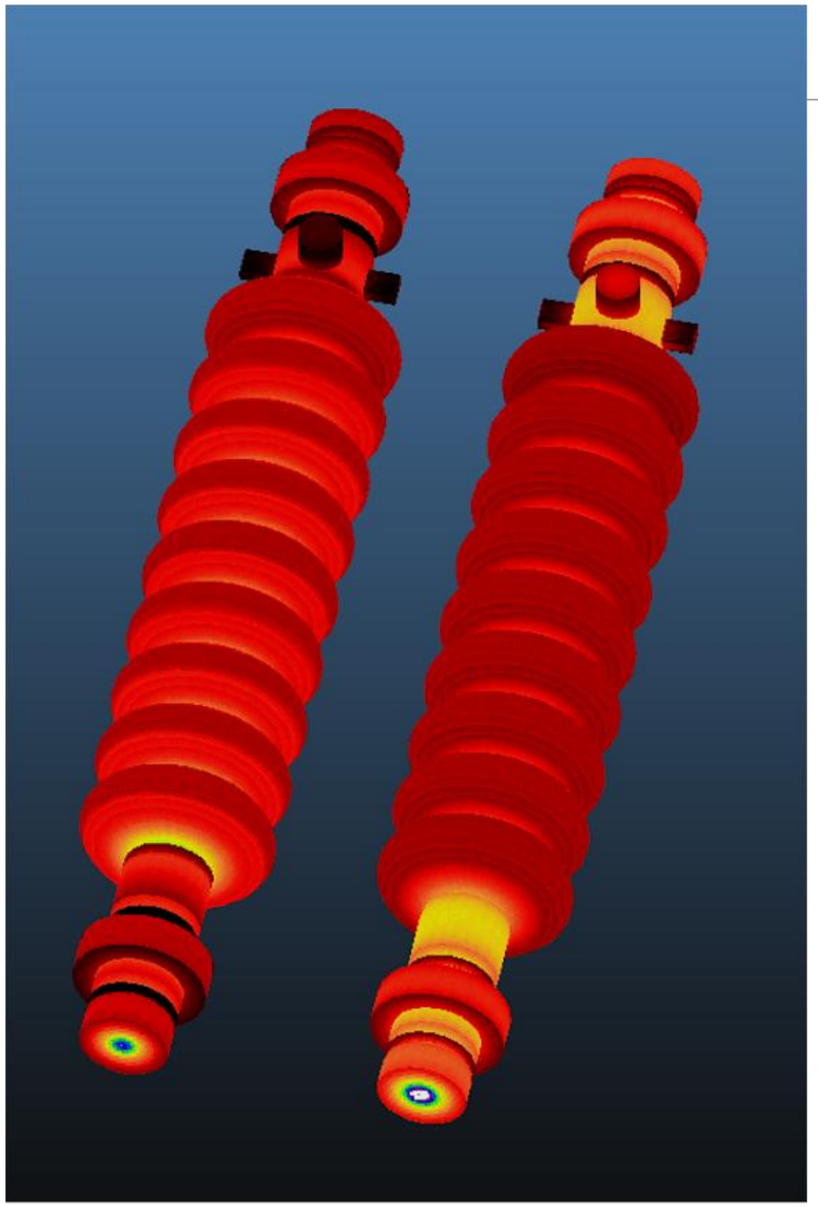
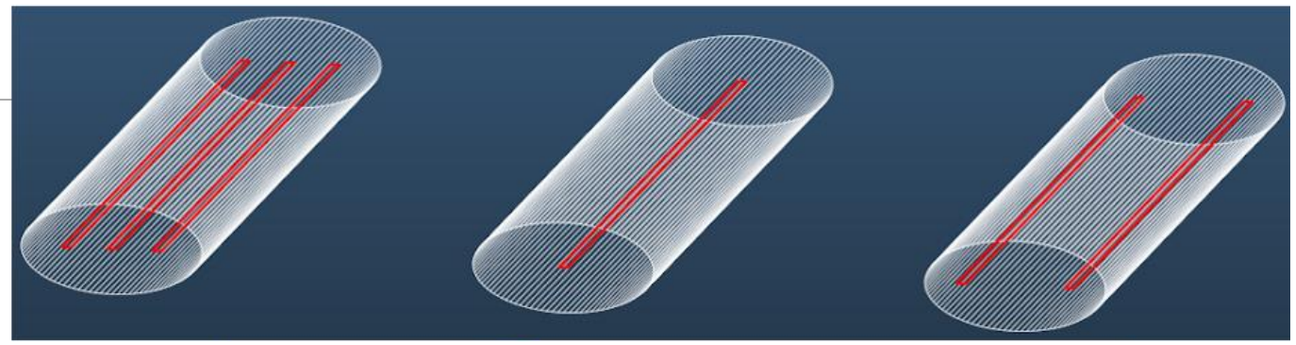
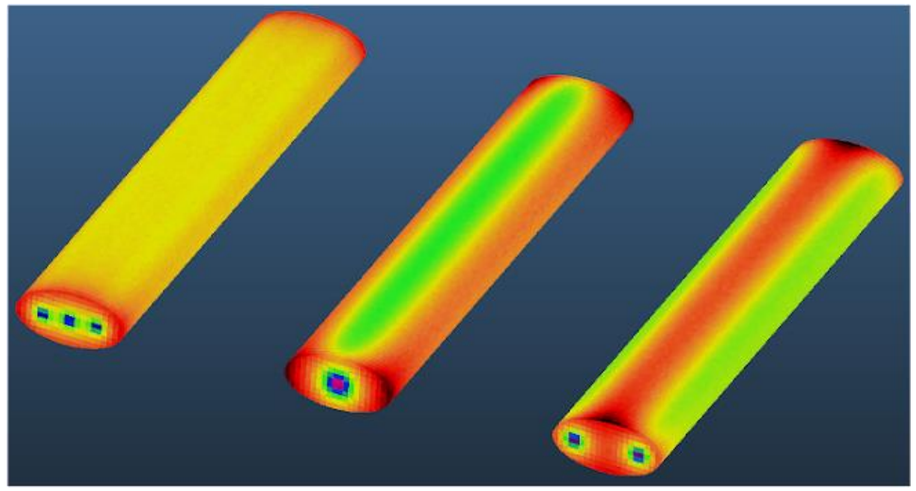
