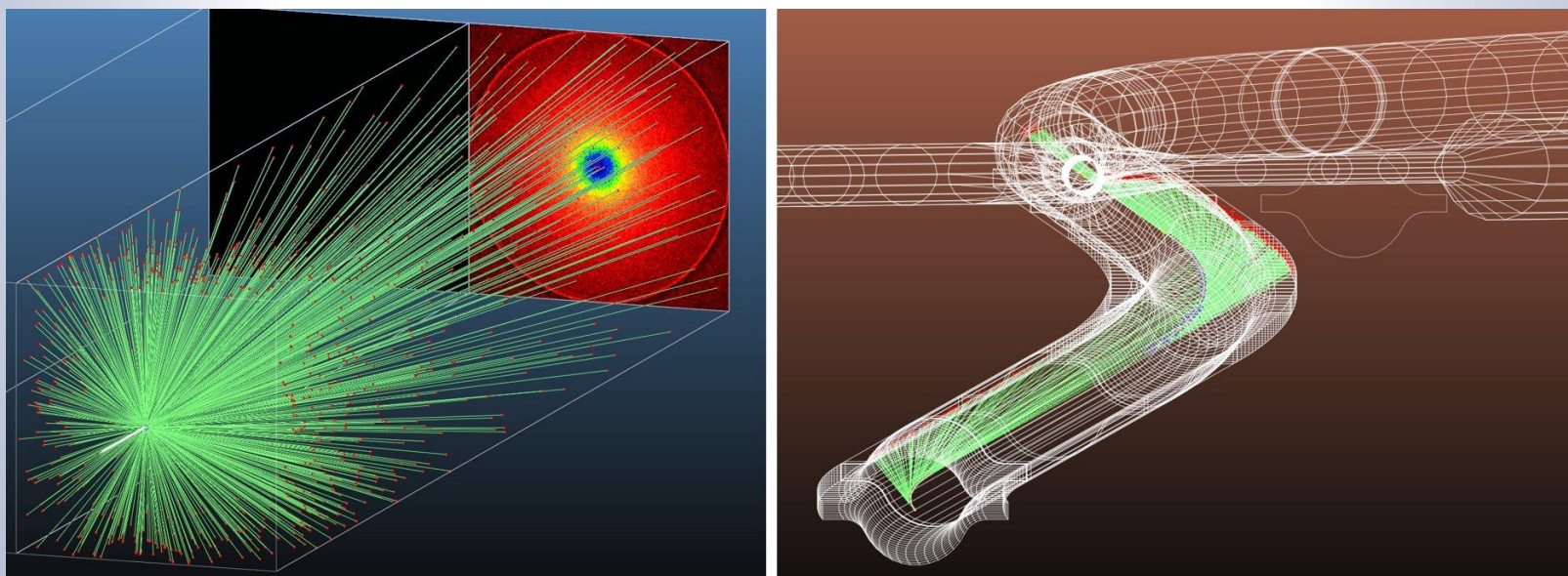
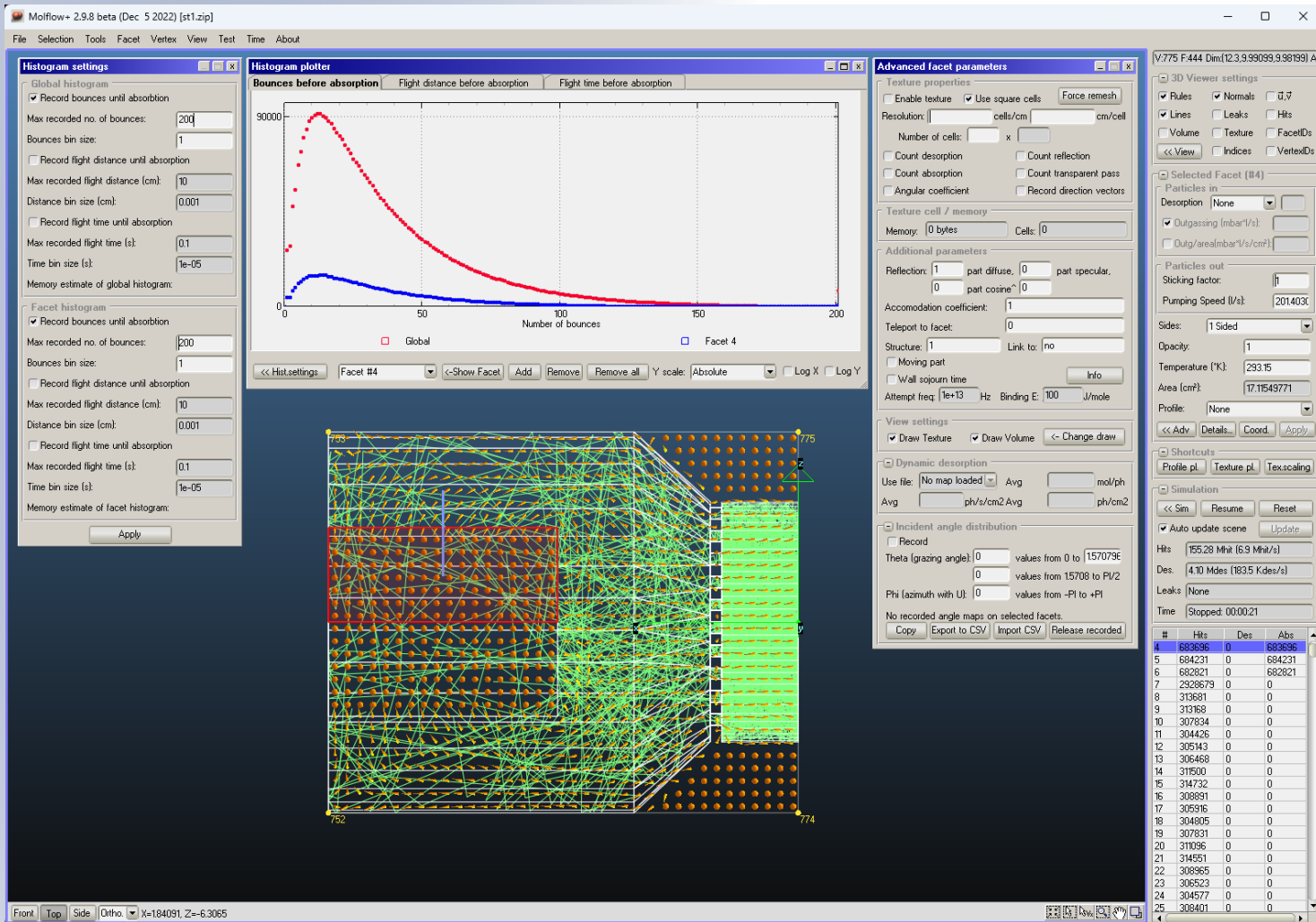


MolFlow and SynRad development update



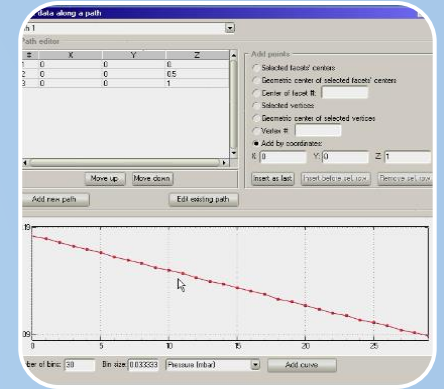
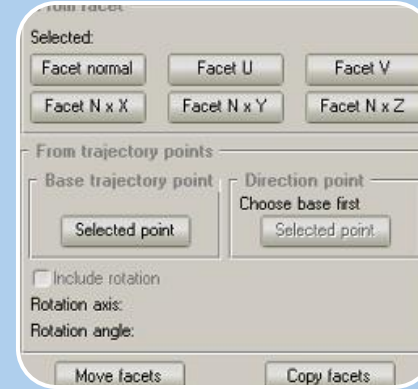
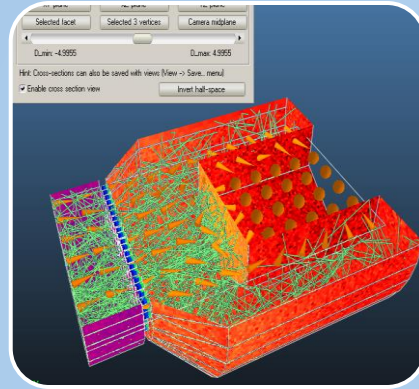
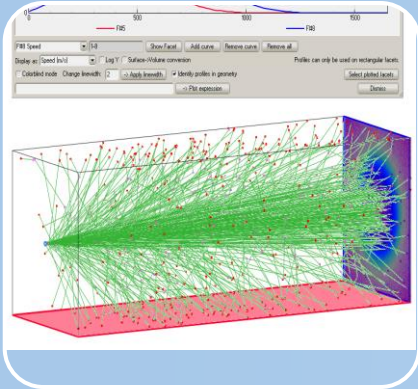
2025-02-25 TE-VSC seminar
Márton Ady, Petar Trifunović

MolFlow in one slide



- Test-particle vacuum simulator
- Uses Monte Carlo test particles
- Assumes molecular flow
- Written by Roberto Kersevan in 1990s
- Modernized at ESRF in 2008
- Developed at TE-VSC since 2012
- Approx. 1000 users

