 10.4: The potential section with **eroded wall** ticked. The eroded outline is drawn in orange, the initial outline dashed, and the removed material hatched. The badge **overlay only** says that the field shown still belongs to the original geometry.

completely empty.

- **Wall from fill level** ticked (default): the outline is drawn where the fill level is one half. This is the wall the calculation used. It is smooth.
- Not ticked: the outline follows the cell occupancy. Cells with a remainder of a few per cent then stand as full cells. The outline shows single-cell teeth that have no physical meaning, and the erosion appears shallower than it was computed.

10.8 Impact analysis

Every lifetime simulation stores, for each step, the complete list of impacts: position, energy, angle of incidence, the electrode struck and the current each impact represents. The list does not contain a sputter yield. The sub-tab **Impact analysis** therefore allows the same bombardment to be evaluated with a different sputter model or scale factor afterwards, without repeating the simulation, and to compare two models directly.

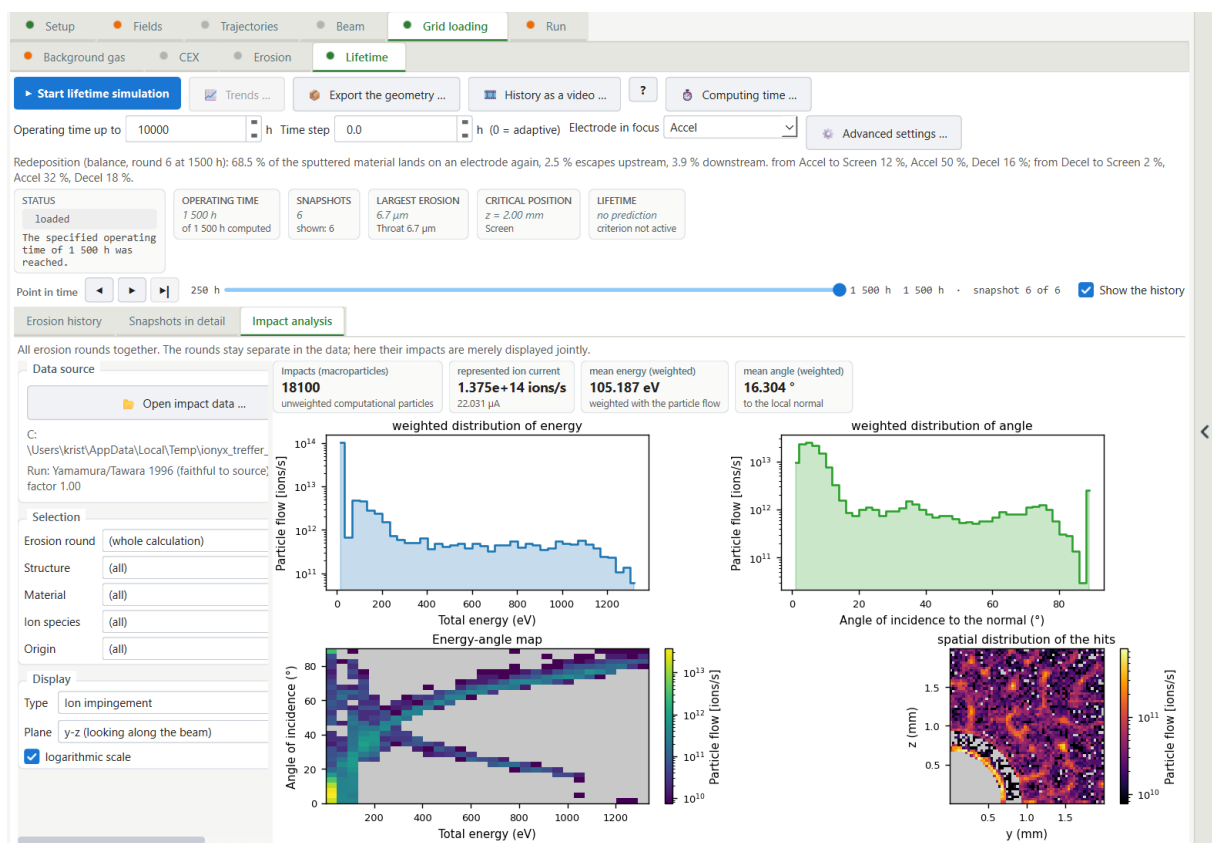


Figure 10.5: Impact analysis: energy and angle distribution of the impacts, the energy–angle map and their spatial distribution.