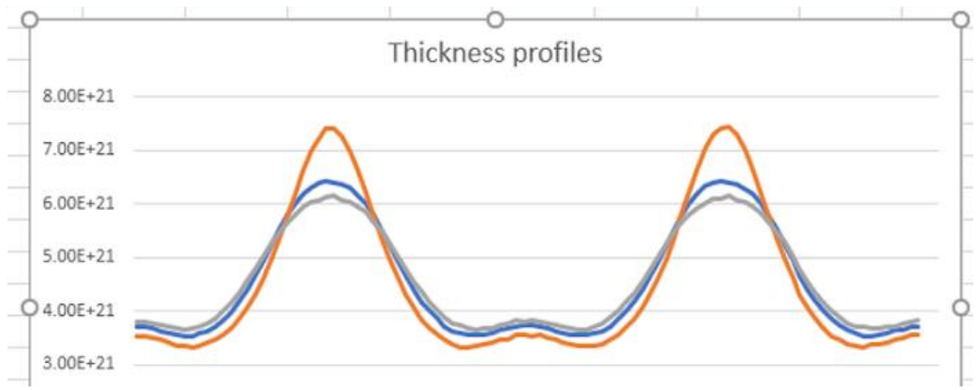
Gas simulations with Monte Carlo methods





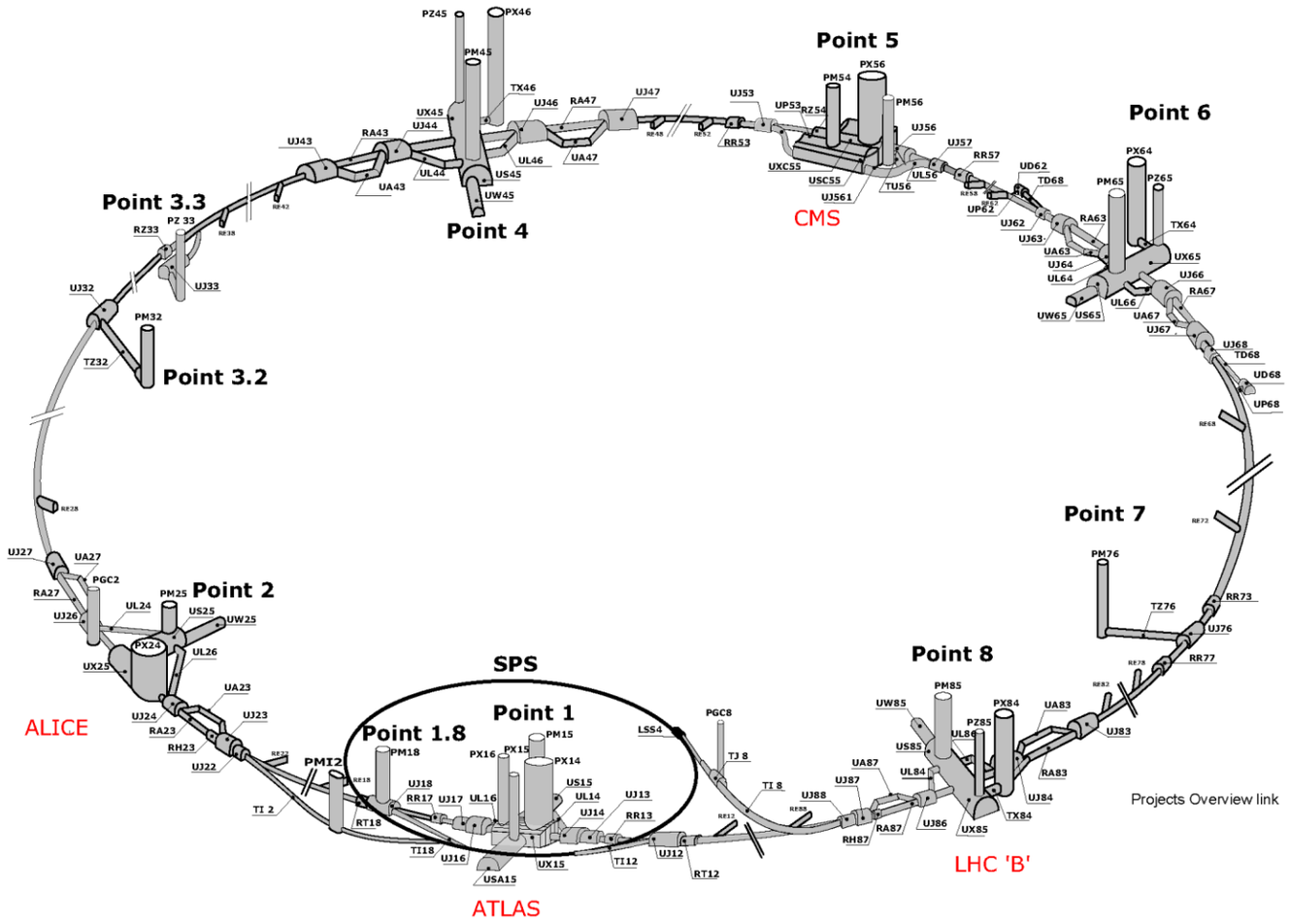