Today: 5 new functions



Physics

Visualization

Contamination

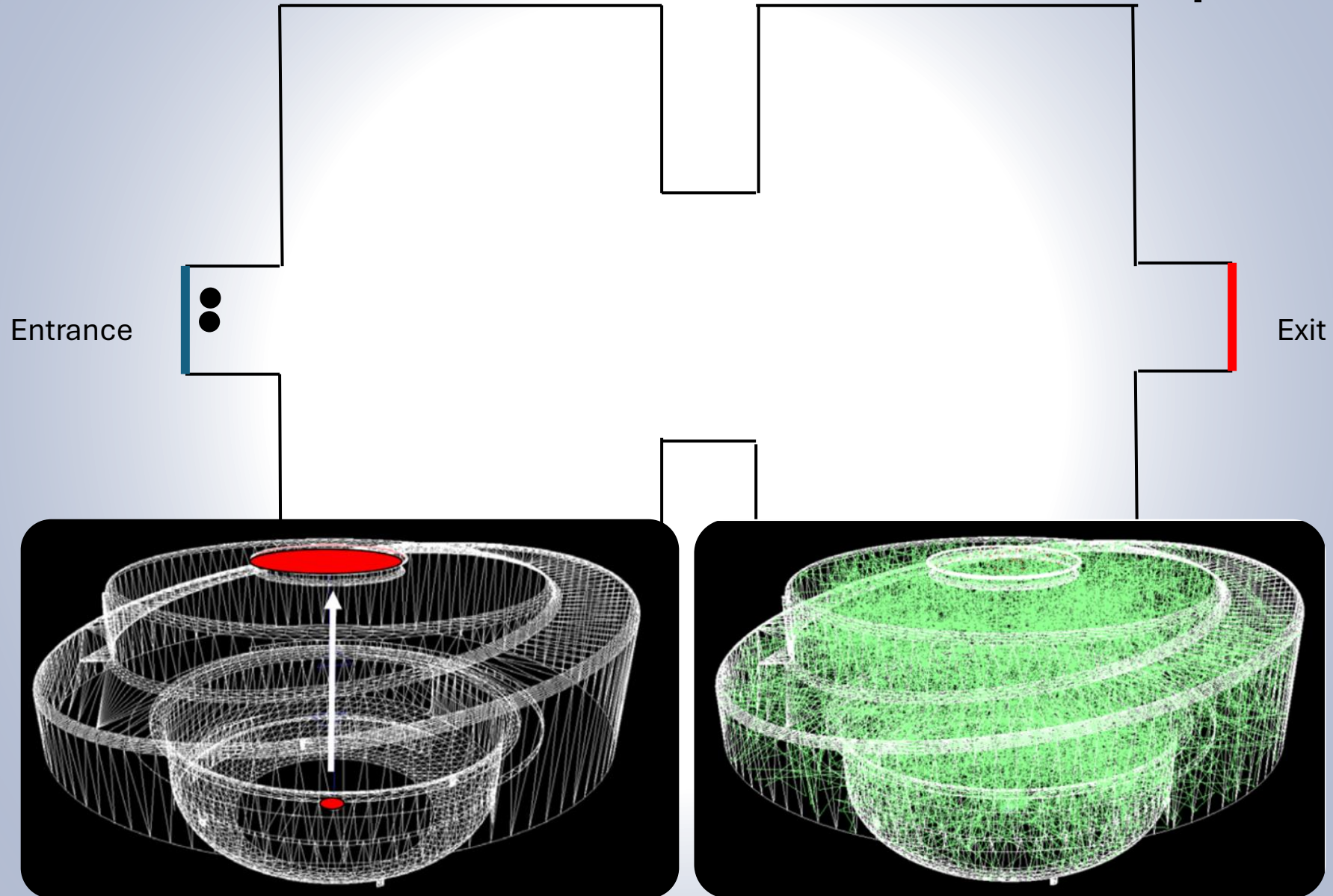
Geometry edit

Data extraction

2024

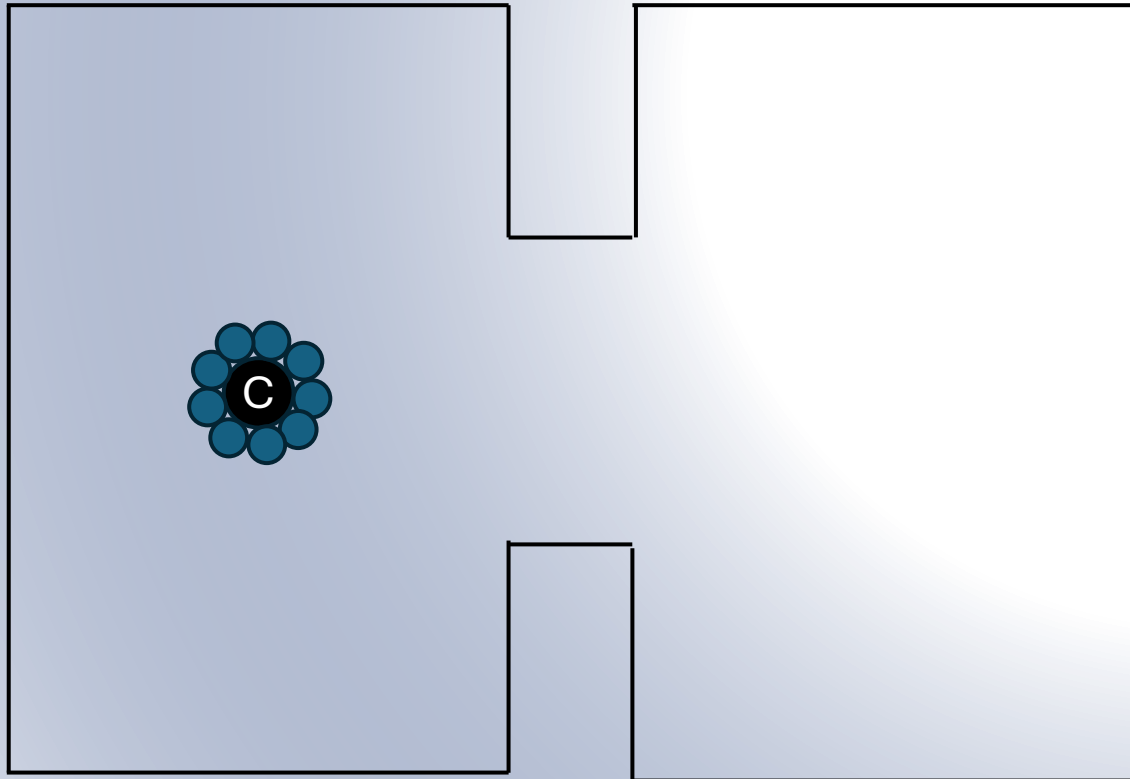
2025

A Monte Carlo simulation: Transmission probability

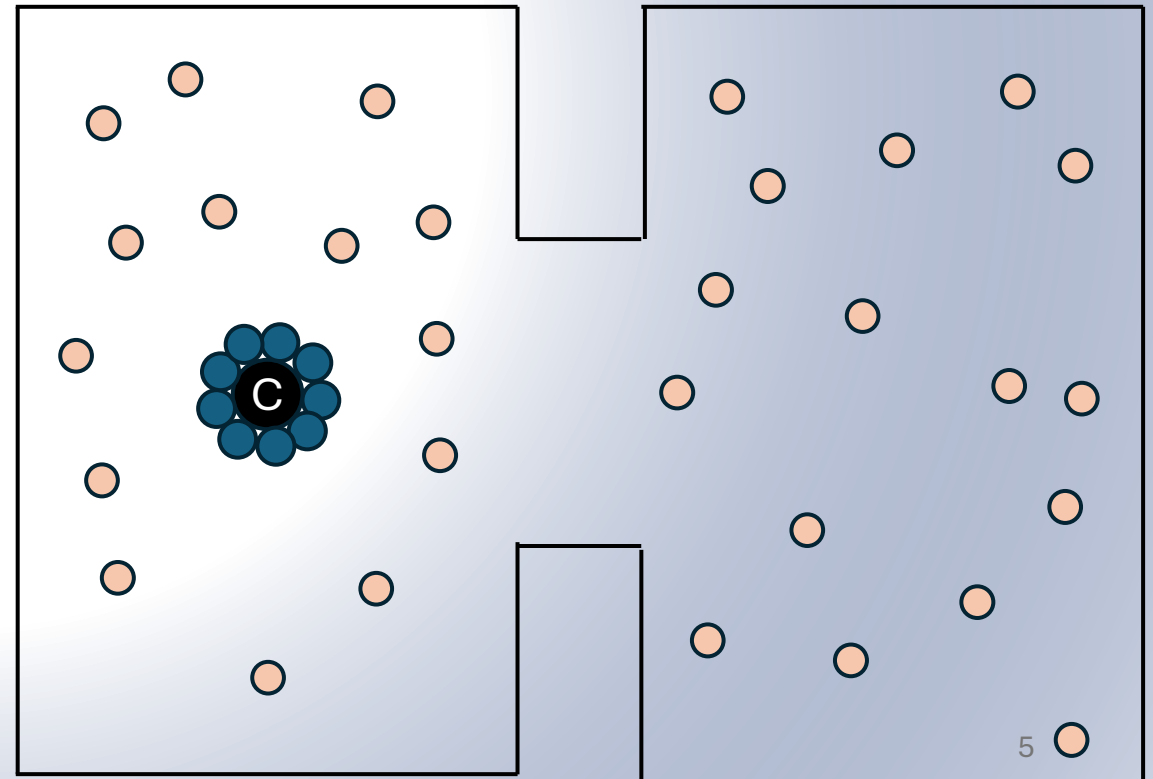


MolFlow for sputtering simulations

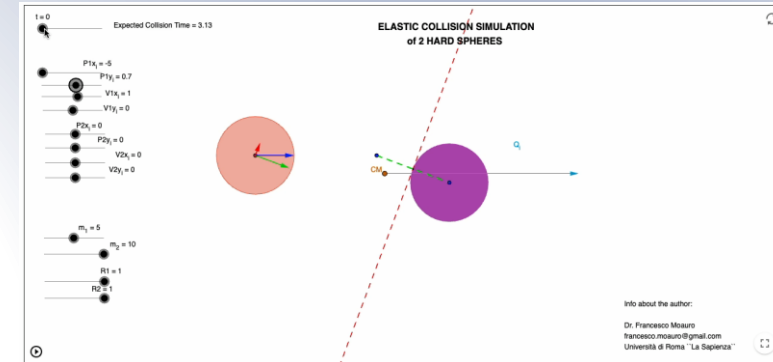
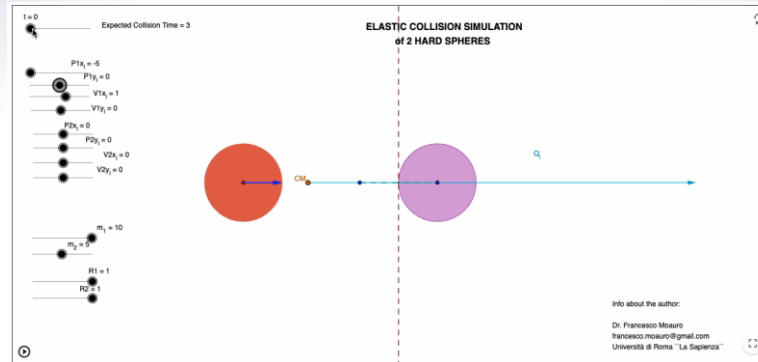
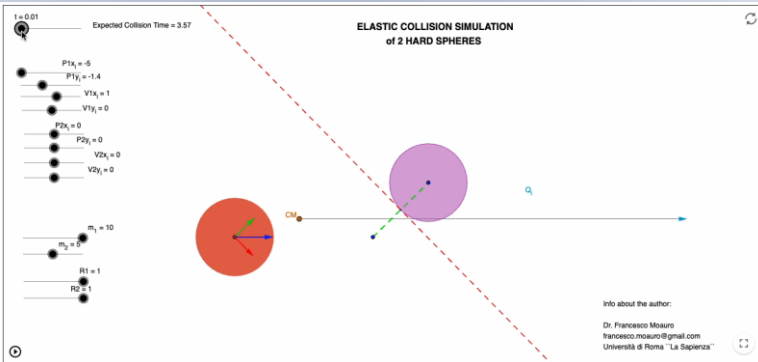
Simple sputtering simulation



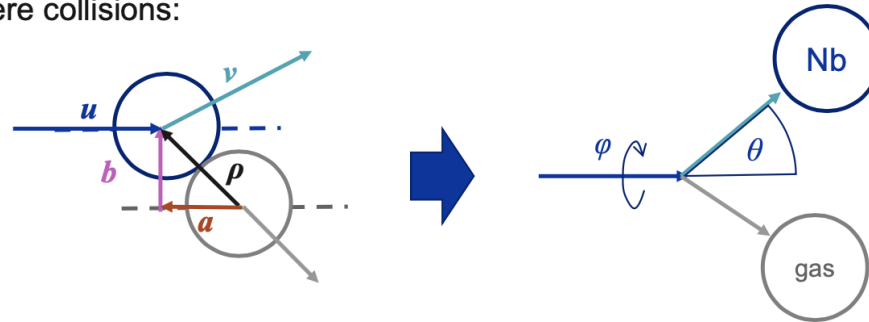
With background gas



Collision between two particles



- Describing hard sphere collisions:



- Azimuthal scattering angle ϕ has uniform PDF due to cylindrical symmetry