Chapter 11

The 3D view

Trajectories → 3D view shows geometry, trajectories and surface quantities in space. The view is rotated with the left mouse button, moved with the middle button and zoomed with the wheel.

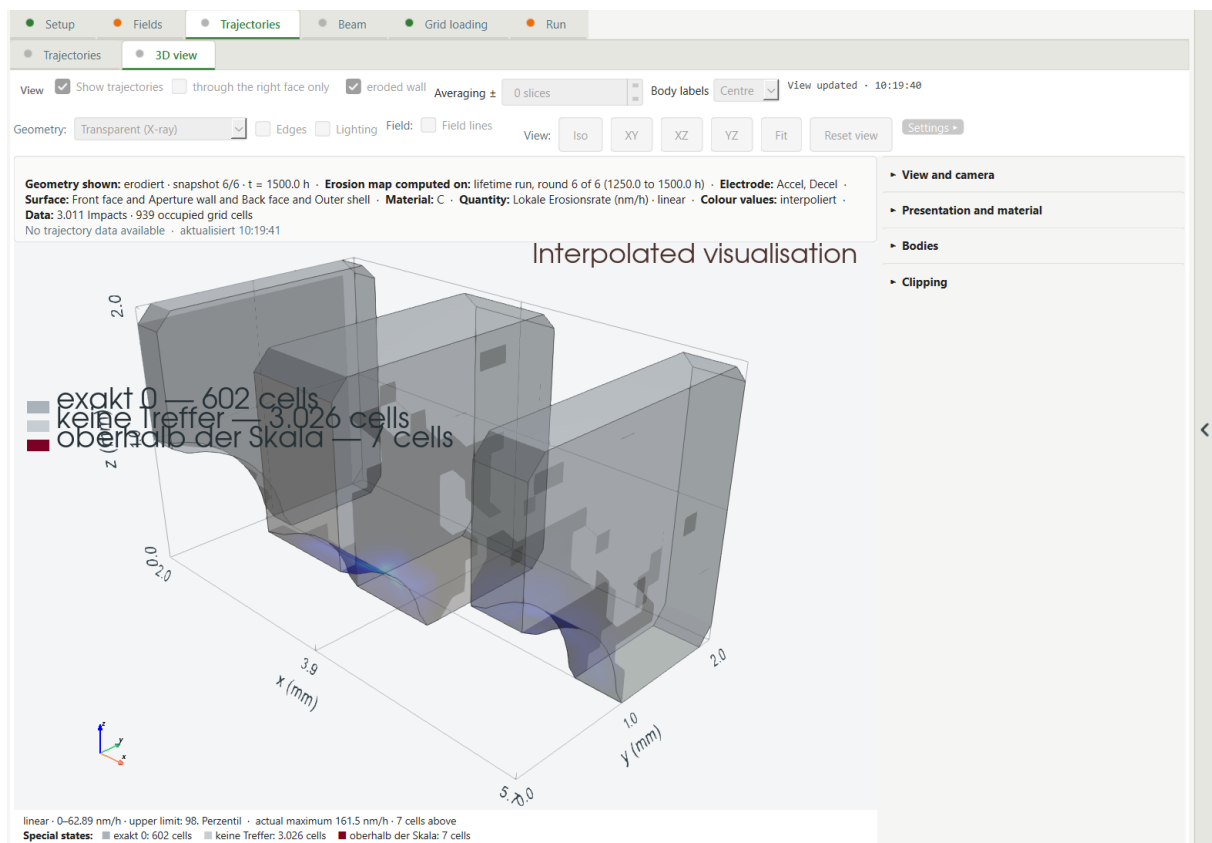


Figure 11.1: The 3D view with the erosion map of the lifetime simulation. The status lines above the picture state which geometry is shown and where the map comes from.

11.1 Toolbar and settings

The toolbar above the picture holds the switches that are needed constantly, in groups: **Geometry** (how the bodies are drawn), **Field** (field lines), **Trajectories**, **Erosion**, **Mesh** and **View** (camera directions, **Fit**, **Reset view**).

All further settings are in the foldable sections on the right:

View and camera

Camera directions and projection.

