

# INTRODUCTION TO THE LATEST VERSION OF THE TEST-PARTICLE MONTE CARLO CODE MOLFLOW

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## Abstract

The Test-Particle Monte Carlo code Molflow+ is getting more and more attention from the scientific community needing detailed 3D calculations of vacuum in the molecular flow regime mainly, but not limited to, the particle accelerator field. Substantial changes, bug fixes, geometry-editing and modelling features, and computational speed improvements have been made to the code in the last couple of years. This paper will outline some of these new features, and show examples of applications to the design and analysis of vacuum systems at CERN and elsewhere.

## INTRODUCTION

Molflow+ is a test-particle Monte Carlo simulator for Ultra-High Vacuum (UHV) systems. The original algorithm was written in the 1990s. It simulates gas particle motion in molecular flow in a vacuum chamber that is described by planar polygons with user-defined physical properties (facets). By tracing the trajectory of virtual test particles from gas sources to the pumping locations, the transmission probability and therefore the conductance of any vacuum element can be calculated. Moreover, the number of simulated collisions on facets are counted and can be converted to pressure, allowing engineers to determine the vacuum profile in a system.

Molflow+ was rewritten [1] from the ground in 2007 at ESRF, keeping the original algorithm but creating a modern program that uses multiple processor cores and hardware accelerated graphics. This new version also introduced profiles and textures on facets that perform part of the post-processing within the program: they visualize pressure in real time in the form of plots and surface colors.

Since 2012 Molflow+ development is continued at CERN. A website [2] has been set up where the software can be downloaded, along with documentation and tutorials. This article presents some of the more important improvements along with examples for their application.

## DIRECT PRESSURE CALCULATION

In previous versions of Molflow+, test particles were created on one single facet which the user defined as desorption point. They were then traced until they hit a pump represented by a facet with a certain capture probability. To calculate the pressure, the number of collisions on facets had to be exported and converted to pressure outside of the program.

Since the goal is to create an UHV simulator targeted for general engineering audience, it is preferable to hide internal computational variables (such as number of virtual collisions, capture probability) and replace them

with real-life quantities, such as impingement rate, pumping speed and outgassing rate. It is also desirable to automate the conversion process so that the user can read the pressure directly in the program. In the recent version this has been implemented the following way:

Once the outgassing rate  $d(pV)/dt$  is set at one point by the user, using the ideal gas equation, it is possible to calculate the molecule flux  $dN_{real}/dt$  entering the system. Therefore, for each traced test particle, a conversion ratio to the flux of real molecules  $\frac{dN_{real}/dt}{N_{virtual}}$  can be determined.

Assuming local isotropy, the capture coefficient of facets that represent the pumps can be converted into volumetric pumping speed. For this, the user specifies the gas molecular mass  $m$  and temperature  $T$ , and the average molecular speed  $v_{avg} = \sqrt{8RT/\pi m}$  is calculated. Using this speed, the conversion between capture coefficient  $s$  and volumetric pumping speed  $S$  is given by the formula

$$S = A \cdot \frac{1}{4} v_{avg} \cdot s,$$

where  $A$  is the pump aperture size.

Having performed the above conversions, every virtual collision can be converted to a precise number of physical collisions per unit time. From this, the impingement rate (collisions per area per second) is calculated, which – assuming isotropy – converts to pressure.

As a result, the user can work with real-life physical units and get the pressure in the system directly.

## TIME-DEPENDENT SIMULATIONS

In the most recent version, the original Molflow algorithm is extended with a time-dependent mode. This allows the simulation of gas propagation and pumpdown processes, as long as the length of the process is only a few orders of magnitudes larger than the time between wall collisions (typically: processes up to a minute). Other Monte Carlo simulators [3-5] have been previously written for this task. They use volumetric meshes to split the vacuum chamber into a finite number of cells, where the number of residing particles are counted at given time intervals (time-driven algorithm). That approach usually requires simplifying the geometry or importing the mesh from a CAD program which prevents later geometry edits.

Molflow+ extends its original algorithm by keeping it event-driven: only collisions with walls are simulated, therefore the geometry can still be described by the boundaries, keeping compatibility with the STL universal CAD format, allowing geometry edits and the use of the original, highly optimized ray-tracing algorithm.

When creating or colliding test particles, they are assigned a speed based on the velocity distribution of gas

molecules. Keeping track of the particle flight time and path, the time when each collision happens can be calculated.

To avoid storing an excessive number of hits along with the time they happened in memory, before the simulation is started, the user defines *time bins*, that is,  $N$  given moments  $t_1, t_2 \dots t_N$  with a time window  $t_{window}$ . Therefore, to calculate the pressure at moment  $t_1$ , all the hits that happen in the interval  $[t_1 - \frac{t_{window}}{2}, t_1 + \frac{t_{window}}{2}]$  are stored. That means that  $N$  different pressure profiles are calculated simultaneously. Each can be viewed independently, or it is possible to use built-in tools that show the evolution of the pressure with time at a given point.