- Polar scattering angle θ based on linear PDF of “impact parameter” b (cf “differential cross sections”)
- New speed v is defined uniquely by θ (b)

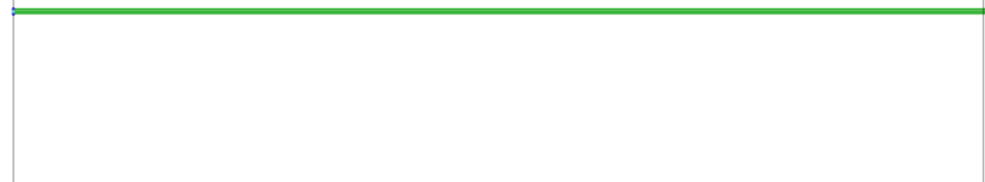
$$P(b) = \frac{2b}{\rho^2} \quad \Rightarrow \quad \cot(\theta) = \frac{1}{2ab} \left(\rho^2 \frac{m_{Nb}}{m_{gas}} + b^2 - a^2 \right) \quad \Rightarrow \quad v^2 = u^2 \left(1 + \frac{m_{Nb}^2 \rho^2}{m_{gas}^2 b^2} \sin^2(\theta) \right)^{-1}$$

green lines: particle trajectories

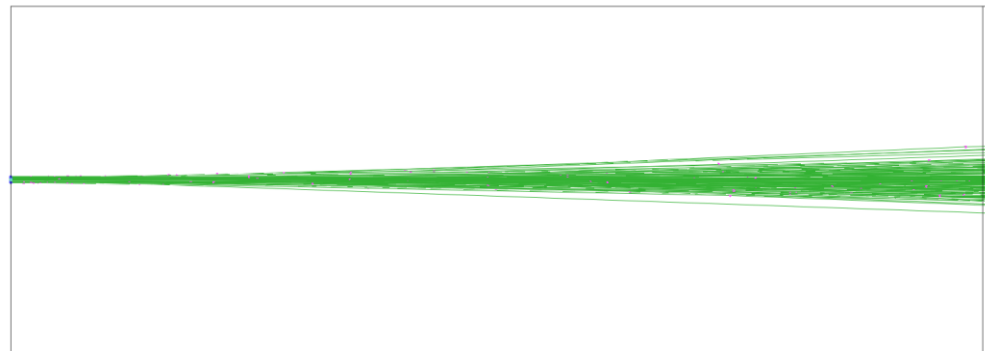
purple dots: collision locations

red dots: absorption locations on walls

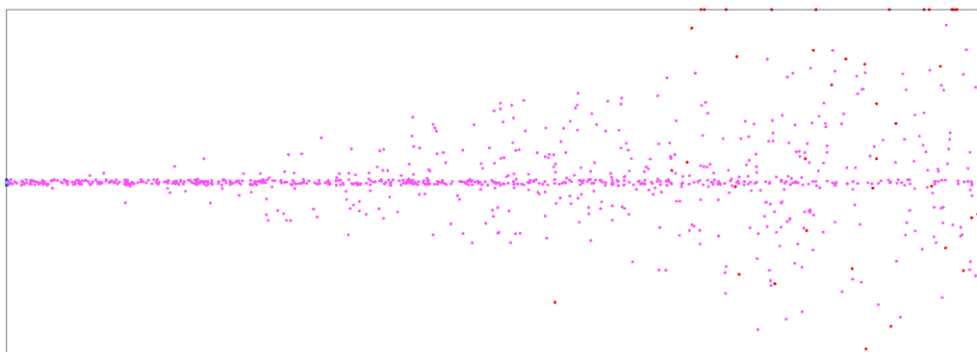
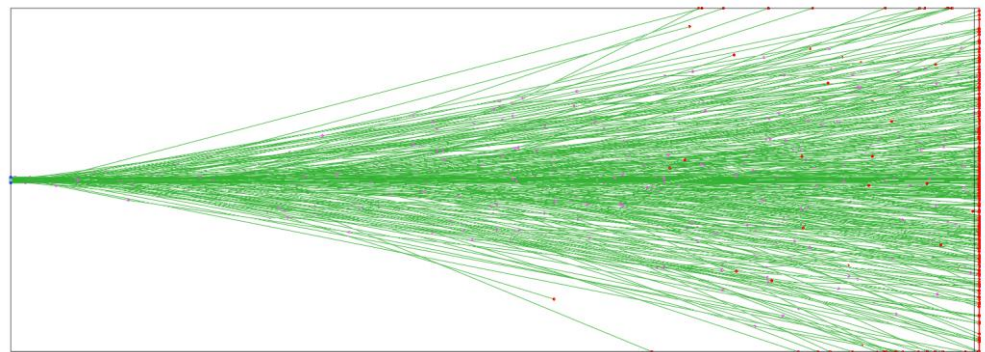
collisions off



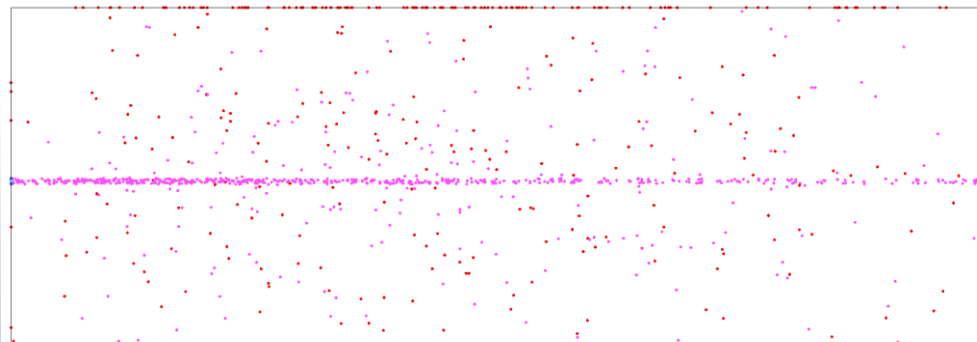
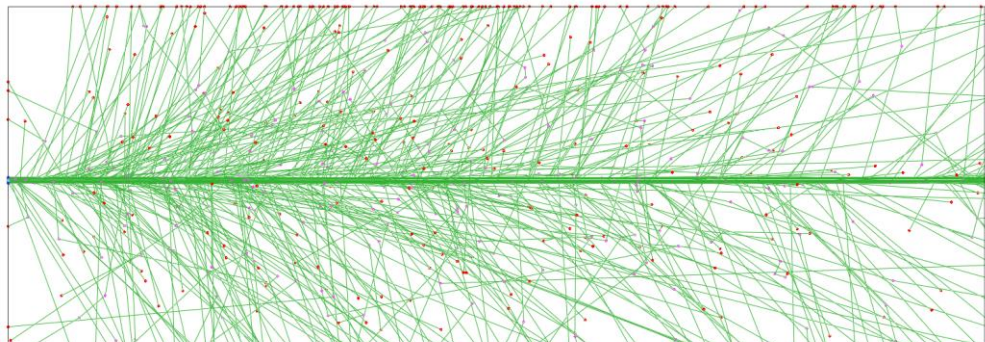
mass ratio = 50

