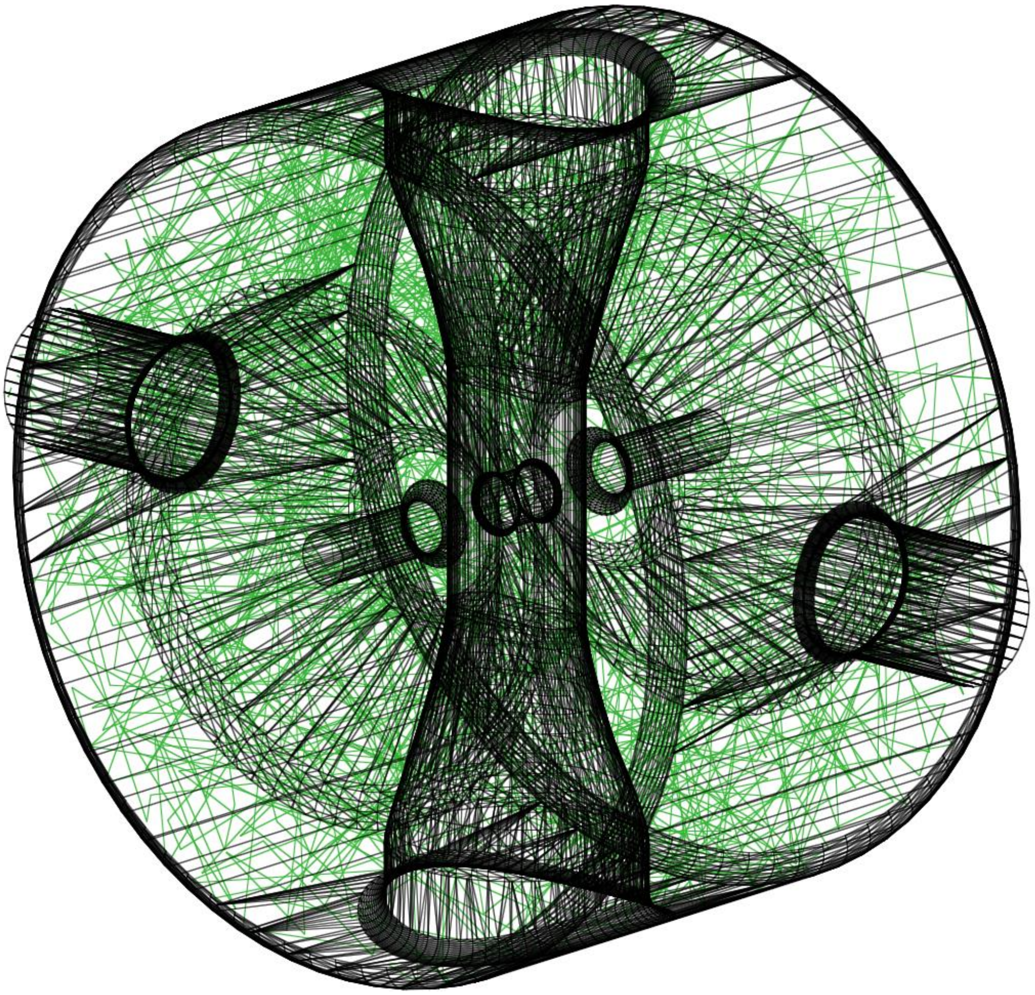
MolFlow+ user guide

for versions 2.4 and before

This user guide was not updated since 2014. To use Molflow, check the articles on the website, which has quick start videos, tutorials, and function-specific descriptions:
https://molflow.web.cern.ch/



For version 2.4.1 – 3 June 2014

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1. About Molflow

Molflow+ is a Windows program that allows you to calculate the steady-state pressure in an arbitrarily complex geometry when ultra-high vacuum condition is met. The name comes from *mol*ecular *flow*, the condition when the mean free path of molecules is so long compared to the geometry size that collisions can be neglected. In this case, particles fly independently, which makes this physics particularly suitable for Monte Carlo simulations. The first version of this program was written by Roberto KERSEVAN in 1990 (see this reference article). In 2007 a new version called MolFlow+ was written in ESRF (Grenoble, France), that uses the original algorithm in a modern environment: it takes advantage of OpenGL acceleration for the 3D display and it can use multiple cores for the calculations. In 2012, the further improvements were added in CERN, and also a website was created. Geometries can be imported from most CAD programs that support the STL file format, and the development is still underway, with current focus on being able to simulate time-dependent processes.

2. Basic concepts

This chapter is a general overview of the program and of the expressions later used.

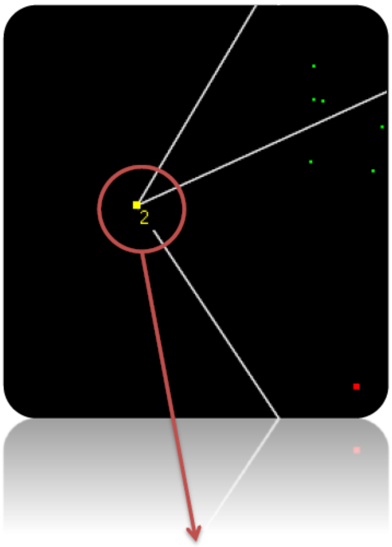
2.1. Working with Molflow

Using Molflow to simulate a vacuum system will in most cases consist of four distinct steps:

1) **Importing the geometry.** To begin, we need a geometry in which particles will fly. This will most likely originate from a CAD program (Autodesk Inventor, Solidworks, Catia, etc.). There is a standard STL file format (STereoLithography or Standard Tessellation Language) that all CAD programs can export to. Molflow is able to open these files and merge (collapse) the list of triangles to a geometry delimited by polygons, referred to as *facets*.
2) **Setting up simulation parameters.** Once we have the geometry, we have to define physical properties of its boundaries through *facet parameters*. Such a parameter is the temperature or the reflective property of the facet. Also, in this phase we execute the important step of defining where the particles come from (outgassing and desorption) and also the location and properties of pumps.
3) **Setting up what to measure.** After the second step, our simulation is ready to run. However, we want to derive useful results of the whole process. Although some physical quantities are measured by Molflow out of the box (average pressure on each facet, etc.), we will most likely want to obtain *formulas* that calculate a given quantity, *profiles* that show the evolution of a quantity along the length of a facet, or *textures* that show us the pressure directly in the form of colors on our geometry.
4) **Running the simulation.** Once we have set up everything, Molflow will trace the trajectories of particles in our system from their insertion until they are being pumped away. Every second, displayed results are being updated. The longer you run a simulation, the smaller the statistical fluctuation becomes.

2.2. Elements of the geometry

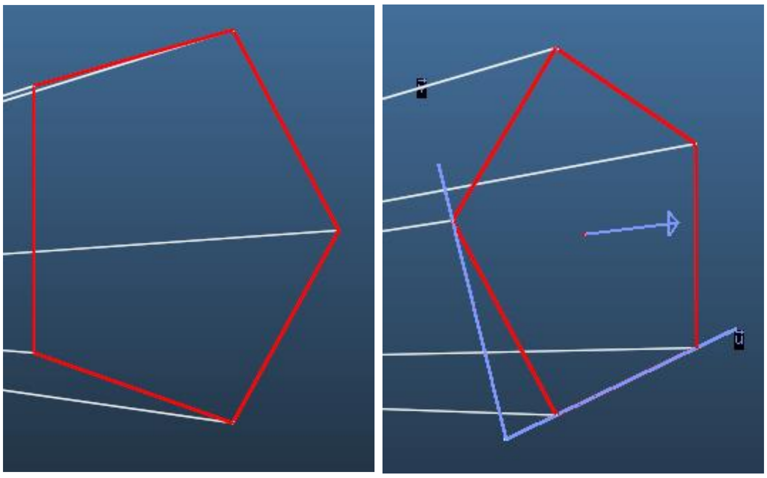
2.2.1. Vertex



A vertex is a point in the 3D space. In Molflow, they are interesting for two reasons:

- All facets have an outline that consists of vertices (vertexes of a given facet are referred to as its *indices*)
- Some geometry operations (such as creating a facet) require creating and selecting vertices first

2.2.2. Facet



A facet and its normal and U, V vectors

Facets are polygons that are the elementary constituents of the geometry. They have *indices,* ie. the vertices they consist of, and they have a *normal vector* defining the direction they are looking to. They also have a local U,V coordinate system, where the U vector points from the first to the second index, and the V vector is perpendicular to it. The normal vector's direction can be swapped, and the U,V vectors can be rotated by the user.

Significance of facets is that their physical parameters can be specified one by one. Therefore a facet can serve as a pump, as a gas inlet, as a teleport gate for boundary conditions and it can also have profiles and textures.

2.2.3. Structures (advanced)

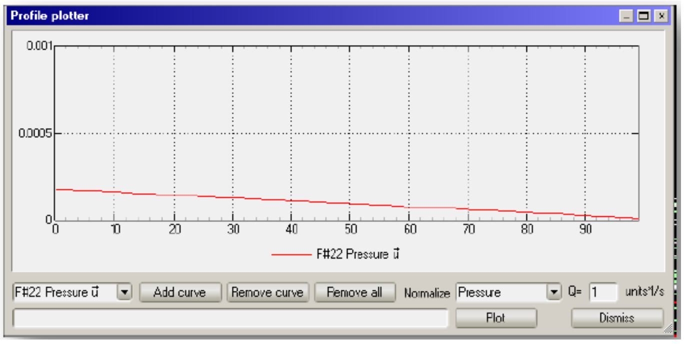
Structures, also called *superstructures* are a set of facets that are specified by the user to be distinct from the rest of the geometry. Structures are connected by *link facets*. They were introduced to Molflow to make geometry handling easier (for example, you can restrict visibility or facet selectability to a given structure only), but their real role is to speed up simulation: ray-tracing algorithms will only look for collisions within the current structure (instead of with every facet in the geometry).

Please note that whereas the computing time can be reduced by using structures, the time to set them up can be long. Experience shows that unless the geometry consists of a lot of facets (in the order of hundreds of thousands), not splitting the geometry to structures might be just fine.

2.3. Post-processing within Molflow

To interpret simulation results (notably the pressure at certain points of the geometry), facets in Molflow can have profiles and textures.

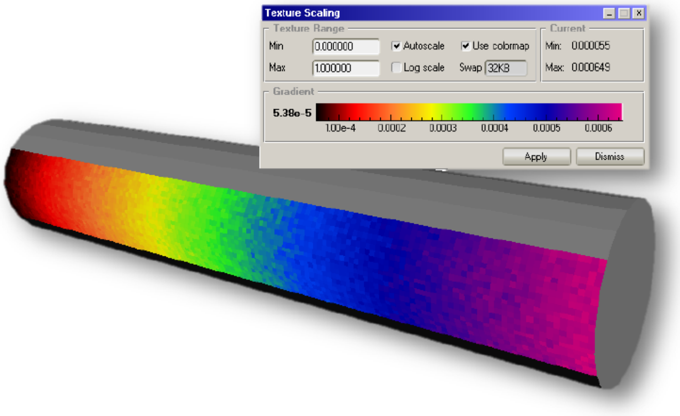
2.3.1. Profiles



Profiles are quick measuring tools if the user wants to see the pressure along a facet. When a profiling is enabled on a facet, it is divided into 100 equal parts along the U or V vector, and for each slice the pressure is calculated.

The advantage is that the pressure evolution can be visualized within Molflow, and several profiles can be plotted on the same *Profile Plotter* window for comparison. The disadvantage is that it only works on rectangular facets, and sometimes the 100 element split is not enough.

2.3.2. Textures



Texture Scaling

Texture Range

Min 0.000000 ☑ Autoscale ☑ Use colormap

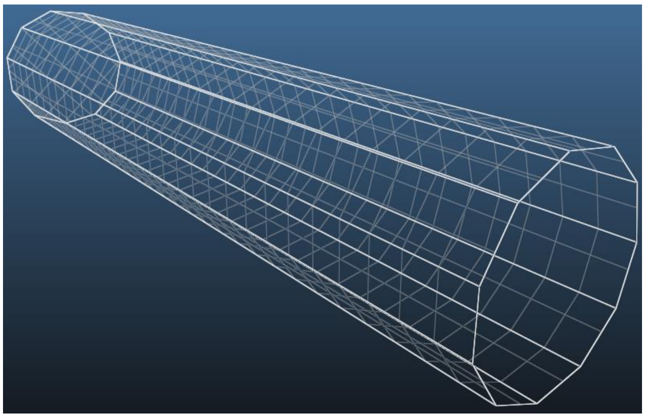
Max 1.000000 □ Log scale Swap 32KB

Current

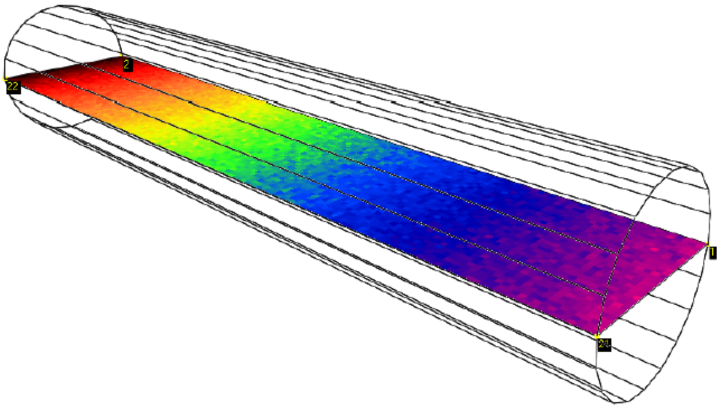
Min: 0.000055

Max: 0.000649

Textures are tools to locally visualize the pressure on given facets with the help of a color scale that the user can customize. To calculate them, the user has to create a *Mesh* first, which is the division of a facet to squares (cells) of arbitrary size. Then the pressure is calculated individually for each of these squares and can be displayed with colors chosen in the *Texture Scaling* dialog.

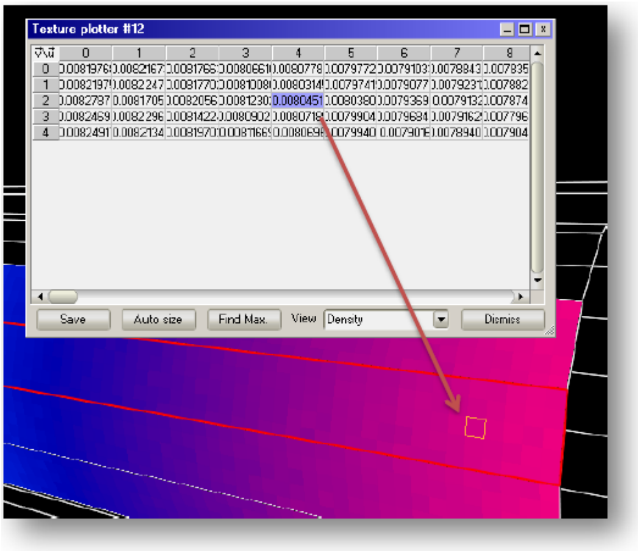


Whereas adding textures to existing facets is sufficient in many cases, it is possible to create *transparent facets* whose only purpose is to hold a texture. These transparent facets serve as tools to visualize the pressure in the middle of the geometry, for example.



Transparent facet to measure the pressure in the middle of a tube

Apart from the visual appearance, it is possible to read and export pressure values cell by cell using the *Texture Plotter*.



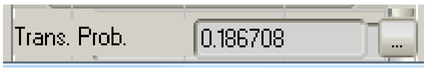
Texture plotter #12

v\u	0	1	2	3	4	5	6	7	8
0	0.0081976	0.0082167	0.0081766	0.0080661	0.0080778	0.0079772	0.0079103	0.0078843	0.007835
1	0.0082197	0.0082247	0.0081770	0.0081008	0.0080314	0.0079741	0.0079077	0.0079231	0.007882
2	0.0082787	0.0081705	0.0082056	0.0081230	0.0080451	0.0080380	0.0079369	0.0079132	0.007874
3	0.0082469	0.0082296	0.0081422	0.0080902	0.0080718	0.0079904	0.0079684	0.0079162	0.007796
4	0.0082491	0.0082134	0.0081970	0.0081166	0.0080698	0.0079940	0.0079018	0.0078940	0.007904

View: Density

Texture Plotter: cell values can be read and exported

2.3.3. Formulas



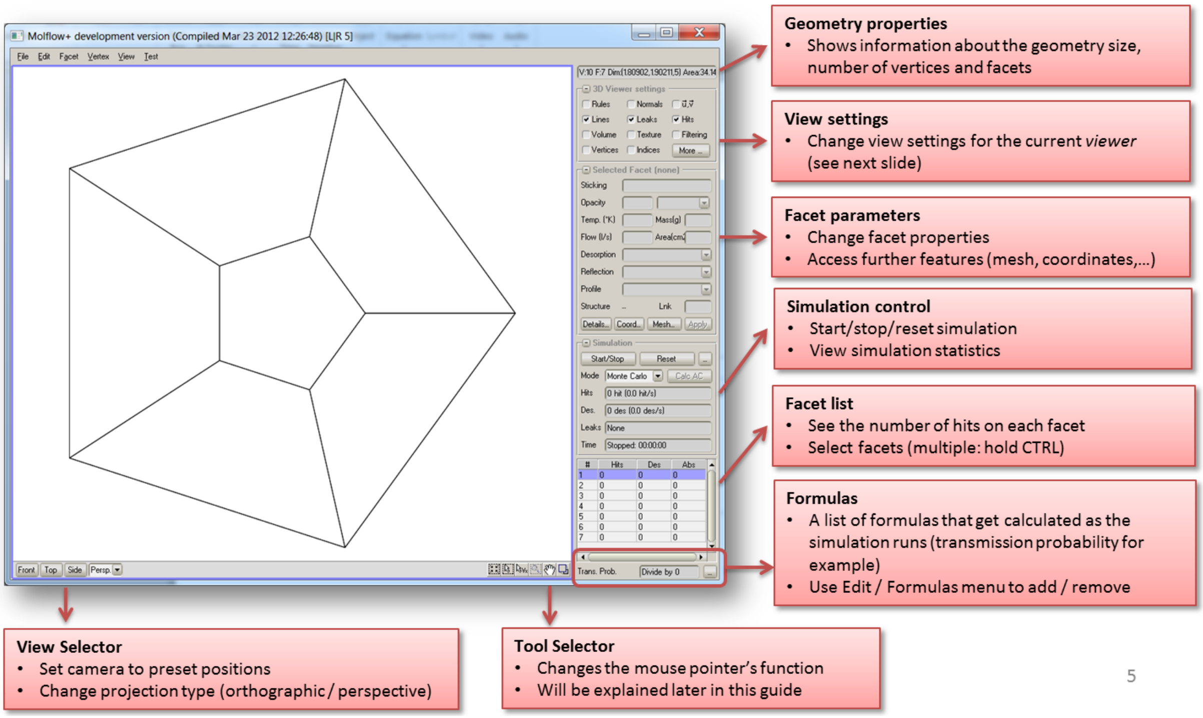
Trans. Prob. 0.186708

Molflow offers the user to set up custom formulas, which are expressions containing internal values as variables. One could, for example, derive the transmission probability for a pipe from the number of particles on its two sides. These formulas are then updated in real-time as the simulation is running.

3. MolFlow+ functions one by one

3.1. Interface overview

When you open MolFlow, you will see an empty geometry window, with the menu bar on its top and panels on the right. Most functions will be unavailable because there is no geometry loaded until you import a file or use the Test -> Quick Pipe command (ALT+Q).



Geometry properties

- Shows information about the geometry size, number of vertices and facets

View settings

- Change view settings for the current *viewer* (see next slide)

Facet parameters

- Change facet properties
- Access further features (mesh, coordinates,...)

Simulation control

- Start/stop/reset simulation
- View simulation statistics

Facet list

- See the number of hits on each facet
- Select facets (multiple: hold CTRL)

Formulas

- A list of formulas that get calculated as the simulation runs (transmission probability for example)
- Use Edit / Formulas menu to add / remove

View Selector

- Set camera to preset positions
- Change projection type (orthographic / perspective)

Tool Selector

- Changes the mouse pointer's function
- Will be explained later in this guide

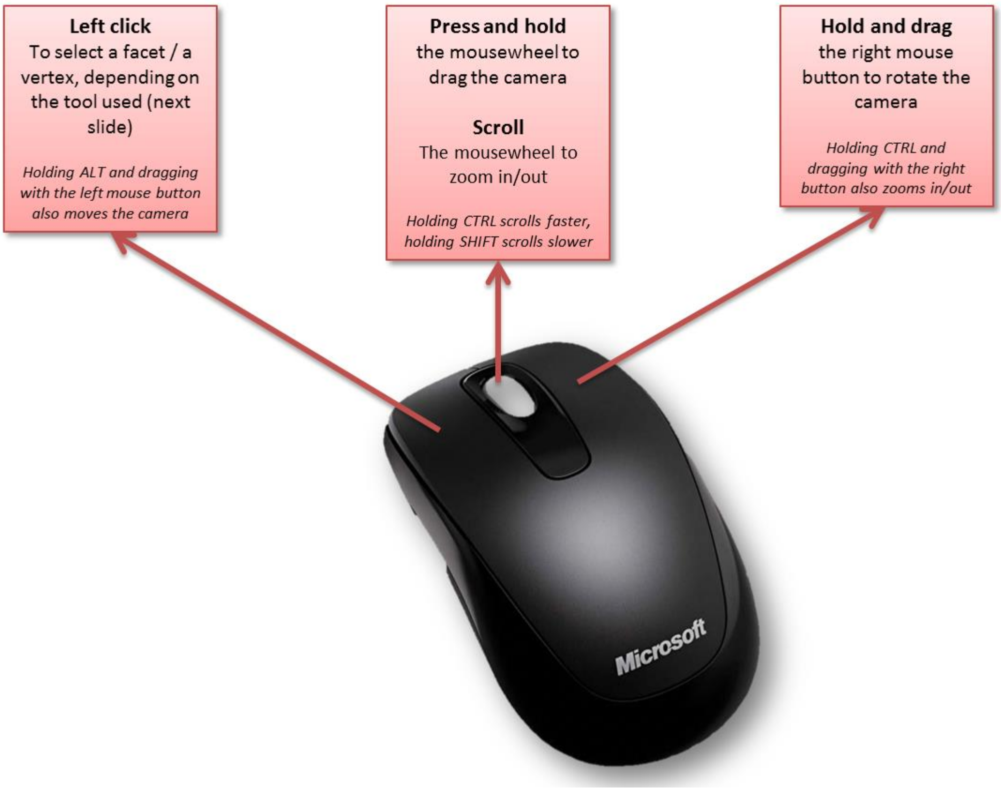
The MolFlow window and functions of different panels

3.2. Camera controls

Once you have the geometry in MolFlow, you must be able to move the camera so you can access facets in every part of the geometry.

The most important things to note are:

- **Selecting** a facet: left-click
- **Scrolling**: move mouse with middle button pressed
  (no 3-button mouse? Hold ALT and the left button to scroll)
- **Rotating**: move mouse with right button pressed
- **Zooming**: mouse wheel



Left click
To select a facet / a vertex, depending on the tool used (next slide)

Holding ALT and dragging with the left mouse button also moves the camera

Press and hold
the mousewheel to drag the camera

Scroll
The mousewheel to zoom in/out

Holding CTRL scrolls faster, holding SHIFT scrolls slower

Hold and drag
the right mouse button to rotate the camera

Holding CTRL and dragging with the right button also zooms in/out

Mouse controls in MolFlow

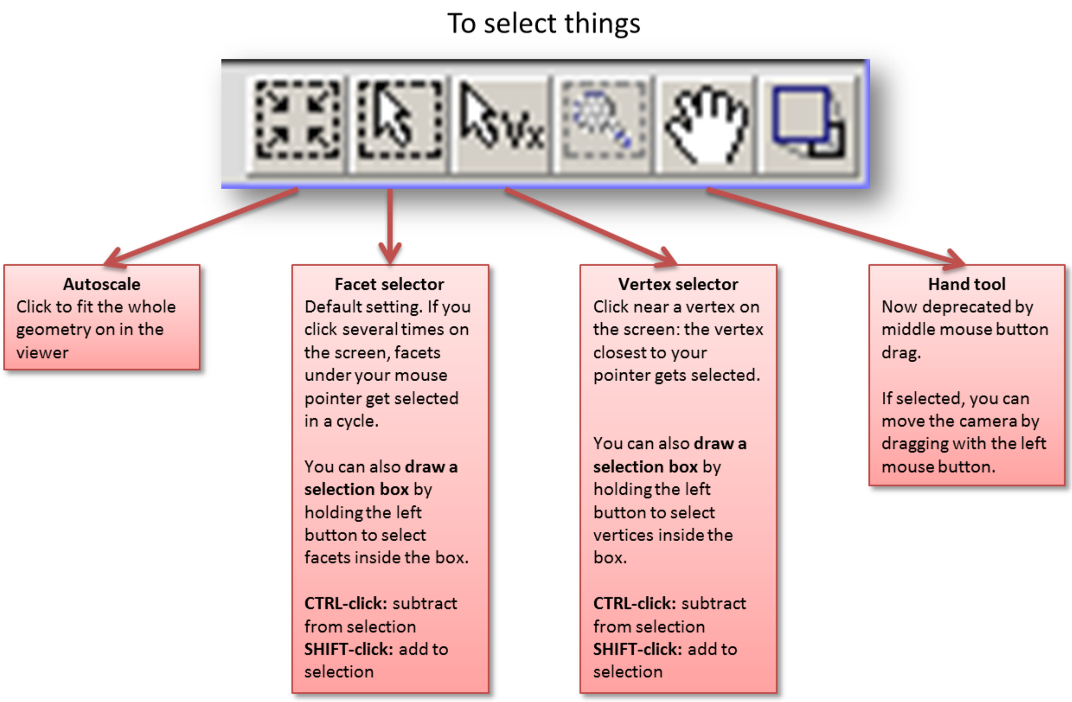
Additional features are:

- Rotate slower: hold SHIFT
- Scroll slower: hold SHIFT
- Zoom slower: hold SHIFT, zoom faster: hold CTRL

3.3. Selecting facets

3.3.1. Selector tools

Switching between these tools will determine what your mouse actions will do on the screen. The default setting is facet selector.


To select things

Autoscale
Click to fit the whole geometry on in the viewer

Facet selector
Default setting. If you click several times on the screen, facets under your mouse pointer get selected in a cycle.

You can also **draw a selection box** by holding the left button to select facets inside the box.

CTRL-click: subtract from selection
SHIFT-click: add to selection

Vertex selector
Click near a vertex on the screen: the vertex closest to your pointer gets selected.

You can also **draw a selection box** by holding the left button to select vertices inside the box.

CTRL-click: subtract from selection
SHIFT-click: add to selection

Hand tool
Now deprecated by middle mouse button drag.

If selected, you can move the camera by dragging with the left mouse button.

The facet selector explained

3.3.2. Selecting facets

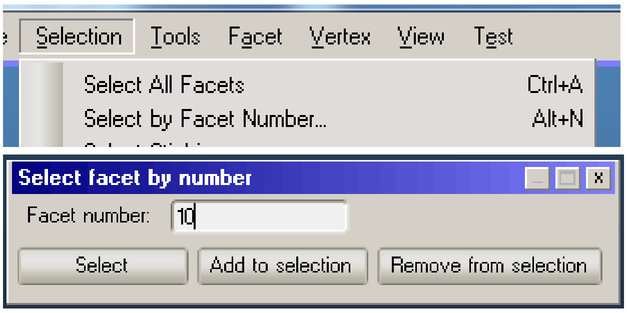
Using left-click

Clicking on any part of the geometry will select a facet under your mouse **that has at least one vertex visible in the viewer**. (ie. large facets filling your whole screen won't be selected unless you zoom out).

Very important: if you keep clicking without moving the mouse, the selection will **cycle** through all facets below your mouse cursor. So if you want to select a particular facet, keep clicking over it without moving your mouse. This is a function that most new users need some time to get used to, but then it becomes really useful. Just remember, don't move your mouse between clicks.

Using the facet number

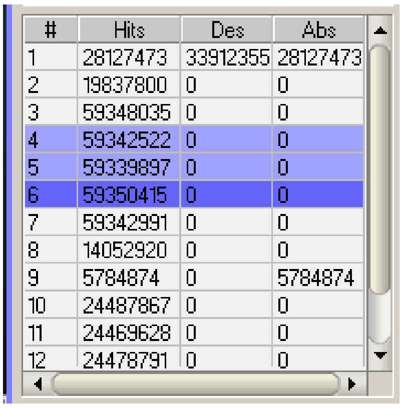
You can also select a facet by entering its number in the selection menu's *Select Facet by Number* dialog:



Facet number: 10

The *Select Facet by Number* dialog

Using the facet hit list



#	Hits	Des	Abs
1	28127473	33912355	28127473
2	19837800	0	0
3	59348035	0	0
4	59342522	0	0
5	59339897	0	0
6	59350415	0	0
7	59342991	0	0
8	14052920	0	0
9	5784874	0	5784874
10	24487867	0	0
11	24469628	0	0
12	24478791	0	0

The *Facet Hits List* panel

Clicking on any row of the facet hit list will select the corresponding facet.

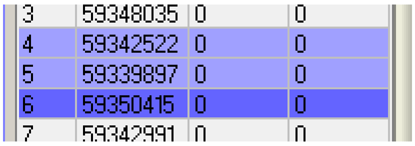
3.3.3. Selecting multiple facets

With your mouse

Hold the SHIFT key to add to a selection, the CTRL to subtract from it (CTRL-clicking will deselect **all** facets under your cursor). You can also **draw selection rectangles** by holding your left mouse button, and SHIFT and CTRL keys also add and subtract them.

In the facet hits list

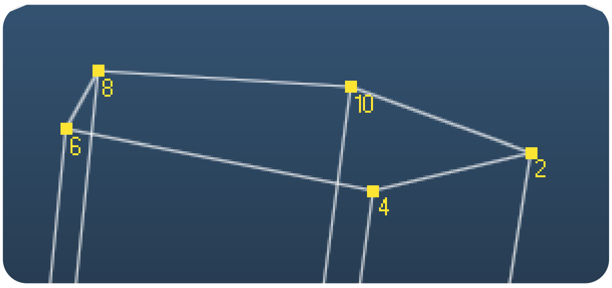
Hold the CTRL key to add/remove the clicked row to the selection.



3	59348035	0	0
4	59342522	0	0
5	59339897	0	0
6	59350415	0	0
7	59342991	0	0

Click on any row (to set the focus), then holding the SHIFT key scroll up or down to select many facets that follow each other.

3.3.4. Selecting vertices

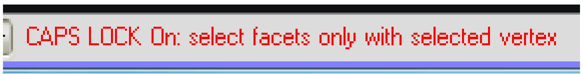


With the vertex selector tool, you can click near a vertex, and Molflow will select the closest vertex to your mouse pointer. Use SHIFT and CTRL to add/subtract from the selection, and you can also use selection areas (drawing selection rectangles).

3.3.5. The CAPS LOCK trick

Sometimes, in complex geometries, it might be very difficult to select the facet we want.

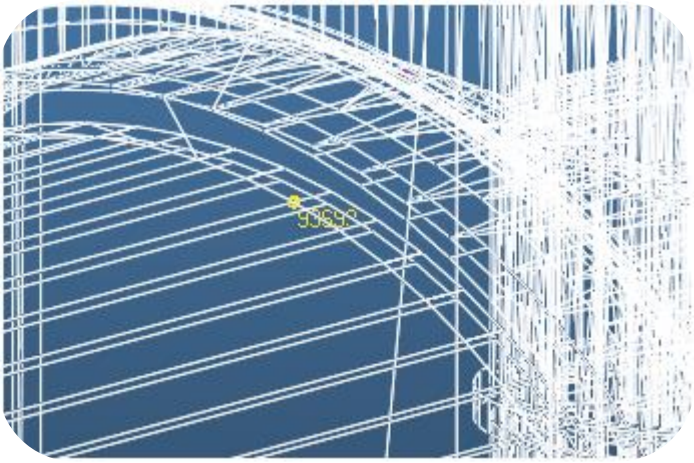
Just select any vertex of the desired facet (which is, in practice, much easier), then turn on the **CAPS LOCK** key:

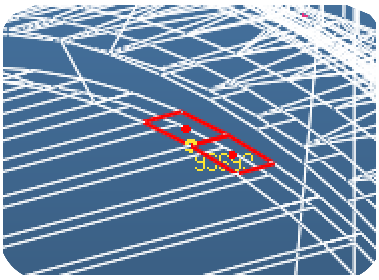


CAPS LOCK On: select facets only with selected vertex

Message on the bottom of the viewer reminding you of the CAPS LOCK mode

This will **restrict** the selectable facets to those that have a vertex selected. Therefore your next click (or selection rectangle) will select directly those whose vertex you just selected:





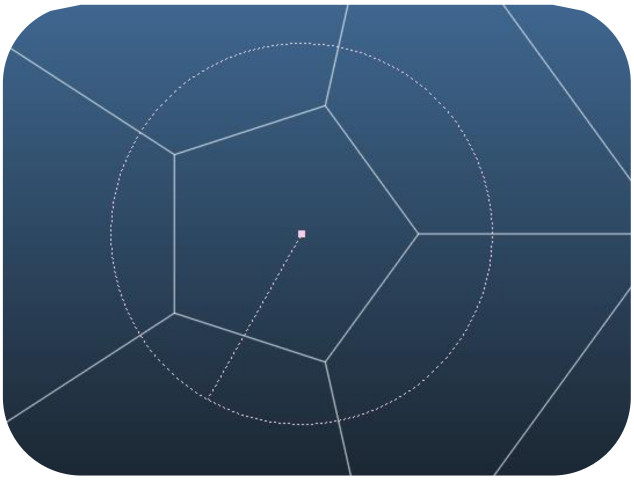
3.3.6. Selection groups

You can also select facets through your memorized selection groups. Once you have made a selection, you can memorize it and recall later. Refer to section 3.11.1

3.3.7. Selecting with a circle

Holding the **ALT** button will change the selection rectangle to a circle.