Presentation and material

Lighting, edges, legends, and **Colour**: what the surfaces of the bodies are coloured by — body, material, potential, field strength or erosion rate.

Bodies

Visibility, colour and opacity of each body.

Clipping

A section plane that cuts the scene open.

Result filter

Which trajectories are shown.

Selection and local values

The data cursor: click a surface cell to read its value.

Presentation of the erosion

Settings of the erosion map (below).

Export and film

Pictures, videos and the erosion data as a table.

11.2 The erosion map

The erosion map colours the electrode surfaces with the local erosion rate in nm/h. It is switched on with **Erosion map** in the toolbar.

Note. The controls under **Presentation of the erosion** and the selector **Surface** are greyed out as long as **Erosion map** is not ticked. They only have a meaning for the map.

Where the map comes from. There are two sources, and the status line above the picture always states which one is shown.

- **eroded wall** *not* ticked: the map is built from the impacts of the single calculation and drawn on the original geometry. A single calculation follows only a few hundred slow ions, so the map is thinly populated: most cells have no impact at all, and the few that have show very high values. This map is not suitable for reading off erosion rates.
- **eroded wall** ticked and a lifetime simulation loaded: the map is built from the complete impact list of the lifetime step that led to the selected snapshot, and drawn on the eroded geometry of that snapshot. This is the map to use.

Cell values or interpolated. **Colour values** selects between **per cell (cell values)**, which shows exactly one value per wall cell as it was computed, and **interpolated**, which smooths the values over neighbouring cells and draws them on a smooth surface. The interpolated picture is easier to read; the cell values are the reference.

Special states. Cells that carry no meaningful rate are not put on the colour scale but drawn in neutral colours and counted in the legend:

- *exactly zero*: ions arrived, but with an energy below the sputter threshold;

- *no hits*: no ion arrived in this cell;
- *above the scale*: a valid value beyond the upper limit of the colour scale.

Periodic display. For a hexagonal unit cell the computed cell can be continued to show one aperture with its six neighbours. The copies are mirror images of the computed values, not separate results. The option is available only when the program recognises the arrangement as hexagonal: two aperture centres in opposite corners of a box with the side ratio $1 : \sqrt{3}$. For a single quarter aperture it stays greyed out, and the text beneath gives the reason.

Chapter 12

Parameter studies, export and batch runs

12.1 Parameter studies

Parameter studies ... opens Run → Parameter studies. A study repeats the single calculation for a series of voltages of one electrode and collects the currents. Typical uses are the perveance limit (beam current against screen voltage) and the onset of direct impingement on the accel grid (accel current against a voltage). The voltage of an electrode is the only quantity a study can vary.

The tab has the list of studies on the left and four sections on the right: **Configuration**, **Progress**, **Results** and **Data table**.

Defining and running a study

New study creates an entry in the list. Under **Configuration** (Fig. 12.1):

- **Name.** If the field is left empty, the name is formed from the electrode and the range and follows later changes.
- **Parameter to be varied:** the **Electrode**, and the values as **Start value (V)**, **End value (V)** and **Step size (V)**. **Several value ranges with their own step size** replaces this by a list of ranges, for example coarse steps far from a limit and fine steps close to it. **Value list** shows the resulting voltages.
- **Analyse currents at the following electrodes:** the electrodes whose currents appear as curves.
- **Save diagnostic plots for every variant:** writes pictures of the chosen fields, with or without trajectories, for the last round of each variant into a folder, optionally with one video per kind of picture at the end.
- **Execution:** **Coupling rounds per variant** is the largest number of PIC rounds of each variant (default 6). **Variants at a time** computes several variants in parallel, each in its own process; the live monitor is then not available.

Check lists what prevents the start or needs confirmation, **Summary** the study as it will run. **Start the parameter study** starts it; **Apply and start later** only stores the definition.