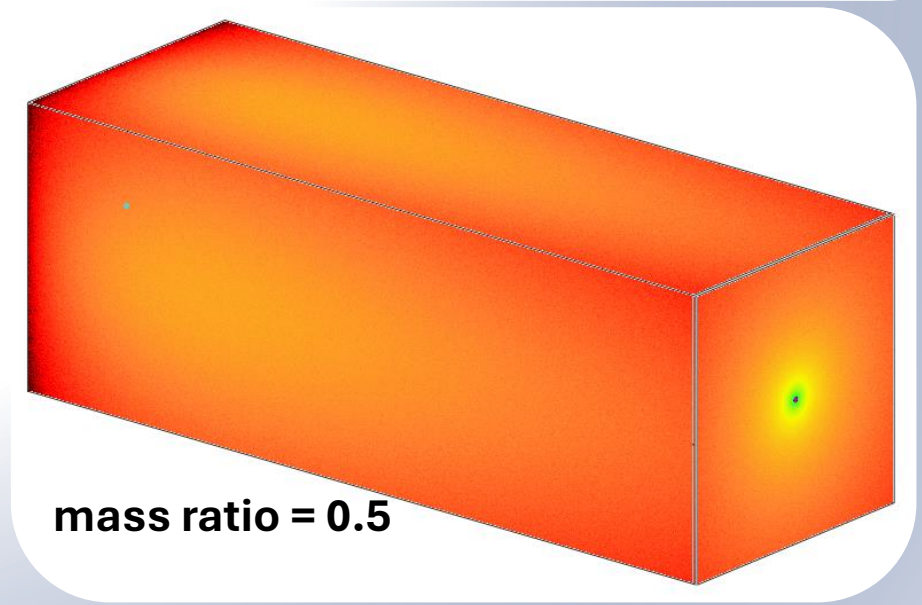
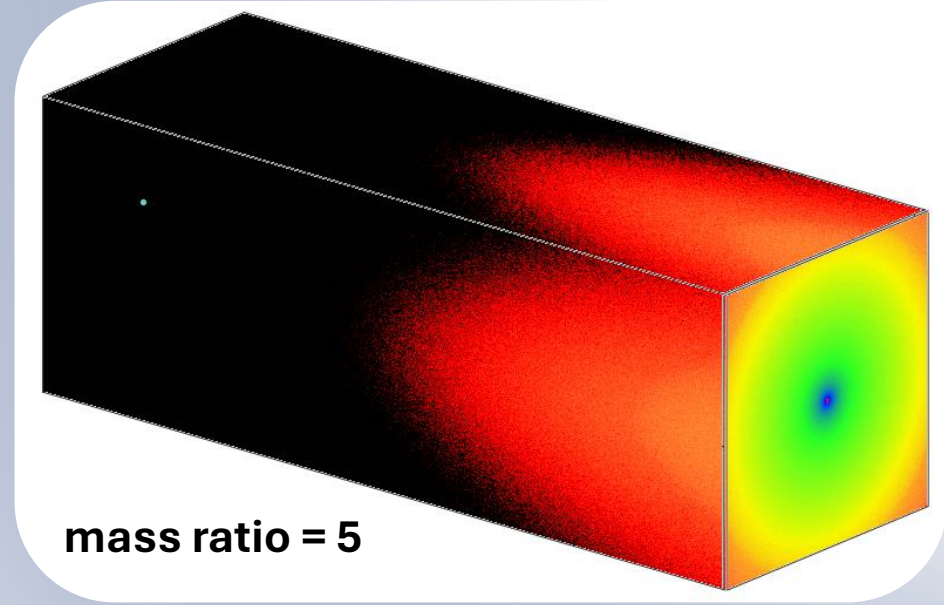
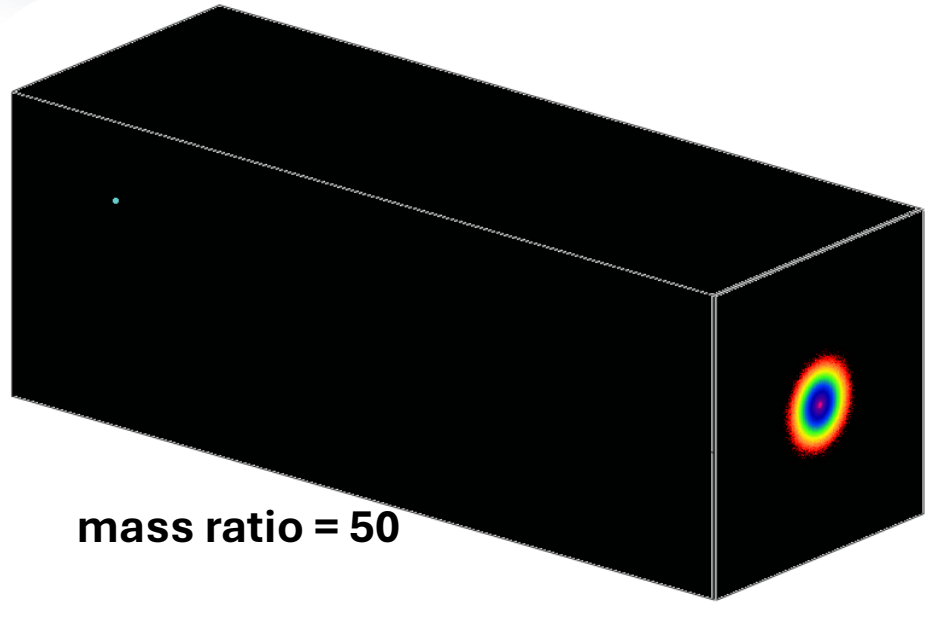
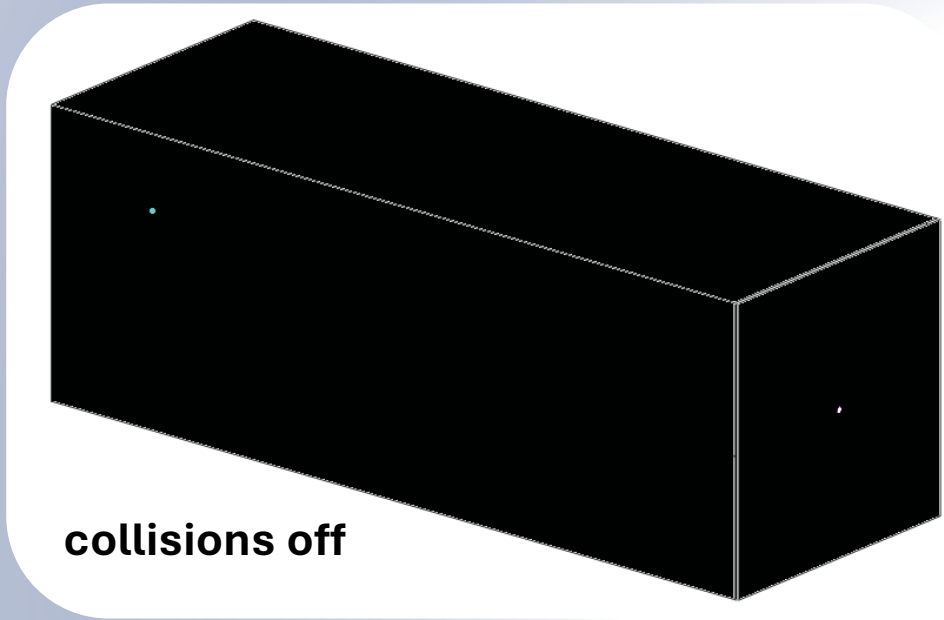
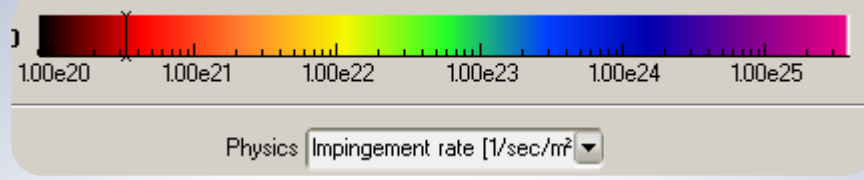