PBC workshop, CERN

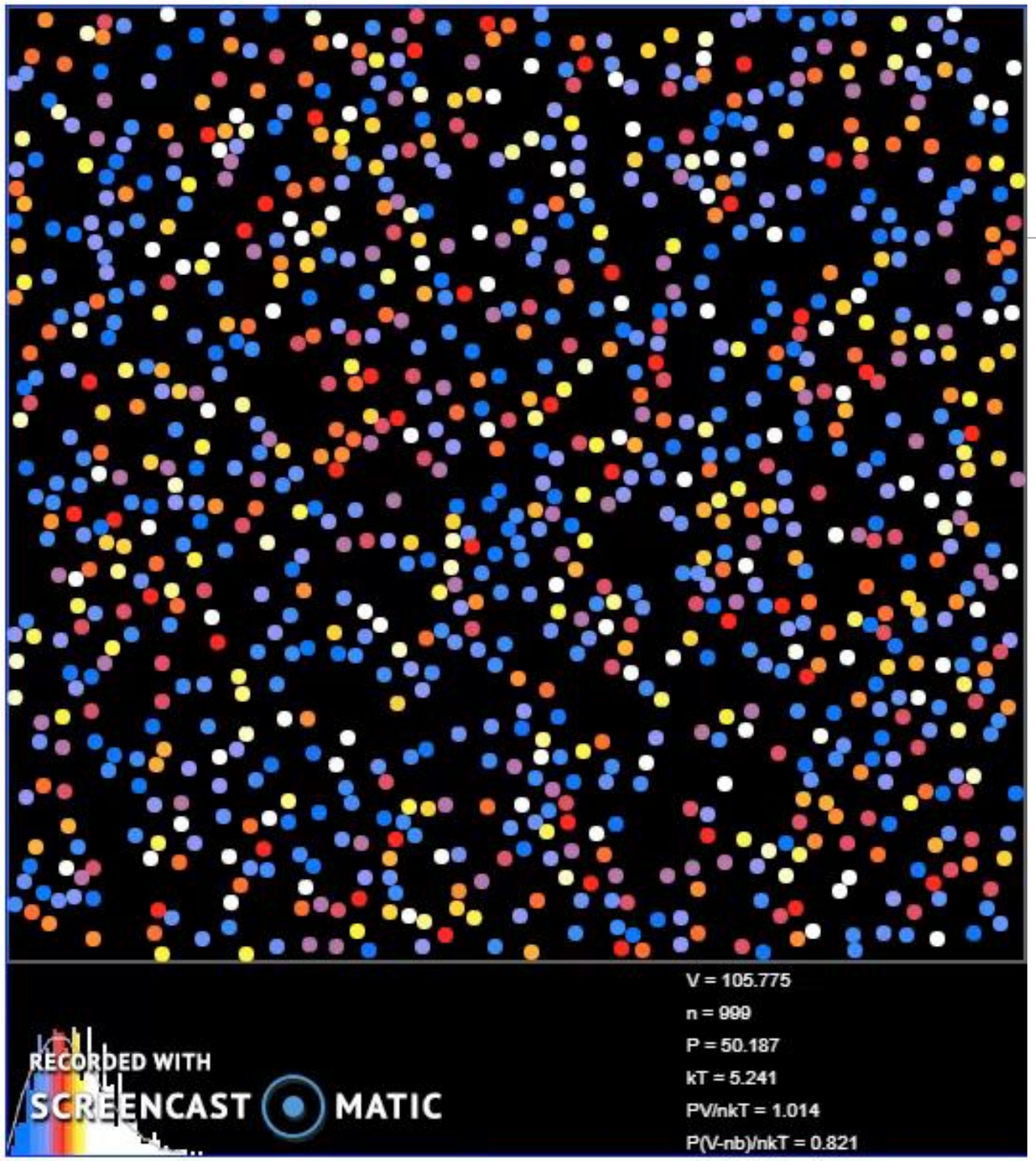
6 April 2022 - Marton Ady

The problem