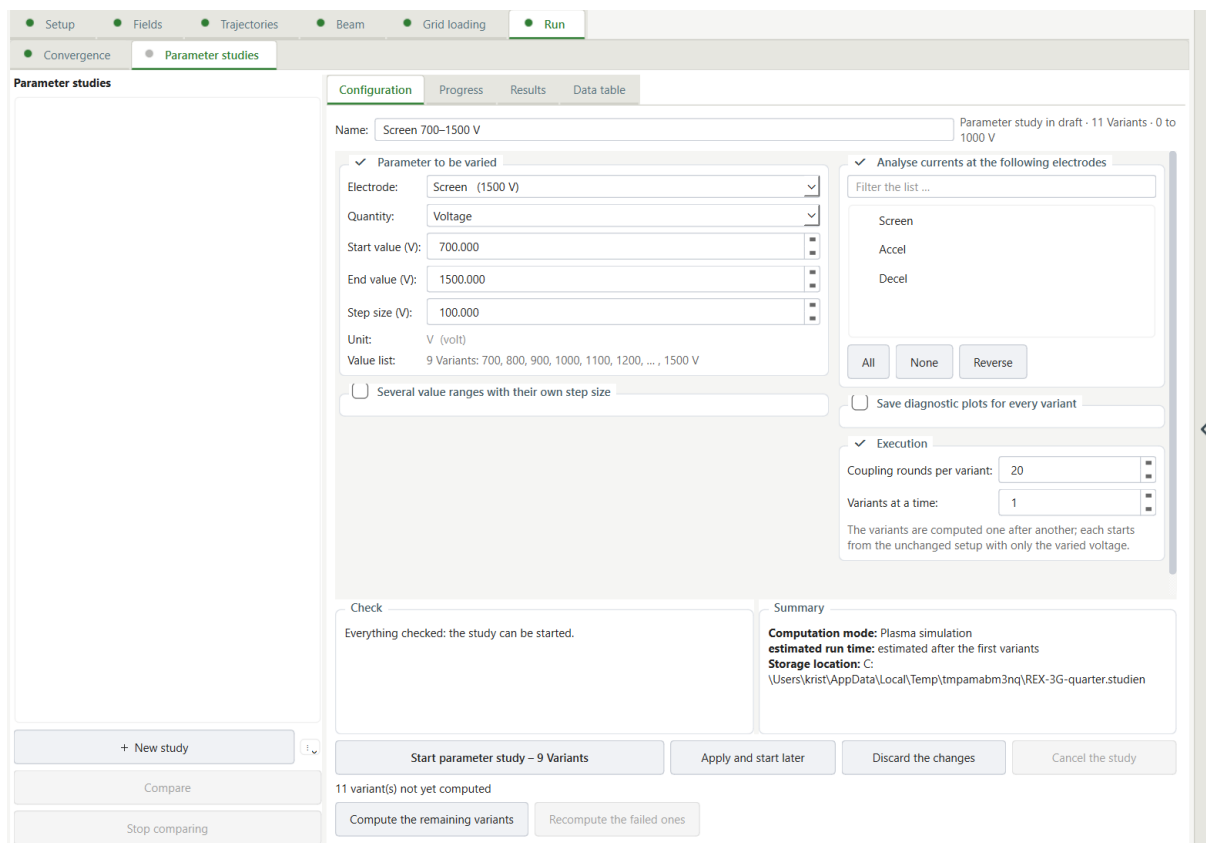


Figure 12.1: Run → Parameter studies, section **Configuration**: a study of the screen voltage of the example from 700 to 1500 V. Below the entries, the check and the summary.

Each variant starts from the unchanged setup with only the one voltage altered; no variant uses the result of another. A variant that fails is recorded with its error message, and the study continues with the next.

Caution. The number of rounds per variant is set here, independently of the **Simulation** dialog. It is an upper limit, as in a single calculation. The default of 6 is fewer than a single calculation usually needs to converge; the bundled example needs 16 at its nominal voltages (Table 2.1). Check with single calculations at both ends of the range how many rounds are required, and set **Coupling rounds per variant** with some reserve. The study of Figs. 12.1 and 12.2 allows 20. A study records the currents of each variant, not its reason for termination. Whether the variants converge is seen in the live monitor while they are computed one at a time, or from single calculations at selected voltages.

Cancel the study ends it after the variant that is running; the variants already computed are kept. A study that was cancelled or interrupted is completed with **Compute the remaining variants**, and **Recompute the failed ones** repeats only the variants that ended with an error. To repeat a whole study, or to run it with another range, use **Duplicate (as a template)** in the menu of the list entry: it copies the definition without the results.

The section **Progress** shows the state of the current variant and of the whole study with an estimate of the remaining time. **Open the live monitor in a separate window** opens a window in which the curves of the study grow with every finished variant; a failed variant appears as a gap with a mark.