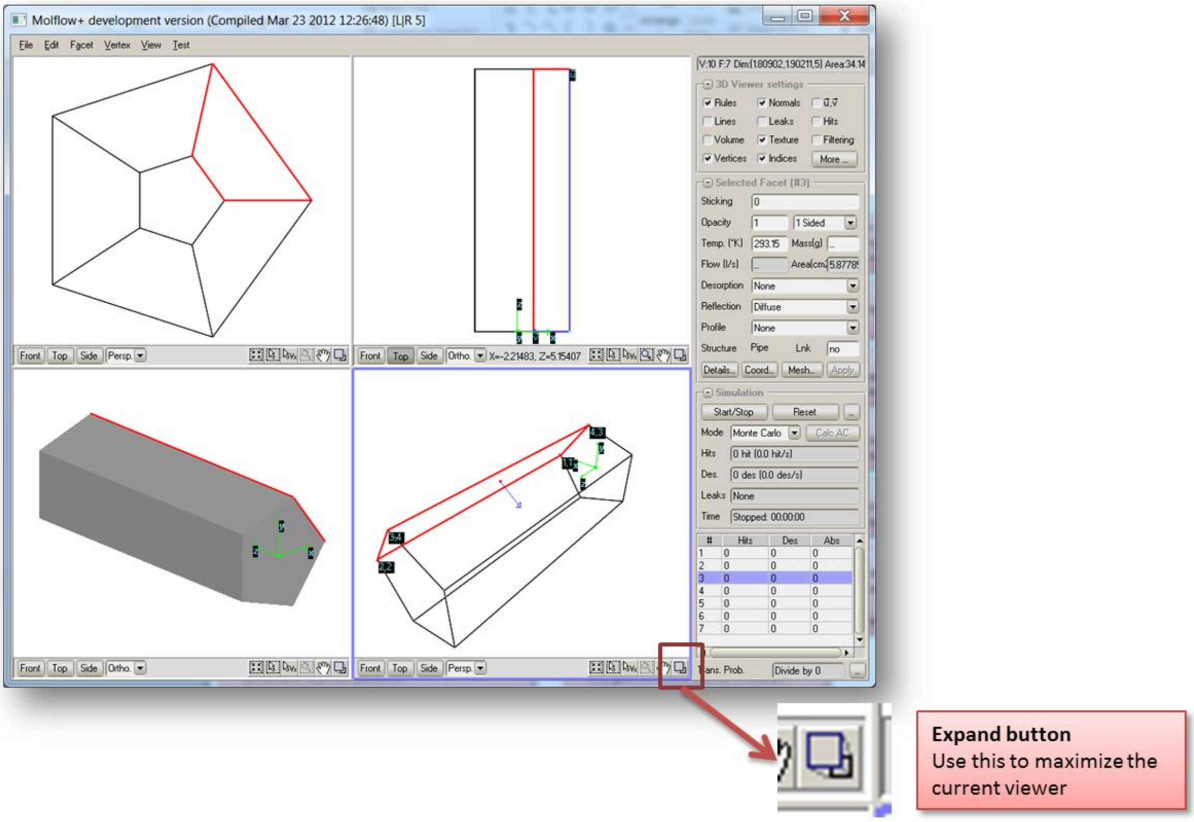
This will work together with both facet and vertex selectors, as well as with the SHIFT and CTRL (add and subtract) modifiers.



Holding ALT will change the selection to a circle

3.4. Viewers

MolFlow offers you to have four different *viewers*, each of which can have different view parameters. For example, camera angles can be different, and you can also decide to display the textures on the first viewer, the hits on the second, and so on.



Molflow+ development version (Compiled Mar 23 2012 12:26:48) [L|R 5]

V:10 F:7 Dim:(180902,190211,5) Area:34.14

3D Viewer settings

☑ Rules ☑ Normals □ u,v
□ Lines □ Leaks □ Hits
□ Volume ☑ Texture □ Filtering
☑ Vertices ☑ Indices

Selected Facet (#3)

Sticking: 0
Opacity: 1, 1 Sided
Temp. (°K): 293.15 Mass(g): ...
Flow (l/s): ... Area(cm²): 5.87785
Desorption: None
Reflection: Diffuse
Profile: None
Structure: Pipe Lnk: no

Simulation

Mode: Monte Carlo
Hits: 0 hit (0.0 hit/s)
Des.: 0 des (0.0 des/s)
Leaks: None
Time: Stopped: 00:00:00

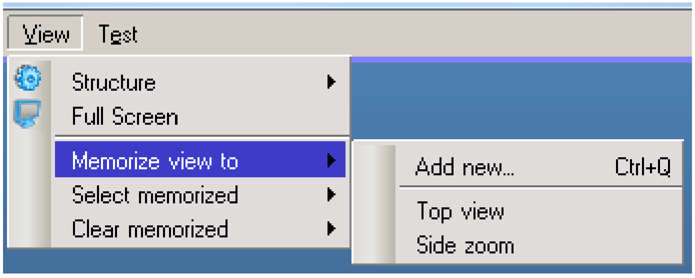
#	Hits	Des	Abs
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	0	0	0
7	0	0	0

Trans. Prob.: Divide by 0

Expand button
Use this to maximize the current viewer

By default, the first viewer is maximized, but you can collapse and expand any of them using the button on the bottom right.

Also, you can save and recall camera positions, so-called *views* with the View menu:

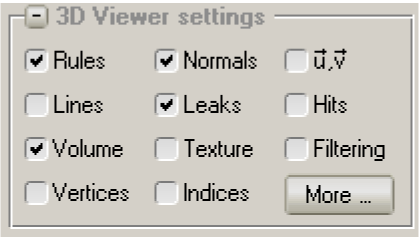


To save a camera view, use View -> Memorize View -> Add new… (CTRL+Q). Give the camera position a name.

To recall a camera view, the easiest way is to press ALT+F1, ALT+F2, … or you can optionally use the *Select Memorized* submenu.

3.5. Viewer parameters

To decide what and how to display in a viewer, we have a panel with the *viewer parameters.* Below we'll go through all the functions.



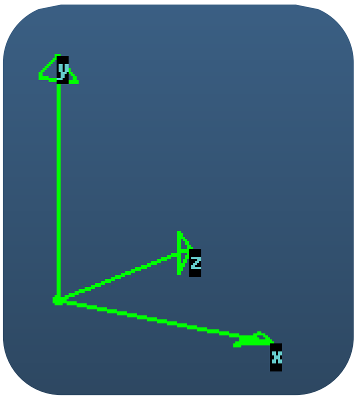
3D Viewer settings

☑ Rules ☑ Normals □ u,v
□ Lines ☑ Leaks □ Hits
☑ Volume □ Texture □ Filtering
□ Vertices □ Indices [More ...]

The viewer parameters panel

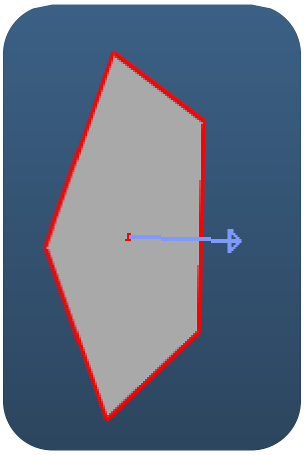
This dialog box customizes what you want to display on the currently selected viewer. Each of the four viewers can have different view settings.

3.5.1. Rules



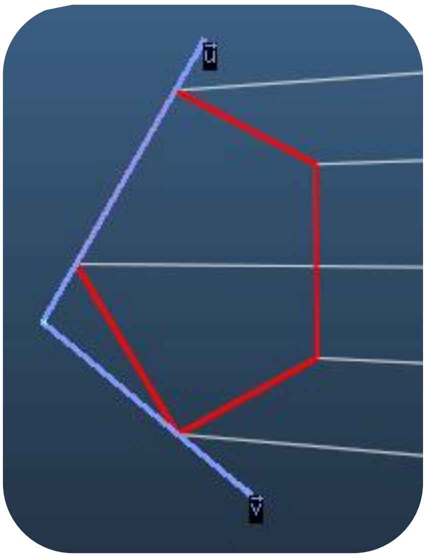
Rules display the origin position and the direction of X,Y,Z base vectors.

3.5.2. Normals



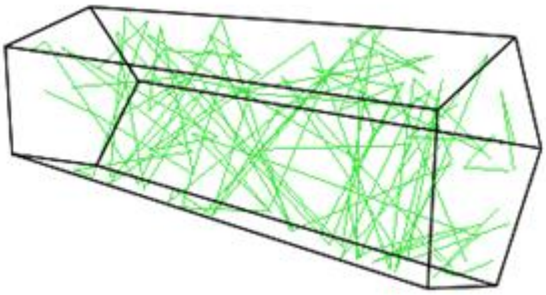
Displays the normal vector of the facets, which is important to define their orientation.

3.5.3. U,V vectors



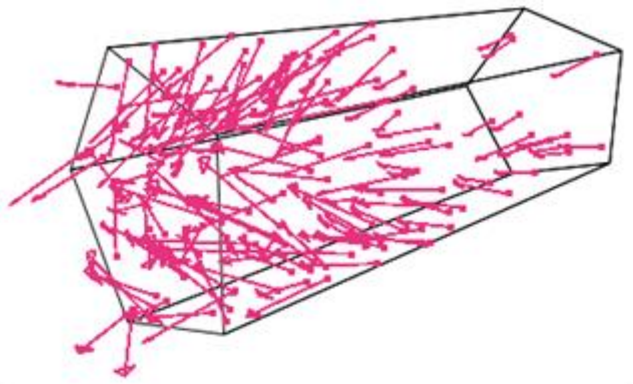
Displays the facet's own coordinate system. Useful when defining profiles and mesh, which follow the orientation of the U vector.

3.5.4. Lines



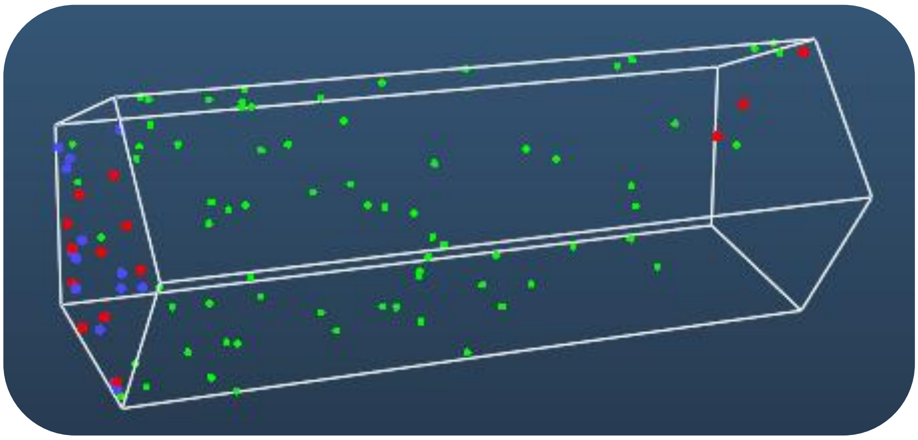
Particle trajectories. Note that at each second the last 2048 lines in cache are displayed, so their position might appear randomly. You can change the displayed number in the *More...* dialog, see later.

3.5.5. Leaks



Visualizes particles escaping from the system. A dot marks the last hit's position, and then the arrow points in the direction where the particle was relaunched, and in which direction it didn't find any collisions thus left the system.

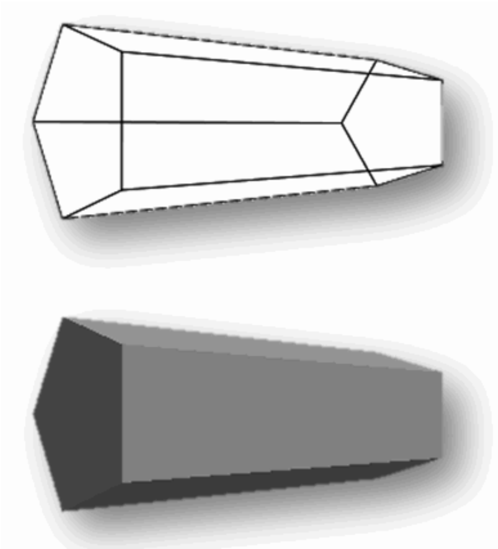
3.5.6. Hits



Shows the positions where hits were registered.

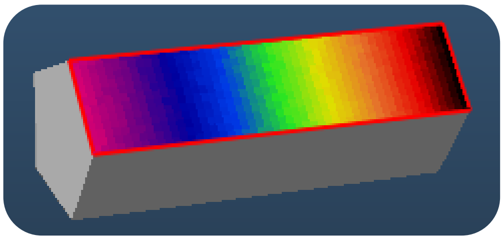
Red hits show absorbed (pumped) hits, blue show desorbed (created) hits, green show reflections, light blue show transparent passes and orange shows teleported particles. You can make the dots small or large in the *More...* dialog.

3.5.7. Volume



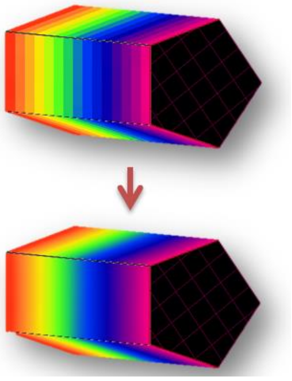
Toggles filling the facets (wireframe / filled polygon modes).

3.5.8. Texture



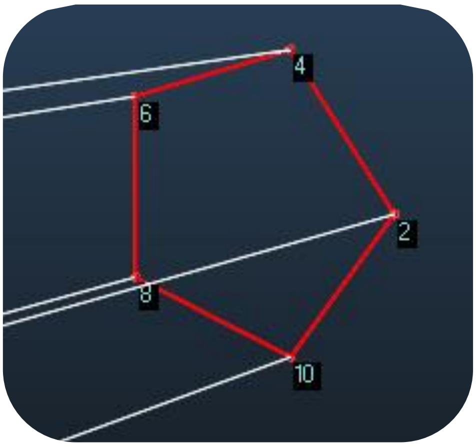
Toggles texture display on those facets where a mesh is set.

3.5.9. Filtering



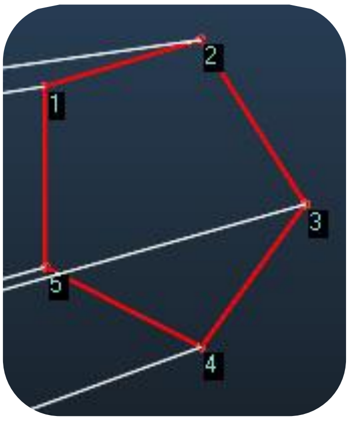
Applies a Gauss filter (smoothing) to the textures.

3.5.10. Vertices



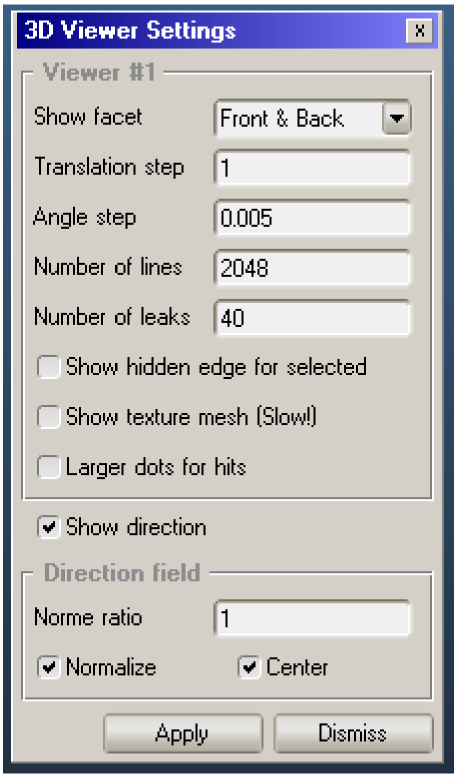
All vertices in the system have a unique ID, starting from 1. You can visualize these IDs on selected facets with this option.

3.5.11. Indices



All facets have an order of vertices (referring to the system-wide vertices). The order defines where the U vector is pointing (always from indice 1 to indice 2), and which direction the normal is pointing (left-hand rule). You might want to visualize these when using the *Shift Vertex* and *Swap Normal* commands.

3.5.12. The *More…* dialog



3D Viewer Settings

Viewer #1

Show facet: Front & Back

Translation step: 1

Angle step: 0.005

Number of lines: 2048

Number of leaks: 40

☐ Show hidden edge for selected

☐ Show texture mesh (Slow!)

☐ Larger dots for hits

☑ Show direction

Direction field

Norme ratio: 1

☑ Normalize ☑ Center

Pressing the *More…* button opens a new dialog that enables you to set additional viewer options.

Show facet (front / back)

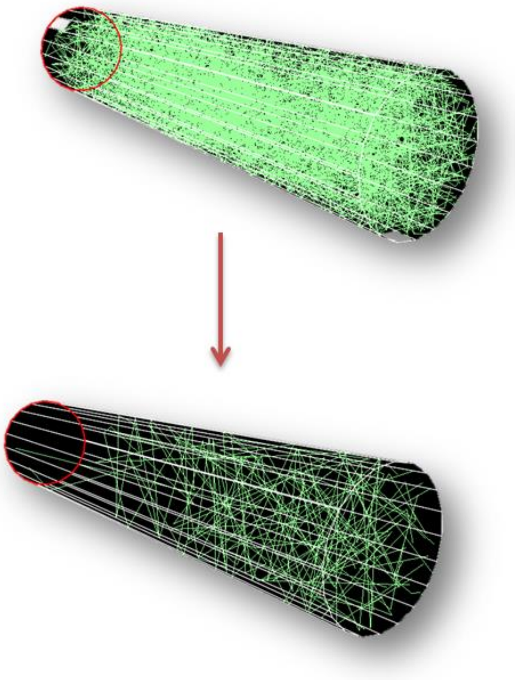
Has effect when *Volume* viewer option is enabled. Front side is the one where the normal is pointing to. Here you can set if you want both sides painted (default), or make one of them transparent.

Translation step / Angle step

Camera movement / rotation speed when using cursor keys to navigate (rotation: SHIFT + cursor keys)

Number of lines

Max. number of displayed lines and hits.

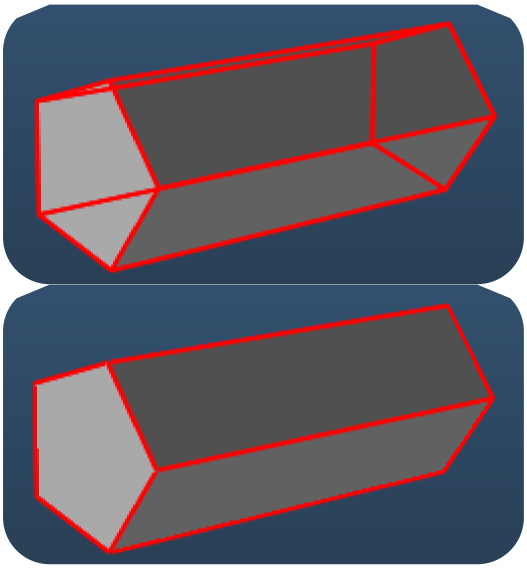


When too many trajectories are displayed, it is a good idea to reduce this number

Number of leaks

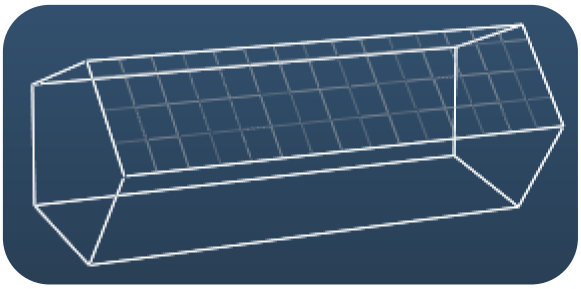
Max. number of displayed leaks.

Show hidden edge for selected



In *Volume* display mode, toggle whether outlines of selected facets should be displayed when hidden by the object's volume.

Show texture mesh



When *Texture* display is disabled (ie. colors of the texture are not painted), the mesh outlines can still be displayed with this option. As large grids consist of many lines to paint, at large texture sizes this can slow down the rendering (making menus, etc. respond slowly to mouse clicks).

Larger dots for hits

As its name suggests, makes the hit points larger (easier to spot).

3.6. Importing geometry

3.6.1. Design guidelines

Whereas it convenient to simply import a vacuum system from a CAD program, several simplifications can be made that make handling of our structure easier in Molflow, and also reduce the number of facets thus the simulation speed.

Therefore it is recommended to create a simplified geometry for Molflow, with the following considerations:

1) Use only necessary parts in your geometry. Remove flanges, holes for screws and mechanical parts that are not hit by particles thus are irrelevant to vacuum. Since CAD programs export geometries in form of triangles, one single hole can severely complicate your geometry. If you have a grid or a dense part of holes, it might be adequate to replace them by a single facet with partial transparency (ie. instead of including 100 holes that take up 20% of the surface, it is equivalent to create a single facet with 80% opacity).
2) Use solid structures, „inside out”. Molflow only sees facets as the boundary of your vacuum chamber, and doesn't know which part of your geometry is solid or empty. (You can define this by the orientation of the facets' normal vectors and by launching particles in the correct part). Therefore, instead of defining a cylinder, that has a wall and a cavity, you can only use half as much facets by creating a solid cylinder. Then the solid part will take the role of the vacuum chamber.
3) Once your simulation has run long enough, you can remove parts that are not necessary, i.e. which are never going to be hit. Choose *Select Hits>0* from the selection menu, then the *Invert selection* command, that way you will have all the facets selected that are never hit. Then you can remove them.

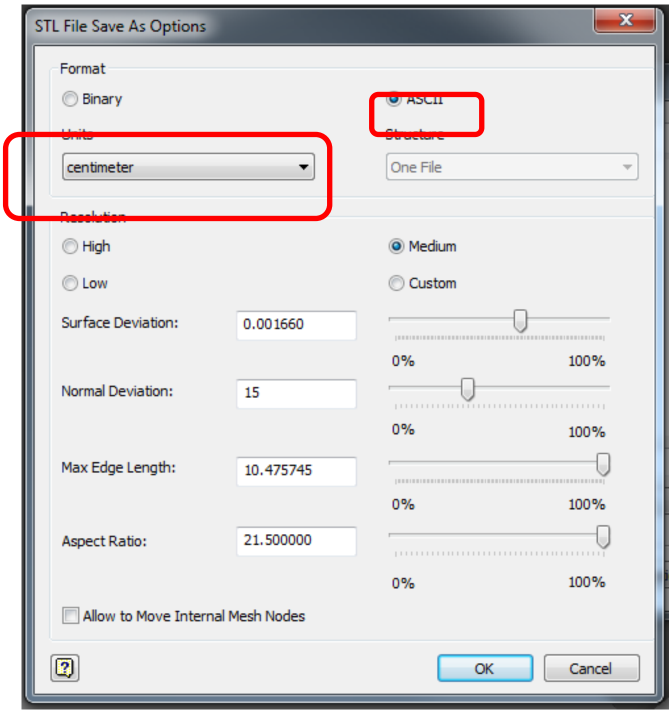
3.6.2. STL files

STL or STereoLithography files describe the 3D geometry. They become more and more popular since all CAD programs support them, and they also happen to be the format recognized by 3D printers. They consist of a list of triangles: each triangle is described by its 3 vertices and the direction of the unit normal vector. A typical block of an STL file is:

```
facet normal 1.095466e-001 8.361753e-001 -5.374108e-001
  outer loop
    vertex   2.436354e+000 3.140374e+000 1.876282e+000
    vertex   2.409825e+000 3.141942e+000 1.873313e+000
    vertex   2.431962e+000 3.152828e+000 1.894764e+000
  endloop
endfacet
```

All CAD programs can export to this format, but one has to be careful when doing this, as STL files can be **binary** or **ASCII**. While the first option results in a smaller, more compact file, the latter is readable, and is the only format that Molflow can interpret.

For example, in Autodesk Inventor, the user can decide the format in the export settings dialog:



STL File Save As Options

Format

○ Binary ● ASCII

Units: centimeter

Structure: One File

Resolution

○ High ● Medium

○ Low ○ Custom

Surface Deviation: 0.001660 0% 100%

Normal Deviation: 15 0% 100%

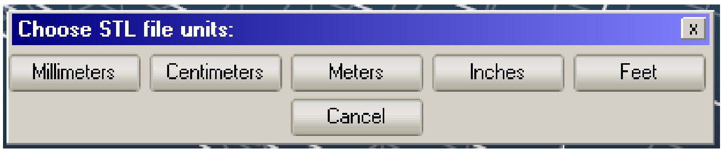
Max Edge Length: 10.475745 0% 100%

Aspect Ratio: 21.500000 0% 100%

□ Allow to Move Internal Mesh Nodes

OK Cancel

Another important setting is the **unit** of the STL file. As you can see on the above snippet, the coordinates don't contain units. Therefore, upon opening an STL file, Molflow will ask for the units it was created with. The thumb rule is to use the same as when exporting. If a mistake is made, one can use the *Facet scale* command later to resize everything.



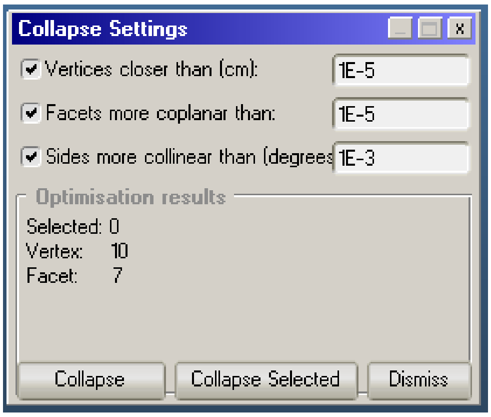
Choose STL file units:

One last advice: To avoid geometry problems (notably the leak of the particle due to an incorrect joint), you can feel free to use a **relatively high resolution** when exporting the STL file. Don't worry: the first thing you'll do upon importing the file is collapsing it in MolFlow, which will reduce the number of facets used.

3.6.3. Collapse

When you import an STL file, it will consist of triangles. Now, adjacent triangles that are in the same plane can be merged, resulting in faster simulation and easier geometry handling. Moreover, each vertex of the system is described several times (if 3 adjacent facets have it, then 3 times); therefore we can unify them.

In short, collapsing geometry means making a geometry use just as many facets as required and no more. This is very important since the time required calculating a "hit" is proportional to the number of facets in the system (except if you use structures). Collapsing is recommended in all scenarios, therefore the Collapse dialog appears after each geometry import:



Collapse Settings

☑ Vertices closer than (cm): 1E-5

☑ Facets more coplanar than: 1E-5

☑ Sides more collinear than (degrees 1E-3

Optimisation results

Selected: 0
Vertex: 10
Facet: 7

Collapsing consists of three steps:

1. Finding **vertices** that are at the same coordinate and merging them
2. Finding **facets** that are
   - Coplanar
   - Adjacent to each other
   - Have the same outgassing, temperature, etc. parameters

   and merging them.
3. Finding **consecutive** edges that are collinear, i.e. if a straight line is divided to 6 different sections and merging them.

Therefore you can toggle which of these steps you want to perform, and for each of them you can set a *tolerance* parameter that can be fine-tuned to the size and detail level of your geometry.

Vertices option

This is **required** to run at least one time, otherwise facet collapsing won't work.

It operates **on all vertices of the geometry**, regardless of what is selected.

The tolerance value is the maximum distance in centimeters, within which two vertices are considered to be at the same coordinates.

Facets option

Each facet's plane can be defined by an Ax+By+Cz+D=0 equation. The tolerance value is the maximum coefficient difference within which two facets are considered coplanar.

Hint: to speed up collapsing large systems, select a smaller part of the system, turn off vertex collapse (after it has run for at least once!) and use the *Collapse Selected* command. Since the collapse function performs an all-to-all comparison, dividing the system to (let's say) three parts and collapsing by groups will be exactly three times faster than the *Collapse All* command. (1000*1000 comparison versus 3*333*333 in a 1000-facet system...) This is because you are *helping Molflow* to decide which facets are next to each other.

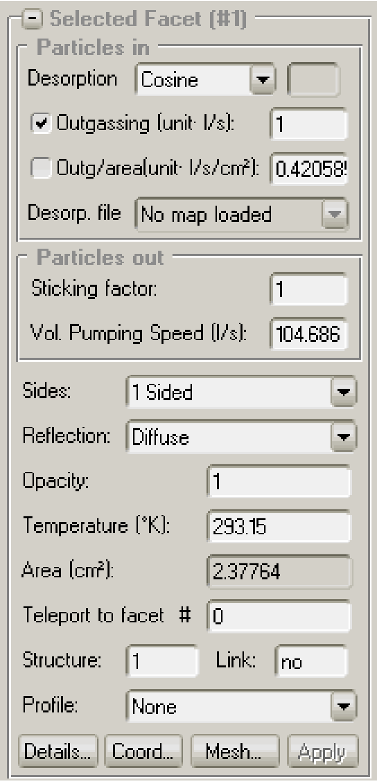
Collinear edges option

Since it is very fast, you can leave it on all the time. The tolerance value is in degrees, the maximum degree of turn under which two consecutive edges are considered collinear.

3.7. Setting up the simulation - facet parameters

Once your geometry is in MolFlow, you have to define where particles are inserted or created in the system and also the pumps/coatings with sticking where they will be absorbed. Most of this work will consist of changing *facet parameters*, whereas some parameters have to be set up in *Global Settings*.

The *facet parameters* expandable panel is on the right side, showing the properties of selected facet(s). In this paragraph we'll go through each option:



Selected Facet (#1)

Particles in

Desorption: Cosine

☑ Outgassing (unit: l/s): 1

□ Outg/area(unit: l/s/cm²): 0.42058

Desorp. file: No map loaded

Particles out

Sticking factor: 1

Vol. Pumping Speed (l/s): 104.686

Sides: 1 Sided

Reflection: Diffuse

Opacity: 1

Temperature (°K): 293.15

Area (cm²): 2.37764

Teleport to facet #: 0

Structure: 1 Link: no

Profile: None

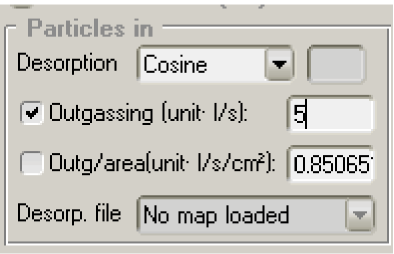
3.7.1. Selected facet indicator

Selected Facet (#1)

Selected Facet (7 selected)

Each facet has an ID, starting from 1. The top of the panel shows how many facets are selected, and if only one, then it will show its ID.

3.7.2. Particles in



Particles in

Desorption: Cosine

☑ Outgassing (unit: l/s): 5

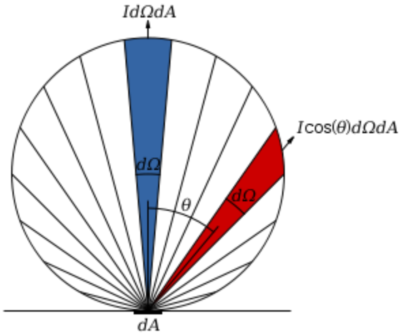
□ Outg/area(unit: l/s/cm²): 0.85065

Desorp. file: No map loaded

This part serves to create particles in your system.

If the **desorption** is enabled, particles will be desorbed from randomly chosen points of the facet's surface. If the facet is *1-sided*, they will fly in the direction of the facet normal, otherwise, for *2-sided* facets, they will fly in both directions. The angular distribution is determined by the chosen desorption type:

- **Uniform** desorption: particles will fly out to every direction with equal probability for every (spatial) angle.



- **Cosine** desorption: corresponds to a Lambertian radiator where the probability of the angle of radiation is proportional to the cosine of that angle. This means in practice that particles are more prone to leave a facet perpendicular to its plane.
- **Cosine^N** desorption: The same as above, but the probability is proportional to a chosen power of the cosine of the angle. In practice, the higher the exponent is, the more perpendicular the gas will flow to the facet.

The **outgassing and outgassing per area** numbers are taken into account for two purposes: to calculate the pressure (that is proportional to the outgassing rate), and also to help MolFlow determine the ratio of the desorption density (when desorption happens at several surfaces).

The two parameters (outgassing and outgassing/area) are linked together, and calculated upon typing.

The **units** for outgassing are "arbitrary_pressure_unit * liter / sec", where you can substitute that arbitrary pressure unit with your preferred one. But you have to keep in mind your unit choice for interpreting the pressure results: for example, if you have used mbar*l/s, then MolFlow will display the pressure in mbars.

Defining outgassing for a single facet:

If only one facet is selected, then the outgassing and outgassing/area values are calculated as you type, taking into account the area of the selected facet. In this case, the checkboxes don't have any meaning.

Defining outgassing for multiple facets:

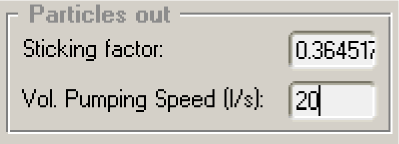
The conversion between the outgassing and outgassing/area uses the **sum area** of the selected facets. The checkboxes define which of the two values will be kept fixed, when outgassing is applied to multiple facets.

Examples:

- You want to set the outgassing of 10 facets to **0.5mbar*l/s each**: type 0.5 to the outgassing field, and apply the parameters keeping the "Outgassing" checkbox ticked
- You want to set the outgassing of **100 different-sized copper facets** to 1E-9 mbar*l/s/cm^2 uniformly: type 1E-9 to the "Outgassing/area" field, and apply parameters with the checkbox ticked next to it.
- You have an outgassing structure, for example a hemisphere consisting of a lot of facets. You want a **total outgassing of 10mbar*l/s distributed between the facets**, proportional to the element areas: select all facets of the hemisphere, enter 10 to the "outgassing" field, that will calculate the necessary "outgassing/area" value, then apply parameters with the **outgassing/area** checkbox ticked.

The **desorption file** area in recent versions is only available if you use the *Import desorption file* option, most likely exported from SynRad. If such a desorption map is loaded for a facet, this field allows you to choose between actually using the map file or override it with a manual value.

3.7.3. Particles out


Particles out

Sticking factor: 0.364517

Vol. Pumping Speed (l/s): 20

A facet that has a sticking factor other than zero will absorb (pump away) particles. Pumping can be set by two parameters that are linked together: the sticking factor and the volumetric pumping speed.

Sticking factor is the probability (0..1) that a particle that hits this facet will be absorbed.

Volumetric pumping speed is converted to sticking factor before being applied. Note that **if multiple facets are selected,** the sum is taken into account at the conversion (i.e. you have to specify the total pumping speed for the facets).

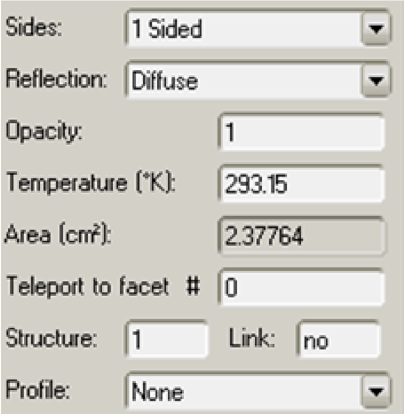
The proper way of defining volumetric pumping speeds for multiple pumps is to calculate the corresponding sticking factor on one facet, then applying the *sticking factor* on all selected facets. This function might change with the upgrades to be more like the desorption definition (two checkboxes).

