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MONTE CARLO SIMULATIONS OF MOLECULAR GAS FLOW :
SOME APPLICATIONS IN ACCELERATOR VACUUM TECHNOLOGY
USING A VERSATILE PERSONAL COMPUTER PROGRAM

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Monte Carlo Simulations of Molecular Gas Flow: Some Applications in Accelerator Vacuum Technology using a versatile Personal Computer Program

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Abstract

The Monte Carlo technique has been used extensively in the past to solve the problem of molecular flow through vacuum pipes or structures with specific boundary conditions for which analytical or even approximate solutions do not exist. Starting from a specific program written in 1975, the idea germinated over the years to produce handy, rather general, problem solving applications capable of running efficiently on modern microcomputers, mainly for ease of transportability and interactivity. Here the latest version is described. The capabilities and limitations of these tools are presented through a few practical cases of conductance and pumping speed calculations pertinent to accelerator vacuum technology.

1. Introduction

When the molecular flow in a vacuum structure is non Maxwellian due to beaming effects, as for instance in limited conductance^{1,2} ducts of various cross sections, or when one wants to assess pumping speeds of devices of various geometries using normalized test domes³, the Monte Carlo method has to be used. In the large majority of these cases, the problem needed to be solved once, and the program code was designed specifically, and not as a general problem solving tool.

Particle accelerators have large vacuum and UHV systems, often complex, necessitating developments such as : new pumping techniques, vacuum structure optimizations in terms of large or low conductance for a given beam configuration, characterization of surfaces submitted to particle bombardment, precise estimates of gas flow rates, etc.. In many of these circumstances the Monte Carlo method has been used with success, also specifically⁴.

The specificity of programs pertained partly to the fact that the method is very demanding in terms of computation power, even for relatively simple problems. This imposed the use of large mainframes not easily accessible and reserved to specialists.

With the advent of cheap Personal Computers, powerful and easy to use, a certain number of applications usually reserved for large mainframes could be democratized. Starting from a specific program⁵, the idea therefore germinated over the years to produce a

rather general problem solving package, allowing easy and practical uses of the method for every day problems in accelerator vacuum technology.

2. Programs history

The software was primarily developed for an Apple Macintosh⁶. In this way a stand alone portable software package has been produced. This software is user friendly and no computer training is necessary for the user. The structure description and the simulation parameters are easily set using windows, dialog boxes, pull down menus and buttons. The performance of the Macintosh hardware, however, limits the complexity of the structure to be simulated (a whole night of simulation is often necessary before the program produces reliable results). For this reason the same program has later been translated into standard FORTRAN 77 and is now also available on VM/CMS (IBM 3090-600E-VF) at CERN. However, using the mainframe computer, the software loses its friendly user interface. In order to avoid this, two other Macintosh programs have been developed allowing pre- and post-processing of the data sent to or received from the mainframe and producing automatic upload / download of information files. In this way, it has been possible to maintain the same (Macintosh) user friendly interface while still benefiting from the performances of the VM/CMS systems, which are ~500 times faster.

The version for the Apple Macintosh was limited in both speed and capabilities. This is why a new version running on an IBM PC-Compatible and on a IBM Mainframe has been developed. The performances obtained on an Intel 80386/20 MHz based machine are more than 10 times better than on the Apple Macintosh and there is now no limitation to the geometry of the structure to be simulated. Of course, complicated geometries will still require several hours of simulation.

3. Algorithms

The program "Molecular Conductance" traces molecular trajectories in a vacuum structure with molecular flow. The structure (fig 1) is composed of flat facets and each facet has a sticking, a transparency and a plane attribute.

The attributes of each facet determine if the particles which cross it have to be reflected, adsorbed or just ignored and counted. This is shown in figures 2,3 and 4.

The law of reflection can be chosen between specular or diffused (cosine law) type. The case of

interest is of course the diffused reflection, but it is foreseen to implement the possibility of doing a weighted average between the specular and diffused reflection to

simulate flows which are *semi-molecular* (Fig 5).

The simulation consists of introducing particles through the structure from a random point uniformly

distributed on the first facet of the structure, with a direction distributed according to the cosine law (i.e.

molecular effusion from a large volume). The program then computes in Cartesian coordinates the trajectory of the particle and finds the intersections with the first facet which the particles encounter. If the particle is transmitted, then an intersection with another facet is searched. If the particle is reflected, the new direction is computed according to the selected law of reflection. If the particle is adsorbed, a new particle is introduced in the structure (Fig 6).

The molecular flow formulae are used⁵. Inter-particle interactions are neglected and in diffused reflection, the cosine law (Fig 7) is applied to determine the new direction of the particle.

All estimated values (x), such as the transmission, sorption or rejection probability, are given with their standard deviations (s) in the form $x \pm s$ (ex 140.7 ± 3.6). This means that the real value is inside the estimated

$$\vec{U}_2 = \begin{bmatrix} \sqrt{\eta} \cos 2\pi\gamma \\ \sqrt{\eta} \sin 2\pi\gamma \\ \sqrt{1-\eta} \end{bmatrix} \quad \vec{U}_n = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Fig 7: Eta and Gamma are random variables uniformly distributed between 0 and 1. If the normal to the surface is not $[0,0,1]$ a rotation has to be applied to the found vector

interval $[x - s, x + s]$ with a probability at least equal to the one given by the Tchebytcheff's inequality⁷. If we suppose the estimated values to have a *normal distribution* (which is the case because we estimate a mean that is asymptotically normal), the interval giving 95 % confidence is $[x - 1.96 s, x + 1.96 s]$. The interval of confidence at 99 % is $[x - 2.58 s, x + 2.58 s]$.