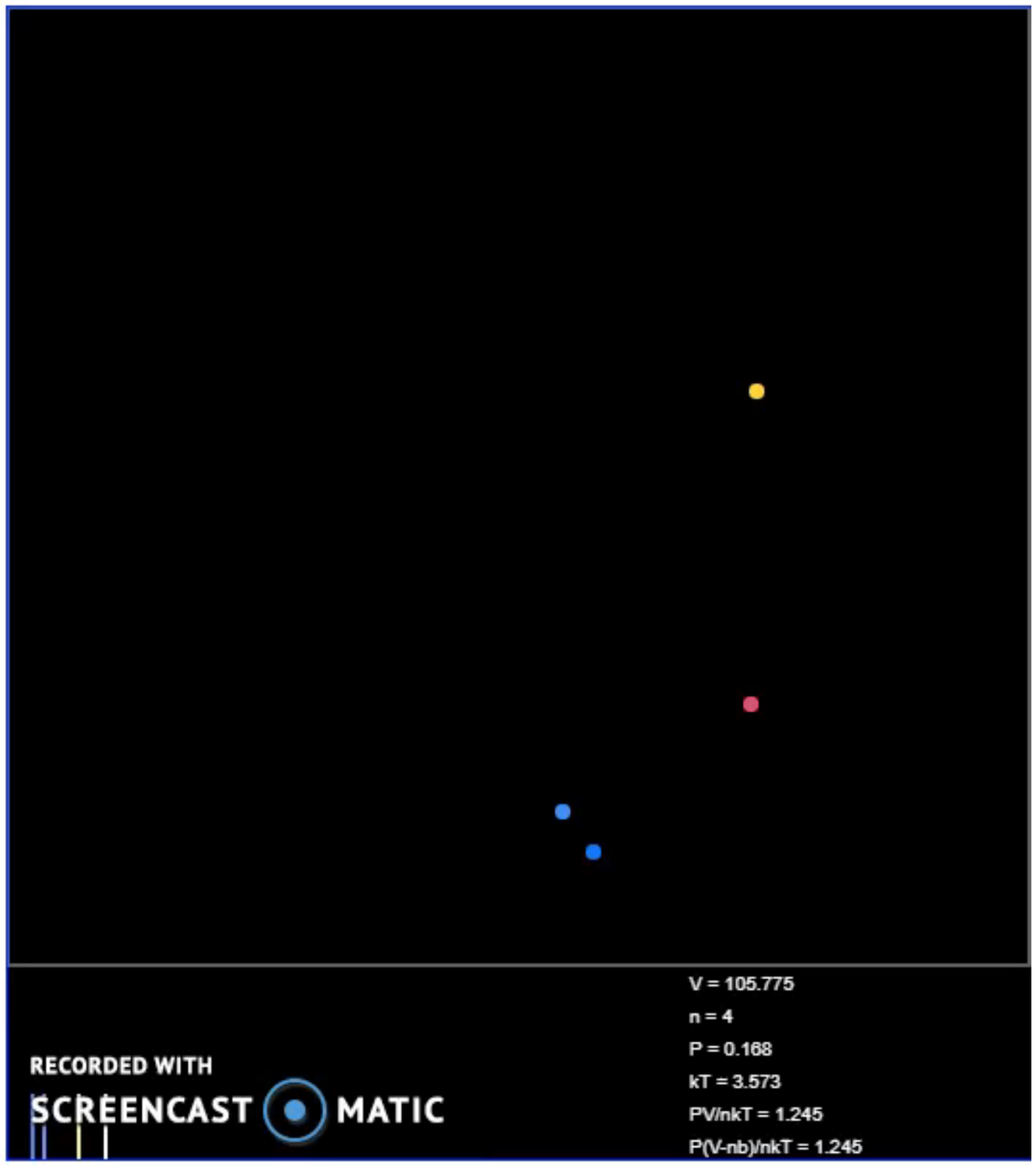
LHC: Pressure below 1E-9 mbar (0.000000 000001 * atmospheric)

High pressure: fluid dynamics