The formula used for the conversion is:

$$volumetric\_pumping\_speed = \frac{facet\ area * average\ molecule\ speed * sticking\ factor}{4}$$

where the average molecule speed depends on the gas mass and temperature, so if you change it, don't forget to update the sticking factor to correspond to the desired pumping speeds.

3.7.4. Additional facet parameters



Sides: 1 Sided

Reflection: Diffuse

Opacity: 1

Temperature (°K): 293.15

Area (cm^2): 2.37764

Teleport to facet #: 0

Structure: 1 Link: no

Profile: None

Sides – allows you to define whether a facet is one- or two-sided. The difference is important and new MolFlow users have to get used to the concept.

> **One-sided facets** are opaque from the side where their *normal vector* is pointing (you can display the normal vector of selected facets by ticking the Normals option in viewer parameters). They are **transparent from the other side**, that is, particles will fly through them.
>
> The area of one-sided facets is the actual geometrical area of the polygon.
>
> Desorption from one-sided facets will happen in the direction of the normal vector.
>
> **Two-sided facets** are opaque from both sides.
>
> Their calculated are is double of the polygon area, meaning that when calculating pressure, it is assumed that they receive hits from both sides!
>
> They desorb particles on both sides (that is, in both directions).

Reflection type – allows you to choose whether particles should be relaunched mirror to the incident direction, or if they should be launched randomly at a cosine-weighed (Lambertian) directional distribution. To simulate vacuum systems, use the latter (see Theory of Molflow chapter for reference paper).

Opacity - The probability (0..1) that a particle going through the facet hits it. Useful for defining transparent facets for measuring the pressure in arbitrary planes.

An example usage might be to simulate a plane which has holes on 20% of its surface by a 0.8 opacity facet.

Temperature – Facet temperature in Kelvins. Currently the support for non-isothermal systems is limited (only textures are weighed taking temperature into account). However, it is recommended to set the temperature of the system (on all facets at the same time), since the conversion between the sticking factor and the volumetric pumping speed, and also the pressure calculation contains the average molecular speed, that depends on the temperature.

Area field - Displays the selected facet's area in cm^2. This is the sum area if multiple facets are selected.

Teleport to facet # - This field allows you to set up a teleport, which means that an incident particle will be transported to the facet whose ID you set here. See the relevant section (3.13) for instructions to do this. The default value is 0, which means that the facet is not a teleport.

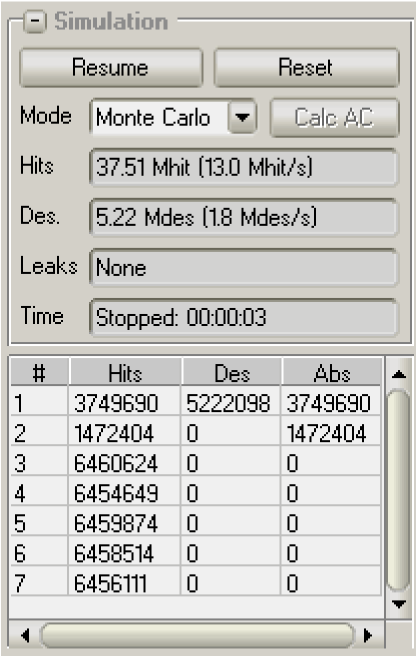
Structure – Defines the ID of the superstructure the selected facet belongs to. See the Superstructures section for information about this function.

Link – A link is a gate facet that connects superstructures. In this field, you enter the number of the superstructure that particles crossing the facet will belong to. For example, if the field value is 3, then a particle that will cross this facet will look for collisions with facets that are in structure 3. For more info on setting up structures, see section 3.14.2.

Profile – Enables calculation of pressure profiles on the selected facet. For that, the facet is divided into 100 slices of equal length along the vector U or V. The U vector is the one pointing from vertex index 1 to vertex index 2, so the user can actually change the orientation of the U vector (and thus the profile direction) by using the Shift Vertex command in the Facet menu.

3.8. The simulation panel

This panel allows you to start/stop the simulation and displays information of its state.



Mode: Monte Carlo

Hits: 37.51 Mhit (13.0 Mhit/s)

Des.: 5.22 Mdes (1.8 Mdes/s)

Leaks: None

Time: Stopped: 00:00:03

#	Hits	Des	Abs
1	3749690	5222098	3749690
2	1472404	0	1472404
3	6460624	0	0
4	6454649	0	0
5	6459874	0	0
6	6458514	0	0
7	6456111	0	0

Begin / Resume / Pause

When these buttons are pressed, MolFlow checks if changes have been made since the last simulated save, if yes, the new geometry is passed to the subprocesses. Then the simulation resumes from where it is left.

Mode

Allows choosing between the **Monte Carlo** and **Angular Coefficients** method. Note that for the moment, the latter is experimental and is not documented.

Hits

Shows the total number of the hits on all facets, and the simulation speed. Note that the hits/sec value is the main indicator of your computer's speed and the simplicity of the geometry. As a thumb rule, a geometry that contains 10 times more facets will be 10 times slower. Defining Superstructures (section 3.14) can speed up simulation.

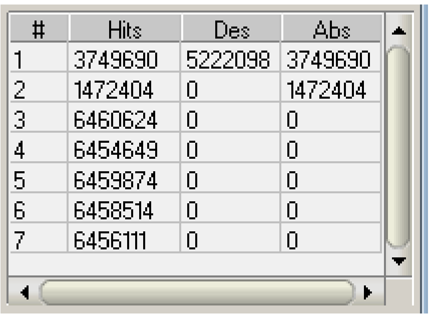
Des.

A particle is kept in the system until it is either leaked or is pumped away. This number shows how many particles were created (desorbed) during the simulation. If the number doesn't increase, that is probably an indicator that the particles are stuck somewhere, thus they can't be pumped away. (Each subprocess creates and traces one molecule at a time, so if you have 4 subprocesses and they are stuck, this number will stay at 4)

Leaks

Indicates that some particles escaped from your system (went in a direction where they didn't collide with any facet). These lost particles represent a geometry error, probably due to too coarse collapsing or improperly oriented one-sided facets.

Facet hit list



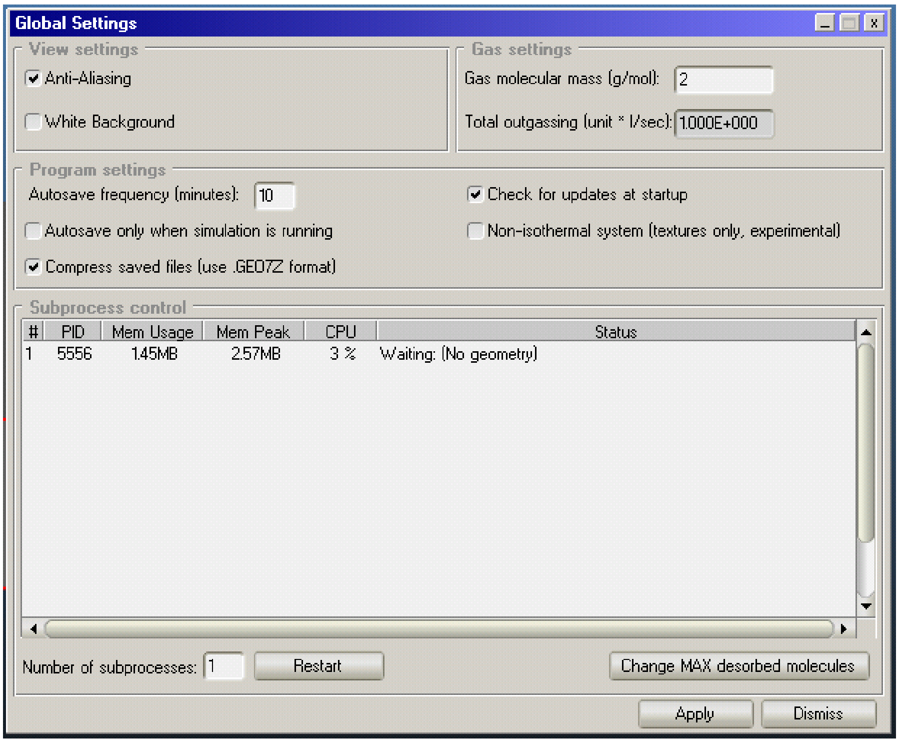
#	Hits	Des	Abs
1	3749690	5222098	3749690
2	1472404	0	1472404
3	6460624	0	0
4	6454649	0	0
5	6459874	0	0
6	6458514	0	0
7	6456111	0	0

This list displays the hit, desorption and absorption number of all facets, and allows you to find and select facets.

The list is sortable. Click on the column label of Hits, Des. or Abs and the facets will be listed based on that number. Click again on the same column to switch between ascending/descending order. This is a good way to find which facets are hit the most of times, for example. To reorder the list based on facet numbers, simply click on the # column label.

The facets are selectable. Click on any row to select a facet. Once the list has the focus, you can scroll and change selection with the UP and DOWN keys. Holding down SHIFT and using the UP and DOWN allows you to select multiple consecutive facets. If you want to select/deselect multiple facets by the mouse, hold down the CTRL key.

3.9. Global settings



Global Settings

View settings

☑ Anti-Aliasing

□ White Background

Gas settings

Gas molecular mass (g/mol): 2

Total outgassing (unit * l/sec): 1.000E+000

Program settings

Autosave frequency (minutes): 10

□ Autosave only when simulation is running

☑ Compress saved files (use .GEO7Z format)

☑ Check for updates at startup

□ Non-isothermal system (textures only, experimental)

Subprocess control

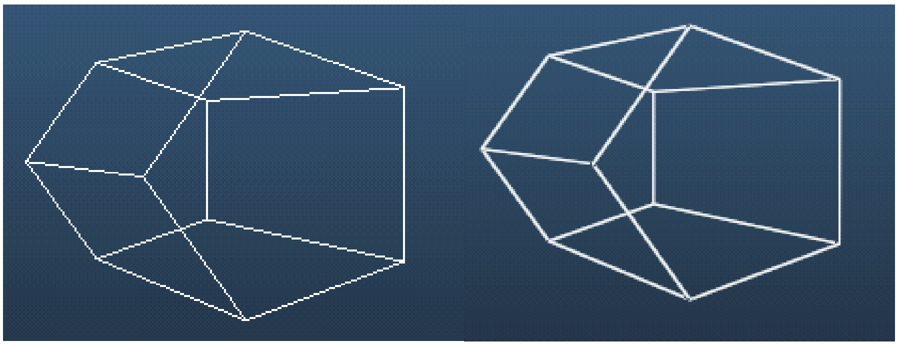
#	PID	Mem Usage	Mem Peak	CPU	Status
1	5556	1.45MB	2.57MB	3 %	Waiting: (No geometry)

Number of subprocesses: 1

The Global Settings panel allows you to toggle simulation parameters that are not part of a facet. These are mostly program settings, but this is also where you can define the molecular mass of the gas in your system.

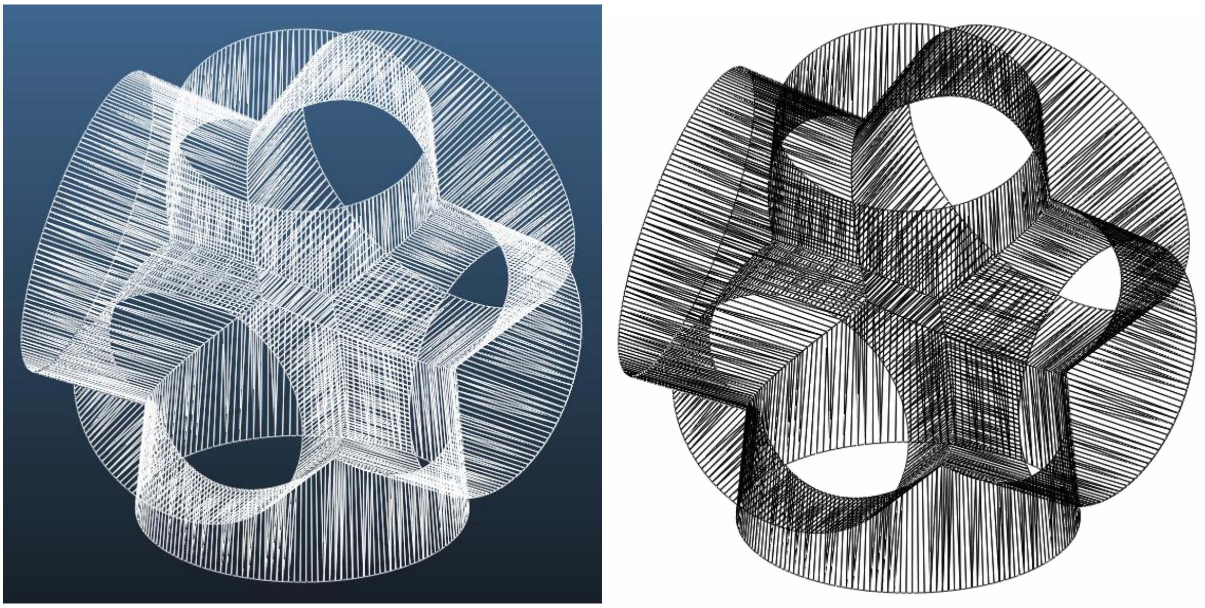
3.9.1. View settings

Anti-aliasing



It is a function that gives your geometry a nicer look on the screen by smoothing lines. In theory, disabling it might increase performance, however, practice shows that the difference is negligible.

White background



Although a blue-black gradient background looks nice on the screen, if you want to print the geometry or insert a screenshot in a document, it is better to invert colors and remove the background.

3.9.2. Gas settings

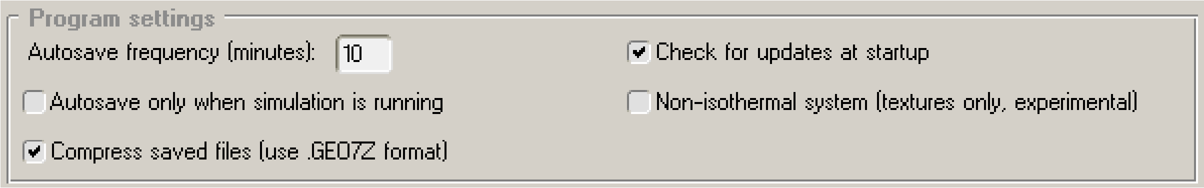
Gas molecular mass

This is the field where you can define the mass of the gas molecules in your system. Molecular mass is used to determine the average molecule speed, and has therefore a role in pressure calculation and the sticking factor/volumetric pumping speed conversion.

Total outgassing

Sum of the outgassing rate of all facets in the system. Useful to verify if outgassing / area values add up to a total outgassing as expected or not.

3.9.3. Program settings



Program settings

Autosave frequency (minutes): 10

☑ Check for updates at startup

□ Autosave only when simulation is running

□ Non-isothermal system (textures only, experimental)

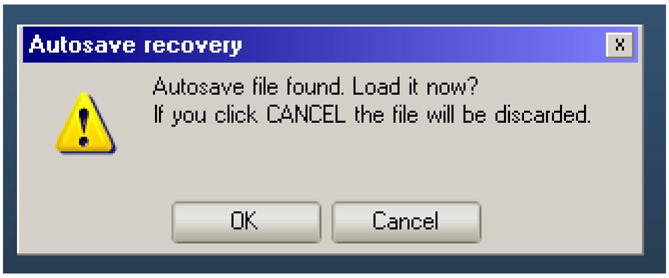
☑ Compress saved files (use .GEO7Z format)

Autosave

This feature will save an autosave.geo file in the program directory at a given interval. If the program is closed normally, this autosave file is deleted upon exit. If not, the file will remain in the directory, and upon next launch, MolFlow will detect it and offer the user to load it.

You can enter any value in the frequency field, including fractions (like saving every 0.5 minutes). Keep in mind though that autosaving will interrupt your work, and that is why the *Autosave only when* *simulation is running* option has been added: it is assumed that the user is not interacting with MolFlow while it's simulating.

When Molflow exits normally, this autosave file is deleted. Thus, if Molflow finds an autosave file in its directory upon startup, it will assume that the previous instance did not exit normally, and the option to reload the autosave file will be offered to the user:



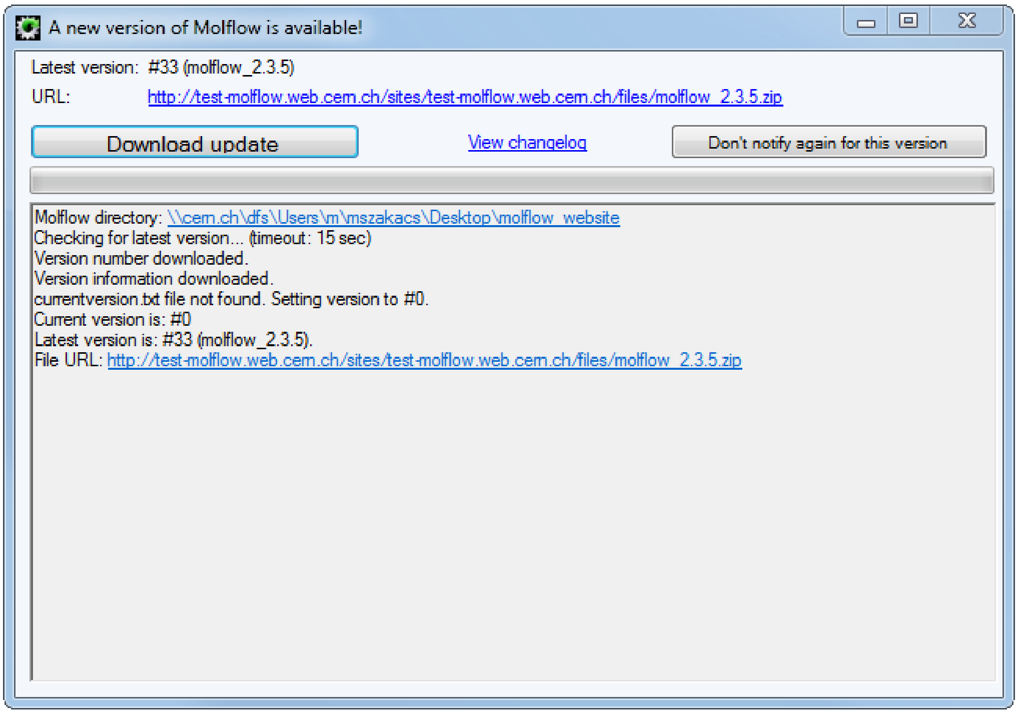
Autosave recovery

Autosave file found. Load it now?
If you click CANCEL the file will be discarded.

If you want to disable this functionality, just enter a big number, like 9999 as autosave frequency.

Updates (see section 5.6)

MolFlow has an own updater module that checks for new versions on startup. The updater process starts minimized along with MolFlow, and quits after 5 seconds if it determines that your version is up to date, otherwise a window pops up allowing you to update automatically.



A new version of Molflow is available!

Latest version: #33 (molflow_2.3.5)
URL: http://test-molflow.web.cern.ch/sites/test-molflow.web.cern.ch/files/molflow_2.3.5.zip

```
Molflow directory: \\cern.ch\dfs\Users\m\mszakacs\Desktop\molflow_website
Checking for latest version... (timeout: 15 sec)
Version number downloaded.
Version information downloaded.
currentversion.txt file not found. Setting version to #0.
Current version is: #0
Latest version is: #33 (molflow_2.3.5).
File URL: http://test-molflow.web.cern.ch/sites/test-molflow.web.cern.ch/files/molflow_2.3.5.zip
```

The auto-updater module

Turn it off if you don't want MolFlow to connect to the internet. Otherwise it is recommended to keep it on.

Compression (see section 5.7)

MolFlow compresses geo files and renames them to geo7z in the background. Therefore saved files are much smaller and can be attached to an email, for example. It is recommended that compression is left enabled.

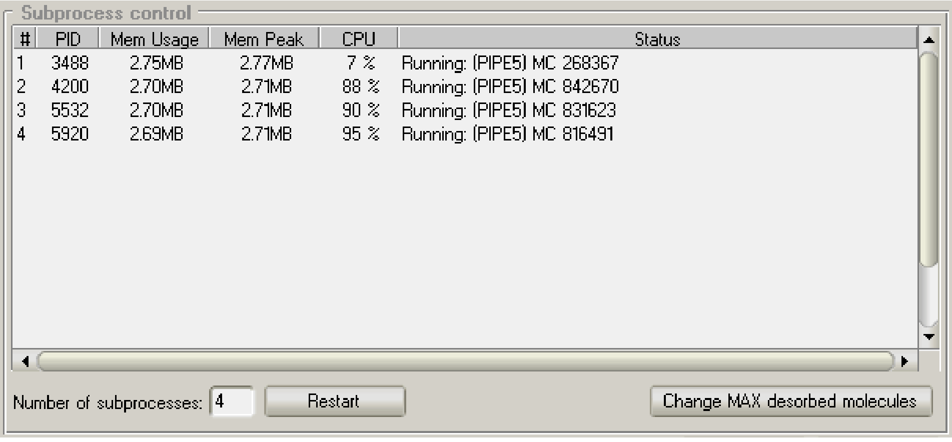
Non-isothermal system

This experimental feature hasn't been fully verified so interpret results with caution. If enabled, molecules will have a temperature, initially that of the desorption facet, and after each collision they are thermalized to the wall's temperature that they hit.

The difference is that on **textures**, each hit is taken into account with a $\sqrt{\frac{T_{source}}{T_{wall}}}$ factor, where T_{source} is the temperature (in Kelvins) of the facet the particle is coming from, and T_{wall} is that what the facet where the collision occurs and where the texture is.

Note that only textures will be different, profiles are incompatible with this calculation mode.

3.9.4. Subprocess control



#	PID	Mem Usage	Mem Peak	CPU	Status
1	3488	2.75MB	2.77MB	7 %	Running: [PIPE5] MC 268367
2	4200	2.70MB	2.71MB	88 %	Running: [PIPE5] MC 842670
3	5532	2.70MB	2.71MB	90 %	Running: [PIPE5] MC 831623
4	5920	2.69MB	2.71MB	95 %	Running: [PIPE5] MC 816491

Number of subprocesses: 4

MolFlow uses workers called subprocesses (molflowSub.exe) to do the actual simulation calculations, whereas the main program serves as an interface to handle geometry, set up parameters and display results.

Reasons to run a lot of processes:

- On a multi-core system, for maximum performance, you should run at least as many processes as the number of cores in your CPU
- Each process uses a different random number generator seed. Thus, running 4 processes, for example, will eliminate repetitions of the random-number generator. Molflow uses the Mersenne-Twister algorithm to generate random numbers.

Reasons to restrict the number of processes:

- Each process keeps the geometry in the memory. Thus, running 16 processes will keep 16 copies of your geometry in the memory.

In the subprocess control panel, you can define the number of workers running in the background, and view the state of these subprocesses as well. Please note that on some architectures the subprocesses might appear to be in "dead" state (Status column), whereas it's simply a false warning message. The bug is known but a solution is yet to be provided.

The main interest for the user here is the number of subprocesses: it is advised to set it **to the number of CPU cores in your computer.** To do that, enter a number in the Number of subprocesses field, and then click Restart. This will reset your simulation. (To continue in the state where it was before changing the number of processes, you have to manually save the file, change the number of processes and then load it again.)

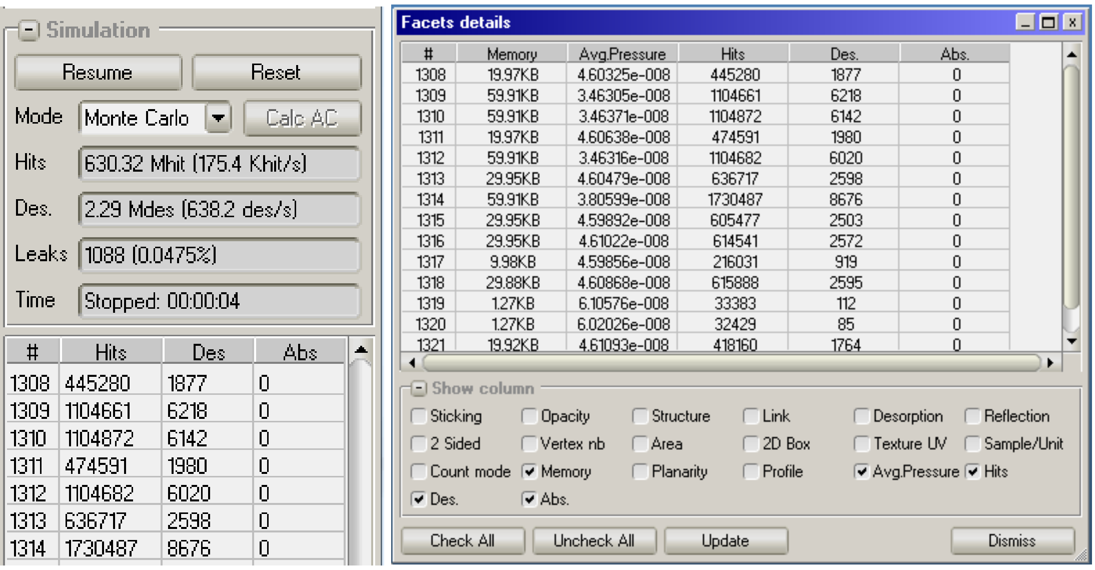
Hint: clicking the Apply button in Global Settings won't change the number of subprocesses. You have to actually click on Restart to do it.

Changing the number of desorption molecules serves as a software limit to stop the simulation after desorption molecules reach a certain number. If set to 0, the simulation will run until stopped by the user. This function might be useful if we change parameters and want to compare results after a given number of desorbed molecules. Therefore, entering 100000 here will pause the simulation after 100K desorbed molecules.

3.10. Processing results

When your simulation is set up and has been running for some time, you can immediately see some results, for example, the number of hits in the simulation and on certain facets.

Opening the Facet Details window will also show you a column where the average pressure on a facet is calculated.



Mode: Monte Carlo

Hits: 630.32 Mhit (175.4 Khit/s)

Des.: 2.29 Mdes (638.2 des/s)

Leaks: 1088 (0.0475%)

Time: Stopped: 00:00:04

#	Hits	Des	Abs
1308	445280	1877	0
1309	1104661	6218	0
1310	1104872	6142	0
1311	474591	1980	0
1312	1104682	6020	0
1313	636717	2598	0
1314	1730487	8676	0

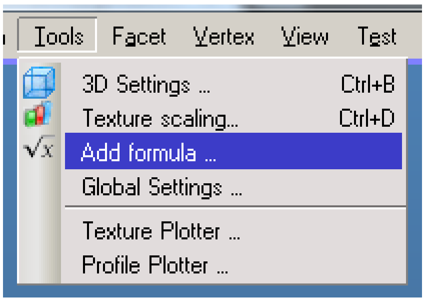
#	Memory	Avg.Pressure	Hits	Des.	Abs.
1308	19.97KB	4.60325e-008	445280	1877	0
1309	59.91KB	3.46305e-008	1104661	6218	0
1310	59.91KB	3.46371e-008	1104872	6142	0
1311	19.97KB	4.60638e-008	474591	1980	0
1312	59.91KB	3.46316e-008	1104682	6020	0
1313	29.95KB	4.60479e-008	636717	2598	0
1314	59.91KB	3.80599e-008	1730487	8676	0
1315	29.95KB	4.59892e-008	605477	2503	0
1316	29.95KB	4.61022e-008	614541	2572	0
1317	9.98KB	4.59856e-008	216031	919	0
1318	29.88KB	4.60868e-008	615888	2595	0
1319	1.27KB	6.10576e-008	33383	112	0
1320	1.27KB	6.02026e-008	32429	85	0
1321	19.92KB	4.61093e-008	418160	1764	0

□ Sticking □ Opacity □ Structure □ Link □ Desorption □ Reflection
□ 2 Sided □ Vertex nb □ Area □ 2D Box □ Texture UV □ Sample/Unit
□ Count mode ☑ Memory □ Planarity □ Profile ☑ Avg.Pressure ☑ Hits
☑ Des. ☑ Abs.

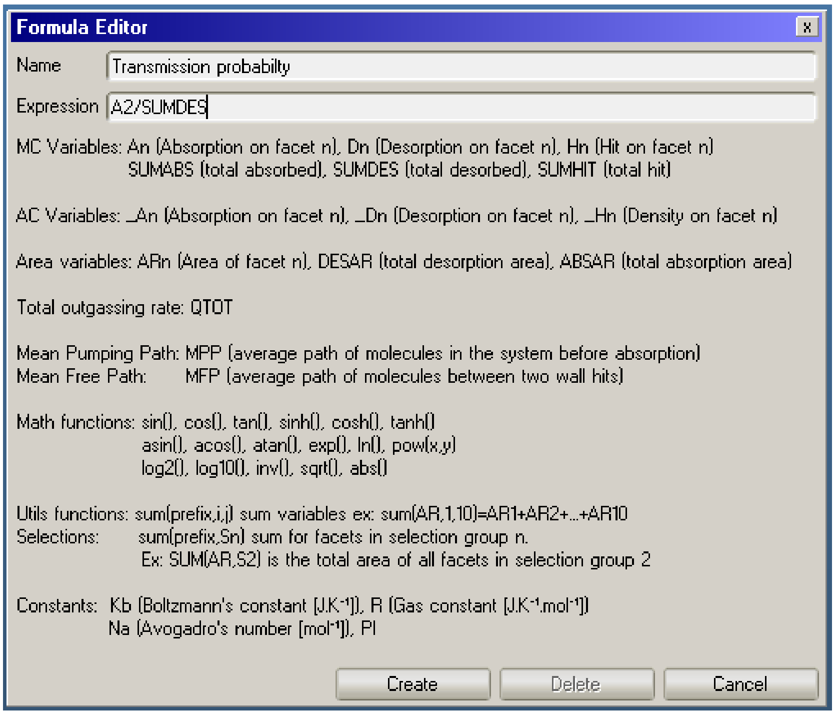
However, usually we need more details, and we can take advantage of the visualization and post-processing options in MolFlow to display our results directly. For memory and speed considerations, the counting of Profiles and Textures must be enabled manually on every facet of our interest:

3.10.1. Formulas

To add a new formula, use the Tools menu:



Then you will be offered a dialog window where you can define a *Name* for your formula (to remember its content), and also to define the formula itself:



Formula Editor

Name: Transmission probabilty

Expression: A2/SUMDES

MC Variables: An (Absorption on facet n), Dn (Desorption on facet n), Hn (Hit on facet n)
SUMABS (total absorbed), SUMDES (total desorbed), SUMHIT (total hit)

AC Variables: _An (Absorption on facet n), _Dn (Desorption on facet n), _Hn (Density on facet n)

Area variables: ARn (Area of facet n), DESAR (total desorption area), ABSAR (total absorption area)

Total outgassing rate: QTOT

Mean Pumping Path: MPP (average path of molecules in the system before absorption)
Mean Free Path: MFP (average path of molecules between two wall hits)

Math functions: sin(), cos(), tan(), sinh(), cosh(), tanh()
asin(), acos(), atan(), exp(), ln(), pow(x,y)
log2(), log10(), inv(), sqrt(), abs()

Utils functions: sum(prefix,i,j) sum variables ex: sum(AR,1,10)=AR1+AR2+...+AR10
Selections: sum(prefix,Sn) sum for facets in selection group n.
Ex: SUM(AR,S2) is the total area of all facets in selection group 2

Constants: Kb (Boltzmann's constant [J.K^{-1}]), R (Gas constant [J.K^{-1}.mol^{-1}])
Na (Avogadro's number [mol^{-1}]), PI

The majority of the formula dialog is a reference to the variables that you can use. For clarity, we go through them:

Constants

Kb – Boltzmann's constant – 1.38065*10^{-23}

R – Gas constant – 8.3144621 J/mol*K

Na – Avogadro constant – 6.022*10^{23}

PI – 3.14159

Global simulation variables

SUMABS – The number of all MC particle absorptions in the system. (This number is not saved in a GEO file)

SUMDES – The number of all MC particles created (desorbed) during the simulation.

SUMHIT – Total simulated hits in the simulation.

DESAR – The total area (in cm^2) of all facets that have a desorption set up

ABSAR – The total area (in cm^2) of all facets that have a desorption set up

QTOT – The total outgassing rate in the system (sum f outgassing rate on all facets)

MPP - Mean pumping path, that is, the average flight distance of a particle in the system before it is being pumped away (Total flight path divided by the number of absorptions. Not saved with a GEO file)

`MFP` – Mean free path, that is, the average distance a particle flies in the system between two collisions with a wall (Total flight path divided by the number of hits).

Facet variables

`An`, `Dn`, `Hn` – The number of absorptions, desorptions or hits on facet #n, respectively. Example: `A5`, `D80`, `H101`

Sum variables

It is sometimes necessary to calculate the sum of the above facet variables over a group of facets. To avoid adding the individual variables one by one in the formula, there are two types of SUM variables:

- Sum by facet number: `SUM(prefix,i,j)` sums the variables from facet I to J.
  Example: `SUM(A,5,8)` is `A5+A6+A7+A8`, and `SUM(AR,1,3)` is the area of facets 1, 2 and 3.
- Sum by selection group: in section 3.11.1, you learn how to create *selection groups*, that is, a group of facets. To perform SUM operations on facets that are part of an above group, the syntax is: `SUM(prefix,Sn)` where n is the number of the selection. ***Example***: `SUM(AR,S3)` is the area of all facets in selection group 3 and `SUM(A,S1)` is the total number of MC particles absorbed on facets of selection group 1.

> **Hint:** calculating SUM operations of a large number of facets might be slow. As formulas are updated constantly (even when the simulation is not running), use them with caution: they might slow down the entire program.

To edit an existing formula, click the … button next to it, change the name and the expression, and click Apply.

To delete a formula, click on the … button next to it and then the delete button.

Formulas are saved with GEO files, and facets reference numbers are automatically updated when you perform geometry operations and when you insert a GEO file to your existing geometry.

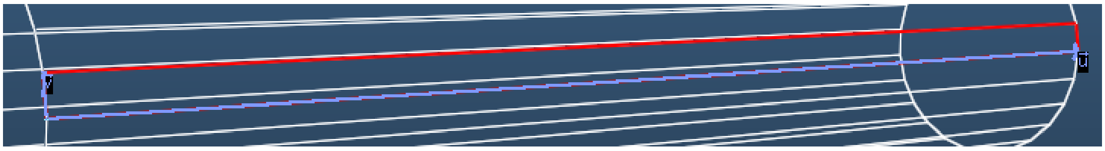
3.10.2. Profiles

Profiles offer you to immediately display the pressure distribution along a certain direction on a certain facet. The direction can be either the local U vector (pointing from a facet's first to second vertex) or the V vector (perpendicular to U). These two vectors can be rotated by the **Shift Vertex** command (CTRL+H) in the Facet menu.