The value of the standard deviation s is computed according to the binomial distribution laws⁷.

Sources of errors in the Monte Carlo calculations are not only limited by the non-infinite number of experiments. Numerical approximations and the cosine law model produce errors which have to be added to the width of the estimated interval. Unfortunately these errors (especially those related to the reflection model) cannot be reduced and affect the estimated value by at least 1 %. For example it would be naïve to extend a simulation with two outcomes (transmission or rejection) to more than 10 - 20 - 30 thousands experiments. A simulation of 10^6 particles would not give better results.

5. Applications and examples

To illustrate the use and practicability of the program, a few applications are briefly presented.

- **Assessment of pumping speeds**

Getter, condensation or cryo sorption pumps are widely used in accelerator systems, commercially standard or tailor-made to a particular application. Pumping speeds are measured with a test dome (Fischer-Mommensen or ISO) which may not be well adapted to the pump characteristics (flange diameter or pumping principle). The program can be used to simulate the flow in the dome, to find the correction factor (usually small) to apply to the pump pressure measurement.

When the intrinsic sticking coefficient on the gettering surfaces is known, the pumping speed S can be calculated from the apparent pumping coefficient at the pump orifice (A):

$$S = 11.6 \cdot 10^{-4} A N_s / N_m \text{ (in l/sec for air)}$$

with N_s and N_m respectively the adsorbed and total number molecules traced.

Conversely, from a pumping speed measurement, the intrinsic sticking coefficient can be determined by trial and error, by simulating the complete pumping process of a gas injected through a given dome and reproducing the dome pressure gradient.

- **Optimization of getter pumps**

Workhorse of UHV systems, the flashed titanium sublimation pump (SU) is very efficient in providing large pumping speeds at low pressure for getterable gases. However the intrinsic sticking probability of an hydrogen atom on a fresh titanium layer is low, typically 0.06^8 . The program has been used to simulate the gettering action of the surfaces of a standard pump with and without a multilayer fine stainless steel mesh covered with titanium. The mesh is represented in the program

Figure 7: Example of a Ti SU pump pumping speed calculation, with enhanced performance of the gettering surface covered with a multilayer fine mesh. Measurements are very preliminary results.

by a surface with transmission probability equal to the ratio of void surface to unit area (aspect ratio, 80% in the following example, mesh wire diameter 0.05 mm):

In the realm of UHV for particle storage rings, Non Evaporable Getters (NEG) have recently made a massive appearance as a powerful and convenient mean of pumping active gases at room temperature⁹. Lumped pumps using NEG activable at temperatures slightly above normal bakeout temperatures have been used to

solve some specific problems of high gas throughputs in UHV⁴, and to reduce the gas conductance between high and low pressure parts of systems. The program allows a very large variety of NEG arrangements, among which annular wrappings fitted around the beam channels, which have found applications on the CERN Low Energy Antiproton Ring (LEAR)¹⁰.

- **Special beaming effects: parallel molecular beams**

Gases such as H₂, N₂ may serve as Internal Beam targets in accelerators (LEAR JetSET experiment), or may have to be injected into the UHV system as a necessary ingredient to a particular device (LEAR Carbon jet target). In these two examples, the gas jet is perpendicular to the beam and passes through a cascade of orifices interleaved with differential pumping chambers (Ti SU, ion and NEG pumps), and should be fully beamed in its interaction with the particles. Such arrangements allow order of magnitudes gas pressure gradients, which can only be calculated with a flow simulation program. In addition the average number of hits of transmitted gas atoms with the walls is easily obtained, and this may be of use in assessment of eventual depolarization.

- **Conductance calculations**

Exactly as we proceed for pumping speed, it is possible to compute the air conductance C of any piped structure. Once the transmission probability N_t/N_m and the entrance orifice surface A are known, we have

$$C = 11.6 \cdot 10^{-4} A N_t / N_m \text{ (in l/sec for air)}$$

with N_t and N_m respectively the adsorbed and total number molecules traced.

This measurement is useful to design the pumping

Fig 10: VESSEL ESRF Grenoble

No 1: Transmission Probability 0.0182 +/- 0.00190
 No 2: Transmission Probability 0.0554 +/- 0.00324
 No 3: Transmission Probability 0.0334 +/- 0.00254
 No 4: Transmission Probability 0.0374 +/- 0.00268
 No 5: Transmission Probability 0.0280 +/- 0.00232

layout in the vacuum structure

6. Conclusion and future trends

The availability of powerful and cheap personal computers with extended graphics capabilities and user friendly interfaces allows the *democratization* of the computer time consuming Monte Carlo method used to evaluate molecular flows. Over the last few years, several programs with growing capabilities and generality have been developed for use as every day application solving

Table 1: Summary of performances

Computer	Geometric Applicability	CPU Time	Input Definition Time
Hewlett Packard 9845	Axisymmetric 10 Segments Max	Several Hours	Short (Simple Geometry)
Apple Macintosh Plus	Any cross sectional shape of revolution 10 Segments Max	Several Hours ~ 5.5	Short (Easy and nice User interface)
Olivetti 80386/20 MHz	No limitations	72' --	Long (Complex Geometry)
Olivetti 80386/16 MHz 80387 coprocessor	No limitations	15'	Long (Complex Geometry)
IBM 3090	No limitations	5".2	Long (Complex Geometry)

tools in Accelerator Vacuum technology. Table 1 illustrates semi-qualitatively the trend in extended applicability and performance on the specific example of conductance calculation (10000 particles in a cylindrical tube, 2 m long, 0.10 m diameter). The clear and fast evolution of the applicability of the method follows the trend of modern micro computers. No doubt the programs will continue to evolve and be more powerful, for the benefit of Accelerator Vacuum Systems.

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