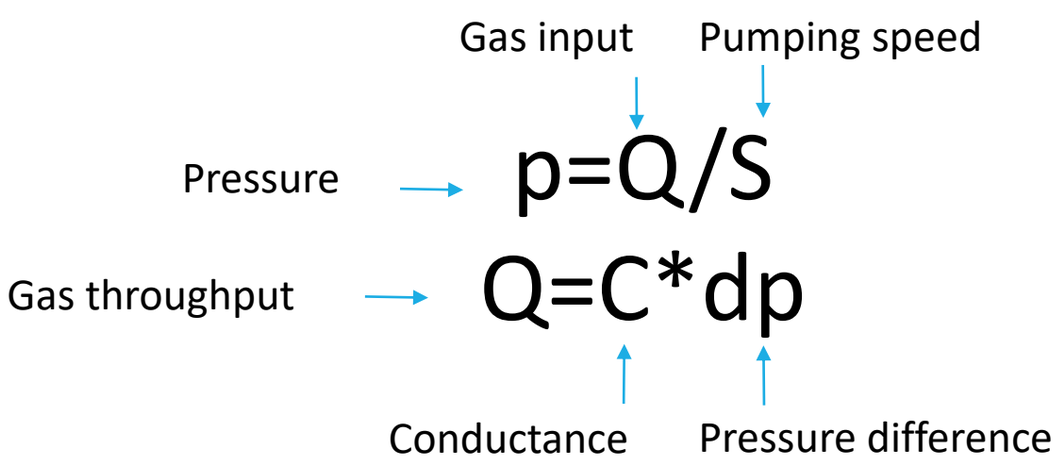
Pumping by **suction**

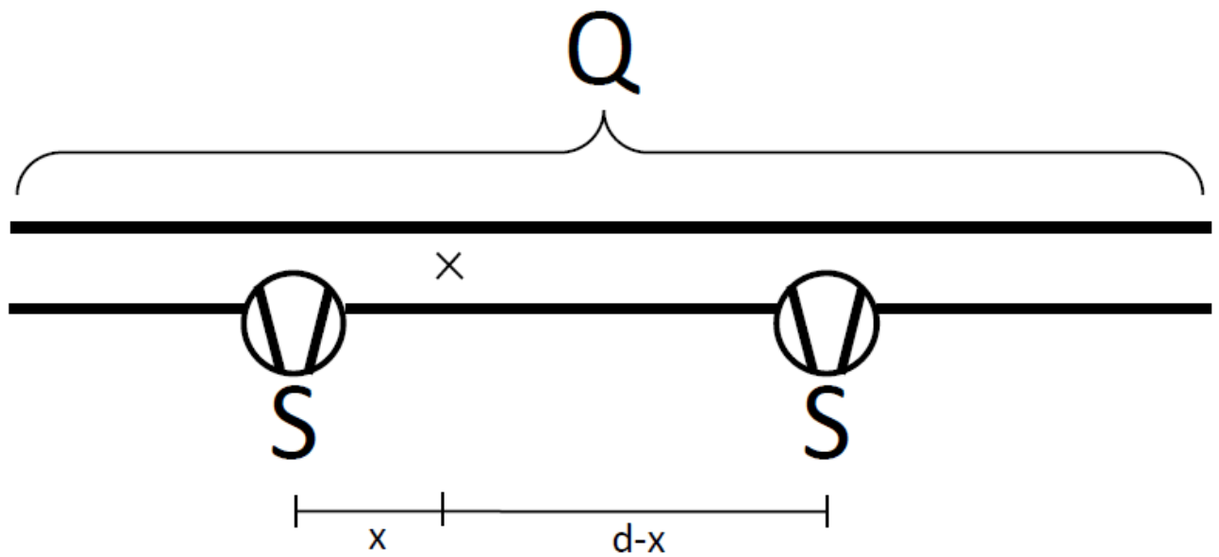
High vacuum: random walk