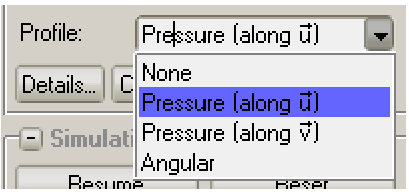
To set up profiling on a Facet, go through the following process:

1. Select the facet(s) to profile

2. Verify the U and V vector orientation

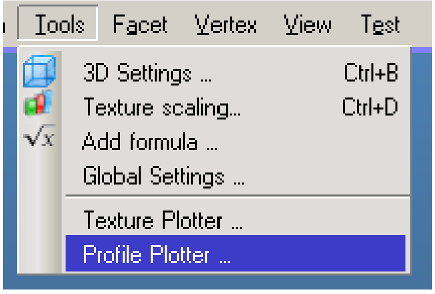


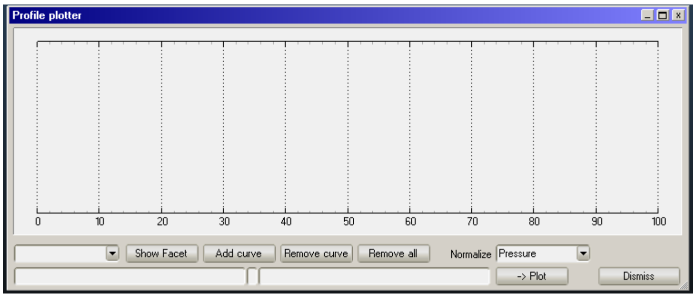
3. In the Facet Parameters panel, choose Pressure along U (or V) and click apply.



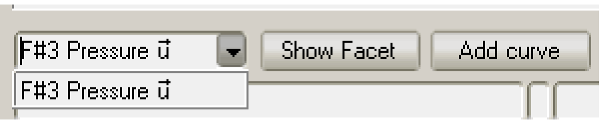
4. From now on, profiling is set up. It means that your facet is divided into 100 slices of equal length along the U vector, and hits (thus pressure) is calculated for each slice.
Note: To get correct pressure results, your slices have to be of equal area, thus **profiling works only on rectangular facets.**

5. To visualize the pressure, open the Profile Plotter window in Tools menu:

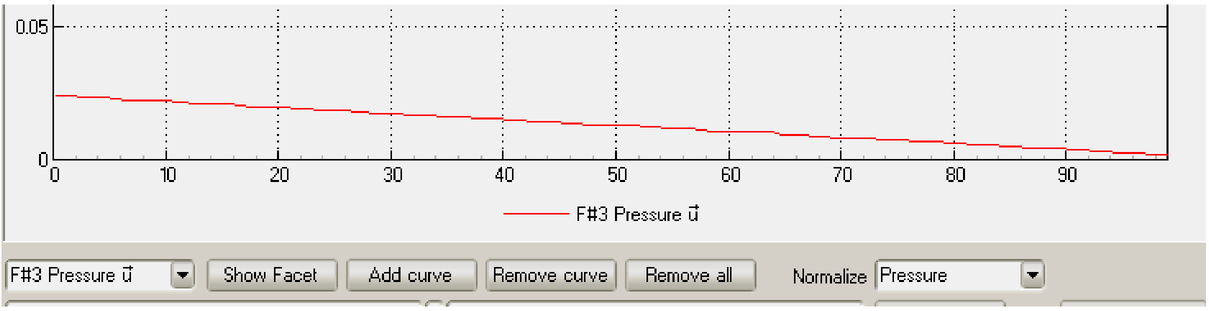




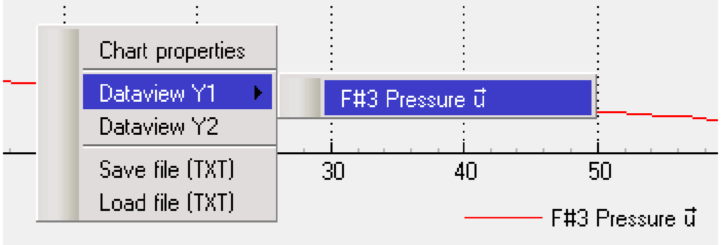
6. By default, nothing is plotted, so you have to add the curve(s) manually. In the left/hand drop-down list, select the facet that you want to add to the plot:

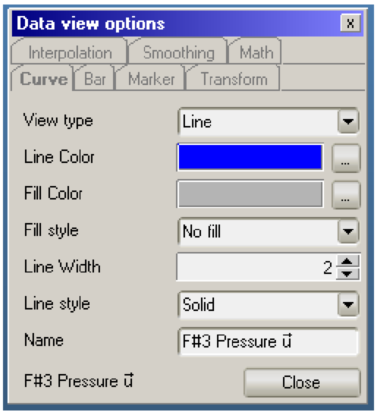


Show Facet will select the facet in your geometry (so that you can identify it), and **Add Curve** will display the pressure values in the 100 slices as a graph:



7. Finally, you can customize the look of your graph by right-clicking on the graph area.





In this menu, you can also customize graph appearance, including axis properties, such as enabling **logarithmic Y scale**.

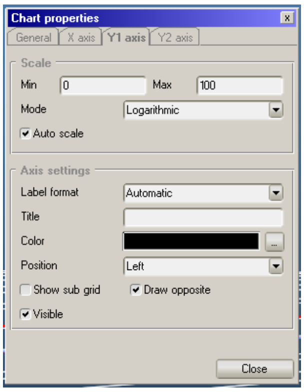


Chart properties

General | X axis | Y1 axis | Y2 axis

Scale

Min: 0 Max: 100

Mode: Logarithmic

☑ Auto scale

Axis settings

Label format: Automatic

Title:

Color: ■

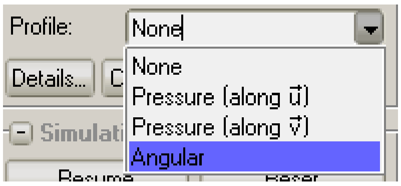
Position: Left

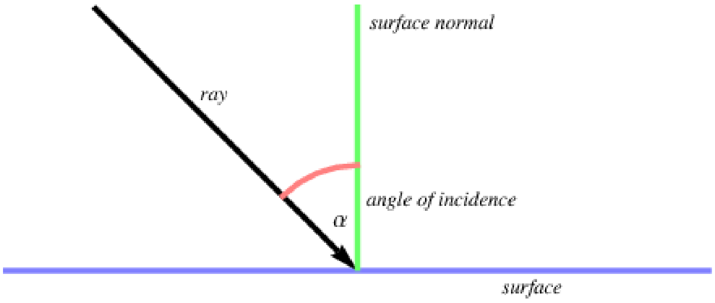
☐ Show sub grid ☑ Draw opposite

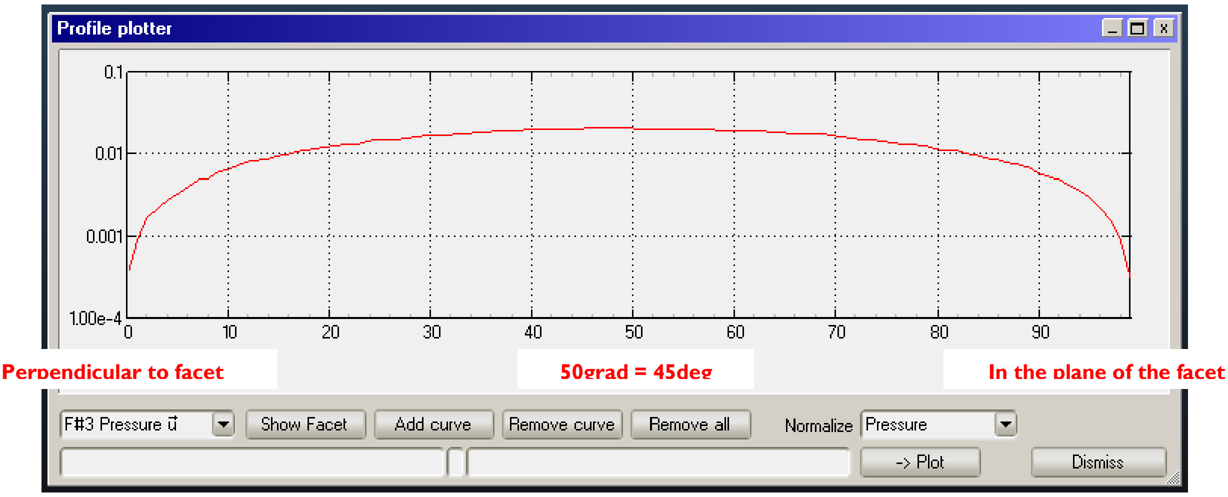
☑ Visible

Angular profiles

Angular profiles allow you to view the angle distribution of incident molecules on a 0-100 degree (gradient) scale on any facet. Setting it up goes the same way as setting up pressure profiles, but in this case, the orientation of the U and V vectors don't have significance.


Profile: None

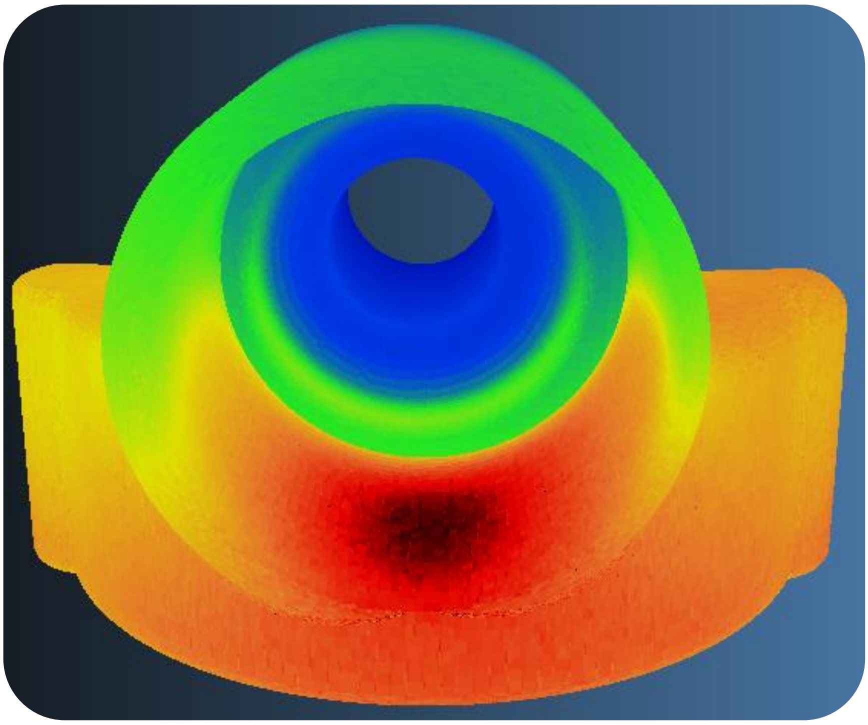




Exporting profiles

Right-clicking on the plot will offer you to save the plots in a TXT file for further processing in external programs.

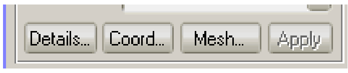
3.10.3. Textures

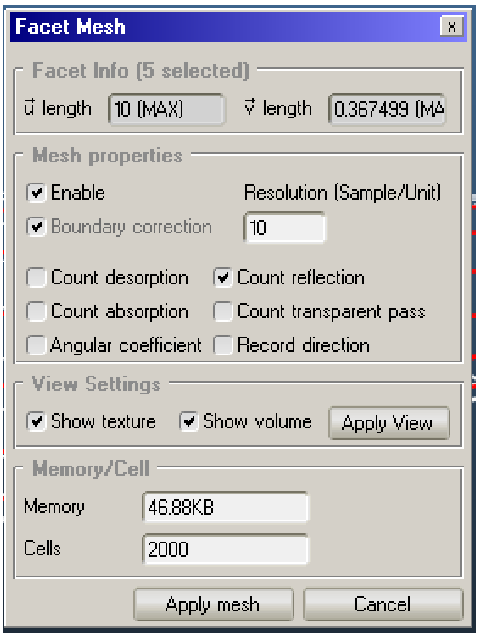


Whereas profiles are used because they immediately show a graph within MolFlow, their shortcomings were mentioned before: they always consist of 100 slices and they can only be used on rectangular facets. In general, they can be regarded as a legacy of the old MolFlow version, so the use of textures is recommended.

To add textures to your geometry, first you have to create a *Mesh*, which is a grid of rectangular elements on the facet that you want to color.

1. Select the facet(s) where you want to add a Mesh. In the Selected Facet panel, click the Mesh… button.





Facet Info (5 selected)

u length 10 (MAX)   v length 0.367499 (MA

Mesh properties

☑ Enable   Resolution (Sample/Unit)

☑ Boundary correction   10

□ Count desorption   ☑ Count reflection

□ Count absorption   □ Count transparent pass

□ Angular coefficient   □ Record direction

View Settings

☑ Show texture   ☑ Show volume

Memory/Cell

Memory 46.88KB

Cells 2000

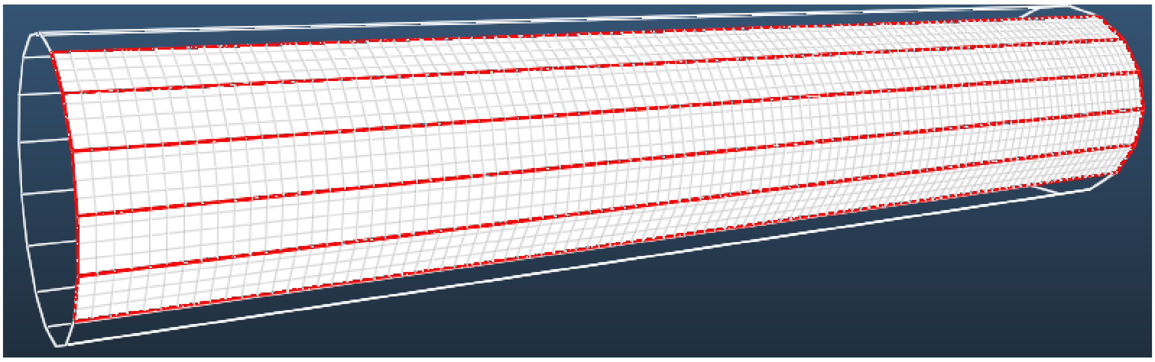
The upcoming Facet Mesh window show you information about the selected facet(s) and allows you to set up a mesh.

The most important parameters are to decide the size of the cell elements, and to define what to count.

The resolution field determines how many cells there will be per cm length (the default length unit in MolFLow). That is, if you enter 10 as resolution, it will mean that each square cm will be divided into 10x10 elements. (And accordingly, one cell will have 0.1cmx01.cm size).

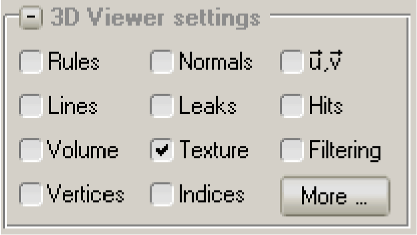
To help you decide the correct density for your geometry (that you can later refine), the total number of cells in your system is calculated upon typing. Usually you don't need more than a few hundreds of thousands of cells.

2. **You have to decide what to count.** For most cases, you want to visualize the pressure on a wall in the system, in that case, pressure is derived from **reflections** on the wall. If your facet is transparent, to know the pressure, you have to record the **transparent passes**. That's the two parameters you have to set up, click **Apply Mesh**.



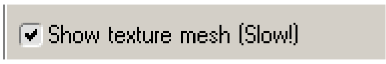
3. Your texture is now set up. You can see it in white color (default texture color) and you can see the cell boundaries.

   Hint: To show cells and textures, you have to tick the Texture toggle in Viewer settings and enable the Show Mesh with the More… button.



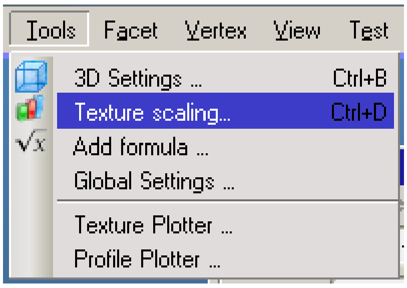
⊟ 3D Viewer settings

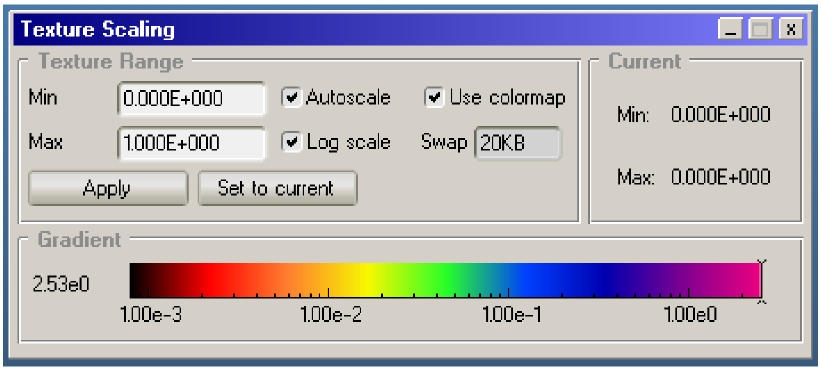
□ Rules □ Normals □ u⃗,v⃗
□ Lines □ Leaks □ Hits
□ Volume ☑ Texture □ Filtering
□ Vertices □ Indices More ...



☑ Show texture mesh (Slow!)

4. If you launch the simulation, your textures should new get their color. Note that coloring options, and most importantly, scaling can be set in the Texture Scaling dialog in the Tools menu:





Min 0.000E+000
Max 1.000E+000
☑ Autoscale
☑ Log scale
☑ Use colormap
Swap 20KB

Current
Min: 0.000E+000
Max: 0.000E+000

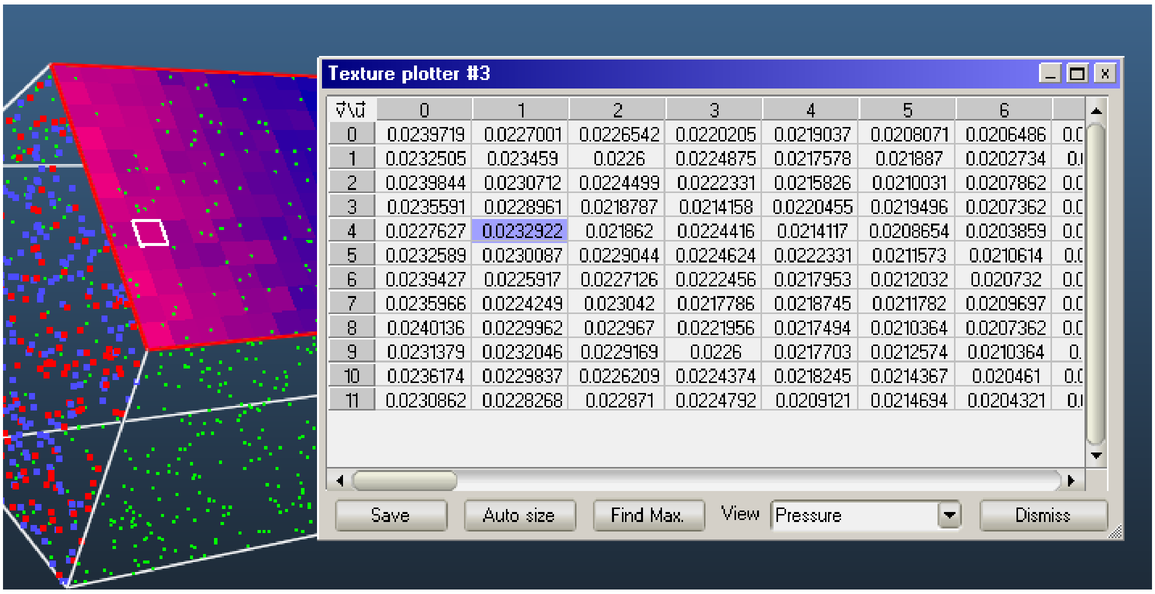
Gradient 2.53e0

On the bottom of this dialog, you can see the color scale that maps different pressures to different colors. Hovering you mouse pointer over the scale will display you the pressure corresponding to the color under your pointer.

The **Autoscale** option will try to extend this scale over all pressure values present in your system (ignoring cells with 0 hits). Note that very small cell elements might have very high displayed pressures (difficulty normalizing over the very few incoming hits), so you might manually set the scale.

The **Set to current** button will disable autoscaling, but before that it will set the Texture Range textboxes to the currently measured values (so it serves to "lock" autoscaling).

Often we need to read the actual cell values. There is a dialog window for this purpose, which also allows the user to copy data on the Clipboard for external processing.

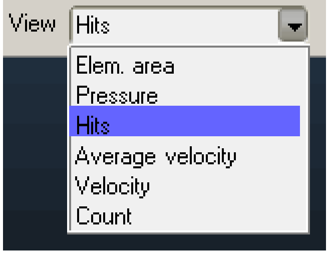


v\u	0	1	2	3	4	5	6	
0	0.0239719	0.0227001	0.0226542	0.0220205	0.0219037	0.0208071	0.0206486	0.0
1	0.0232505	0.023459	0.0226	0.0224875	0.0217578	0.021887	0.0202734	0.
2	0.0239844	0.0230712	0.0224499	0.0222331	0.0215826	0.0210031	0.0207862	0.0
3	0.0235591	0.0228961	0.0218787	0.0214158	0.0220455	0.0219496	0.0207362	0.0
4	0.0227627	0.0232922	0.021862	0.0224416	0.0214117	0.0208654	0.0203859	0.0
5	0.0232589	0.0230087	0.0229044	0.0224624	0.0222331	0.0211573	0.0210614	0.0
6	0.0239427	0.0225917	0.0227126	0.0222456	0.0217953	0.0212032	0.020732	0.0
7	0.0235966	0.0224249	0.023042	0.0217786	0.0218745	0.0211782	0.0209697	0.0
8	0.0240136	0.0229962	0.022967	0.0221956	0.0217494	0.0210364	0.0207362	0.0
9	0.0231379	0.0232046	0.0229169	0.0226	0.0217703	0.0212574	0.0210364	0.
10	0.0236174	0.0229837	0.0226209	0.0224374	0.0218245	0.0214367	0.020461	0.0
11	0.0230862	0.0228268	0.022871	0.0224792	0.0209121	0.0214694	0.0204321	0.

View: Pressure

The Texture Plotter window is available from the Tools menu. It displays the map of the mesh of the currently selected facet. Selecting a cell on it will display its position on the geometry in the form of a white border cell.

In the view drop-down list, we can choose between different quantities to display:



a. **Elem. Area:** shows the area of cells in cm². The value should be the same on all whole cells, and smaller on cells on the border of the facet.

b. Pressure: the pressure on the cell displayed in the arbitrary units you used to define outgassing

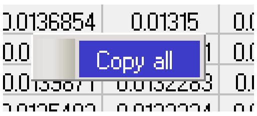
c. Hits: the number of MC hits on the facet. Please note that values are counted from the pressure, therefore sometimes the results are not exactly integer.

d. Average velocity / velocity / count: these functions are for direction counting, see later

3.10.4. Exporting results

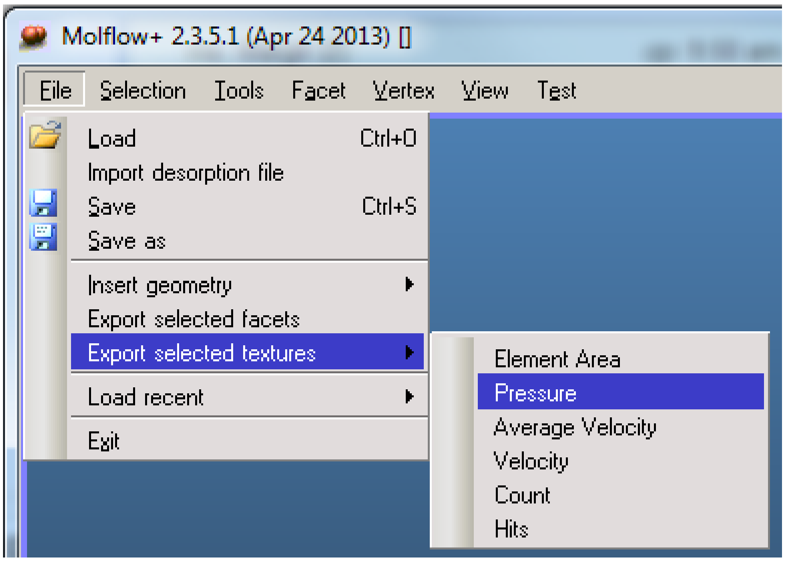
If we need to post-process texture maps in an external program, we have two options:

To export texture for a single facet, we can put it on clipboard by right-clicking and using the *Copy All* function.

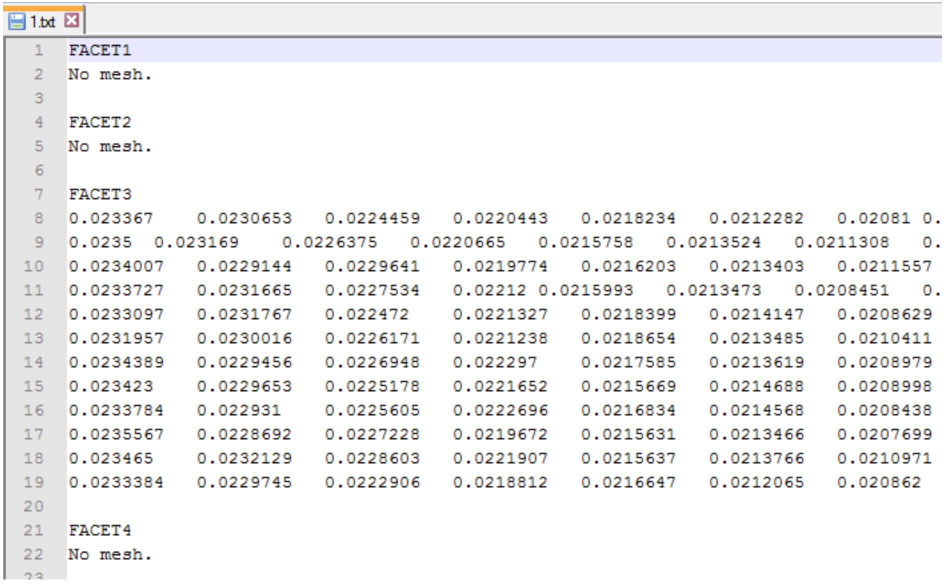


To export textures for multiple facets, we can automate the process:

- Select the facet(s) that you want to export – you can select all, for example
- Use the *Export Selected Textures* option:



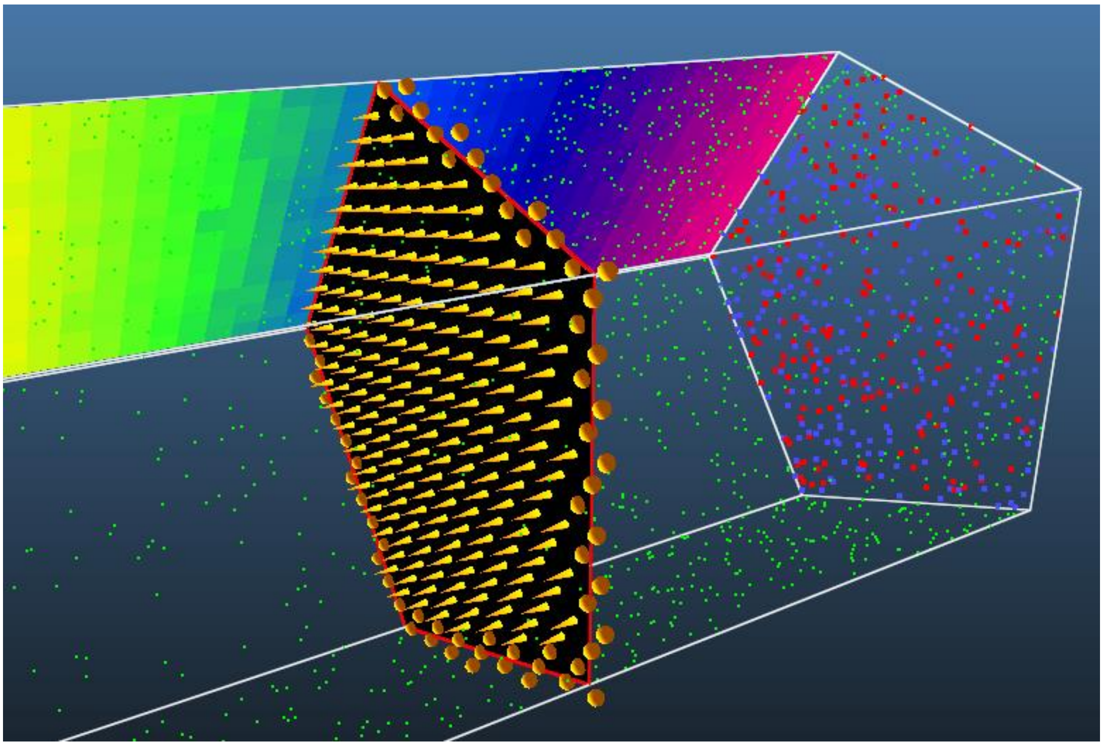
- Choose a TXT file name, and the results will be written in a TXT file, separated by tabs:



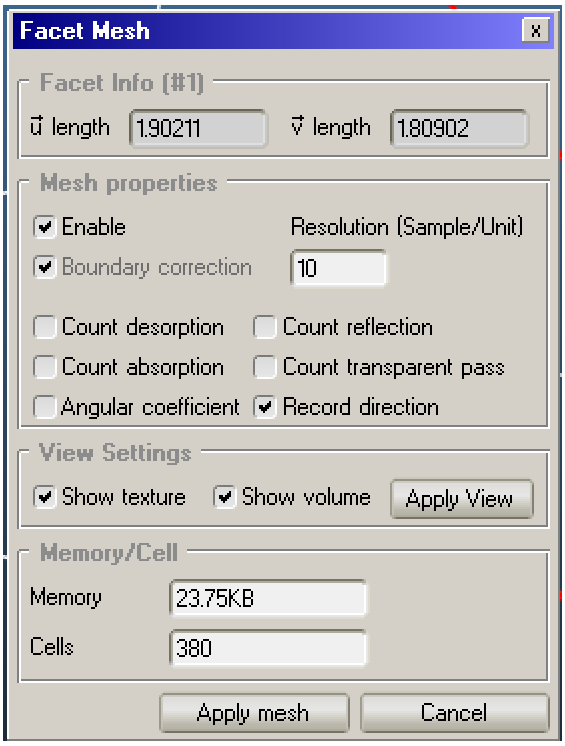
```
FACET1
No mesh.

FACET2
No mesh.

FACET3
0.023367    0.0230653   0.0224459   0.0220443   0.0218234   0.0212282   0.02081 0.
0.0235  0.023169    0.0226375   0.0220665   0.0215758   0.0213524   0.0211308   0.
0.0234007   0.0229144   0.0229641   0.0219774   0.0216203   0.0213403   0.0211557
0.0233727   0.0231665   0.0227534   0.02212 0.0215993   0.0213473   0.0208451   0.
0.0233097   0.0231767   0.022472    0.0221327   0.0218399   0.0214147   0.0208629
0.0231957   0.0230016   0.0226171   0.0221238   0.0218654   0.0213485   0.0210411
0.0234389   0.0229456   0.0226948   0.022297    0.0217585   0.0213619   0.0208979
0.023423    0.0229653   0.0225178   0.0221652   0.0215669   0.0214688   0.0208998
0.0233784   0.022931    0.0225605   0.0222696   0.0216834   0.0214568   0.0208438
0.0235567   0.0228692   0.0227228   0.0219672   0.0215631   0.0213466   0.0207699
0.023465    0.0232129   0.0228603   0.0221907   0.0215637   0.0213766   0.0210971
0.0233384   0.0229745   0.0222906   0.0218812   0.0216647   0.0212065   0.020862

FACET4
No mesh.
```

3.10.5. Counting directions

At certain points of the geometry, it might be required to visualize / determine the average direction of the particles. As pressure calculations assume that molecule speed is isotropic, it is sometimes worth checking it.



Counting directions also requires to create a mesh with the *Record direction* option. To display average directions in the form of cones, the *Show direction* option must be enabled in 3D Viewer Settings (available by pressing the *More…* button in the viewer parameters).



Facet Mesh

Facet Info (#1)

u⃗ length: 1.90211 — v⃗ length: 1.80902

Mesh properties

☑ Enable — Resolution (Sample/Unit): 10

☑ Boundary correction

☐ Count desorption ☐ Count reflection

☐ Count absorption ☐ Count transparent pass

☐ Angular coefficient ☑ Record direction

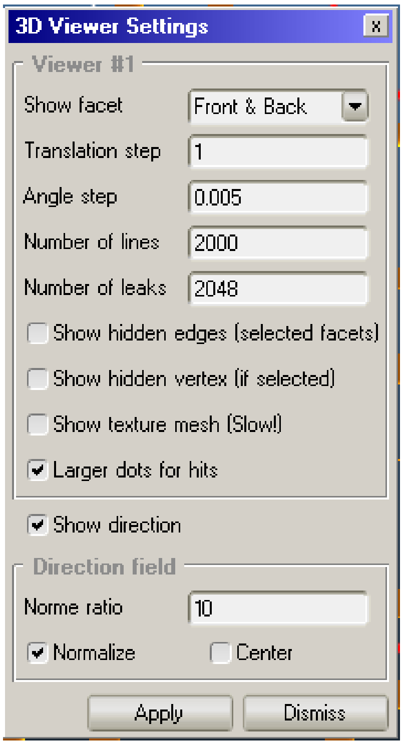
View Settings

☑ Show texture ☑ Show volume

Memory/Cell

Memory: 23.75KB

Cells: 380



3D Viewer Settings

Viewer #1

Show facet: Front & Back

Translation step: 1

Angle step: 0.005

Number of lines: 2000

Number of leaks: 2048

☐ Show hidden edges (selected facets)

☐ Show hidden vertex (if selected)

☐ Show texture mesh (Slow!)