mass ratio = 5

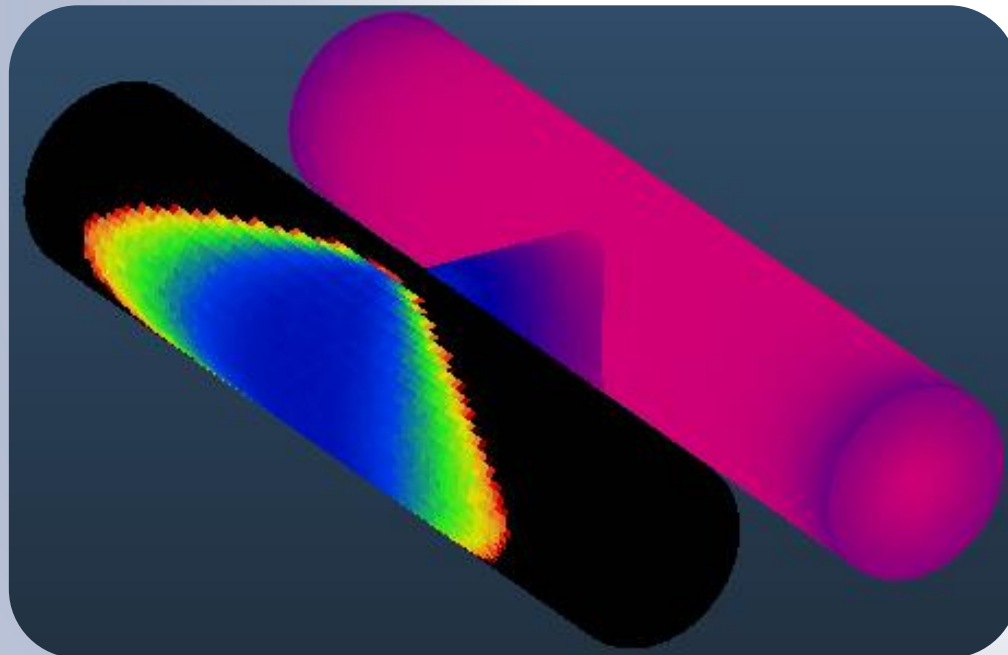
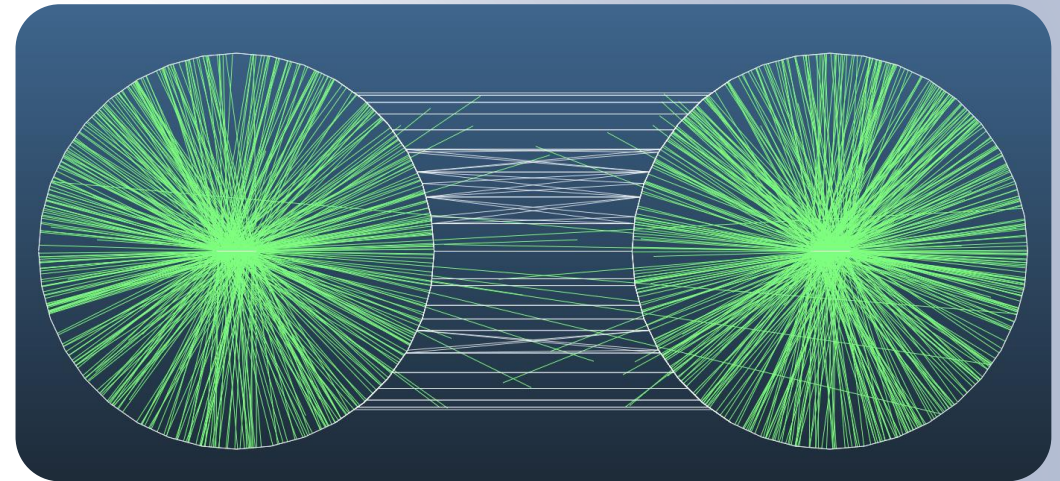
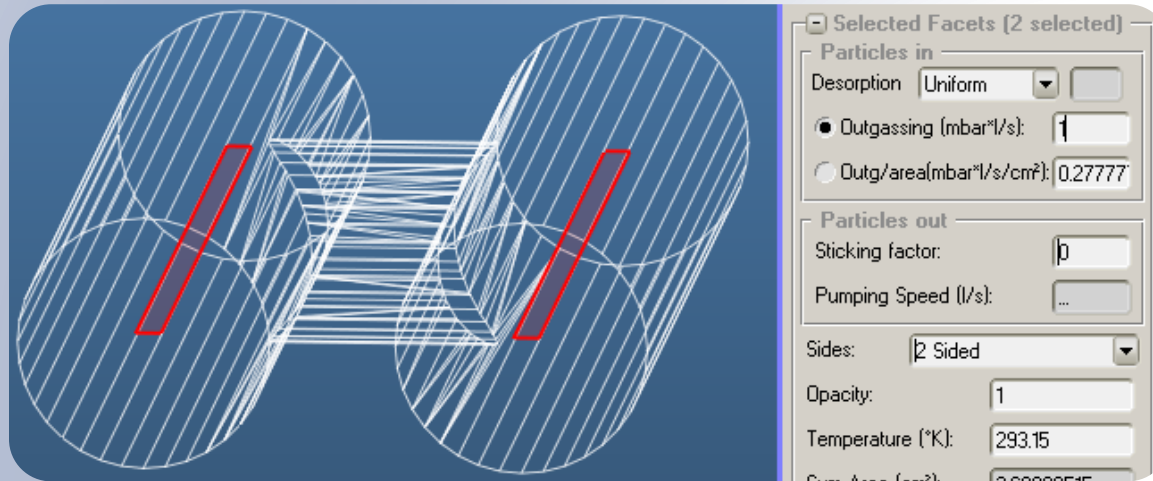


mass ratio = 0.5

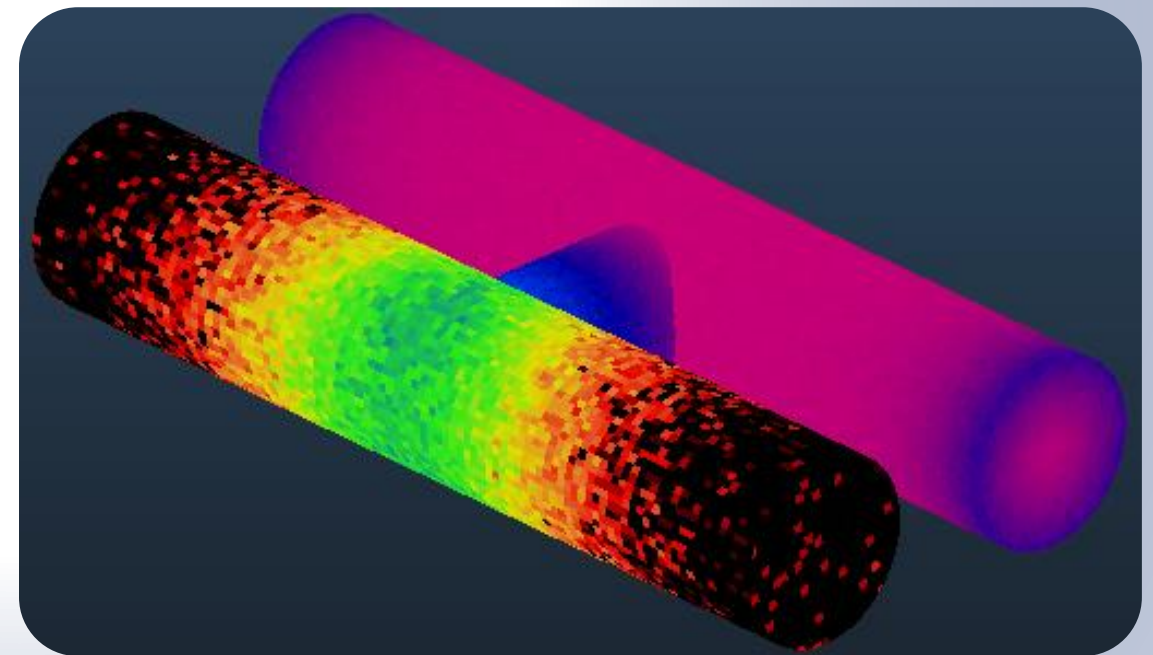




Sputtering seminar for SCC section



reference – no background



with background gas

Water vapor sticking



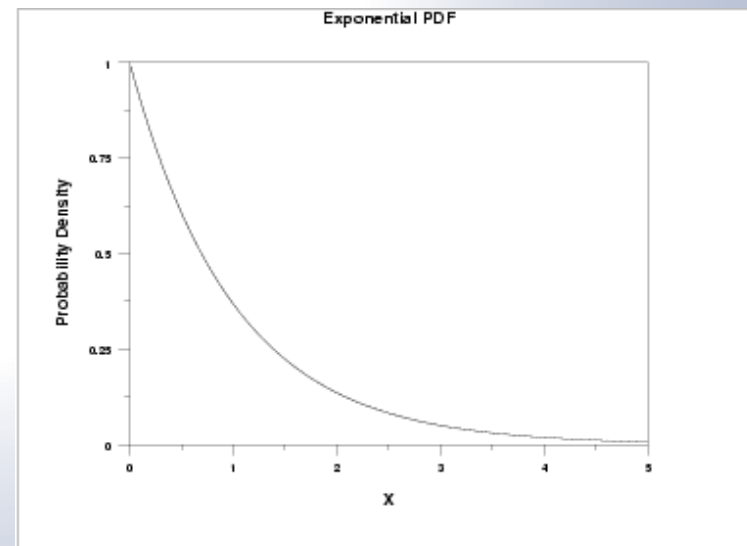
Surface

Probability of sojourn time t:

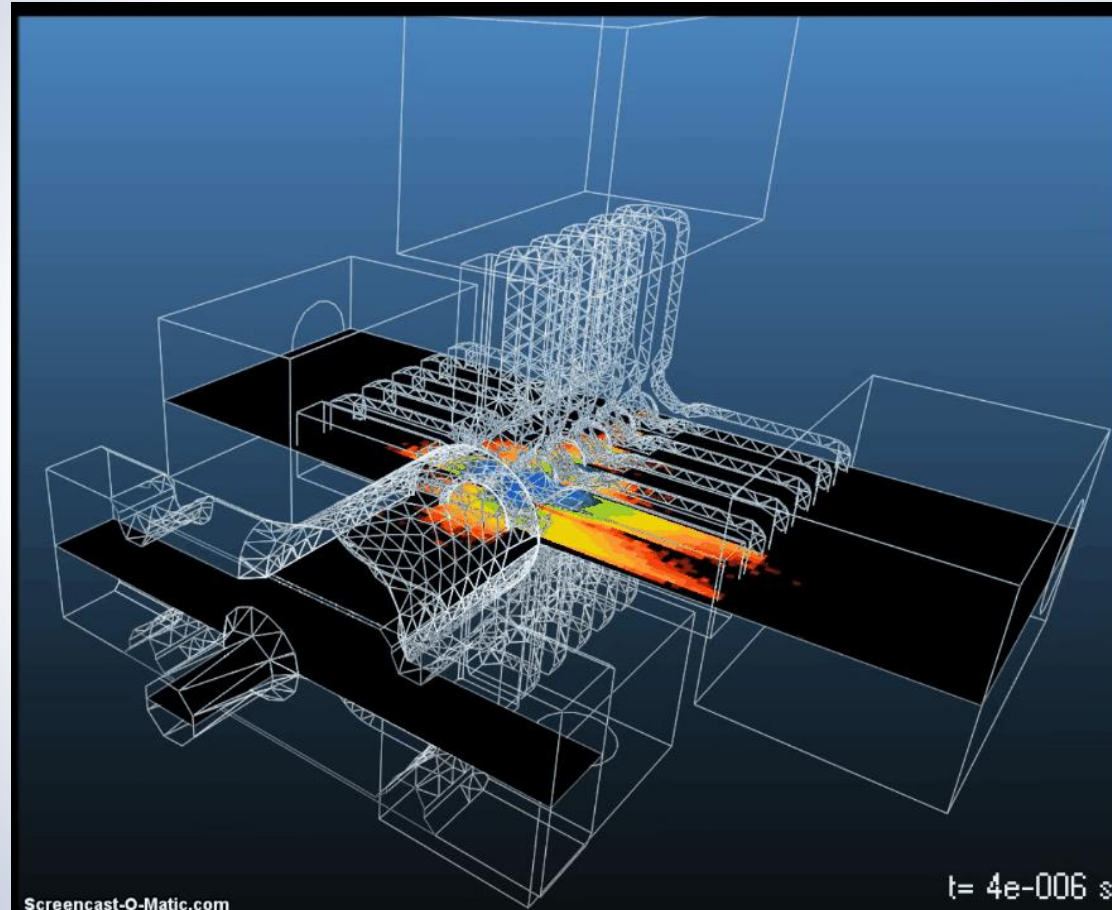
$$p(t) = A f e^{-A f t}$$

where

- f: Molecule's surface oscillation frequency [Hz]
- E: Adsorption energy [J/mole]
- A: Escape probability per oscillation:
 $A = \exp(-E/(RT))$