Studies are stored as one file each in a folder named after the setup, with the ending **.studien**, next to the setup file. They are loaded again with the setup. A study whose setup has been

changed since is marked as no longer matching.

Evaluating a study

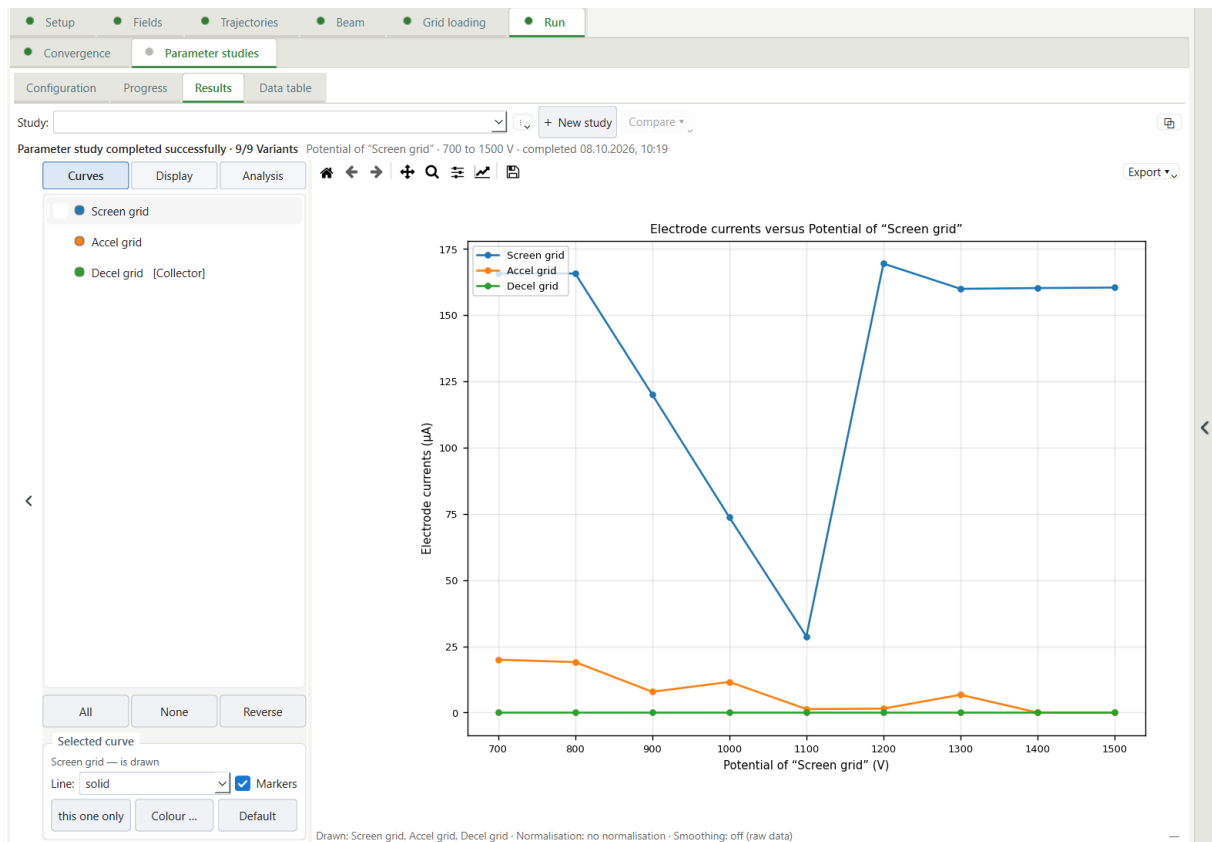


Figure 12.2: Section **Results** of the study of Fig. 12.1: the currents to the three grids against the screen voltage, with the tool column on the left. The jumps of the screen current between 900 and 1100 V are not a property of the grid system: these variants did not converge (see the text).

The section **Results** plots the recorded currents against the varied voltage (Fig. 12.2). The tool column beside the plot has three parts.

Curves

Which currents are shown, and line, marker and colour of each.

Display

The unit of the currents, a logarithmic axis, mesh lines, the legend and manual axis limits.