☑ Larger dots for hits

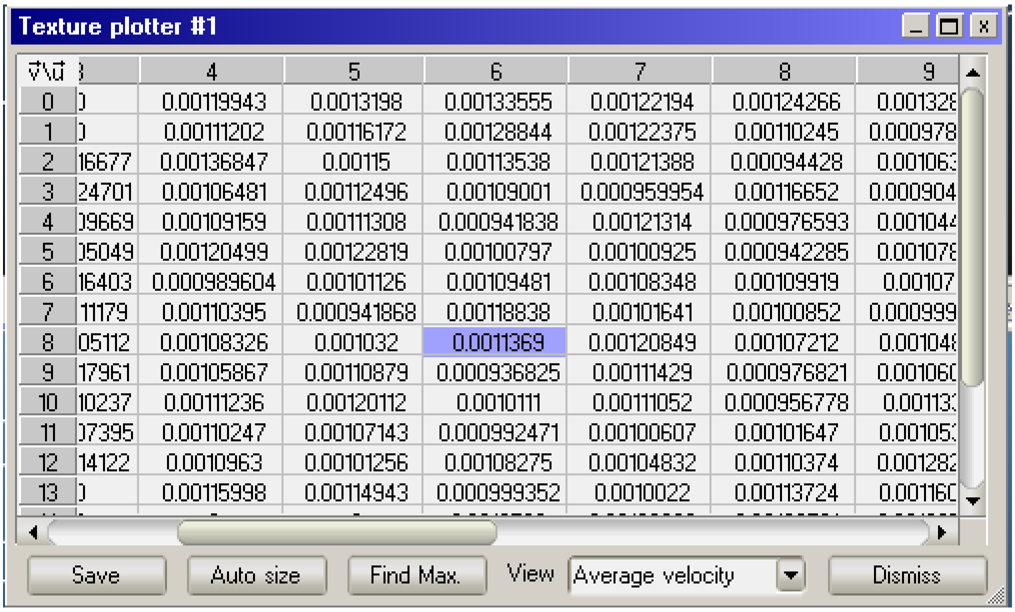
☑ Show direction

Direction field

Norme ratio: 10

☑ Normalize ☐ Center

Using the **Texture Plotter** we can visualize the directions, using the following three options:



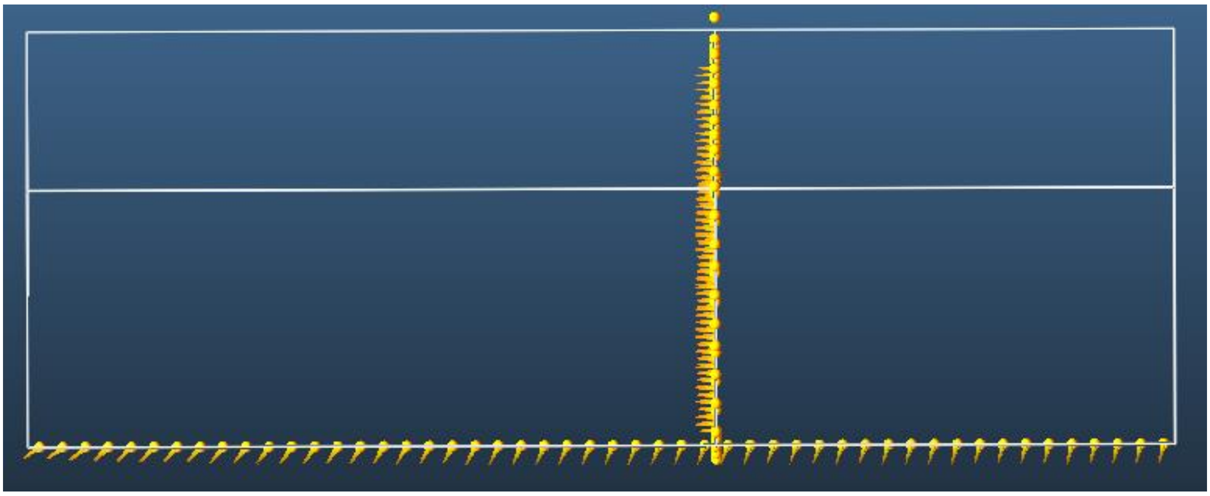
Texture plotter #1

v⃗\u⃗	3	4	5	6	7	8	9
0	0	0.00119943	0.0013198	0.00133555	0.00122194	0.00124266	0.00132
1	0	0.00111202	0.00116172	0.00128844	0.00122375	0.00110245	0.000978
2	16677	0.00136847	0.00115	0.00113538	0.00121388	0.00094428	0.00106
3	24701	0.00106481	0.00112496	0.00109001	0.000959954	0.00116652	0.000904
4	09669	0.00109159	0.00111308	0.000941838	0.00121314	0.000976593	0.00104
5	05049	0.00120499	0.00122819	0.00100797	0.00100925	0.000942285	0.00107
6	16403	0.000989604	0.00101126	0.00109481	0.00108348	0.00109919	0.00107
7	11179	0.00110395	0.000941868	0.00118838	0.00101641	0.00100852	0.000999
8	05112	0.00108326	0.001032	0.0011369	0.00120849	0.00107212	0.00104
9	17961	0.00105867	0.00110879	0.000936825	0.00111429	0.000976821	0.00106
10	10237	0.00111236	0.00120112	0.0010111	0.00111052	0.000956778	0.00113
11	07395	0.00110247	0.00107143	0.000992471	0.00100607	0.00101647	0.00105
12	14122	0.0010963	0.00101256	0.00108275	0.00104832	0.00110374	0.00128
13	0	0.00115998	0.00114943	0.000999352	0.0010022	0.00113724	0.00116

View: Average velocity

- **Average velocity:** the sum of all (normalized) velocity vectors crossing the cell, divided by the number of desorbed particles. If there would be a cell in the system that all particles cross once, its value would be 1.
- **Velocity:** the actual average velocity vector in X, Y, Z coordinates
- **Count:** number of times a molecule passed the cell

Example usage: On the pipe below, we lose isotropy on the left side, where a very strong pump (sticking probability = 1) is located (average direction tends to point to the left):



Direction vectors showing anisotropy near a pump (left side)

3.11. Advanced handling

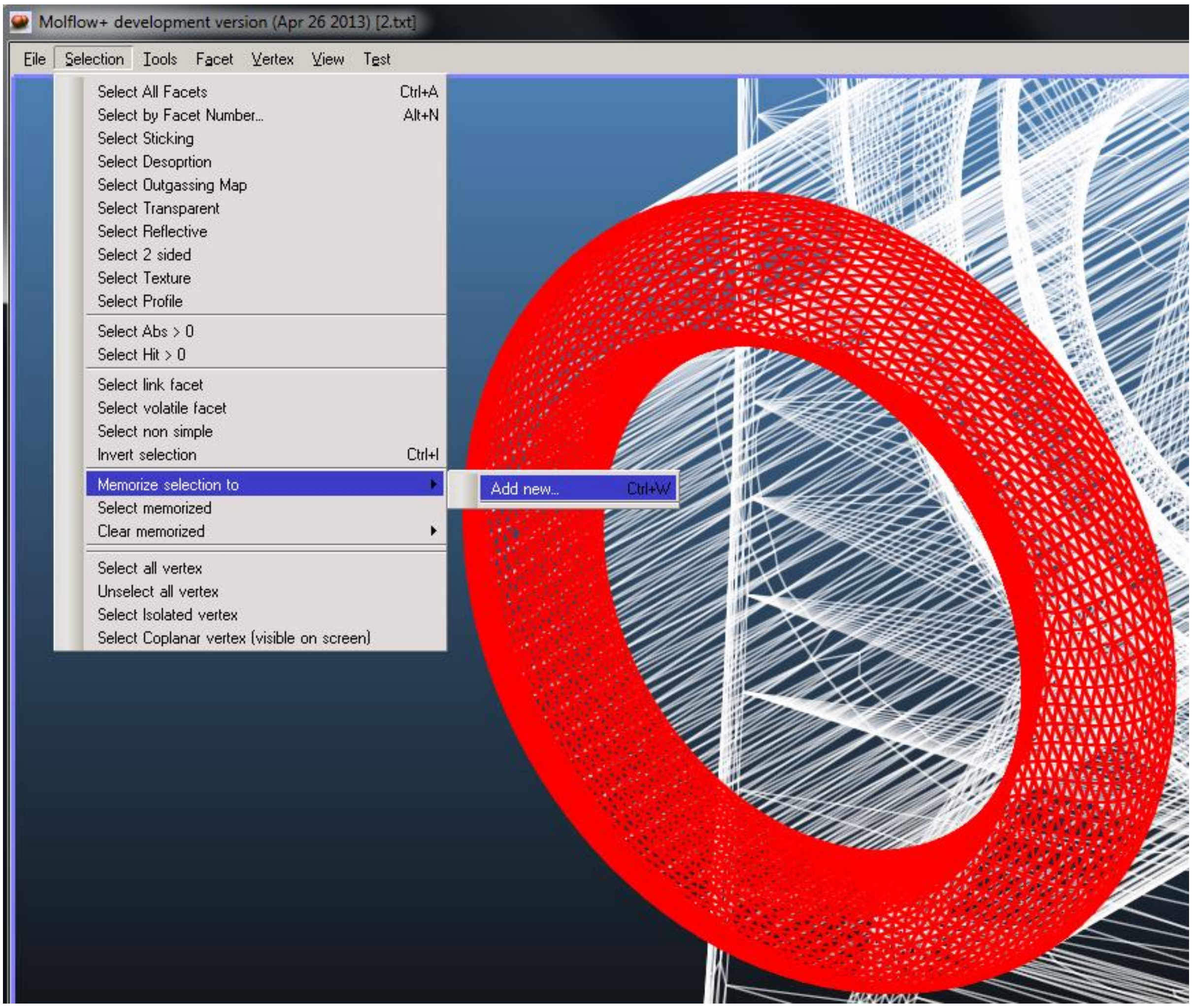
In this chapter we go through functions that make geometry handling easier in MolFlow.

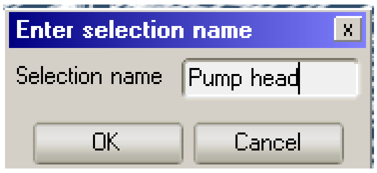
3.11.1. Selection groups

You can memorize selections (that is, a certain group of facets). It is useful to define such groups so you don't have to select them again if you want to change a parameter.

Apart from facilitating the re-selection of the facets in the group, selections also serve as a way to perform SUM operations on all facets that are part of a group when you use *Formulas*.

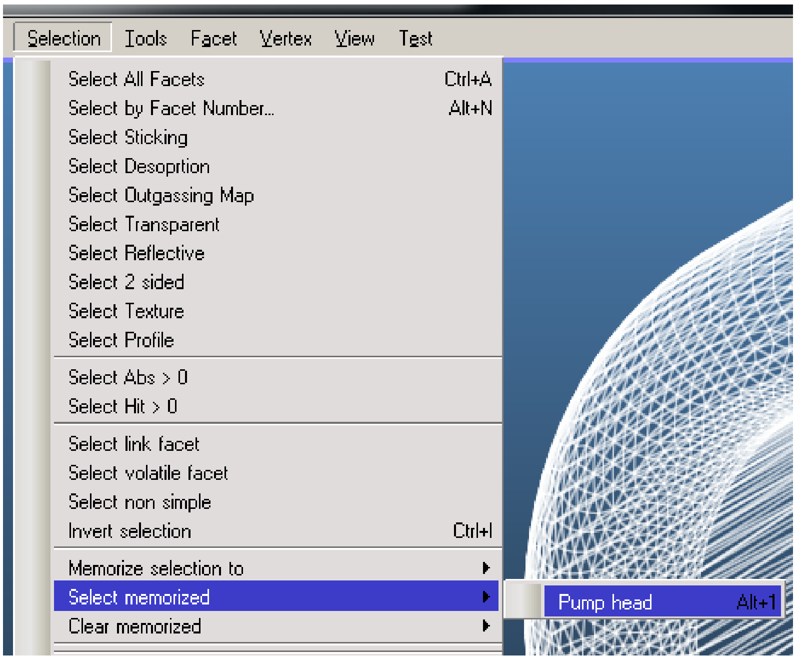
To create selections, select the facets that you want to include, then choose Selection -> Memorize Selection to -> Add new… (or use the shortcut, CTRL+W). Then give a name to the selection.





Selection name: Pump head

To recall (select) selections, press the ALT+1, ALT+2, … combinations, or use the menu:



To redefine selections, use Selection -> Memorize Selection to… then choose the selection group that you wish to overwrite.

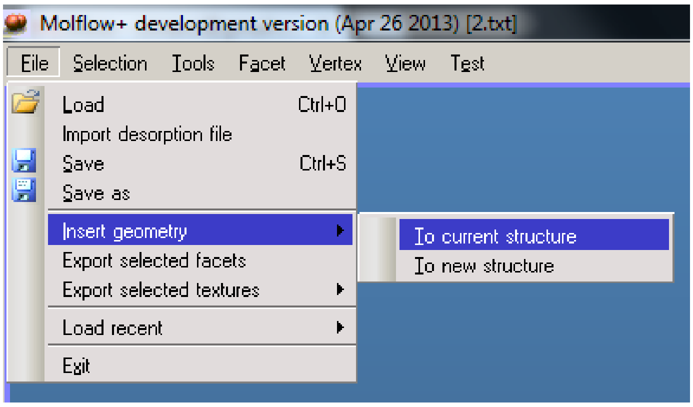
To clear selections, (to free up ALT shortcuts, for example), use the Clear Memorized menu.

To perform SUM operations on selection groups, see the Formulas section.

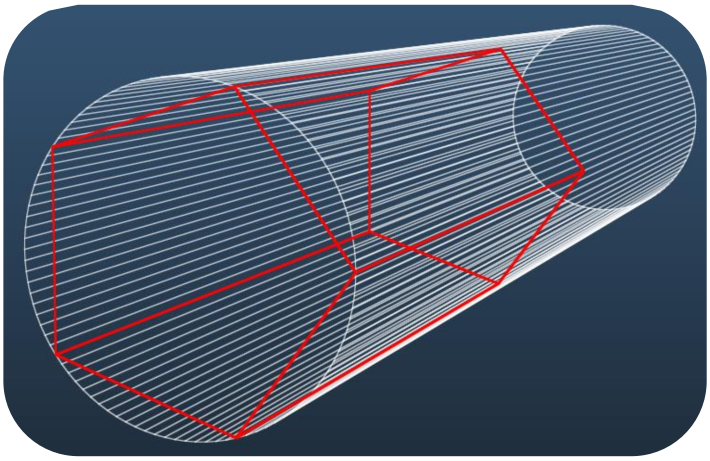
3.11.2. Exporting and Inserting parts

It is possible to assemble a geometry within MolFlow, and it is also possible to save a part of our model in a separate file for re-use. The idea is that you can have frequently used parts (pumps, valves…) in their own files, and then you can attach it to your system.

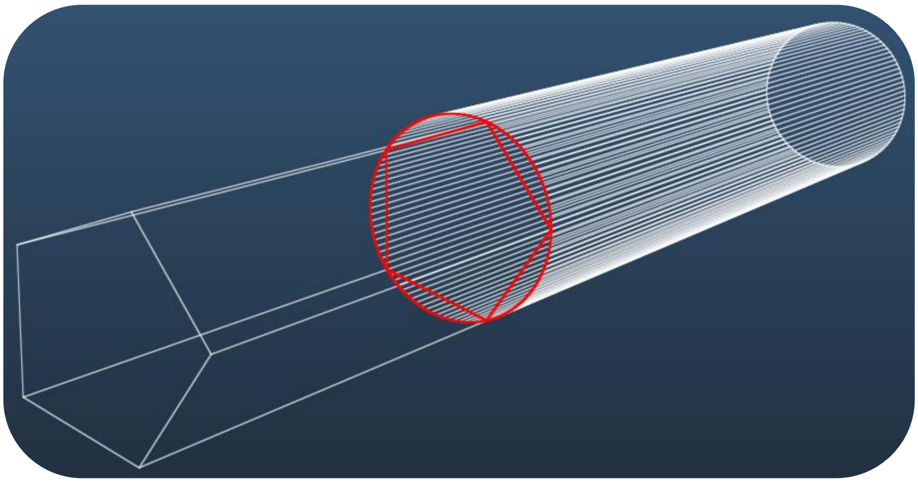
To insert a geometry file (GEO, SYN, TXT or STL), choose *Insert geometry* from the File menu:



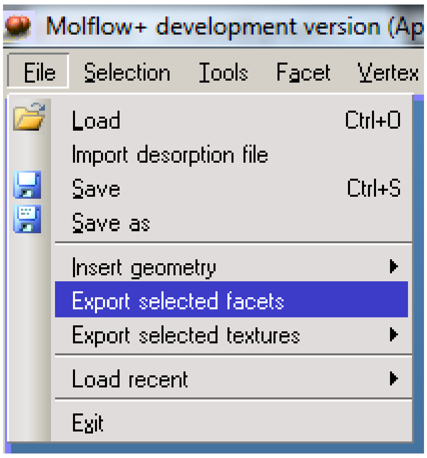
Then you will be offered the usual Open File dialog, and upon opening, the new file will appear in its original position.



As this is probably not its final place, the new facets remain selected, so you can easily apply a geometry operation on them, most probably **aligning** the new body to your existing geometry (see section 3.12.6).



To export a part as a separate file, simply select the facets and use File -> Export Selected Facets:

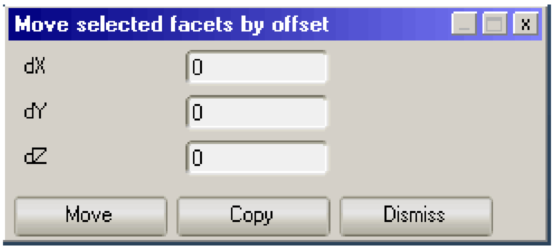


Your part will be saved as a separate geometry that you can later insert in your system.

3.12. Geometry Editor

Whereas it is recommended to use an external CAD program to edit your geometry, MolFlow offers basic operations to make small modifications and to assemble different parts inserted separately. In points 3.12.1-3.12.5 (move, mirror, scale rotate), it is always possible to **apply changes** on the selected facets or **create a copy** at the new position. If you perform a copy, most facet properties (including the mesh) will be copied.

3.12.1. Moving facets



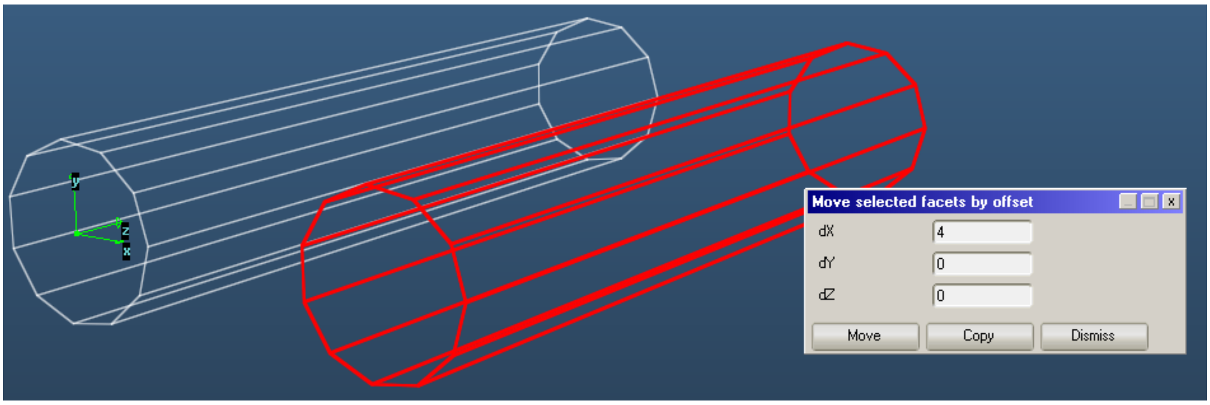
Move selected facets by offset

dX 0

dY 0

dZ 0

A basic dialog window where you enter the offset coordinates in centimeters. If you are not sure of the needed offset, enter a small value (for example, dX=1cm), and every click on the Move button will be performed immediately. Use the copy button to create a copy at an offset location:



Move selected facets by offset

dX 4

dY 0

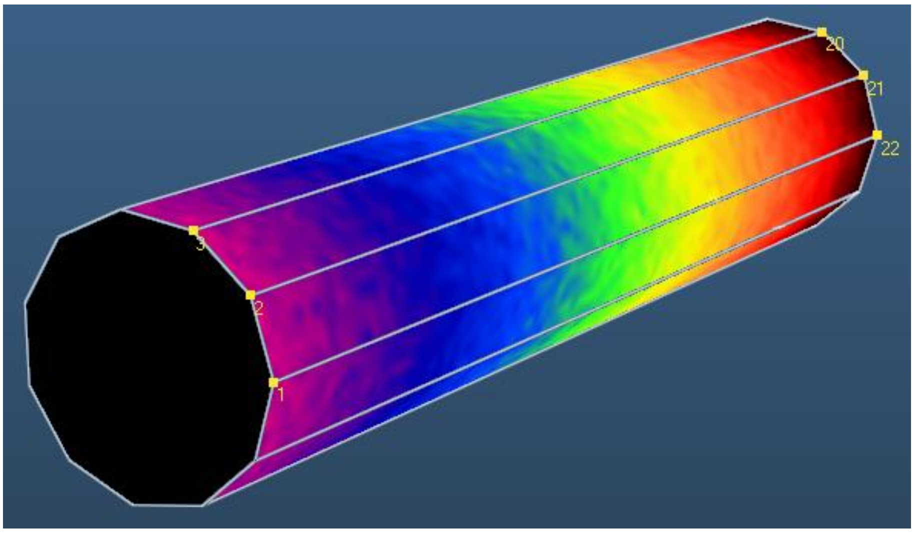
dZ 0

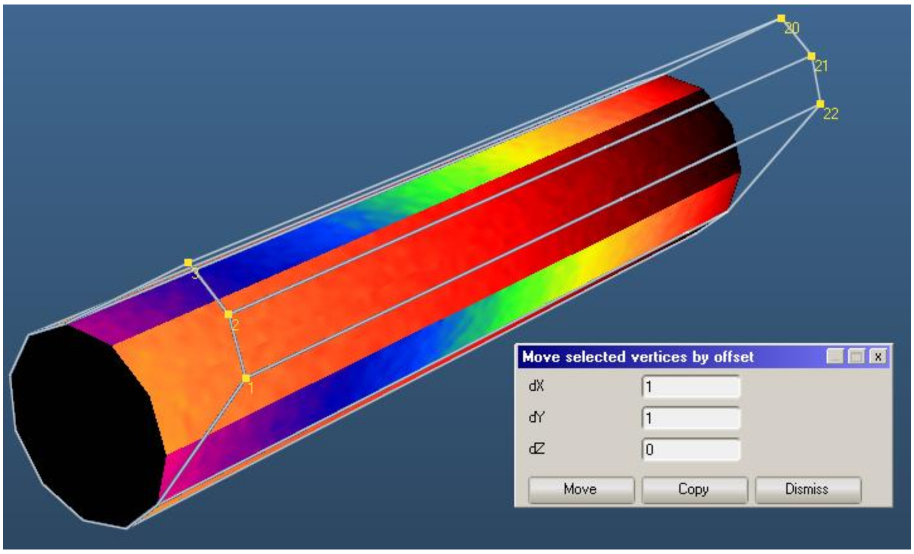
A new tube created 4cm to the X direction from the original. Note that facets of the new copy are selected.

3.12.2. Moving vertices

It is possible to distort the geometry by moving only certain vertices. All facets that contain the given vertices will be updated (area recalculation, etc.) but you need to re-apply the mesh.

Hint: to select vertices, use the tool in the lower right of your viewer.

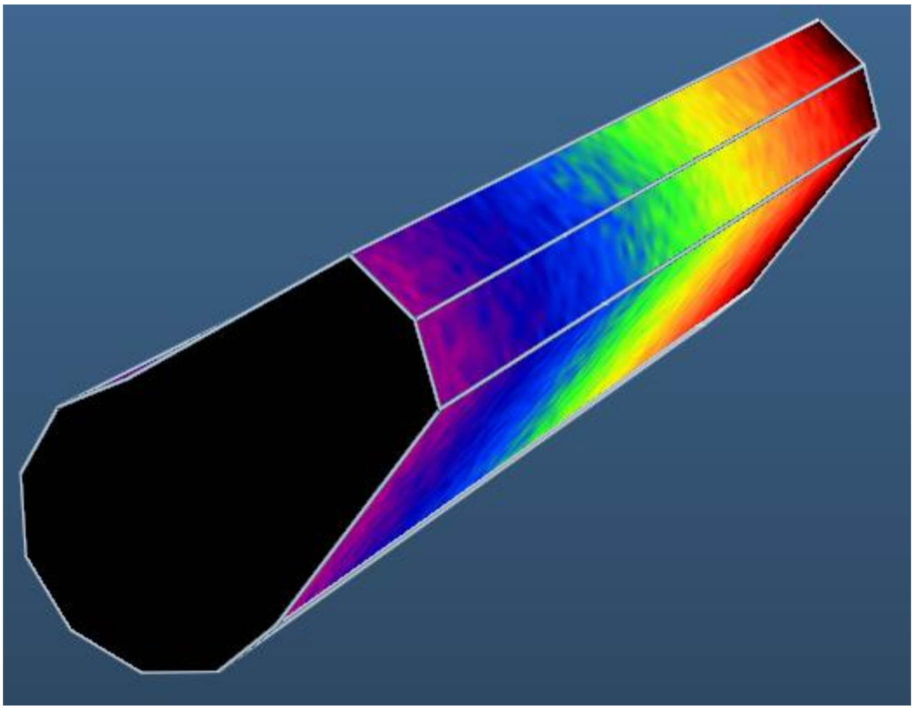




dX 1

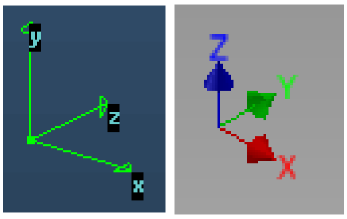
dY 1

dZ 0

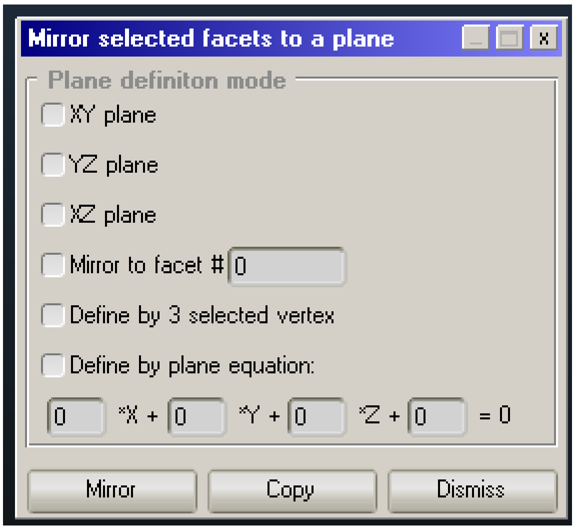


3.12.3. Mirroring facets

This function allows you to mirror parts. This might be useful since MolFlow uses a left-handed coordinate system, whereas most CAD programs use a right-handed one, resulting in a mirrored view upon importing.



Coordinate system axes in MolFlow and AutoDesk Inventor



Mirror selected facets to a plane

Plane definiton mode

□ XY plane

□ YZ plane

□ XZ plane

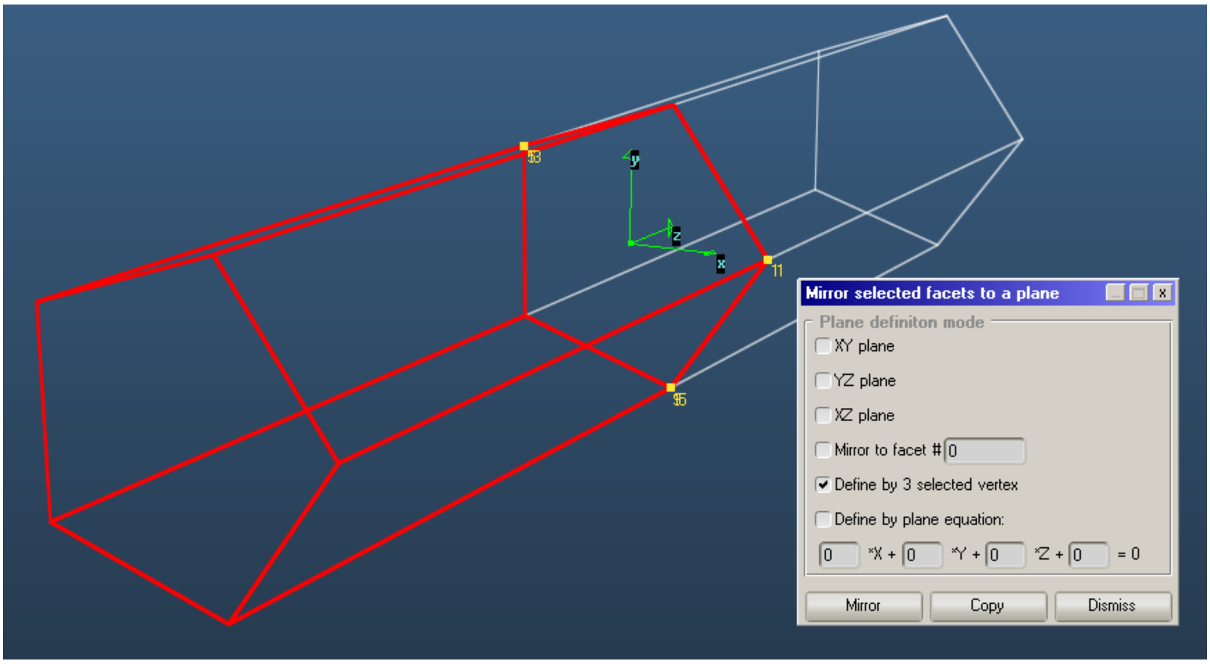
□ Mirror to facet # 0

□ Define by 3 selected vertex

□ Define by plane equation:

0 *X + 0 *Y + 0 *Z + 0 = 0

The purpose of the dialog window is to define the mirror plane. This can be one of the default XY, YZ, XZ planes, or the plane where a facet lies, but you can even define a new plane by selecting 3 vertices or by entering its equation. After mirroring, verify if the normal vectors are pointing in the correct direction.



Mirror selected facets to a plane

Plane definiton mode

□ XY plane

□ YZ plane

□ XZ plane

□ Mirror to facet # 0

☑ Define by 3 selected vertex

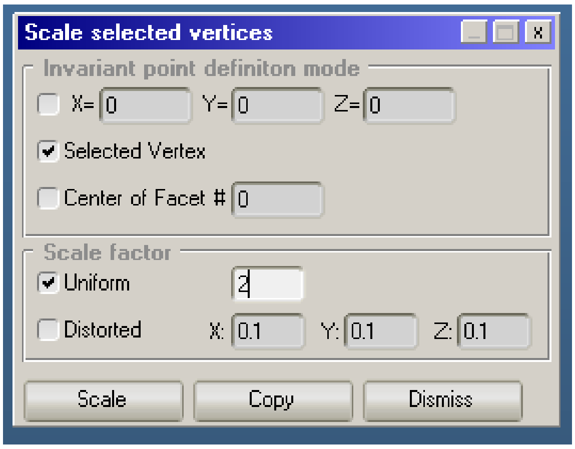
□ Define by plane equation:

0 *X + 0 *Y + 0 *Z + 0 = 0

A tube created by mirroring half of it to 3 vertices

3.12.4. Scaling facets

It is possible to scale or distort facets. This function is useful if there was a unit mistake when importing the STL file, or if we want to make an ellipse out of a tube.



Scale selected vertices

Invariant point definiton mode

☐ X= 0 Y= 0 Z= 0

☑ Selected Vertex

☐ Center of Facet # 0

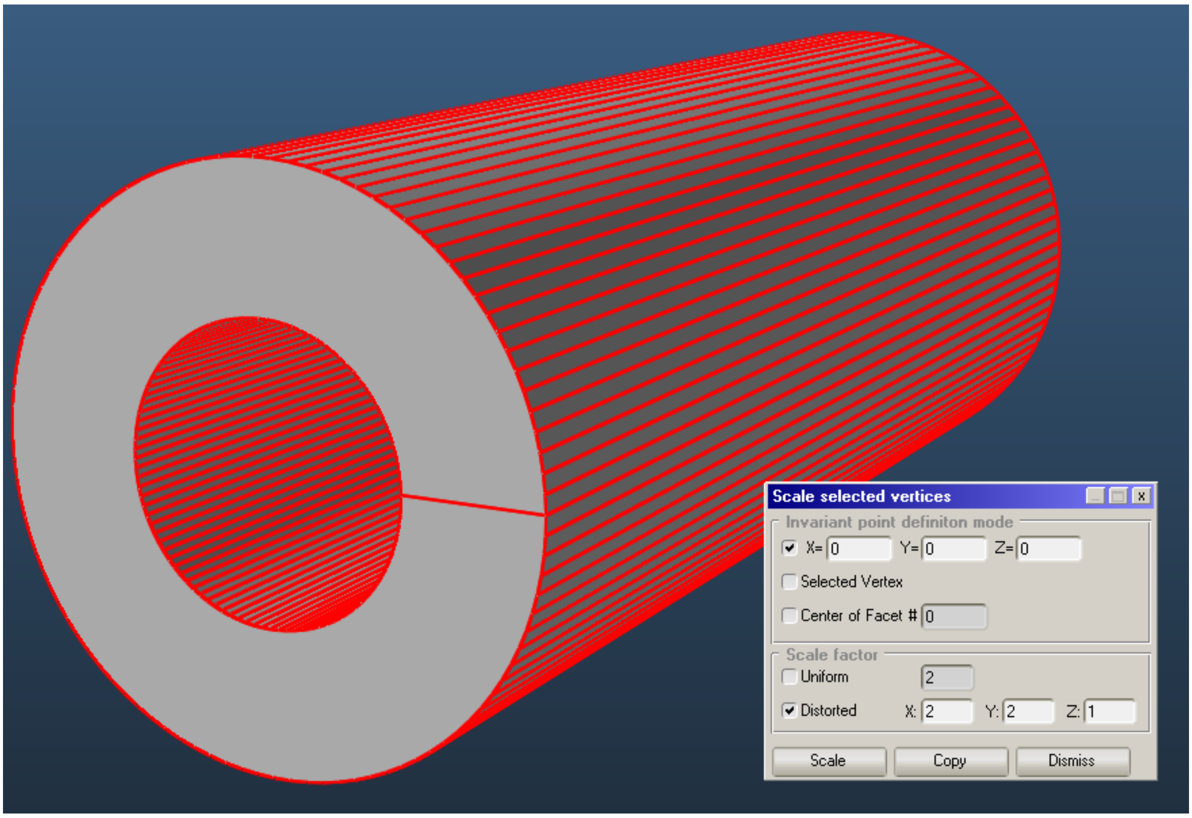
Scale factor

☑ Uniform 2

☐ Distorted X: 0.1 Y: 0.1 Z: 0.1

Scaling an object requires the user two define two parameters:

- **The invariant point:** the centre of the scaling, that is, the point which will stay at the same position. This can be defined by coordinates, by a selected vertex or it can be the centre of a facet.
- **The scale factor:** for the point at X, Y, Z coordinates, the new position will be
  $[\ factor_X * (X-X_0)\ ,\ factor_Y * (Y-Y_0)\ ,\ factor_Z * (Z-Z_0)\ ]$
  Where X_0,Y_0,Z_0 are the coordinates of the invariant, and the factor parameters are the content of the text fields (in uniform scaling, $factor_X$=$factor_Y$=$factor_Z$).