Time-dependent mode in MolFlow



CLIC cavity geometry: Cedric Garion

Problem: No connection between independent time moments

New features

Add temperature-dependent residence time

Wall sojourn time (mean=1.0419e-13 s) Info
 Attempt freq: Hz Binding E: J/mole

 Temperature (*K):

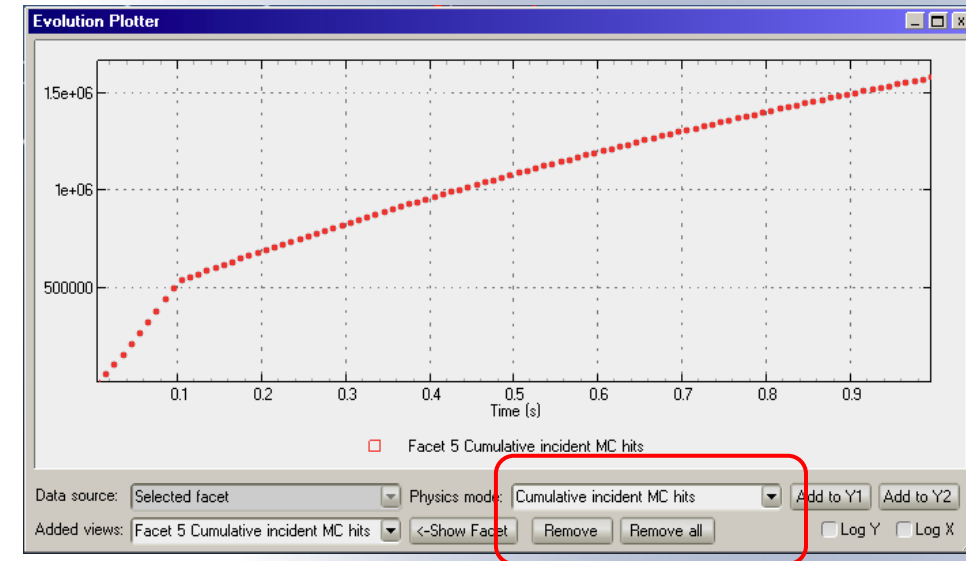
Add reflection counters

#	Hits	Des	Abs	Refl
1	1705444	237	1705	0
2	670154	0	670	0
3	2936831	0	0	2.93683e+06
4	2935478	0	0	2.93548e+06
5	2936135	0	0	2.93614e+06
6	2935874	0	0	2.93587e+06
7	2935099	0	0	2.9351e+06

Integrate over time

Time About
 Time settings... Alt+l
 Edit moments...
 Edit parameters...
 Timewise profiles plotter
 Evolution Plotter
Calculate cumulative quantities

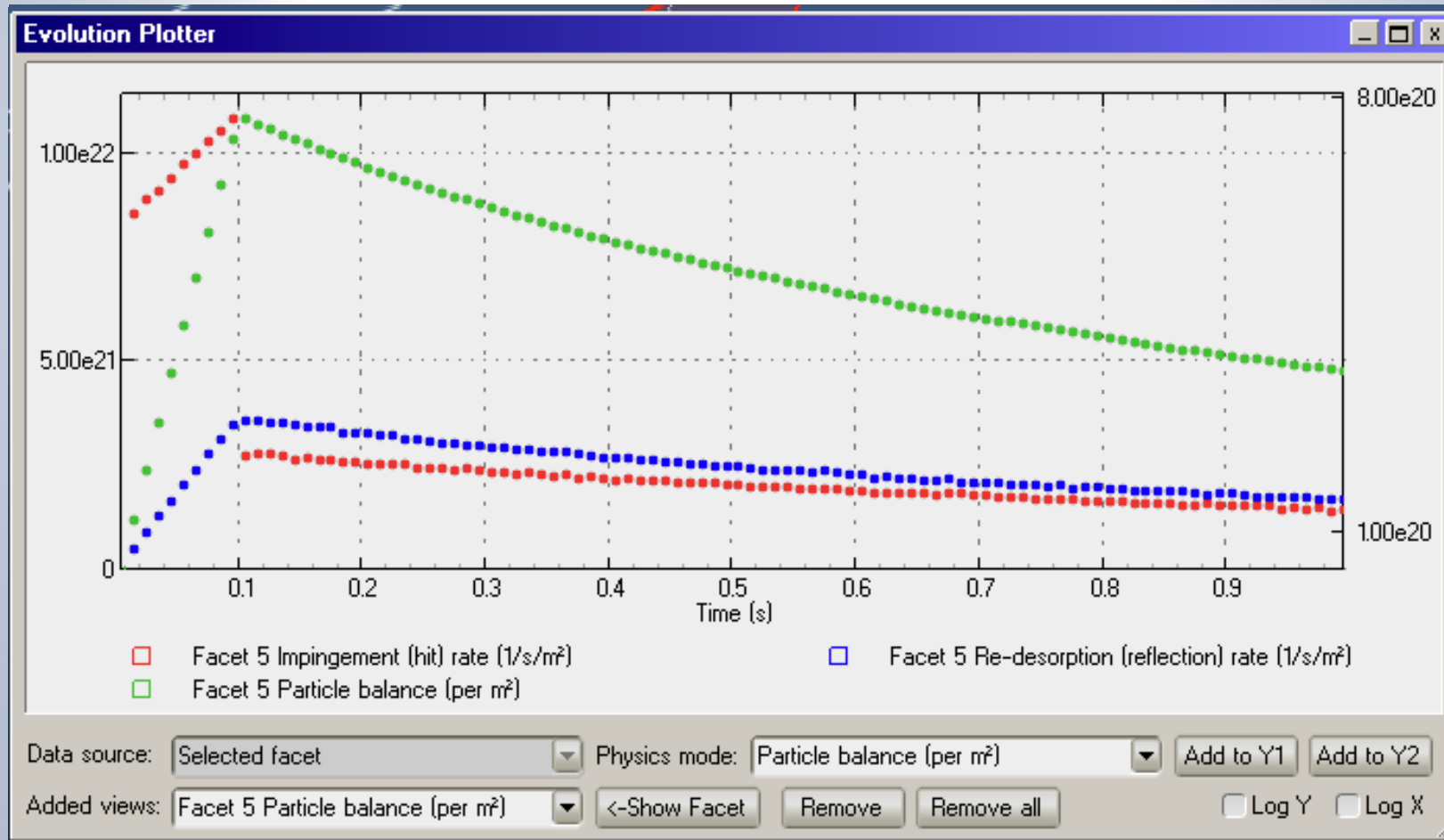
New plotter window



Outgassing (desorption) rate (1/s/m²)
 In-gassing (adsorption) rate (1/s/m²)
 Cumulative incident MC hits
 Cumulative desorbed MC hits
 Cumulative absorbed MC hits
 Cumulative reflected MC hits
 MC hit balance
 Particle balance (absolute)
 Particle balance (per m²)

Particle balance example

- Mean residence time: 0.2s
- Outgassing: from 0 to 0.1s



Automation with MolFlow



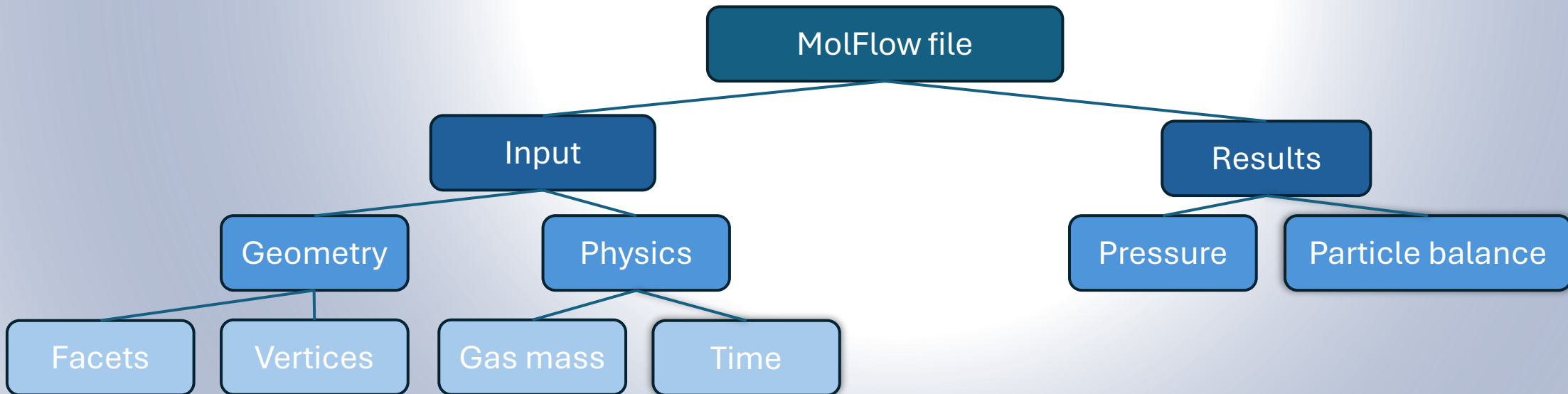
- Parameter sweep
- Iterative simulations
- Result-based optimization