Analysis

Normalisation divides the curves by the emission current, by their first or largest value, or by a reference current. **Smoothing** applies a moving average or a Savitzky–Golay filter of a chosen window width; **Draw the raw data as well** keeps the unsmoothed points visible. **Derivative** adds a second plot with the slope of a curve, from the smoothed or the raw data. (**RPA analysis** belongs to the simulation of a retarding potential analyser and is not needed for extraction studies.)

Caution. A curve is only as good as its variants. In Fig. 12.2 the screen current jumps between 900 and 1100 V. A single calculation of the example with the screen grid at 1100 V shows why: it does not converge within 40 rounds, the change of the potential stays near 20 V and the particle balance alternates between transmission and backflow, the first pattern of Table 6.3. The points of a study in such a range are states of an unfinished iteration. Before a curve is interpreted, check single calculations at the voltages where it jumps or bends (Chapter 13).

The program does not determine a perveance limit or a backstreaming limit by itself; they are read from the curves, the derivative being helpful to find the kink.

Compare lays the curves of other studies, dashed, over those of the current one, for example the same voltage sweep at two plasma densities. **Export** writes the raw data or the processed curves as CSV, the latter with the applied normalisation and smoothing stated in the header, and saves the figure. The section **Data table** lists the values per variant, including the run time and the status of each.

12.2 Saving pictures and data

Save plot opens the export dialog for the plot that is currently shown. It offers PNG, PDF, SVG and EPS, a fixed size in centimetres, font sizes, and profiles for publications and presentations. The preview in the dialog is produced in the same way as the file. Elements such as the legend or the labels can be moved with the mouse before saving.

Data (CSV) writes the numbers behind the current plot. All files use a decimal point and a comma as column separator, and begin with comment lines (#) that state the origin, the units and the program version. Field sections can be written as a matrix or as a list of x , y and value.

ParaView ... writes the three-dimensional fields, the trajectories, the impacts and the electrode surfaces as VTK files for further processing in ParaView.

F12 saves a picture of the whole window.

12.3 Calculations without the user interface

The script `ionyx_run.py` runs a setup from the command line, for example on a compute cluster:

```
python ionyx_run.py setups/REX-3G-quarter.picsetup --out results/rex
python ionyx_run.py my_setup.picsetup --lifetime --tpmc --out results/life
python ionyx_run.py my_setup.picsetup --lifetime --resume --out results/life
```

The first line runs a single calculation and writes a report, the course of the iteration and a `result.picsim` that can be opened in the program. The second runs a lifetime simulation with the settings stored in the setup; `-tpmc` computes the gas map if the setup does not contain one. The third continues an interrupted lifetime simulation in the same folder. `python ionyx_run.py -help` lists all options.

Note. On Windows, set the environment variable `PYTHONIOENCODING=utf-8` before redirecting the output of a lifetime run into a file. Without it the run stops with a character encoding error.

12.4 Sending a calculation to a compute node

HPC → Run on the compute node ... sends the current setup to a compute cluster with the SLURM queueing system, follows the job and fetches the result. The menu is present only when the program is run from its source; the installed Windows version does not contain it.

The window needs a working `ssh` connection to the cluster that logs in without a password (a short name defined in the SSH configuration), and an installation of the program on the cluster. It has four parts:

- **COMPUTE ACCESS.** The SSH name, the partition, the Python environment, the number of cores, the memory, the time limit and the folder on the cluster. **Test connection** and **Check remote side** test the connection and the installation on the other side. **Save access** stores the entries; they are then preset at the next use.
- **RUN DETAILS.** **Kind of run:** **Beam computation** (a single calculation) or **Lifetime**; the number of PIC rounds; and a name for the run. A lifetime run can only be chosen when the setup has a current gas map and charge exchange is switched on. Its operating time, time step and current control are taken from the **Lifetime** tab.
- **RUN STATUS.** Queries the state of the job, shows the end of its log, and downloads the result into a local folder, on request automatically when the job has finished.
- **LOG.** The messages of the window itself. They are German (Section 1.4).

The setup is sent as it is at that moment, including the gas map and the lifetime settings. When a lifetime run reaches the time limit of the queue, a follow-up job continues it in the same folder, and the window follows the new job. Of a lifetime run the result file, the log and the protocol are downloaded; the individual snapshots remain on the cluster. The downloaded `result.picsim` is opened like any other result.