Scale selected vertices

Invariant point definiton mode

☑ X= 0 Y= 0 Z= 0

☐ Selected Vertex

☐ Center of Facet # 0

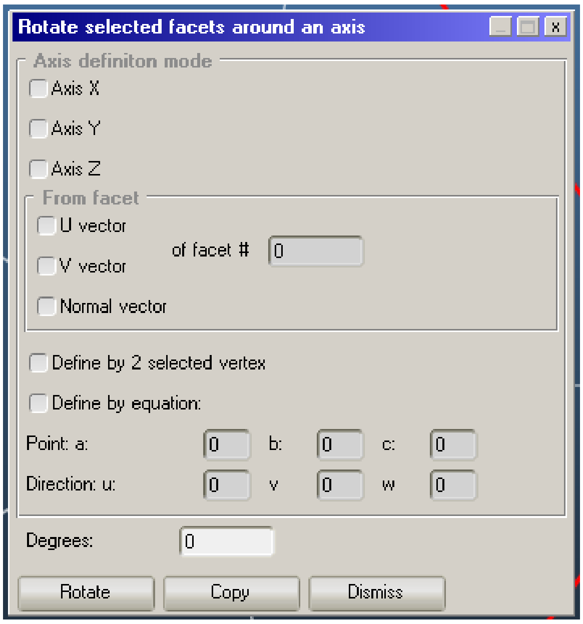
Scale factor

☐ Uniform 2

☑ Distorted X: 2 Y: 2 Z: 1

A concentric tube created by scaling up a single tube in the X and Y directions.

3.12.5. Rotating facets



Rotate selected facets around an axis

Axis definiton mode

☐ Axis X

☐ Axis Y

☐ Axis Z

From facet

☐ U vector

☐ V vector

☐ Normal vector

of facet # 0

☐ Define by 2 selected vertex

☐ Define by equation:

Point: a: 0 b: 0 c: 0

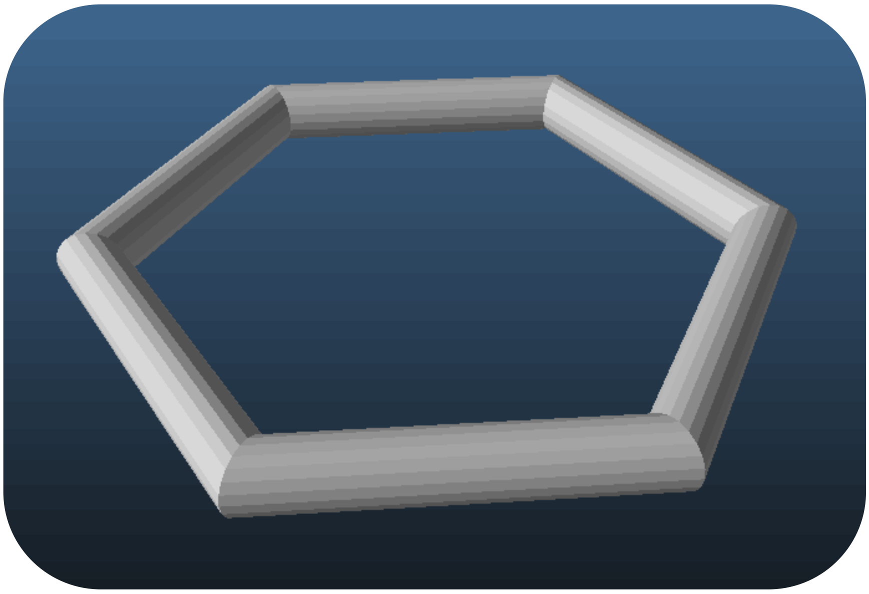
Direction: u: 0 v 0 w 0

Degrees: 0

Rotating facets require a rotation **axis** and the rotation **angle**.

- The axis can be one of the default X, Y, Z axes, it can be a local U,V or N vector a facet. You can also define a new axis by either using 2 vertices or defining a base point and a direction vector with coordinates.
- The rotation angle is in degrees, and it can be negative.

Hint: If you use the '2 vertices' option, the direction is not well defined. Use a positive or negative value for the rotation angle, and see which yields the correct result.



A circular geometry created from a tube and 60 degree facet rotations

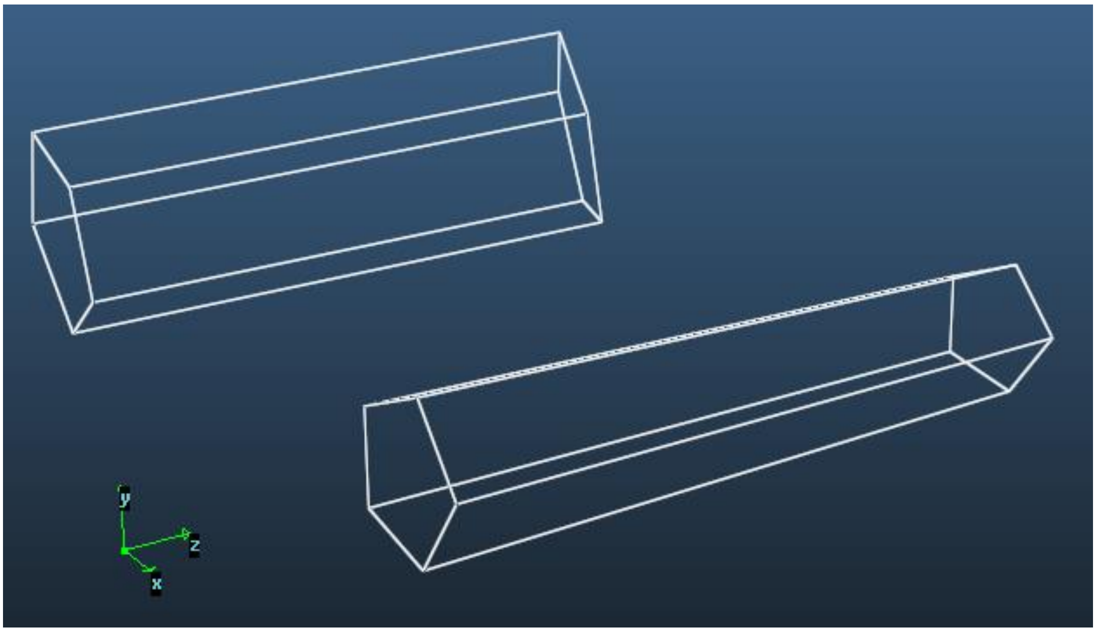
3.12.6. Aligning facets

When you insert a new part or geometry, the most obvious step to do next is to attach it to your existing geometry. This function takes some practice to master, but is very useful once learned.

You have to do essentially three steps:

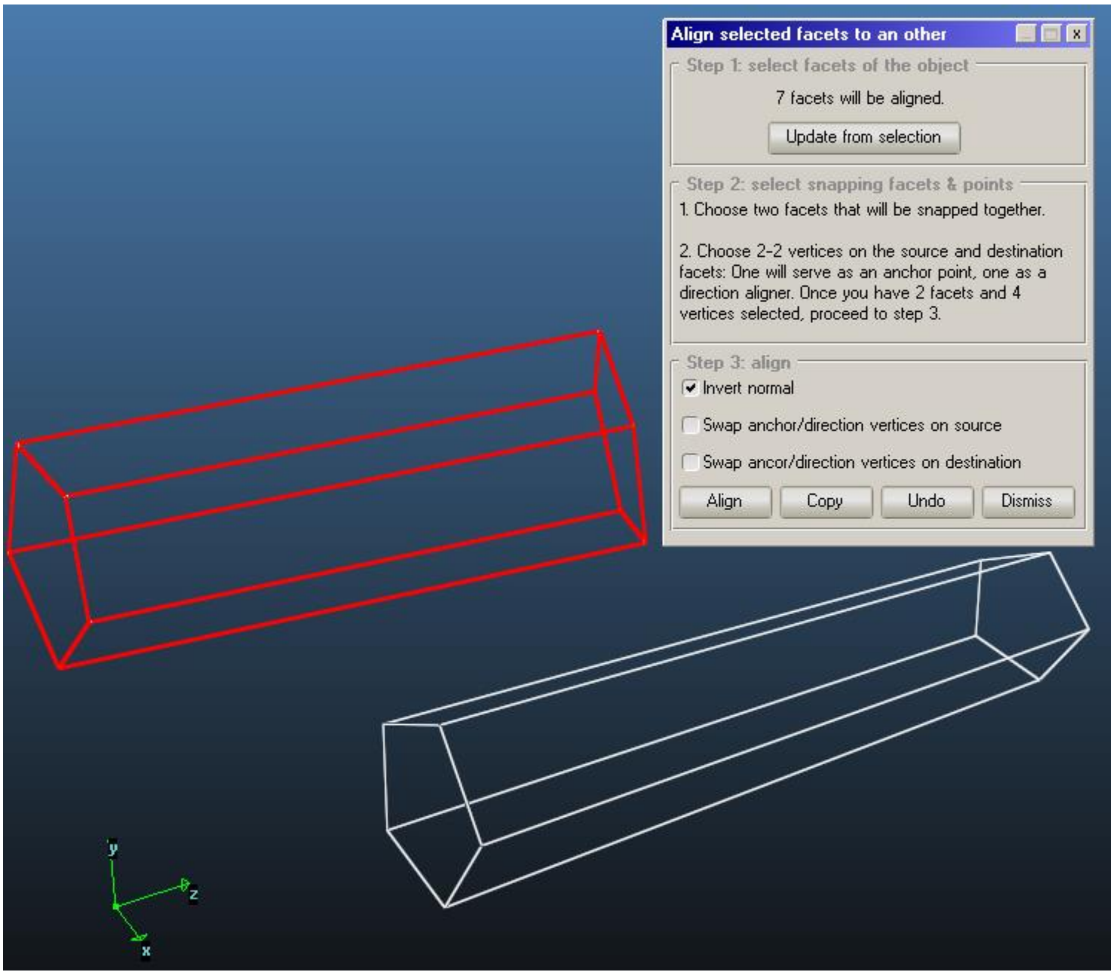
1. Define what to move
2. Define where to move
3. Vary the options in a way that the alignment is as it should be

We'll go through these three steps in detail. As an example, we assume that we just inserted the small pipe, and we want to stick it to the large one:



Step 1: Defining what to move

This is the easy step: select the facets to align (to move) and open the Align… window:



Align selected facets to an other

Step 1: select facets of the object

7 facets will be aligned.

Step 2: select snapping facets & points

1. Choose two facets that will be snapped together.

2. Choose 2-2 vertices on the source and destination facets: One will serve as an anchor point, one as a direction aligner. Once you have 2 facets and 4 vertices selected, proceed to step 3.

Step 3: align

☑ Invert normal

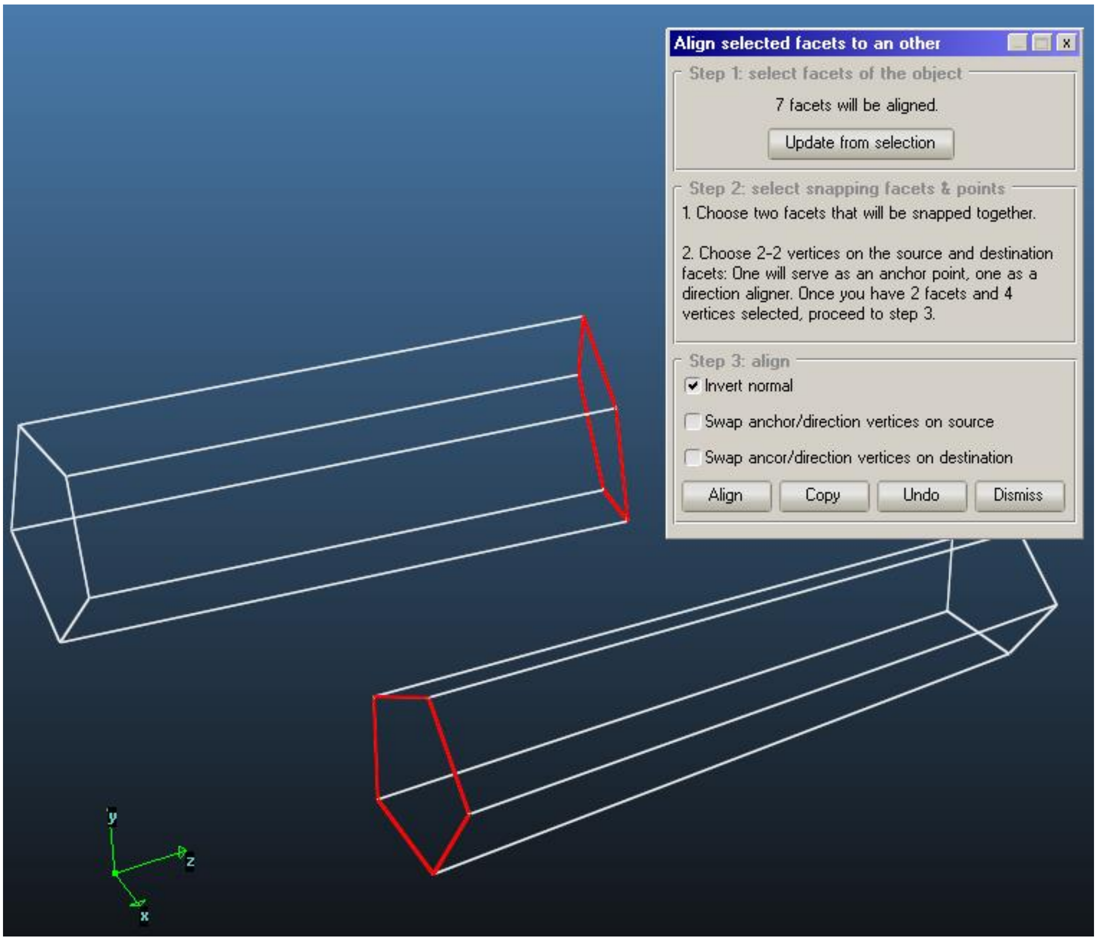
□ Swap anchor/direction vertices on source

□ Swap ancor/direction vertices on destination

When you open the window, the facets that are actually selected will be memorized as the ones to move. If this is not what you want, you can select other facets and click the “Update from selection” button.

Step 2/a: select facets that will snap together

Now you have to tell MolFlow which two facets to snap together. Select them:



Align selected facets to an other

Step 1: select facets of the object

7 facets will be aligned.

Step 2: select snapping facets & points

1. Choose two facets that will be snapped together.

2. Choose 2-2 vertices on the source and destination facets: One will serve as an anchor point, one as a direction aligner. Once you have 2 facets and 4 vertices selected, proceed to step 3.

Step 3: align

☑ Invert normal

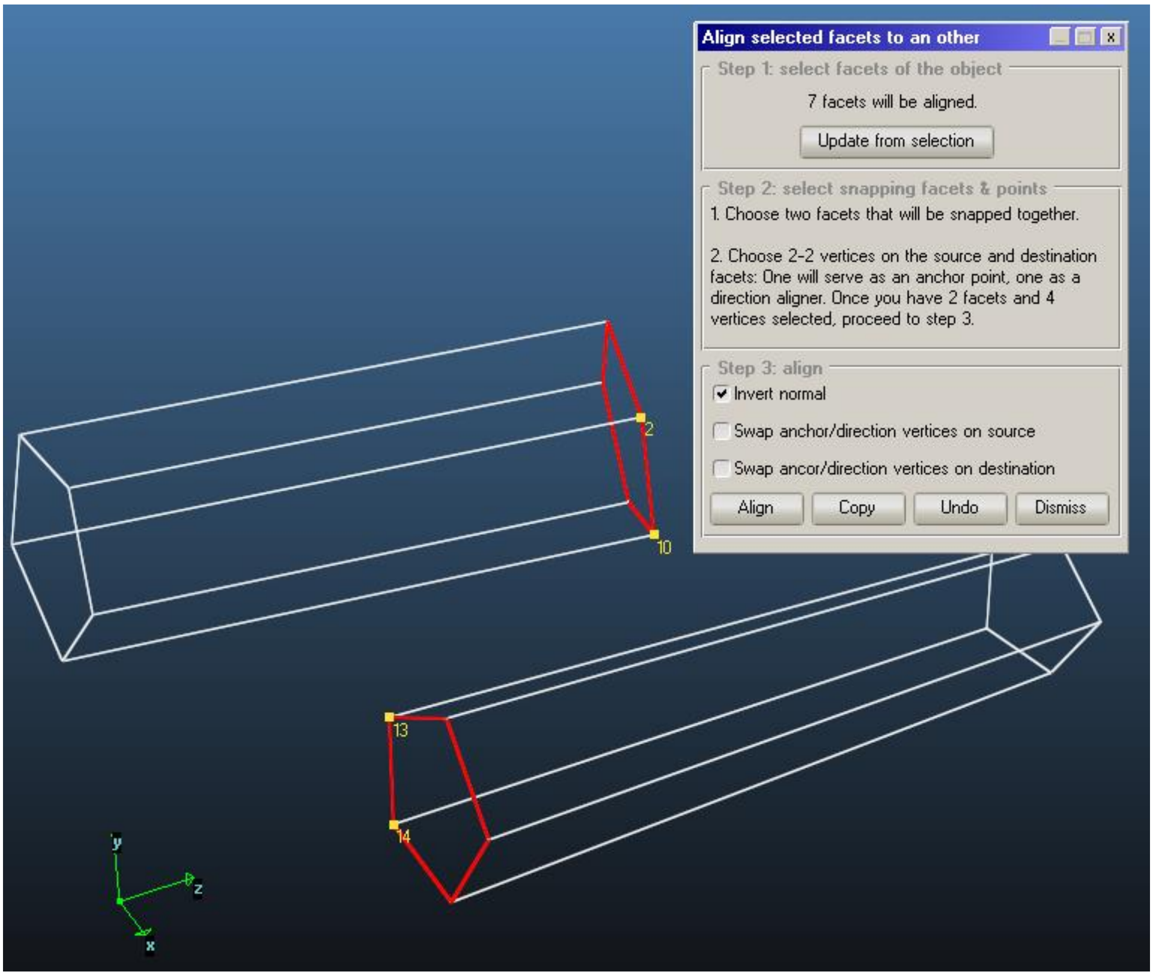
□ Swap anchor/direction vertices on source

□ Swap ancor/direction vertices on destination

Hint: In this example, we already had two facets at the end of the pipe. If the planes to snap together don’t have facets, you can always create some “temporary” facets for defining the plane. Refer to the section 3.12.7 to read more about creating facets.

Step 2/b: select vertices to snap together

Even though the two facets from the previous step will be snapped together, it is necessary to define their direction relative to each other. This is done with two **anchor vertices** that will be on each other, and two **direction vertices** that will define the direction from the anchors. In short, select 2-2 vertices on the source and destination facets and proceed to the next step:



Align selected facets to an other

Step 1: select facets of the object

7 facets will be aligned.

Step 2: select snapping facets & points

1. Choose two facets that will be snapped together.

2. Choose 2-2 vertices on the source and destination facets: One will serve as an anchor point, one as a direction aligner. Once you have 2 facets and 4 vertices selected, proceed to step 3.

Step 3: align

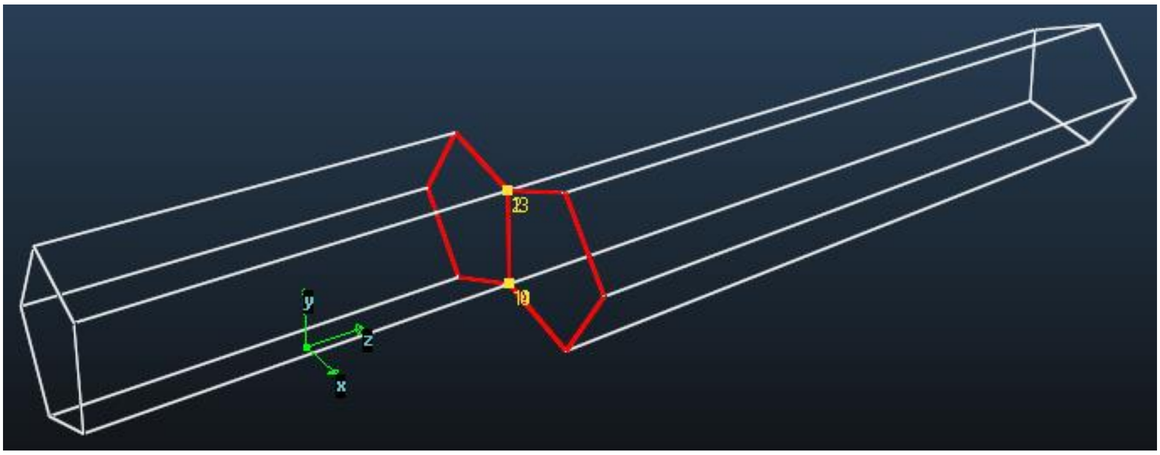
☑ Invert normal

□ Swap anchor/direction vertices on source

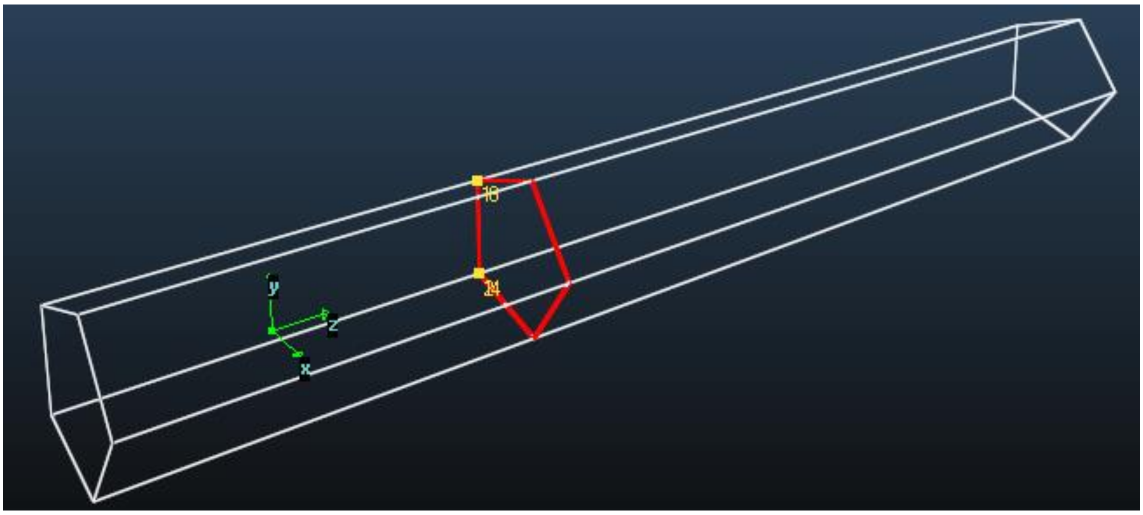
□ Swap ancor/direction vertices on destination

Step 3: performing align

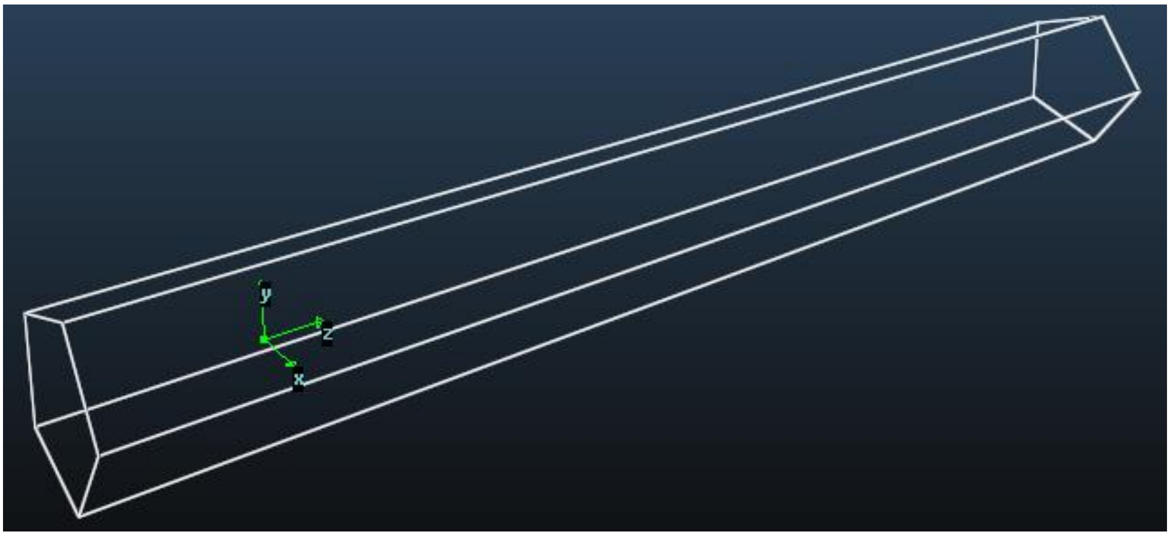
Click the Align button. Now, chances are that the result is not the one you looked for (in the example below, the axis and direction vertices are mixed up):



Change the 3 checkboxes until you have the result you want. You can always use the **undo** button to restore the original position.



Done! Depending on what you want, you can delete the intermediate facets that were used for aligning, and also collapse the geometry to merge collinear lines:



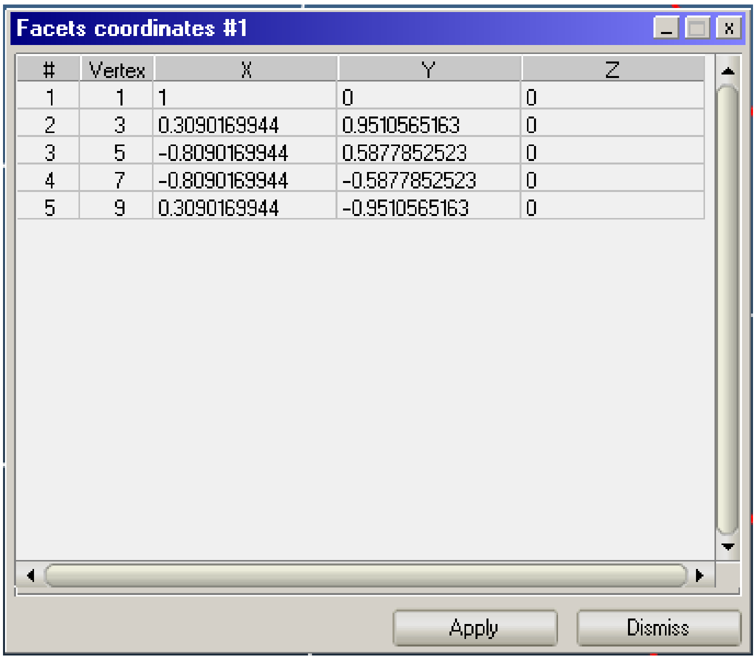
3.12.7. Swap normal of a facet

Swaps the side that the normal vector of selected facets points to. Available in Facet -> Swap normal

3.12.8. Shift vertex

Changes the numbering of the facet's vertices. You can see these numbers by enabling the *Indices* display option and selecting a facet. Use this option if you want to change the U,V vector positions, and also in some cases this option solves the "non simple facet" problem.

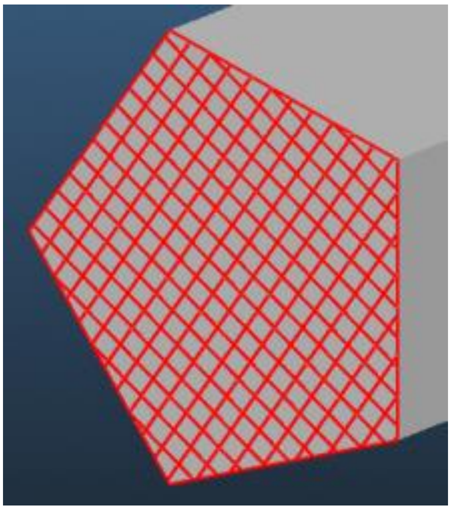
3.12.9. Edit facet coordinates



#	Vertex	X	Y	Z
1	1	1	0	0
2	3	0.3090169944	0.9510565163	0
3	5	-0.8090169944	0.5877852523	0
4	7	-0.8090169944	-0.5877852523	0
5	9	0.3090169944	-0.9510565163	0

Directly view / edit the coordinates of a selected facet. Note that you can also use the *Edit Coordinates* command of the Vertex menu, which will list all selected vertices.

3.12.10. Explode selected



With this option you can divide a facet to new facets, each inheriting their parent's parameters. First, define a mesh on the facet(s), and then this command will create one new facet of each mesh cell.

3.12.11. Delete facets

Available from Facet -> Remove selected (CTRL + DEL)

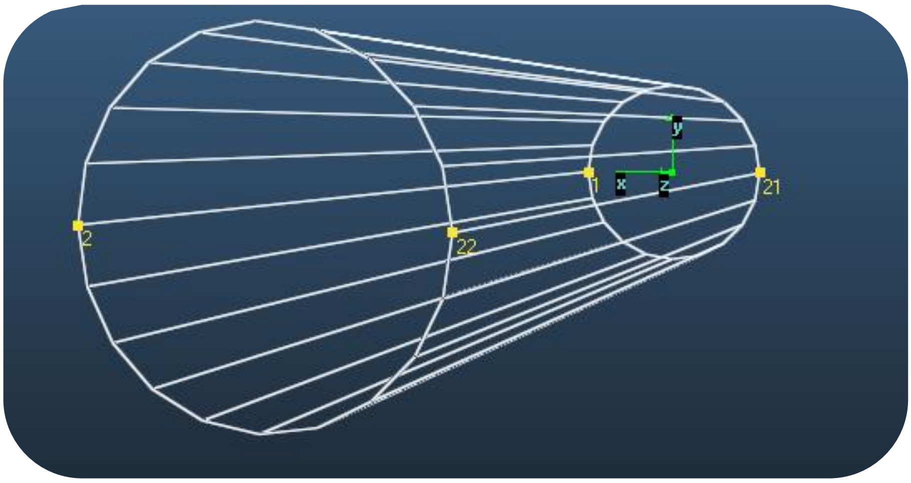
Will delete selected facet(s), and also prompt to delete the liberated vertices.

3.12.12. Creating transparent facets for measurements

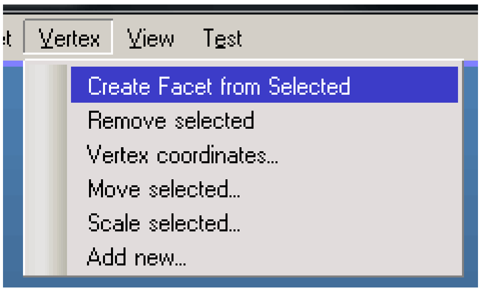
So far, we have seen how to create profiles and textures on facets. These serve to measure the pressure on the wall of your system, however, with MolFlow; it is possible to calculate physics properties at any point in the geometry. For this, you will need to create transparent facets whose only purpose will be to measure.

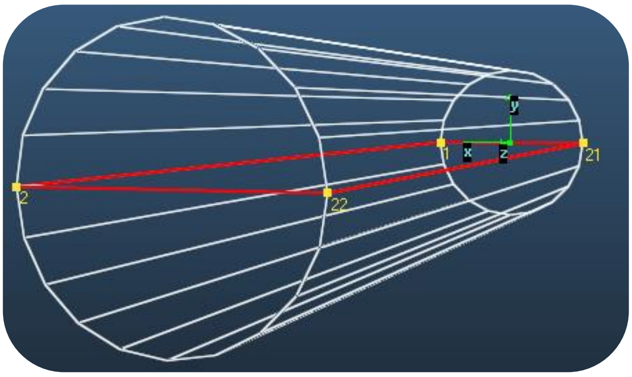
To create facets, you can use the above geometry editor functions (for example, the *Move facets* command with the *Copy* button), but for its multiple uses, we'll use the **create facet from vertices** command.

The idea is to select vertices that exist already or to create new ones with the *Add vertex* or *Move vertices* commands, then use them as the corners (indices) of the new facet that we are about to create. In the following example, we'll select four vertices that are form the cross-section of our pipe:



Then we create a facet using the dedicated command:



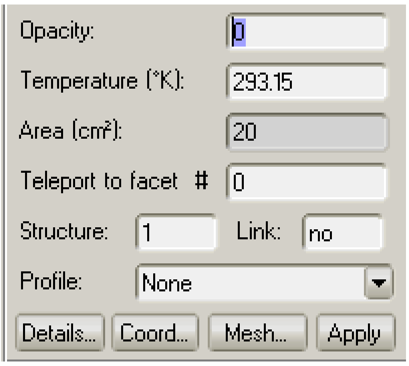


The new facet will be added to the geometry.

Hint: connecting vertices to form a polygon is not always a well-defined operation. MolFlow uses the Graham scan algorithm to construct a convex outline with the largest area for the selected vertices.

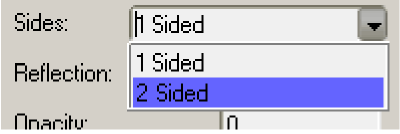
Now that we have created the new facet, we need 3 steps to make it measure the pressure:

1. **Make it transparent**
   We want to measure without disturbing the system. To do that, set the facet's opacity to 0 in the facet parameters panel:



Opacity: 0
Temperature (°K): 293.15
Area (cm²): 20
Teleport to facet #: 0
Structure: 1 Link: no
Profile: None

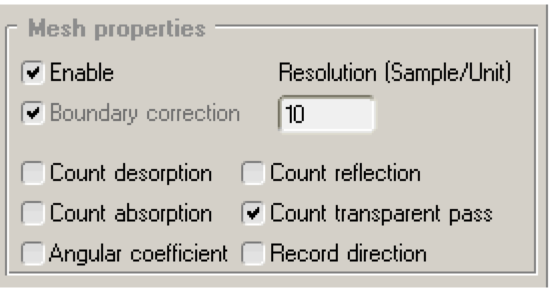
2. **Make it two-sided**
   Two-sided facets count collisions or particle crosses from both sides. Since our facet is in the middle of our system, it can be two-sided:



Sides: 1 Sided
Reflection:
Opacity: 0

   Please note that pressure in molecular flow is not isotropic: it depends on the angle of measurement. Therefore working with two-sided facets is also a good idea since the average of the two pressures from the two sides is calculated.