Two examples of practical applications are presented below.

### Gas Injection and Pumpdown

According to elementary vacuum physics equations, when gas is injected with rate  $Q$  in a high-conductance vacuum vessel of volume  $V$ , which has a pump of volumetric pumping speed  $S$  installed, the pressure evolution is described by the formula

$$p(t)_{injection} = \frac{Q}{S} \left( 1 - \exp\left(-\frac{S}{V}t\right) \right).$$

Once the injection is stopped at moment  $t_{stop}$ , the gas is pumped down following the

$$p(t)_{pumpdown} = \frac{Q}{S} \exp\left(-\frac{S}{V}(t - t_{stop})\right)$$

equation. This process is demonstrated on a simple model of a cylinder of 1cm length and 1 cm radius, with an injection rate of  $Q=1\text{mbar}\cdot\text{l/s}$  on one end, and a pump of speed  $S=1\text{l/s}$  on the other. The pump is constantly operational, the injection starts at  $t=0$  and stops at  $t=30\text{ms}$ .

The Molflow+ model consists of 102 planar facets. 1 million test particles are generated, and pressure is calculated for 120 equidistant moments between 0 and 60ms. The time window for each moment is 0.1ms. The simulation time is about a minute. On Fig. 1 the theoretical pressure evolution is plotted against Molflow+ results and we can see a perfect match.

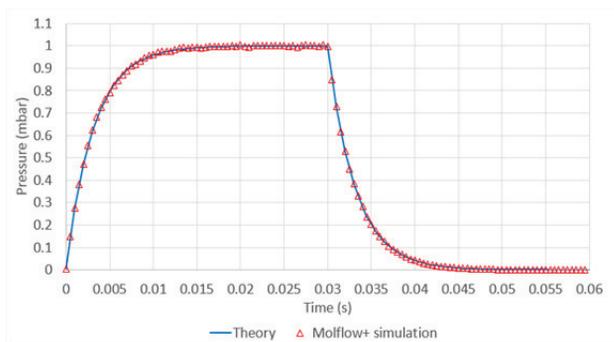


Figure 1: Evolution of pressure during gas injection and pumpdown, theory vs. simulation.

### Gas Propagation in an Acoustic Delay Line

Acoustic delay lines (ADL) are obstacles that introduce a planned delay to a gas inrush. Usually they are designed to work in high pressure regime, introducing turbulences thus slowing down shockwave propagation. However, due to their geometry, they work in UHV regime as well as they force propagating particles to travel along a longer path.

Molflow's ability to help design such a system is demonstrated through a simple example. We have a 1m long, 8cm diameter pipe where gas is expected to leak from one side with a constant rate of  $Q=1\text{E-3mbar}\cdot\text{l/s}$ . We are interested to see if inserting an ADL device can significantly slow down the pressure rise in the opposite, protected side.

Therefore we perform two simulations: one with the bare pipe for reference, and one with two ADL devices inserted at one- and two-thirds of the pipe length. The devices are 5cm long, varying pipe diameter between 8cm and 1.6cm with a period of 1cm.

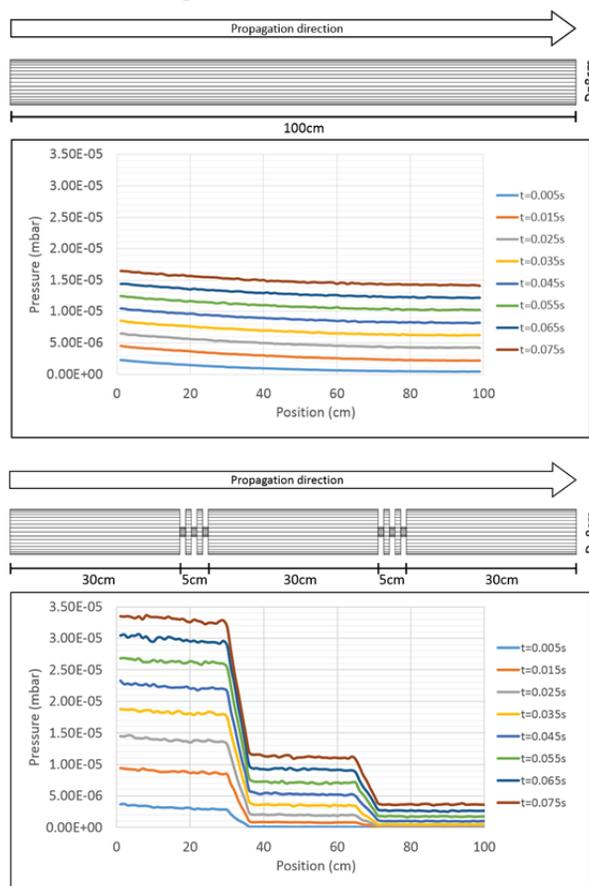


Figure 2: Pressure profiles at different moments in a pipe with and without an ADL device.