Chapter 13

Checking the reliability of a result

A finished calculation is not yet a reliable one. The steps below show how far a result depends on the numerical settings. Each step changes one setting, repeats the calculation and compares the quantities that the result is needed for: for the ion optics typically the beam current, the currents to the grids, the beam radius and the emittance; for the lifetime the erosion at the throat and its rate. Which difference is acceptable depends on the quantity and on the purpose; the manual gives no general limit. State the comparison together with the result.

13.1 Convergence and steadiness

1. Read the reason for termination in Run → Convergence (Section 6.4). Only **Converged** says that the tolerance was met. After **noise floor reached** or **maximum number of rounds reached** follow the checks described there.
2. Look at the quantities themselves, not only at the potential. **View** → **Beam and current** and **Particle balance**, and the table **Values per PIC round**, show the currents, the emittances and the particle counts of every round. They should be flat over the last rounds. A current consists of whole macro-particles, so it changes in steps; in the example one step is 0.34 μA , or 0.8 % of the beam current of the cell.
3. If a quantity still drifts, tighten the tolerance or allow more rounds, and repeat.

13.2 Mesh and number of start points

Change the two separately, so that their effects can be told apart.

1. **Start points.** Keep the mesh and increase **n_beamlets** in the window **Particle start** (Section 5.4), for example to four times the number. Compare the quantities. Those that rest on few macro-particles react most: a small current to a grid, the edge of the beam profile, the 90 % emittance.
2. **Mesh.** Keep the box and reduce the **Cell size h** (Section 4.2). Use **fit** so that the computed box does not change with the mesh, and raise the number of start points to the new suggestion **n_min**, so that every cell of the emitting face still has its start point. Compare again. The tab **Fields** → **Debye h/λ** shows where the mesh is coarse compared with the Debye length; this is a hint where to look, not a proof in either direction.

3. A change of the boundary model or of the symmetry cell is not a convergence test. Comparing a quarter model with the full aperture checks the symmetry assumption, which is a different question.

13.3 Erosion and lifetime

An erosion result rests on the beam calculation, so the checks above come first. In addition:

1. **Number of charge exchange ions.** Repeat with a larger **N_target erosion** (Table 10.2), or, for a single calculation, with more ions in **Compute the erosion distribution**. Compare the erosion rate at the place of interest, not only the total: a map with many cells needs more ions than a total current.
2. **Time step.** Repeat the lifetime simulation with a shorter **Time step**, or with a smaller **Voxel threshold per step** when the step is chosen automatically, and compare the columns **Erosion at the throat** and **Erosion max** at the same operating time (Table 10.3).
3. **Beam calculation within the steps.** The column **I_beam** and the window **Lifetime trends** (Section 10.6) show whether the beam current behaves smoothly from step to step. If it jumps, repeat a section of the run with more **PIC rounds per step**.
4. **Gas map.** The map has a statistical scatter of its own. It is reduced with **n_markers**, or with the **Profile** of the operating-data window (Section 9.3), which states the uncertainty of the transmission.

13.4 Numerical convergence and model uncertainty

The checks above answer one question only: whether the program has solved its equations accurately enough. They say nothing about how well these equations describe the thruster. The second question has to be answered separately, and for erosion it usually dominates:

- **Sputter yield.** The models differ strongly in the energy range of the charge exchange ions, and the general formula itself deviates from measurements by tens of per cent (Section 10.1). The sub-tab **Impact analysis** evaluates the same impacts with another sputter model without a new simulation (Section 10.8); the difference between the models is a direct measure of this uncertainty.
- **Charge exchange cross section.** The cross sections are fits to measurements with their own uncertainty, some are estimates, and for fast beams they are used beyond the measured range (Table 9.2). The number of charge exchange ions is proportional to the cross section.
- **Neutral gas.** The density between the grids follows from the inlet pressure or from the operating data and the assumptions of the channel model (Section 9.3). The number of charge exchange ions is proportional to it as well.
- **Plasma.** j_i and T_e are inputs. The model contains no magnetic field and no collisions in the beam, and it takes the emitted current density as uniform over the emitting face (Section 5.1).
- **What is not modelled.** Redeposited material does not change the geometry (Section 10.3); chemical effects of molecular gases are not included.