3. **Add a texture**
   To make our new facet actually count particles crossing it (and thus the pressure), we have to add a mesh with the *count transparent passes* option enabled:

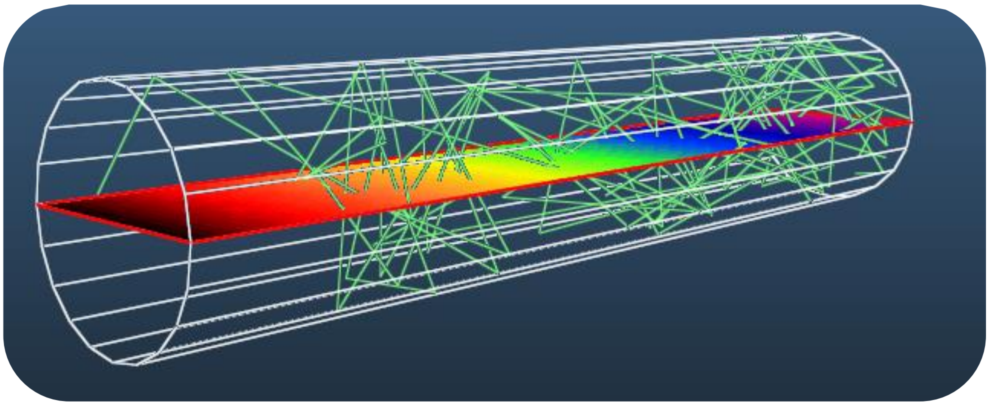


Mesh properties

☑ Enable
☑ Boundary correction
Resolution (Sample/Unit): 10

☐ Count desorption ☐ Count reflection
☐ Count absorption ☑ Count transparent pass
☐ Angular coefficient ☐ Record direction

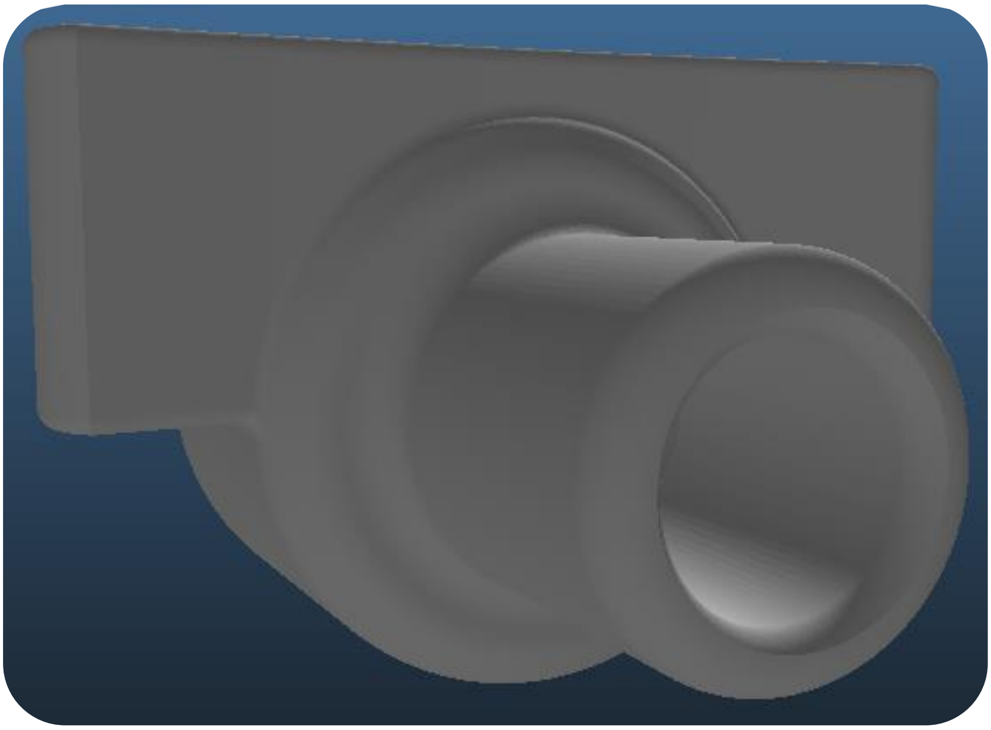
Done! Now our new facet will count the pressure in the middle of our system:



Pressure is measured through the cross-section of a tube while particles cross the transparent facet.

3.12.13. Plugging holes

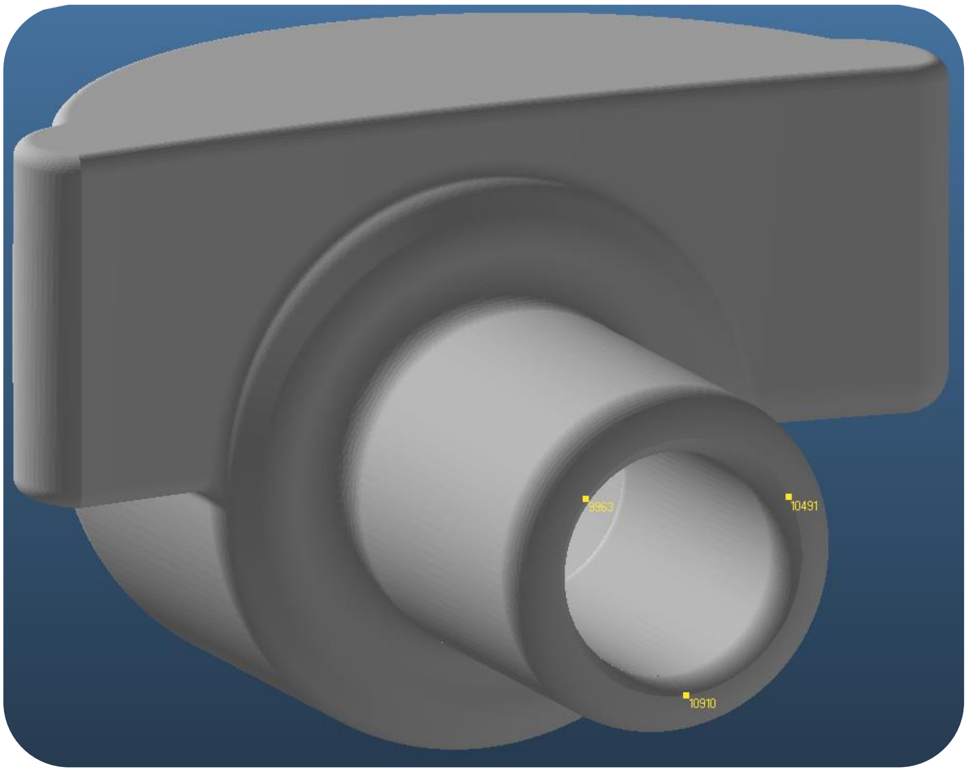
Sometimes we have to create a facet to desorb particles from a circular orifice or to set up a pump where there were no facets upon importing the geometry. For example, in the below object, the hole is “unplugged”, resulting in leaks:



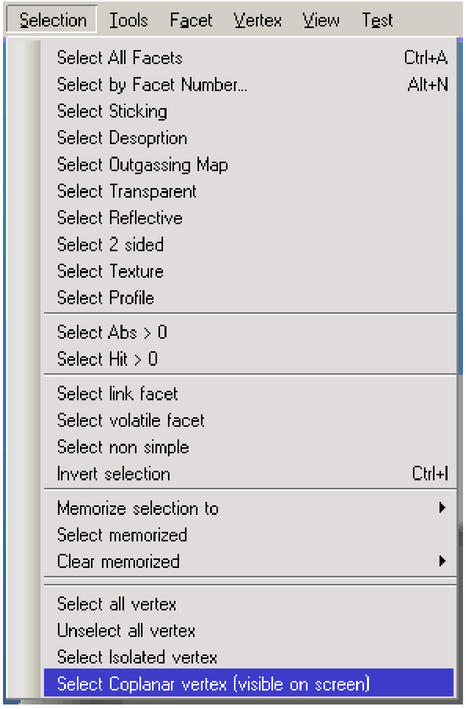
To plug this hole with a facet, we could theoretically select all vertices on the outline, but we’ll use a special command.

Step 1: Define the plane of the hole

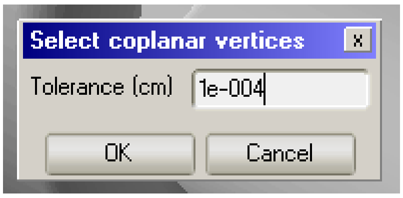
To do that, we’ll select 3 vertices on the hole:



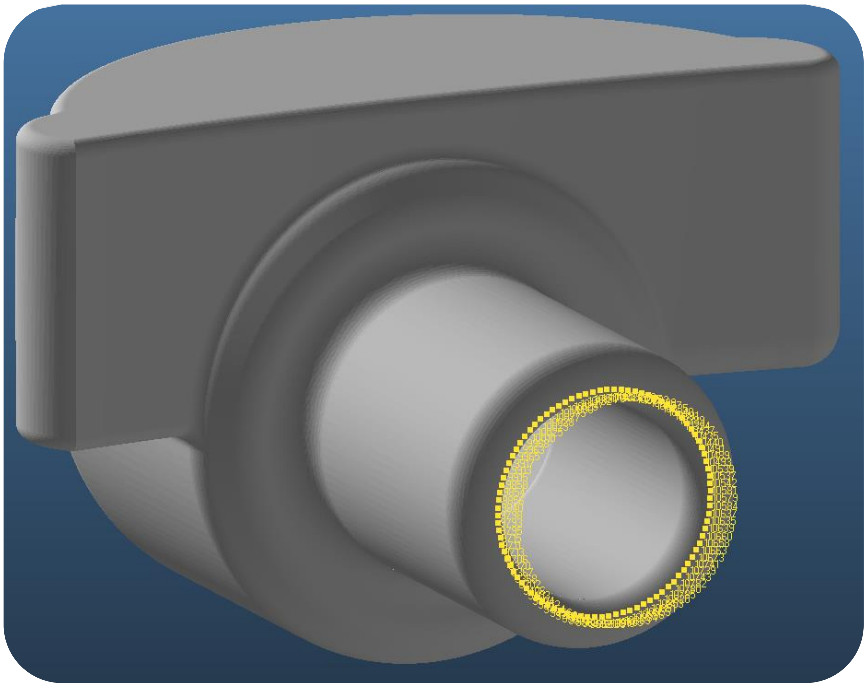
Then we select all vertices on that plane by the special *Select Coplanar* command:



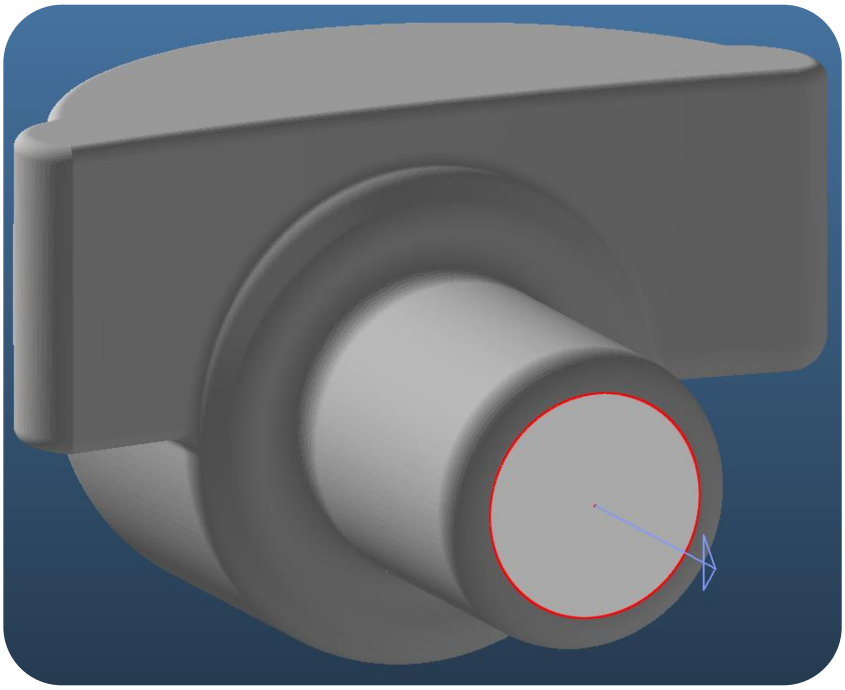
Then select a tolerance value (in centimetres) comparable with your system size:



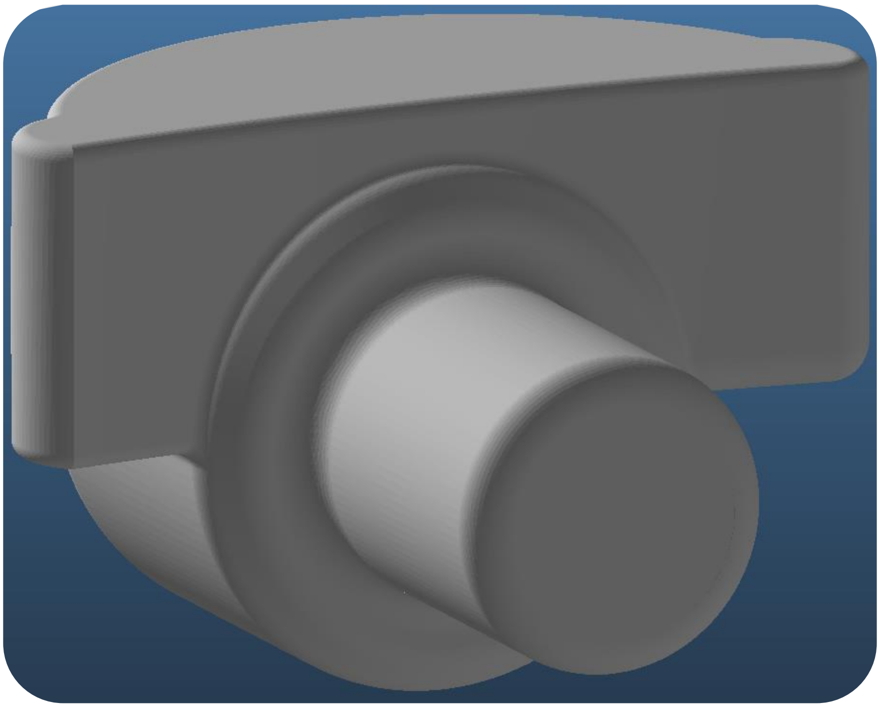
Tolerance (cm) 1e-004



Now you are ready to create the new facet (don't worry if you selected concentric vertices: MolFlow will create the largest possible facet):

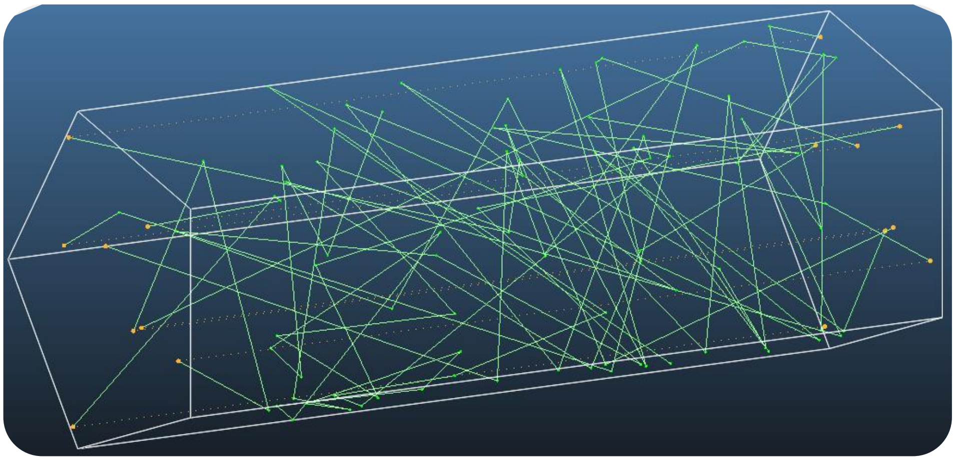


Change the normal vector, if necessary, then your plug is complete:



3.13. Periodic boundary conditions (teleport)

In accelerators, we often deal with periodic structures, for example with circular storage rings. The idea is that it is sufficient to include the repeating part of the geometry only once, and then connect its two ends by defining *teleports*. Therefore, once a particle hits one end of the structure, it is transported back to the other side, thus simulating an infinite loop.



A simple tube with its two ends connected through *teleports*. See the yellow dotted lines which visualize particles that are just teleported.

Though the principle is simple, several conditions have to be met to define such a structure in Molflow.

You have to have two teleport facets, that will teleport particles to each other. For the correct functioning of the teleport, the following conditions have to be met:

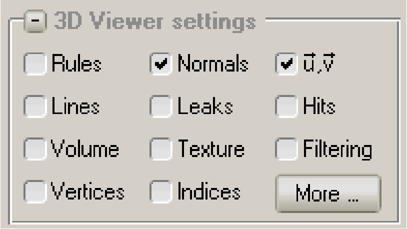
- Both facets have the same shape
- Both **normals** are pointing to the same direction
- Both U,V vectors point to the same direction
- If the above conditions are met, most probably one of the two facets will receive particles from its back side, thus it has to be **two-sided**

- Facet A must be a teleport to facet B (enter facet B's number to the *teleport* facet parameter field)
- Facet B must be a teleport to facet A

In the example below, we'll set up a teleport on a tube consisting of 7 facets. The beginning and the end of the tube are facets number 1 and 2, so we'll essentially work on them.

Step1: selecting facets

Select facets 1 and 2, and turn on normal and U,V vector display:



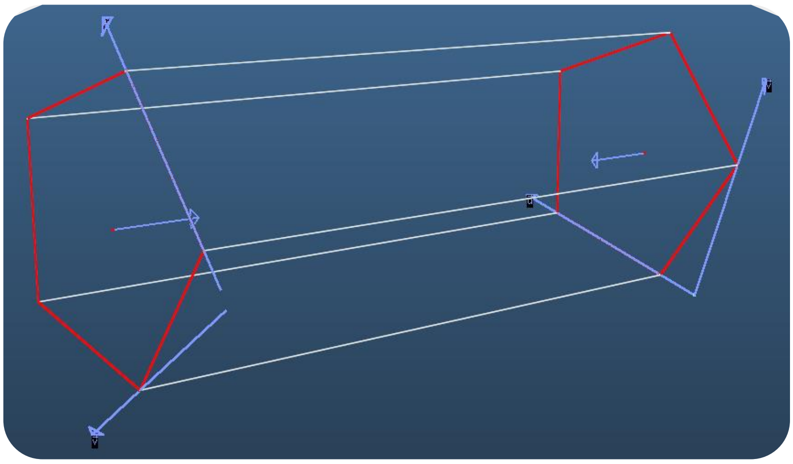
3D Viewer settings

□ Rules ☑ Normals ☑ $\vec{u},\vec{v}$

□ Lines □ Leaks □ Hits

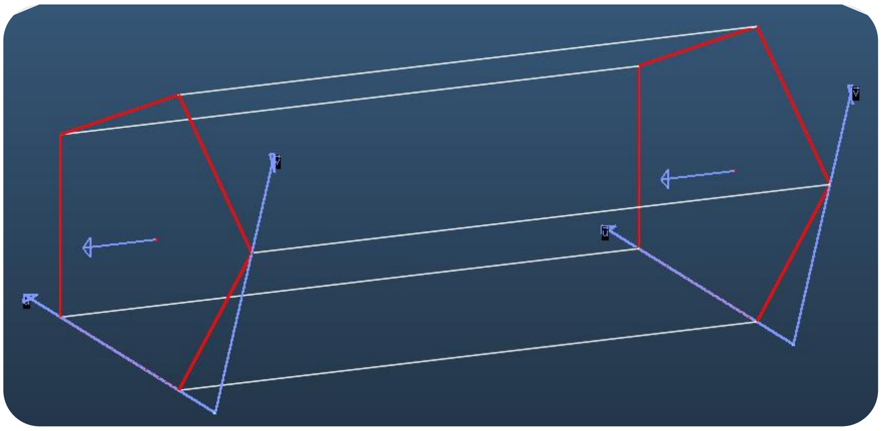
□ Volume □ Texture □ Filtering

□ Vertices □ Indices More ...



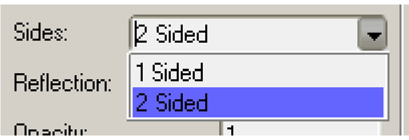
Step2: Align facets

The two facets must be oriented in the same way (to ensure correct flight path after the teleportation). Use the *Swap Normal* and *Shift vertex* commands to rotate one of the facets like the second.



Step3: Setting up teleports

- Make both facets 2-sided (so they can detect particles from the back as well):

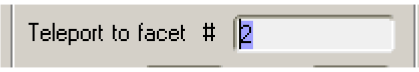


Sides: 2 Sided

Reflection: 1 Sided / 2 Sided

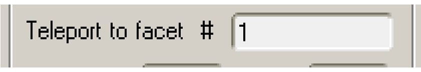
Opacity: 1

- Select facet #1 and fill in the *Teleport* parameter with 2 (the number of the teleport destination)



Teleport to facet # 2

- Select facet #2 and set the *Teleport* parameter to 1



Teleport to facet # 1

Done! Launch a particle from somewhere and your simulation will be running with teleports.

3.14. Superstructures

Superstructures, often simply referred as structures, are smaller parts of your geometry.

3.14.1. Their purpose

After a facet is hit and a particle is rebounded in a new direction, Molflow looks for the next collision with the help of ray tracing algorithms. The program must essentially search for collision with **ALL** of the facets, then decide which collision is closest, thus which will actually happen. Therefore, in a geometry with 10.000 facets, it takes more or less 10 times as much computing time to calculate the next hit as in a system with 1.000 facets only. You might feel that it is not optimal to look for collisions with facets that are very far in the system.

Superstructures help Molflow by defining which parts of the system are together.

Therefore, we do the following:

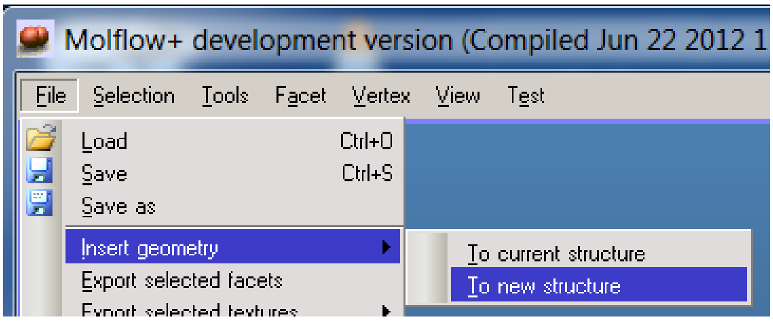
- We split our system to smaller parts, each part belonging to a different structure
- We create *links* between them; these links are "port" facets that all particles going from structure A to structure B will cross.
- When a particle is in structure A (got there through a link or desorbed from a facet in structure A), it will only check collisions with facets in structure A (which is faster than checking with all facets).

In the structure below, we can see two clearly separable parts that are connected via a link facet. The simulation is more or less two times faster.

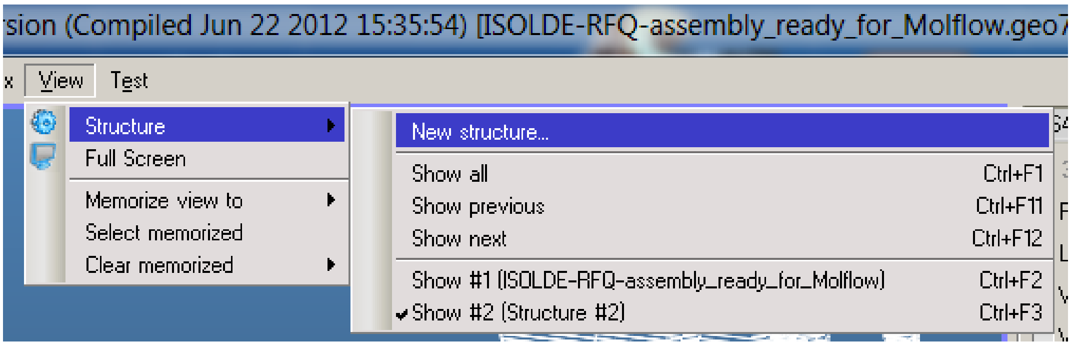
3.14.2. Creating structures

You can define structures by two different methods.

One is by importing different geometry files on each other, using the *insert to new structure* option:



You can **select** different structures in the view menu (cycle through them by CTRL+F11, CTRL+F12):


sion (Compiled Jun 22 2012 15:35:54) [ISOLDE-RFQ-assembly_ready_for_Molflow.geo7
View Test
Structure
Full Screen
Memorize view to
Select memorized
Clear memorized
New structure...
Show all Ctrl+F1
Show previous Ctrl+F11
Show next Ctrl+F12
Show #1 (ISOLDE-RFQ-assembly_ready_for_Molflow) Ctrl+F2
✓Show #2 (Structure #2) Ctrl+F3

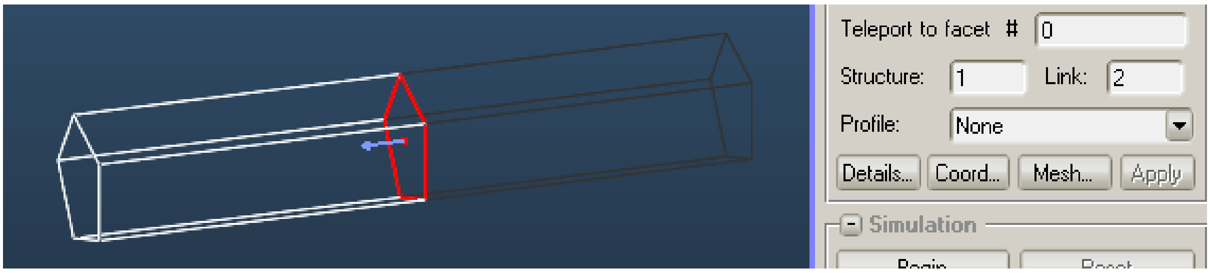
The other method is to edit the facets directly. In the facet parameters, you can see a "structure" field. Each structure has a number, beginning from 1.

If you change this number, the facet will belong to a new structure. You can **add new** structures in the view menu "New structure" command, which will create an empty structure. After you have this new structure, move facets into it by changing their structure numbers in their parameters.

3.14.3. Linking structures

To let particles know that they arrive to a new structure by crossing a “port”, you have to define *links*. Links are **two facets in the same position,** each belonging to its own structure. They have to fulfil the following:

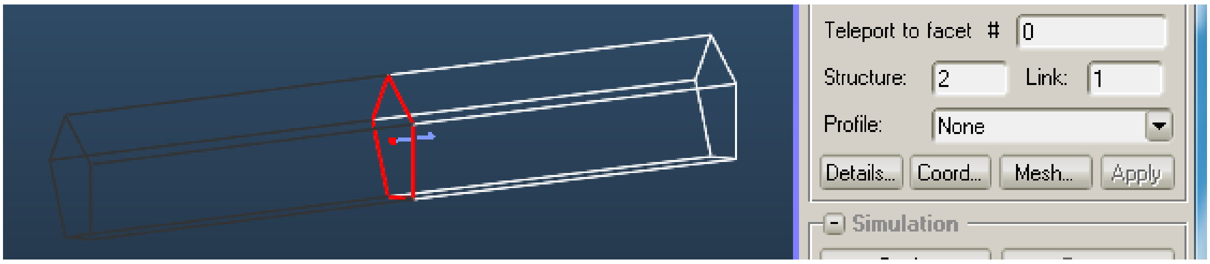
- They have exactly the same shape
- They are in the same position
- Both are **one-sided**
- One belongs to structure A, one to structure B
- The one that belongs to structure A has its normal pointing towards structure A, the other's normal is pointing towards structure B
- The one that belongs to A links to B, the one belonging to B links to A (ie. the facets are "showing their backs" to each other)



Teleport to facet # 0

Structure: 1 Link: 2

Profile: None



Teleport to facet # 0

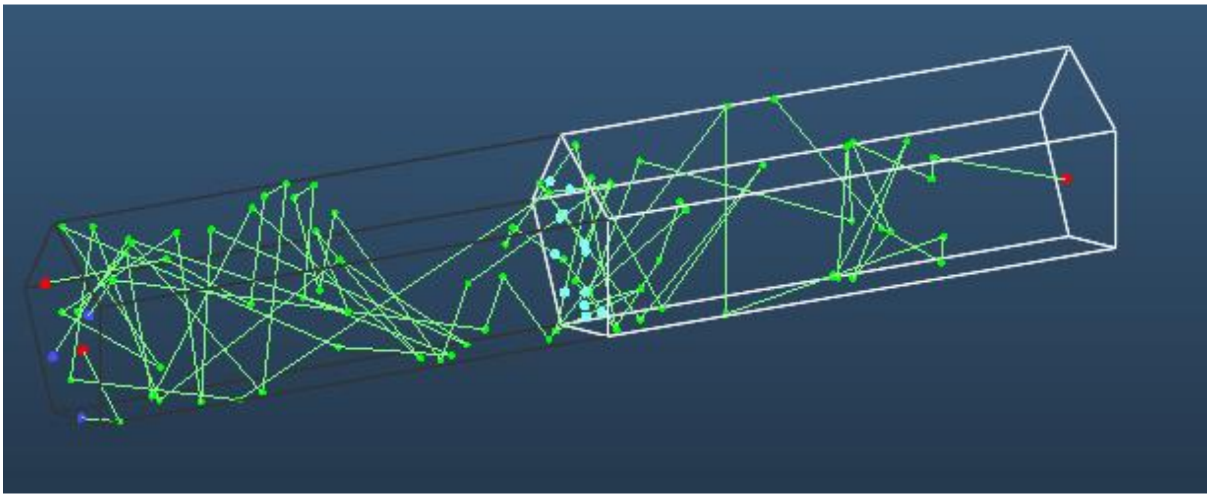
Structure: 2 Link: 1

Profile: None

To make a facet link towards another structure, enter the destination structure's number in the *Link* parameter.

To disable linking, enter 0 as destination.

A link facet **is always transparent.** You can see hits as "transparent passes", colored in light blue.

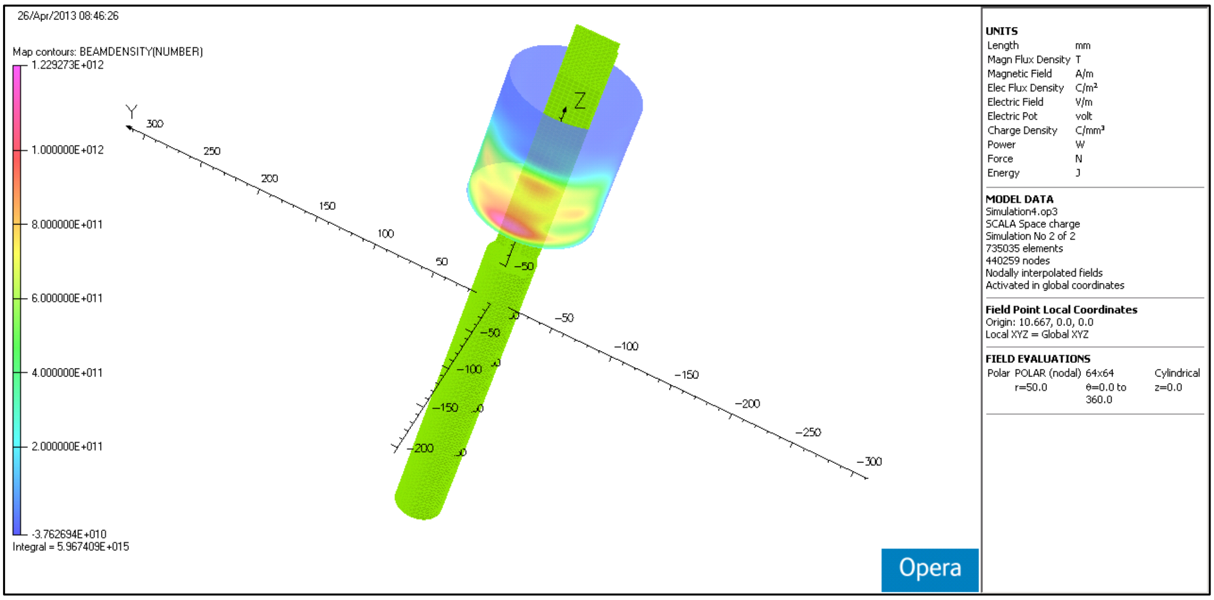


To help understand the concept, download this simple example geometry that contains two structures with their links defined correctly.

Note that if you have the time to run the simulation longer, it is not required to define structures. Putting everything in structure 1 will have the only negative effect of slowing down the simulation.

3.15. Desorption map / Outgassing map

In MolFlow, one Facet can have only one desorption value, and thus the desorption density is always uniform. This is adequate for simulating the gas influx through a port, but if we want to model a finer distribution of desorption, we have to do a few “tricks”.