molflowCLI

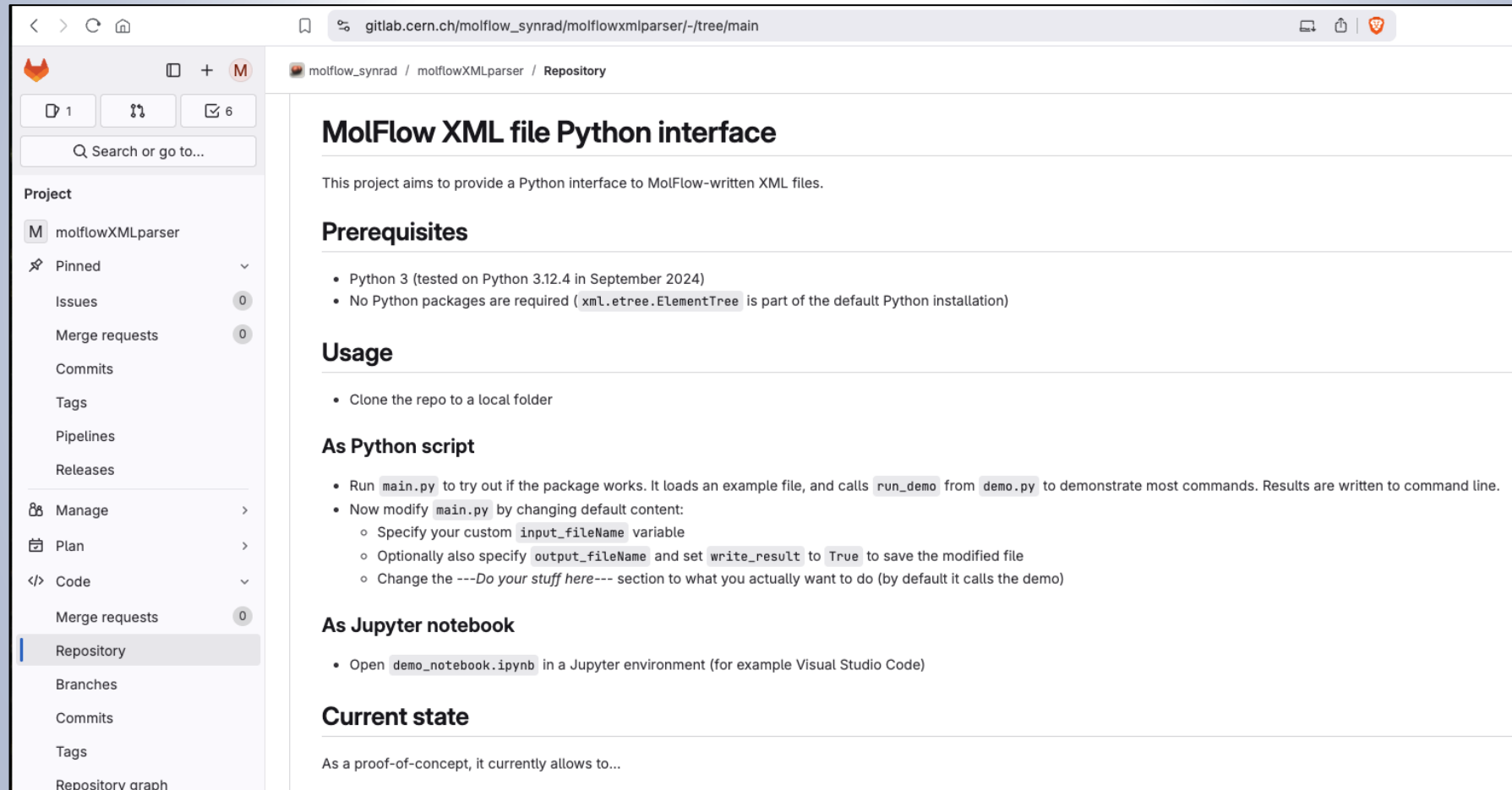
```
molflowCLI.exe --file inputFile.xml -t 3600 -o ./outputFile.xml
```

Python XML interface

- Python is an easy to learn, popular programming language
- XML is a file format – both machine and human-readable
 - Looks like a tree
 - Non-linear, can be searched



Published as Python module or Jupyter notebook



The screenshot shows a GitLab repository page for 'molflowXMLparser' under the user 'molflow_synrad'. The page title is 'MolFlow XML file Python interface'. The main content area is divided into sections: 'Prerequisites', 'Usage', 'As Python script', 'As Jupyter notebook', and 'Current state'. The left sidebar contains navigation options like 'Project', 'Manage', 'Plan', 'Code', and 'Repository'.

MolFlow XML file Python interface

This project aims to provide a Python interface to MolFlow-written XML files.

Prerequisites

- Python 3 (tested on Python 3.12.4 in September 2024)
- No Python packages are required (`xml.etree.ElementTree` is part of the default Python installation)

Usage

- Clone the repo to a local folder

As Python script

- Run `main.py` to try out if the package works. It loads an example file, and calls `run_demo` from `demo.py` to demonstrate most commands. Results are written to command line.
- Now modify `main.py` by changing default content:
 - Specify your custom `input_fileName` variable
 - Optionally also specify `output_fileName` and set `write_result` to `True` to save the modified file
 - Change the `---Do your stuff here---` section to what you actually want to do (by default it calls the demo)

As Jupyter notebook

- Open `demo_notebook.ipynb` in a Jupyter environment (for example Visual Studio Code)

Current state

As a proof-of-concept, it currently allows to...

Examples

Set what to work on:

Specify input and output paths

In this example we don't write the modified file, otherwise set `write_result` to `True`

```
input_fileName = "examples/quickpipe.xml" # .xml or .zip
output_fileName = "out/output.zip" # .xml or .zip
write_result = False # save loaded file at script end
```

Read geometry:

Facet count

```
facet_count = get_facet_count(root)
print(f"The geometry has {facet_count} facets.")
```

The geometry has 7 facets.

```
y_coord_2 = get_vertex(root, 2).y
print(f"The Y coordinate of vertex 2 is {y_coord_2}")
```

The Y coordinate of vertex 2 is 0.9510565162951535

Get results:

Facets

Print pressure on facet at moment 0 (const. flow)

```
print(f"Pressure on facet id {facet_id} is {get_facet_pressure(root, facet_id, moment_id)} mbar")
```

Pressure on facet id 3 is 0.17865621366500498 mbar

Change physics:

Update the temperature on facet to 400K

```
print(f"Temp on facet id {facet_id} was {get_temperature(facet_node)} K")
set_temperature(facet_node, 400.0)
print(f"Temp on facet id {facet_id} is now {get_temperature(facet_node)} K")
```

Temp on facet id 3 was 293.15 K
Temp on facet id 3 is now 400.0 K

Cross-section viewer

Molflow+ 2.9.17 beta (Oct 25 2023) [first exercise.zip]

File Selection Tools Facet Vertex View Test Time About

Cross section view (Viewer #1)

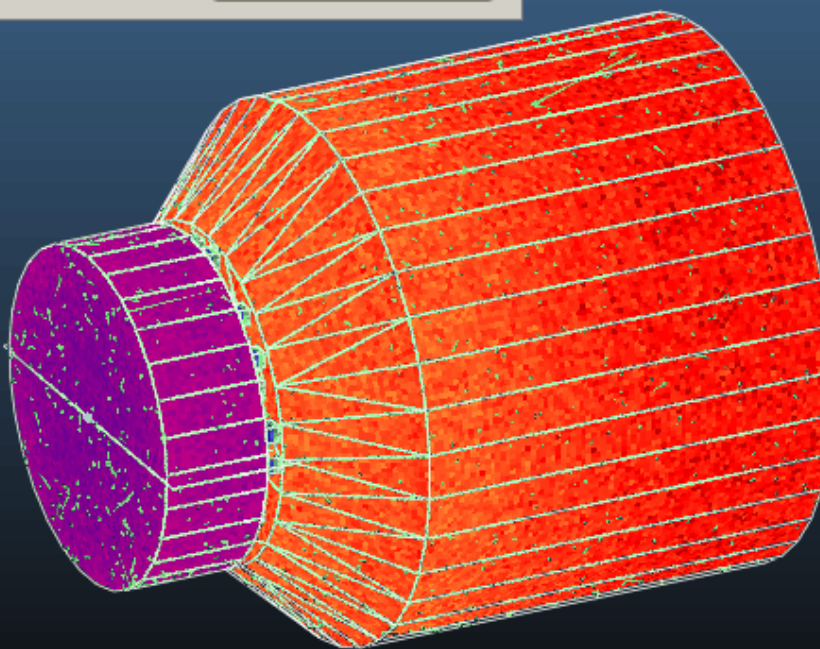
Cut plane
 $-0 *X + -0 *Y + -1 *Z + 4.981987 = 0$

XY plane XZ plane YZ plane
Selected facet Selected 3 vertices Camera midplane

D_min: -5 D_max: 4.98199

Hint: Cross-sections can also be saved with views (View -> Save... menu)

Enable cross section view



V:777 F:444 Dim(12.3,9.99099,9.98199) A

3D Viewer settings

Axes Normals \vec{d}, \vec{v}
 Lines Leaks Hits
 Volume Texture FacetIDs
 Indices VertexIDs

Selected Facet (none)

Particles in

Description

Outgassing (mbar¹/s):
 Outg/area(mbar¹/s/cm²):

Particles out

Sticking factor:
Pumping Speed (l/s):

Sides:

Opacity:

Temperature (*K):

Area (cm²):

Profile:

Shortcuts

Simulation

Auto update scene

Hits 125.08 Mhit (6.1 Mhit/s)

Front Top Side Ortho.

Rich facet and vertex movement

- SynRad movement using beam trajectory points
 - Two points of a trajectory define the movement parameters:
 - Direction,
 - Distance,
 - Rotation.