A calculation that is converged to a per cent can therefore still be uncertain by the factor by which two sputter models differ. Report both: the numerical checks that were made, and the models and inputs that were used. Where a measured erosion is available, the **Scale factor of the sputter yield** calibrates the model against it; this is a calibration and is stated as such.

Chapter 14

Troubleshooting

Observation	Explanation and remedy
Start single calculation is greyed out.	The setup is incomplete. The Readiness list in the Setup tab names the reason; a click on the line opens the dialog concerned.
The header reads Results out of date .	An input was changed after the calculation. The pictures show the old result. Start the calculation again.
The calculation ends with Not converged .	See Table 6.3. First lower sc_relax_omega .
The beam footprint shows a cross or spokes.	A regular start pattern or the staircase boundary model. Use Grid with jitter in Particle start and the boundary model Fractional .
The charge density is streaky.	Too few start points. Use the suggested number in Particle start .
Charge exchange stays inactive.	No current gas map, or ion species and collision partner are not set to a predefined species.
The lifetime simulation does not start.	It needs a finished single calculation with charge exchange and a current gas map.
The eroded outline shows single-cell teeth.	Wall from fill level is not ticked (Section 10.7).
A field tab shows overlay only .	The eroded wall is drawn over the field of the original geometry (Section 10.7).
Controls of the erosion presentation in the 3D view are greyed out.	Erosion map is not ticked.
The 3D erosion map shows only a few scattered coloured cells.	The map comes from the single calculation. Tick eroded wall to use the impacts of the lifetime simulation (Chapter 11).
Periodic display is greyed out.	The setup is not a hexagonal unit cell with two aperture centres.
A thin body does not appear in the field.	It is thinner than a cell. Check with Check the computational domain . . .

14.1 If the program stops unexpectedly

Every start of the program is watched by a second, small process. It records in a session folder what the program was doing, and it notices when the program ends without having been closed properly.

- **After a crash** a message appears that names the kind of termination, the time, the last action and the session folder, and offers to open that folder. If the message could not be shown, it appears once at the next start.
- **If the program does not respond** nothing is terminated and no window appears. A long calculation can make the interface slow without anything being wrong. The watching process notes the standstill in the session folder, where it can be examined afterwards.
- **An error during a calculation** that does not end the program is written as an error report into the same folder; the log in the right column of the main window gives its path.

The session folders are in `%LOCALAPPDATA%\IONTRACE\diagnose`, one per start, named with date and time. A folder contains the events of the session, the output of the program and, after an error, a report with the program version, the place of the error, what was being computed and the technical details. The program does not send anything by itself. To report a problem, pass on the folder of the session concerned, together with the setup if possible. Folders of sessions that ended normally are removed automatically after some time.

Appendix A

Symbols and units

Symbol	Unit	Meaning
x	mm	Coordinate along the beam axis; the plasma is at $x = 0$
y, z	mm	Transverse coordinates
h	mm	Cell size of the mesh
φ	V	Electric potential
$ E $	V/mm	Electric field strength
ρ	C/m ³	Charge density
T_e, T_i	eV	Electron and ion temperature, entered as the energies $k_B T_e$ and $k_B T_i$
T	K	Temperature of the neutral gas or of a wall
n_i	m ⁻³	Ion density of the plasma; reference density of the emitted current (Section 5.1)
U_{plasma}	V	Plasma potential
j_i	mA/cm ²	Ion current density emitted by the plasma
v_B	m/s	Bohm velocity
λ_D	mm	Debye length
ω	—	Mixing factor of the charge density (sc_relax_omega)
$\max \Delta\varphi $	V	Largest change of the potential between two rounds
ε_{rms}	mm mrad	RMS emittance
r_{50}, r_{90}	mm	Radii enclosing 50 % and 90 % of the beam current
n	m ⁻³	Neutral gas density
σ	m ²	Charge exchange cross section
Y	atoms/ion	Sputter yield
E, θ	eV, °	Energy of an ion and its angle of incidence against the surface normal
z, m_i	—, kg	Charge number and mass of the beam ions

Appendix B

Keyboard shortcuts

Key	Action
F5	Start single calculation
Shift+F5	Cancel calculation
Ctrl+S	Save setup
Ctrl+Shift+S	Save setup as ...
F12	Save a picture of the window
Shift+F12	Save a picture of the window, with file dialog
Ctrl+Q	Quit

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