UNITS

Length	mm
Magn Flux Density	T
Magnetic Field	A/m
Elec Flux Density	C/m²
Electric Field	V/m
Electric Pot	volt
Charge Density	C/mm³
Power	W
Force	N
Energy	J

MODEL DATA
Simulation4.op3
SCALA Space charge
Simulation No 2 of 2
735035 elements
440259 nodes
Nodally interpolated fields
Activated in global coordinates

Field Point Local Coordinates
Origin: 10.667, 0.0, 0.0
Local XYZ = Global XYZ

FIELD EVALUATIONS

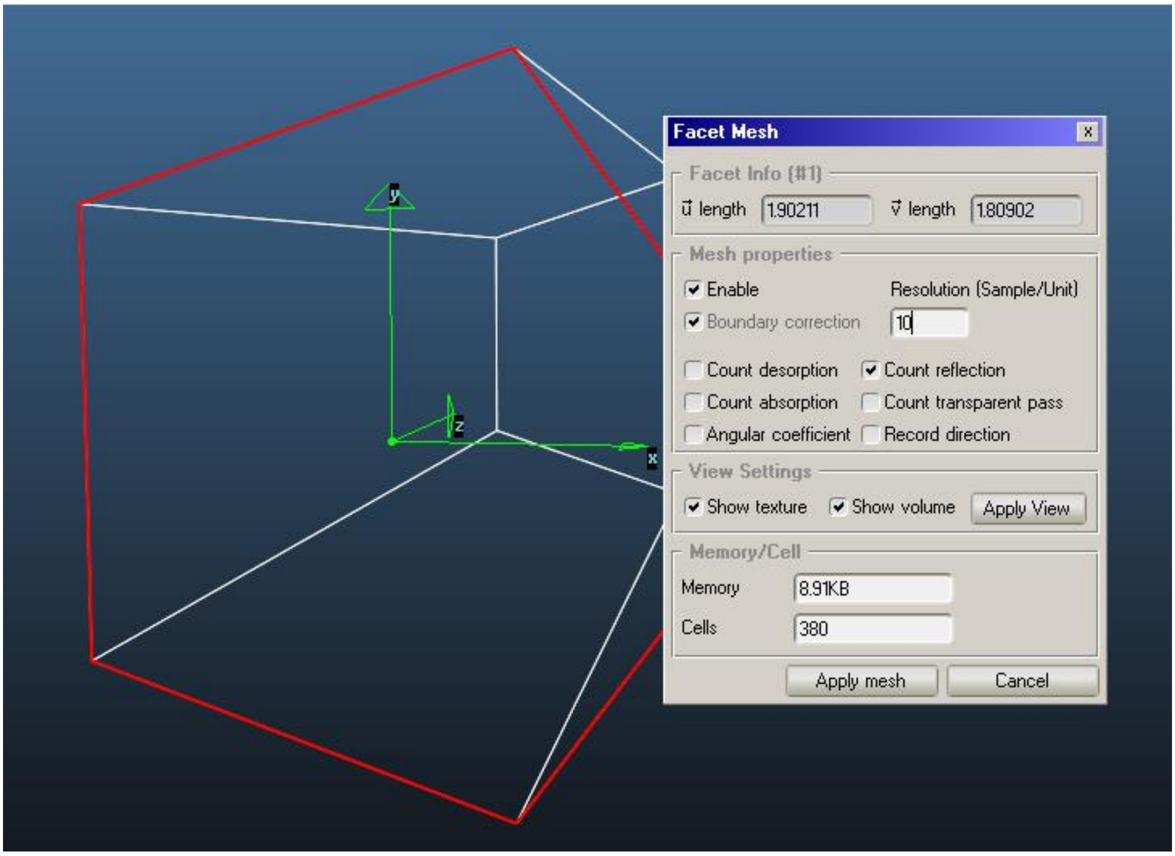
Polar	POLAR (nodal)	64x64	Cylindrical
	r=50.0	θ=0.0 to 360.0	z=0.0

Electron current density map on the wall of a tube, ideally the desorption should follow this distribution

One approach is to **break up the facet** to smaller elements; one would typically do it with the *Explode* command (you add a Mesh to the facet and the command makes the mesh cells become new facets).

Once we have the smaller facets, it is enough to assign a desorption value to them one-by-one. However, there is an automated method to do this faster, which allows you to directly import any data table from the clipboard.

Step1: You have to define how fine the outgassing matrix is by defining adding any kind of mesh to your facet:



Facet Mesh

Facet Info (#1)

$\vec{u}$ length 1.90211 $\vec{v}$ length 1.80902

Mesh properties

☑ Enable Resolution (Sample/Unit) 10

☑ Boundary correction

□ Count desorption ☑ Count reflection

□ Count absorption □ Count transparent pass

□ Angular coefficient □ Record direction

View Settings

☑ Show texture ☑ Show volume Apply View

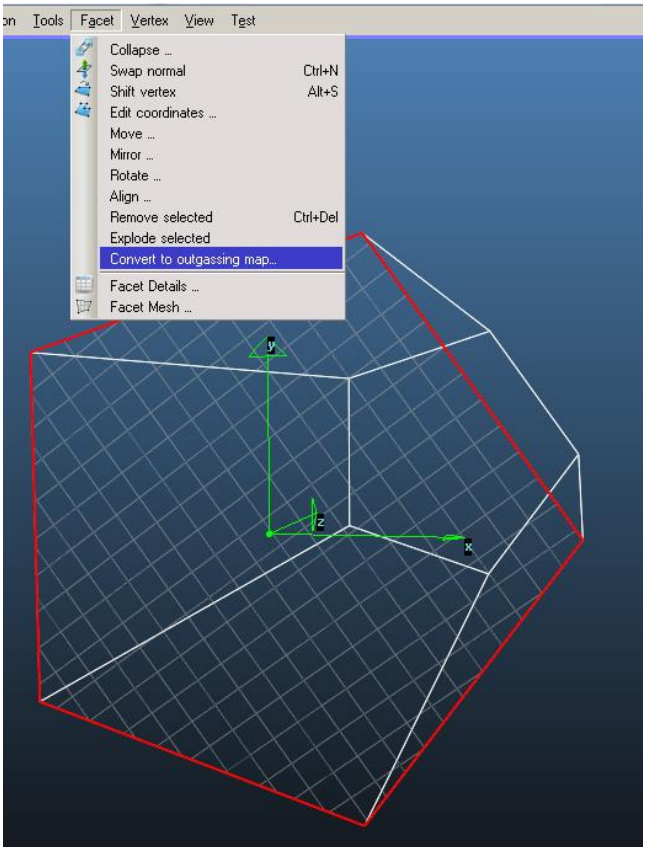
Memory/Cell

Memory 8.91KB

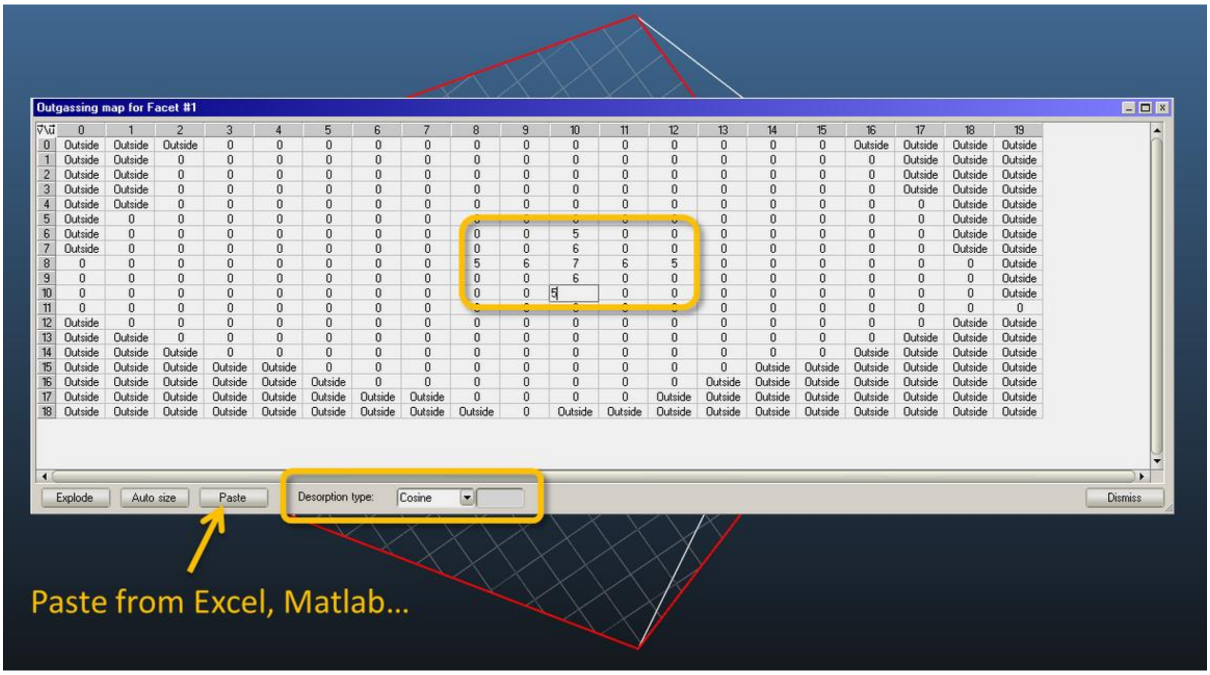
Cells 380

Apply mesh Cancel

Step2: Select the facet and issue the new "create outgassing map" command:



Below you see a map of the facet. For each mesh element, you can manually set the outgassing value. Note that the edited cell's location is highlighted on the geometry (similar to texture plotter):



Outgassing map for Facet #1

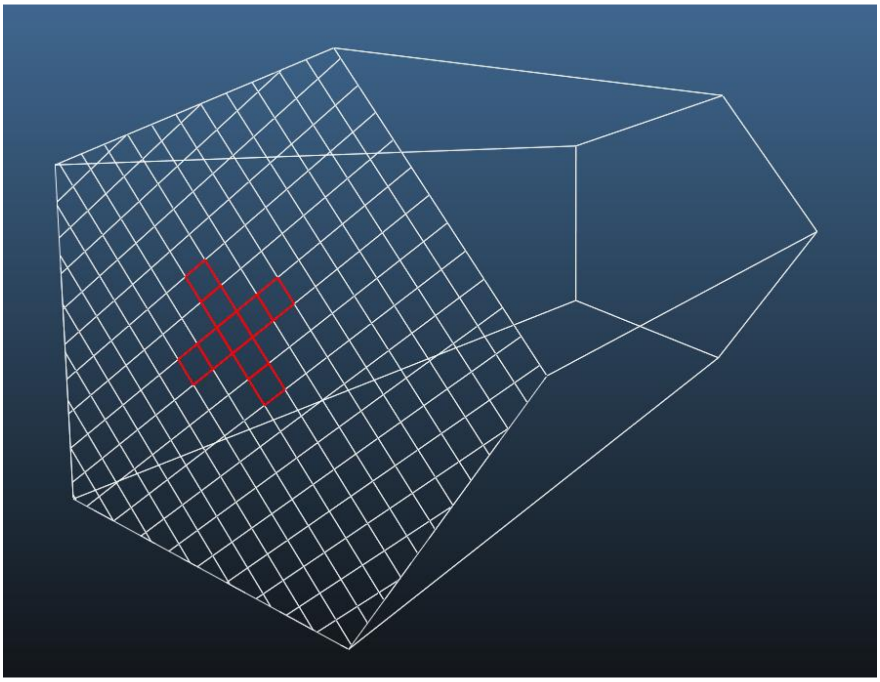
$\vec{v}\backslash\vec{u}$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
0	Outside	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside	Outside
1	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside
2	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside
3	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside
4	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside
5	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside
6	Outside	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	Outside	Outside
7	Outside	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	Outside	Outside
8	0	0	0	0	0	0	0	0	5	6	7	6	5	0	0	0	0	0	0	Outside
9	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	Outside
10	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	Outside
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside
13	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside
14	Outside	Outside	Outside	0	0	0	0	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside	Outside
15	Outside	Outside	Outside	Outside	Outside	0	0	0	0	0	0	0	0	0	Outside	Outside	Outside	Outside	Outside	Outside
16	Outside	Outside	Outside	Outside	Outside	Outside	0	0	0	0	0	0	0	Outside	Outside	Outside	Outside	Outside	Outside	Outside
17	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside	0	0	0	0	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside
18	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside	0	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside	Outside

Desorption type: Cosine

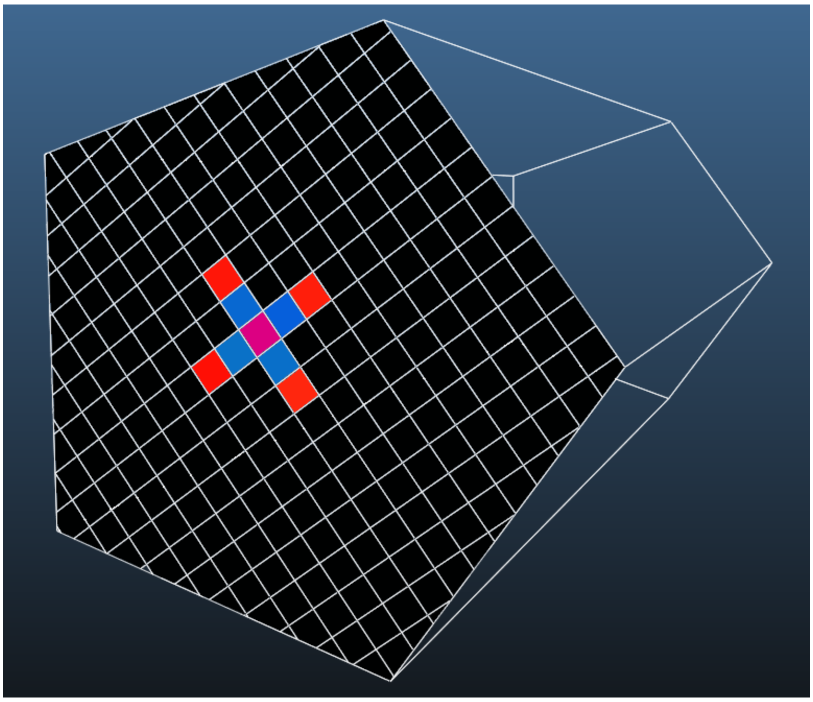
Paste from Excel, Matlab...

You can also **paste values from the clipboard** from Excel. The values are pasted to the right and bottom from the actual cell. Then you can define the desorption type (Uniform, Cosine, Cosine^N). Finally, if everything's ready, click **Explode**.

The exploded geometry highlights those facets that have desorption now:



To test that everything was well defined, add a mesh that counts desorbed molecules, and you'll see a nice color map of the values you just entered:



4. Theory

4.1. Pressure calculation

The pressure calculation described here applied to Molflow 2.4 and before, that assumed isothermal and isotropic conditions. Starting from Molflow 2.5, a direct conversion between the impingement rate (or the proportional Monte Carlo hit count) and the pressure is only valid in the above conditions. Formulas below (pressure as a function of hits) are NOT valid near pumps (strong sticking) or multi-temperature systems. For those cases, see section 1.2.1.8 (calculating physical quantities) of my Phd thesis.

In a vacuum system, the velocity of the gas molecules follows the Maxwell-Boltzmann model. According to this, the mean speed of the molecules is:

$$\langle v \rangle = \sqrt{\frac{8RT}{\pi m}}$$

Where

- v is the average speed in m/s
- R is the universal gas constant
- T is the gas temperature in Kelvins
- m is the molecular mass of the gas (in kg/mol)

The **impingement rate** (collisions on a surface per second on a unit area) is therefore

$$\varphi = \frac{1}{4} n \langle v \rangle = \frac{1}{4} n \sqrt{\frac{8\,RT}{\pi\,m}}$$

When running a Monte Carlo simulation, we have a limited number of "virtual" molecules that our computer can trace; therefore it is necessary to convert the MC "virtual" particle density to the physical density of the real world.

Sticking to SI units, the pressure on a surface in a MC simulation is therefore:

$$p = 4Q\frac{hits}{N}\frac{1}{A * \sqrt{\frac{8\,RT}{\pi\,m}}}$$

Where

- p is the pressure in Pa
- Q is the total outgassing of the system in Pa*m^3/sec
- *hits* is the number MC hits recorded on the surface in question
- *N* is the total number of MC particles our computer has created and traced
- *A* is the area of the surface in m^2
- *m* is the molecular mass in kg/mol

In MolFlow, we prefer to use mbars, cm, liter and g/mol units, moreover, we have some computational aspects to consider, therefore the exact code to calculate the pressure is:

$$p_{calc} = \frac{4 * 10}{\sqrt{\frac{8\,RT}{\pi\,m * 0.001}}}\frac{Q * hits}{N}\frac{1}{A * opacity * 2\_sided}$$

Where

- *p* is the pressure in mbars
- *Q* is the outgassing in mbar*l/sec
- *m* is the molecular mass in g/mol
- *A* is the area in cm^2
- the factor of 10 in the denominator is due to the conversion between cm^2 and m^2, g and kg, litre and m^3
- *opacity* is 1 for transparent and totally opaque facets, and a number between 0 and 1 for partially transparent facets. This is to compensate for less hits being recorded due to transparency
- *2_sided* is 2 for two-sided and 1 for one-sided facets. This is to double the calculated area for facets counting collisions from both sides

5. Computing aspects

5.1. Random generator

MolFlow uses the Mersenne Twister algorithm, grabbed from NumPy (http://numpy.scipy.org). It relies on Knuth's PRNG and some "magic constants". According to the Wikipedia article, its advantages are:

- It has a very long period of $2^{19937} - 1$. While a long period is not a guarantee of quality in a random number generator, short periods (such as the 2^{32} common in many software packages) can be problematic.
- It is k-distributed to 32-bit accuracy for every $1 \le k \le 623$

- It passes numerous tests for statistical randomness, including the Diehard tests. It passes most, but not all, of the even more stringent TestU01 Crush randomness tests.

Amongst its disadvantages, it is mentioned that it is rather difficult to obtain a truly random initial state. That is why each molflowSub.exe worker process uses a different *seed*; therefore initial non-random states cancel out when using multiple processes.

5.2. Area calculation

The area of a polygon is the measurement of the 2-dimensional region enclosed by the polygon. For a non-self-intersecting (simple) polygon with n vertices, the area is given by:

$$A = \frac{1}{2}\sum_{i=0}^{n-1}(x_i y_{i+1} - x_{i+1} y_i)$$

This area formula is derived by taking each edge *AB*, and calculating the (signed) area of triangle *ABO* with a vertex at the origin *O*, by taking the cross-product (which gives the area of a parallelogram) and dividing by 2. As one wraps around the polygon, these triangles with positive and negative area will overlap, and the areas between the origin and the polygon will be cancelled out and sum to 0, while only the area inside the reference triangle remains.

The formula was described by Meister in 1769 and by Gauss in 1795. It can be verified by dividing the polygon into triangles, but it can also be seen as a special case of Green's theorem. [source: Wikipedia article]

5.3. Ray tracing, collision finding

MolFlow uses a highly optimized ray-tracing algorithm that builds an axis-aligned bounding box (AABB) tree of the geometry and then uses the slabs method to find the actual collision distance. The original algorithm had to be modified to take MolFlow particularities into account (like one-sided facets, etc.)

5.4. Graphics, OpenGL, SDL Framework

For all graphics (except the Windows Open/Save) dialogs, MolFlow uses OpenGL acceleration through the SDL (Simple Directmedia Layer) C++ library. This is an open-source, cross-platform library. Since the Windows 7 open/save dialogs offer a lot of advantages over the built-in ones, and since all CERN users run MolFlow under Windows, the cross-platform portability was sacrificed for the improved functionality the built-in dialogs offer.

5.5. Shared memory, worker subprocesses

Molflow uses shared memory for cross-process communication between molflow.exe (the interface, ie. the main process) and the various parallel executed molflowSub.exe subprocesses spawned by the main process.

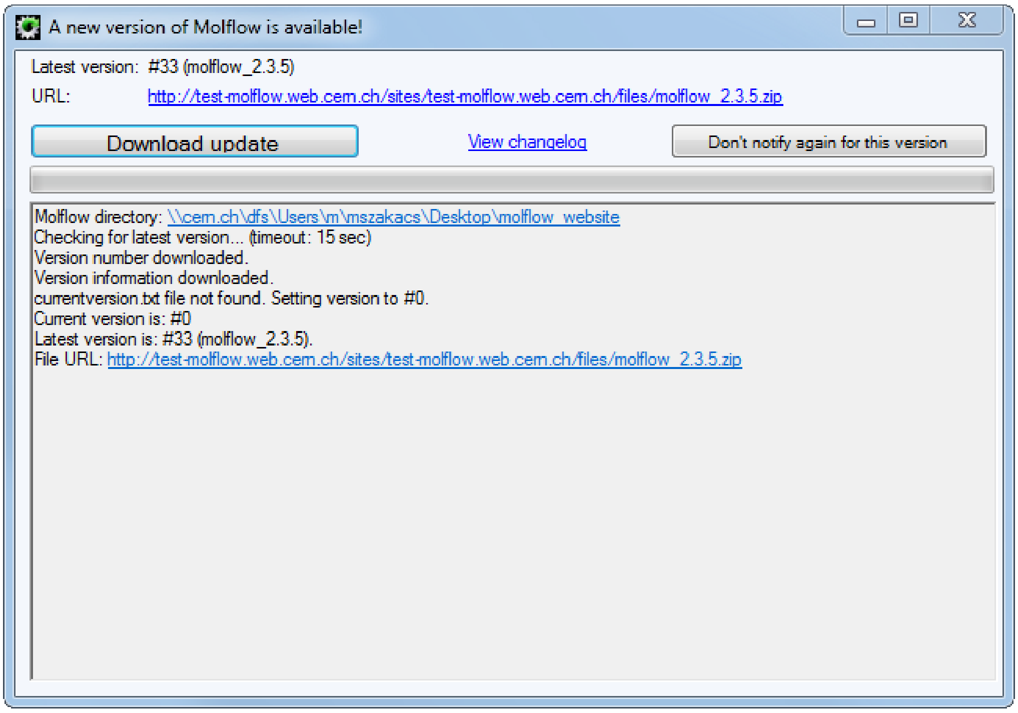
Through the CreateFileMapping and MapViewOfFile commands (default Windows.h library), file mappings are created, and so-called Dataports access the shared memory, granting exclusivity with a Mutex created by the CreateMutex command.

The *dpControl* dataport stores commands from the main process towards its subprocesses (workers), and the workers also use it to report their state. Moreover, workers regularly check if there is at least one process called molflow.exe running, if not, they close themselves (to avoid using resources even after the parent process has crashed or was killed by the user).

Upon launching the simulation, all geometry details are written by the main process to the *loader* dataport in a compact byte sequence, and then a LOAD command is issued through the dpControl dataport to the child processes. Once they load the geometry, the simulation is started, and they regularly update the *dpHit* dataport with simulation results (notable with the hits). This dpHit dataport is then read by the main process, and after post-processing, the simulation state is visualized to the user.

5.6. Auto-updater

MolFlow has a proprietary updater that checks for new version on startup. The updater process starts minimized and quits in 5 seconds if it is determined that MolFlow is up to date, otherwise a window pops up allowing updating automatically.


A new version of Molflow is available!
Download update
View changelog
Don't notify again for this version

Latest version: #33 (molflow_2.3.5)
URL: http://test-molflow.web.cern.ch/sites/test-molflow.web.cern.ch/files/molflow_2.3.5.zip

```
Molflow directory: \\cern.ch\dfs\Users\m\mszakacs\Desktop\molflow_website
Checking for latest version... (timeout: 15 sec)
Version number downloaded.
Version information downloaded.
currentversion.txt file not found. Setting version to #0.
Current version is: #0
Latest version is: #33 (molflow_2.3.5).
File URL: http://test-molflow.web.cern.ch/sites/test-molflow.web.cern.ch/files/molflow_2.3.5.zip
```

Please keep in mind that MolFlow's update server populates anonymous user statistics of its users (using Google Analytics), so by checking for updates you submit the same data (country, network provider, etc.) as you do when you visit webpages. It is for this reason that you can disable checking for updates, but generally it is advised to keep the feature on.

The updates mechanism works the following way:

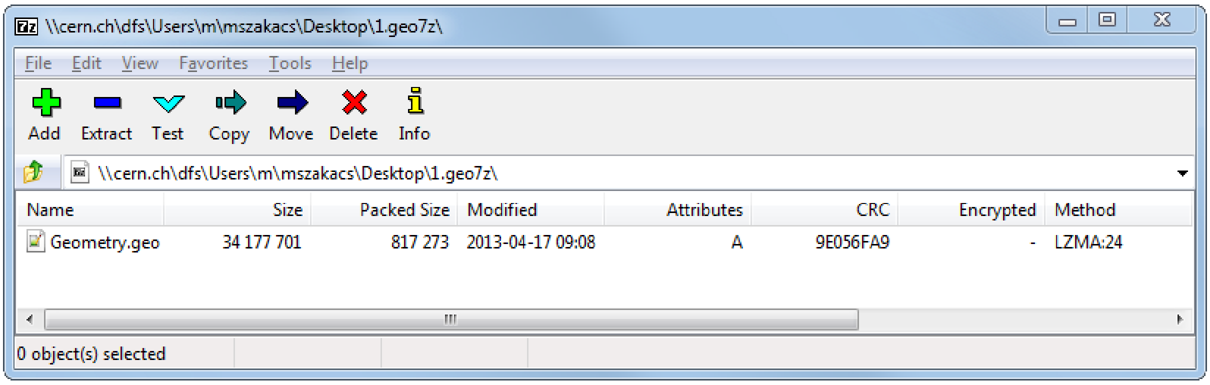
1. The updater downloads the file http://test-molflow.web.cern.ch/sites/test-molflow.web.cern.ch/files/autoupdate.txt
2. This file contains the number of the current version, and also the location where the program can be downloaded
3. Then it compares that number to the currentversion.txt file in MolFlow's directory. (If the file is missing, it is assumed that the current version is 0, therefore an update is forced).
4. If you have the latest version, the updater stays in background and exits after five seconds. If there is a new version, it pops up and offers you to download it. If you choose the "Don't notify again for this version", then the currentversion.txt is updated to reflect the latest online version number: you will only be notified on the next version.

5. If you choose to update, the updater downloads 7za.exe (if missing) to decompress the compressed update, then gets the zip file. If you choose Apply update, running instances of MolFlow will be killed, and the decompressed version will overwrite MolFlow files. As the updater is running, it cannot be overwritten; therefore the next MolFlow launch will update the updater module itself.

5.7. 7-Zip compression

MolFlow uses an open-source compression engine, 7-zip to compress .geo7z files from .geo files. This is beneficial because .geo files are essentially text files with a lot of repeating terms, and thus are prone to good compression.

Because .geo7z files use the 7z format, if you associate them to 7-Zip, you will be able to open them easily in Windows.



\\cern.ch\dfs\Users\m\mszakacs\Desktop\1.geo7z\

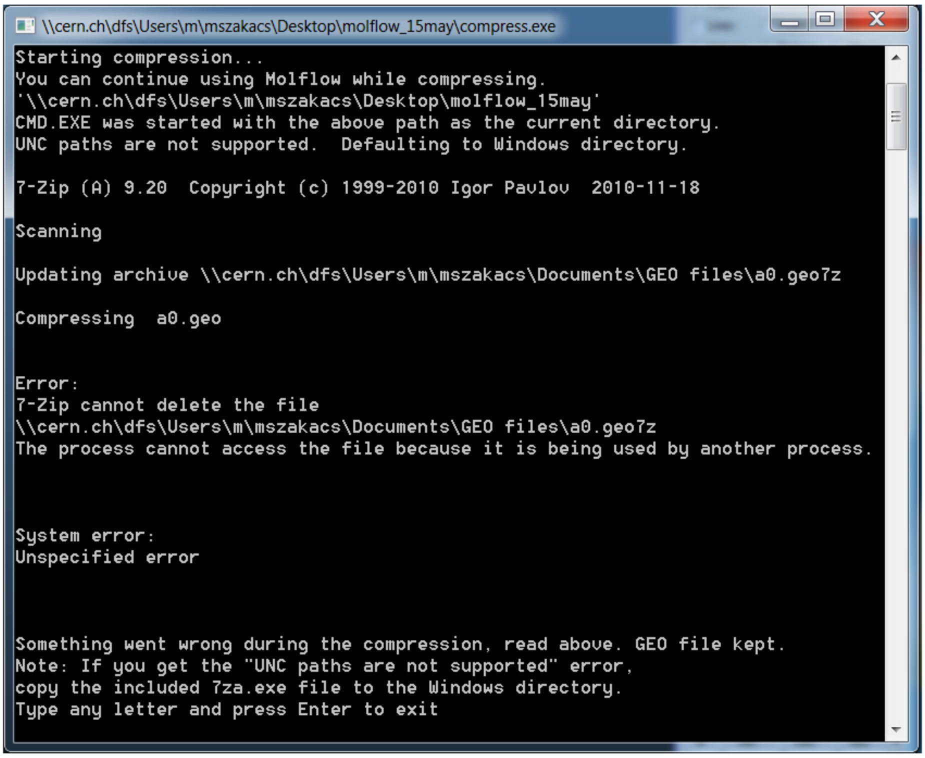
Name	Size	Packed Size	Modified	Attributes	CRC	Encrypted	Method
Geometry.geo	34 177 701	817 273	2013-04-17 09:08	A	9E056FA9	-	LZMA:24

0 object(s) selected

A .geo7z file open in 7-zip viewer. Note that the .geo file was compressed from 34MB to 820kB.

If you use the Compression option, files will be saved in .geo format, and then renamed to Geometry.geo (to allow .geo7z files to be renamed without breaking reference to their content). Then compress.exe (in MolFlow directory) will be called that serves as an interface between MolFlow and the 7za.exe command-line version of 7-zip.

Compress.exe will do the following: it will start minimized as a background process, not interrupting MolFlow. It calls 7-zip with the correct parameters, and then watches the output. If 7-zip returns the “Everything is OK” message, then the original .geo file is deleted (since we have a compressed copy of it), otherwise the file is kept and the error message is displayed to the user by popping up the minimized window.



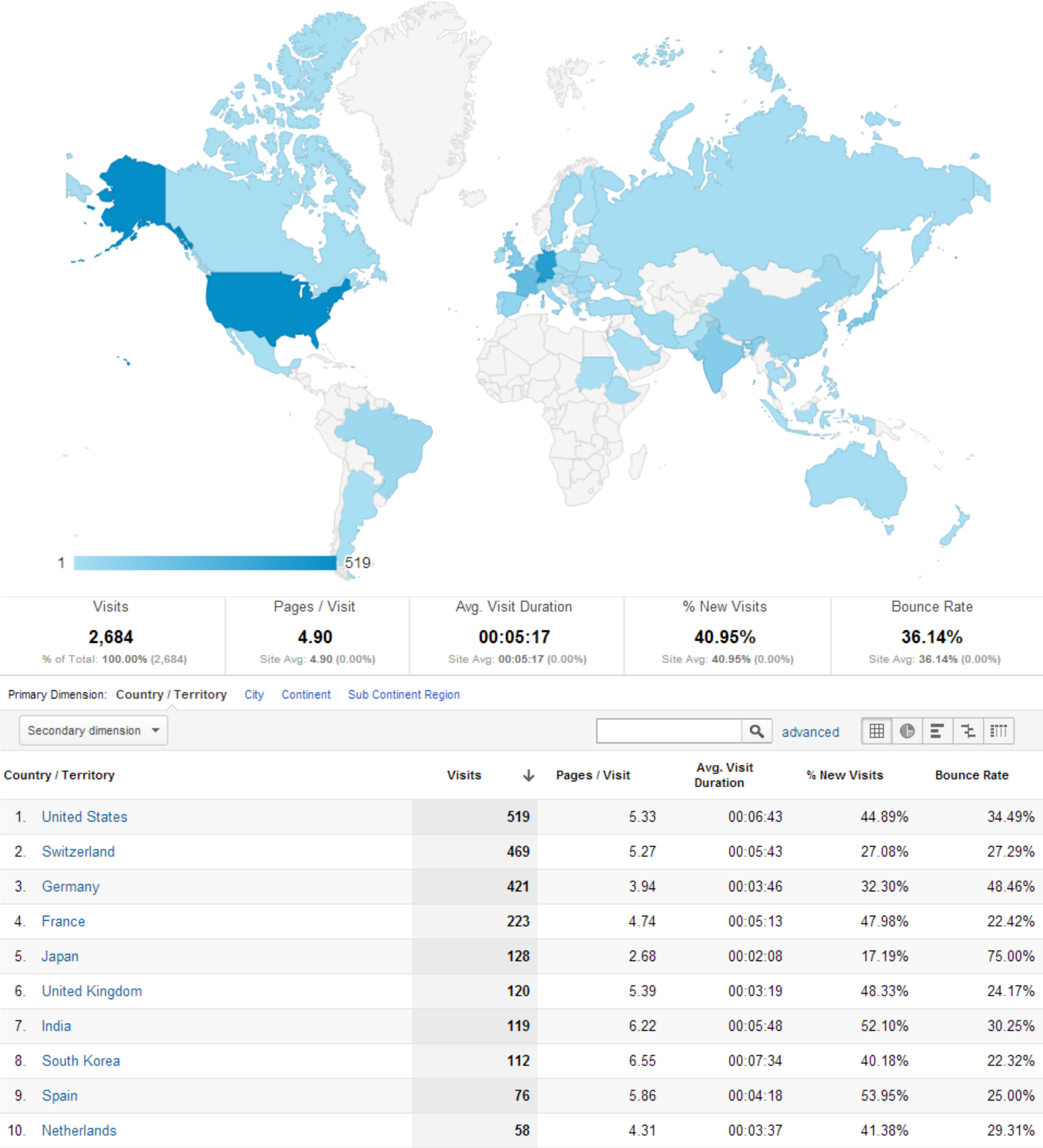
\\cern.ch\dfs\Users\m\mszakacs\Desktop\molflow_15may\compress.exe

```
Starting compression...
You can continue using Molflow while compressing.
'\\cern.ch\dfs\Users\m\mszakacs\Desktop\molflow_15may'
CMD.EXE was started with the above path as the current directory.
UNC paths are not supported.  Defaulting to Windows directory.

7-Zip (A) 9.20  Copyright (c) 1999-2010 Igor Pavlov  2010-11-18

Scanning

Updating archive \\cern.ch\dfs\Users\m\mszakacs\Documents\GEO files\a0.geo7z

Compressing  a0.geo


Error:
7-Zip cannot delete the file
\\cern.ch\dfs\Users\m\mszakacs\Documents\GEO files\a0.geo7z
The process cannot access the file because it is being used by another process.



System error:
Unspecified error



Something went wrong during the compression, read above. GEO file kept.
Note: If you get the "UNC paths are not supported" error,
copy the included 7za.exe file to the Windows directory.
Type any letter and press Enter to exit
```

The users sees this error message (file used by another process) if something goes wrong during GEO file compression

5.8. Website

The current website, http://cern.ch/test-moflow is running on the Drupal CMS service. Hosting and maintenance is fully supported by the CERN infrastructure, to the extent that configuration and user account management modules are integrated by default, and user roles are managed by CERN e-groups.



Visits	Pages / Visit	Avg. Visit Duration	% New Visits	Bounce Rate
2,684	4.90	00:05:17	40.95%	36.14%
% of Total: 100.00% (2,684)	Site Avg: 4.90 (0.00%)	Site Avg: 00:05:17 (0.00%)	Site Avg: 40.95% (0.00%)	Site Avg: 36.14% (0.00%)

Primary Dimension: Country / Territory City Continent Sub Continent Region

Country / Territory	Visits ↓	Pages / Visit	Avg. Visit Duration	% New Visits	Bounce Rate
1. United States	519	5.33	00:06:43	44.89%	34.49%
2. Switzerland	469	5.27	00:05:43	27.08%	27.29%
3. Germany	421	3.94	00:03:46	32.30%	48.46%
4. France	223	4.74	00:05:13	47.98%	22.42%
5. Japan	128	2.68	00:02:08	17.19%	75.00%
6. United Kingdom	120	5.39	00:03:19	48.33%	24.17%
7. India	119	6.22	00:05:48	52.10%	30.25%
8. South Korea	112	6.55	00:07:34	40.18%	22.32%
9. Spain	76	5.86	00:04:18	53.95%	25.00%
10. Netherlands	58	4.31	00:03:37	41.38%	29.31%

As of May 2013, the website had 2700 visits from 1100 unique visitors, and the average user spends 5 minutes on the site.