The two geometries are described by 38 and 411 facets respectively, and pressure profiles are calculated for every 5ms. Results are plotted on Fig. 2, and it can be deduced that at  $t = 75\text{ms}$  the pressure at the end of the tube is approximately 4 times lower in the ADL equipped system than in the bare pipe. In a real design application, since

simulation time is less than a minute for both cases, the user can try several ADL designs and reiterate the simulation until the best result is achieved.

## NON-ISOTHERMAL SYSTEMS

The original algorithm assumes that the system is isothermal and isotropic. This greatly simplifies calculations (pressure is deductible from the number of hits on facets), but obviously limits the areas of application. With recent changes for the time-dependent mode, we already assign speed to the molecules, which allows us to move a step forward and stop assuming isotropy, and calculate instead the pressure in an elementary way from the momentum change rate of molecules that hit the wall.

For this, the user defines the temperature not for the whole system as before, but individually for each facet. Upon collision, a new velocity  $v_{wall}$  is calculated according to the temperature of the collided facet, and the rebounded molecule's velocity  $v_{new}$  is set using

$$v_{new}^2 = v_{old}^2 + A_{thermal} (v_{wall}^2 - v_{old}^2),$$

where  $v_{old}$  is the incident velocity and  $A_{thermal}$  is the thermal accommodation factor, a number between 0 and 1.

When the collision takes place, the components  $v_{\perp old}$  and  $v_{\perp new}$  that are orthogonal to the collided facet's plane are stored in memory. Knowing these and the mass  $m$  of the colliding particle, the orthogonal momentum change for one collision can be calculated:

$$dI = m * (v_{\perp old} + v_{\perp new})$$

Summing these momentum changes, and knowing the collision rate, the pressure is obtained in an elementary way:

$$p = \frac{\sum dI/dt}{A}$$

where  $A$  is the facet area.

Moreover, if we calculate the average of the orthogonal velocity components  $v_{\perp avg}$ , we can obtain the density near a facet:

$$\frac{dN}{dV} = 2 \frac{Z}{v_{\perp avg}}$$

where  $Z$  is the impingement rate and the factor of 2 accounts for the fact that one half of the particles next to the facet moves towards it, while the other half moves away thus does not collide.

### Thermal Transpiration

Results of this non-isothermal extension can be demonstrated through a simple system, shown on Fig. 3, with two vacuum vessels connected by a narrow pipe. One vessel is hot, the other is cold, and the pipe's temperature changes linearly between the two sides.

Gas in this system will exhibit a phenomenon called thermal transpiration: due to higher molecule velocities,

at equilibrium pressure is locally higher on the hot side, while the molecule density is higher on the colder side. The theoretical [6] pressure and density ratios are given by the formulas

$$p_1/p_2 = \sqrt{T_1/T_2}$$

$$n_1/n_2 = \sqrt{T_2/T_1}$$

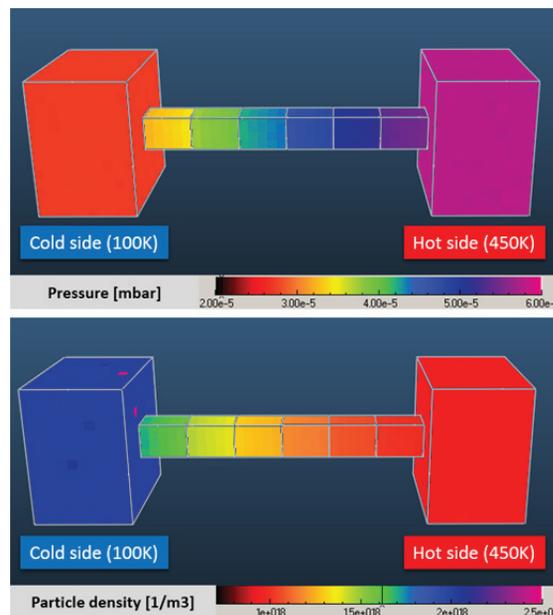


Figure 3: Pressure and density profiles of a non-isothermal system.

Results of the simulation are summarized in Table 1. These non-isothermal calculations can play an important role in applications where vacuum systems with cryogenic and hot parts are close to each other, such as accelerators and also in fusion physics where particle density estimation is important.

Table 1: Molflow+ Estimates the Pressure and Density Ratios precisely.

T1: 100K	p1: 2.75E-5 mbar	n1: 2.0E18 /m <sup>3</sup>
T2: 450K	p2: 5.82E-5 mbar	n2: 9.4E17 /m <sup>3</sup>
Molflow+ ratio: $p_1/p_2 \approx n_2/n_1 = 2.1211$		Analytical ratio: $\sqrt{450/100} = 2.1213$

## REFERENCES

- [1] R.Kersevan, J-L Pons, "Introduction to Molflow+", JVST A27, 1017 (2009).
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