Move facet

Absolute offset Direction and distance

Absolute offset:

dX: 0 cm

dY: 0 cm

dZ: 0 cm

Distance: cm

From two points

Base point

Selected vertex

Facet center

Direction point

Choose base first

Selected vertex

Facet center

From facet

Selected:

Facet normal Facet U Facet V

Facet N x X Facet N x Y Facet N x Z

From trajectory points

Base trajectory point

Selected point

Direction point

Choose base first

Selected point

Include rotation

Rotation axis:

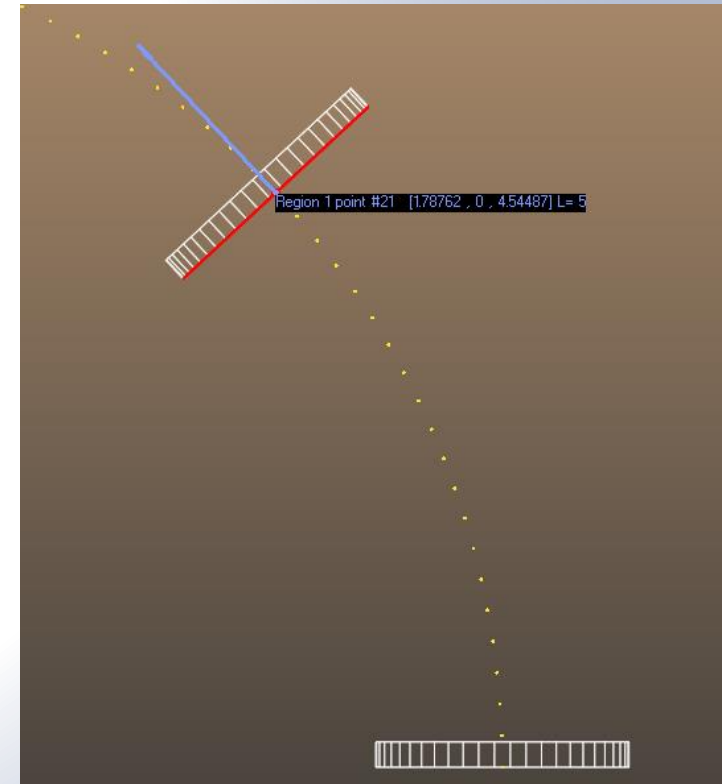
Rotation angle:

Move facets Copy facets

Rich facet and vertex movement

- SynRad movement using beam trajectory points
 - Two points of a trajectory define the movement parameters:
 - Direction,
 - Distance,
 - Rotation.

Example (top view):



Rich facet and vertex movement

- SynRad movement using beam trajectory points:
 - Why add this feature?
- Problem:
 - Moving or duplicating smaller pieces of geometry along longer pipes.
 - Long pipes usually contain beams whose trajectory is aligned with the pipe.
- The old “solution”:
 - Using the *Move* and *Rotate* options separately, manually calculating the rotation.
- The new solution:
 - Selecting the appropriate trajectory points while SynRad does the rest.

Rich facet and vertex movement – a simple demo

Synrad+ 1.5.8 beta (Feb 4 2025) [move_along_traj_pres_end.syn]

File Selection Tools Facet Vertex View Test Regions About

V:500 F:52 Dim:(4.7901,1.99605,6.01704) A

3D Viewer settings

- Rules
- Normals
- \vec{u}, \vec{v}
- Lines
- Leaks
- Hits
- Volume
- Texture
- FacetIDs
- Indices
- VertexIDs

<< View

Selected Facet (none)

Refl:

Rough surface scattering

sigma (nm): T (nm):

Sides:

Opacity:

Sum Area (cm²):

Teleport to facet #:

Structure: Link:

Profile:

Record spectrum

Details... Coord. Mesh... Apply

Simulation

<< Sim Begin Reset

Auto update scene Update

Mode: Fluxwise

Hits: 0 hit (0.0 hit/s)

Des.: 0 des (0.0 des/s)

Leaks: None

Dose: Scn:0.0 F=0 P=0

Time: Stopped: 00:00:00

#	Hits	AbsFlux	AbsPower
1	0	0	0
2	0	0	0

Rotation mode: hold SHIFT to slow down rotation, hold CTRL to rotate around the third axis, and hold ALT to rotate lighting direction of volume view

Front Top Side Ortho X=1.46813, Z=1.28868

Rich facet and vertex movement – FCCee demo

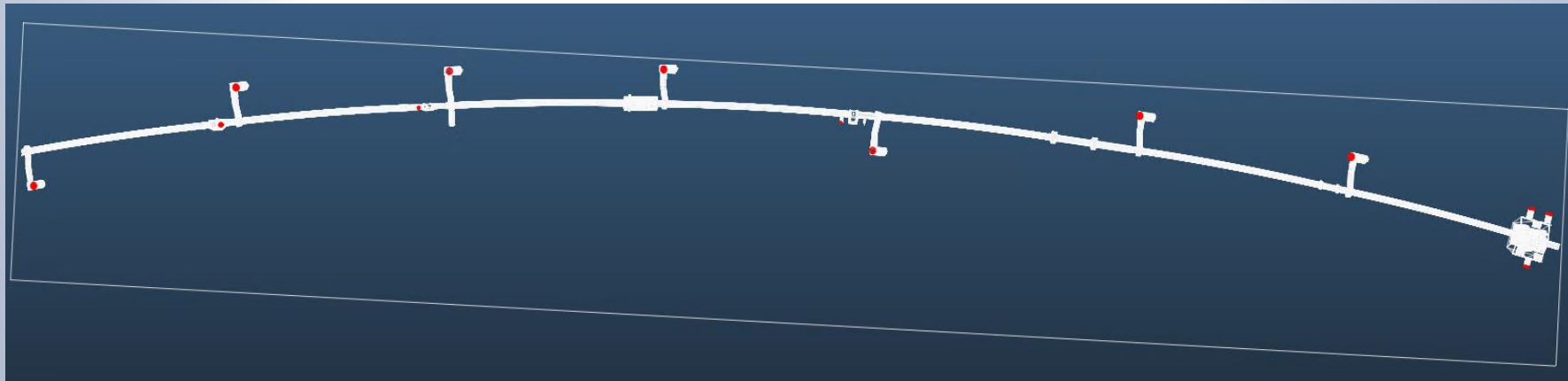
The screenshot displays the Synrad+ software interface. The main window shows a 3D view of a vertical yellow rod. The interface includes a menu bar (File, Selection, Tools, Facet, Vertex, View, Test, Regions, About) and a status bar at the bottom (Front, Top, Side, Ortho, X=-6590.83, Z=1465.18). The right-hand side contains several panels:

- 3D Viewer settings:** Includes checkboxes for Rules, Normals, Lines, Leaks, Hits, Volume, Texture, FacetIDs, Indices, and VertexIDs. A '<< View' button is present.
- Selected Facet [4 selected]:** Shows material 'Ref: 02-Copper', 'Rough surface scattering' options (sigma: 100 nm, T: 10000 nm), 'Sides: 1 Sided', 'Opacity', 'Sum Area (cm²): 59.17031528', 'Teleport to facet # 0', 'Structure: 1 Link: no', 'Profile: None', and 'Record spectrum' checkbox. Buttons for 'Details...', 'Coord.', 'Mesh...', and 'Apply' are at the bottom.
- Simulation:** Features '<< Sim', 'Begin', and 'Reset' buttons. 'Auto update scene' is checked with an 'Update' button. 'Mode' is set to 'Fluxwise'. Statistics show 'Hits: 0 hit (0.0 hit/s)', 'Des: 0 des (0.0 des/s)', 'Leaks: None', 'Dose: Scr:0.0 F=0 P=0', and 'Time: Stopped: 00:00:00'.
- Table:** A table with columns '#', 'Hits', 'AbsFlux', and 'AbsPower'. The data rows are as follows:

#	Hits	AbsFlux	AbsPower
58	0	0	0
59	0	0	0
60	0	0	0
61	0	0	0
62	0	0	0
63	0	0	0
64	0	0	0
65	0	0	0
66	0	0	0
67	0	0	0
68	0	0	0

New feature – extracting data along a path

- Problem:
 - It is often required to extract simulation results (e.g. pressure, impingement rate...) along a certain path in the geometry.
- The old solution:
 - For straight paths, it could be sufficient to add a transparent facet that stretches along the desired path and “records” results.
 - For curved paths, this can be hard:



New feature – extracting data along a path

- **Problem:**
 - It is often required to extract simulation results (e.g. pressure, impingement rate...) along a certain path in the geometry.
- **The old solution:**
 - For straight paths, it could be sufficient to add a transparent facet that stretches along the desired path and “records” results.
 - For curved paths, this can be hard.
- **The new solution:**
 - Allow the user to define a data extraction path by specifying the points in space it consists of.
 - Read simulation results from the surrounding facets.

Extracting data along a path – a preview

MolFlow 2.9.27 (Feb 24 2025) []

File Selection Tools Facet Vertex View Test Time About

V:200 F:102 Dim(2,2,1) Area:12.5612

3D Viewer settings

- Axes
- Normals
- \vec{u}, \vec{v}
- Lines
- Leaks
- Hits
- Volume
- Texture
- FacetIDs

<< View Indices VertexIDs

Selected Facets [9 selected]

Particles in

Desorption: None

- Outgassing [mbar⁴/s]:
- Outg/area[mbar⁴/s/cm²]:

Particles out

Sticking factor: 0

Pumping Speed (l/s):

Sides: 1 Sided

Opacity: 1

Temperature (*K): 293.15

Sum Area (cm²): 0.5653936634

Profile: None

<< Adv Details... Coord. Apply

Shortcuts

Simulation

<< Sim Resume Reset

Auto update scene Update

Hits: 126.20 Mhit (12.5 Mhit/s)

Des.: 63.08 Mdes (6.2 Mdes/s)

Leaks: None

Time: Stopped: 00:00:08

#	Hits	Des	Abs
1	20696110	63082047	2.06961e+
2	42385924	0	4.23859e-
3	631843	0	0

Front Top Side Ortho. v

Extracting data along a path – an important use case

- FCC-ee:
 - Using curved geometries at CERN is a very common practice.
 - The new feature will be useful for simulations for the FCC-ee.
 - The SynRad version will include data extraction along trajectory points