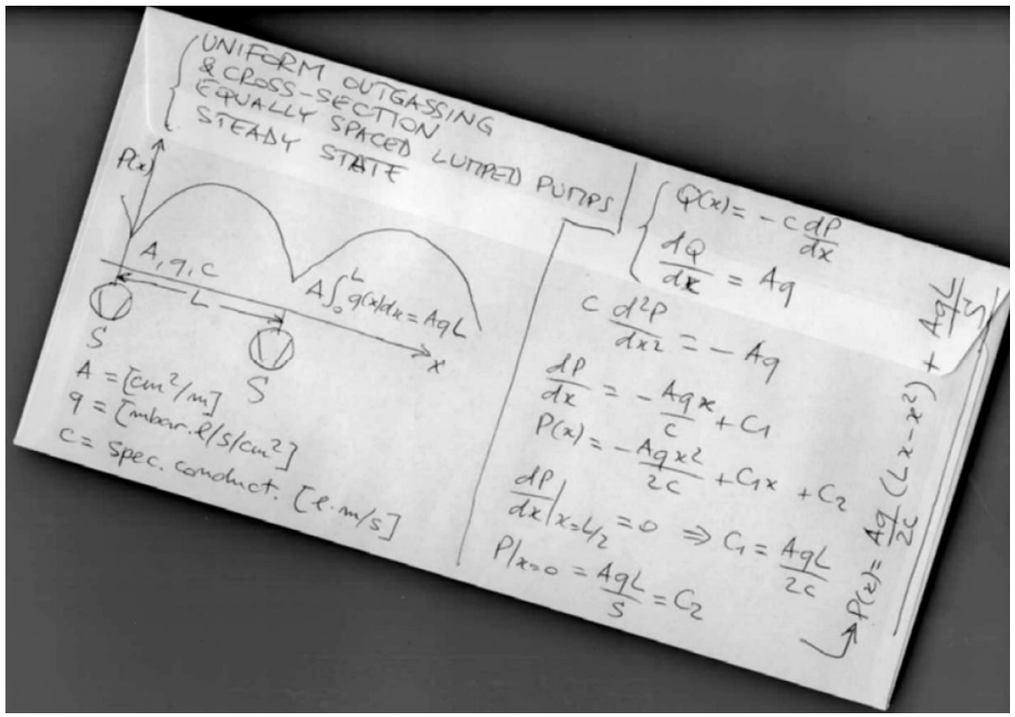


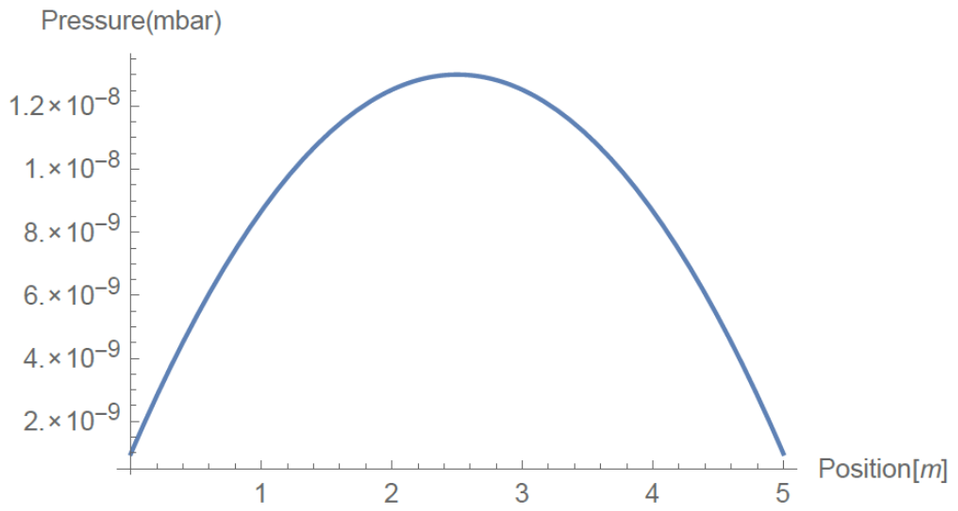
Pumping by **capture**

Analytic methods







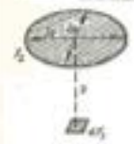
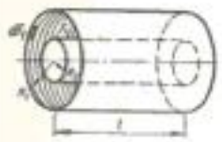
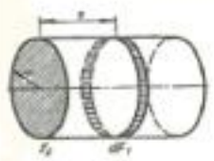
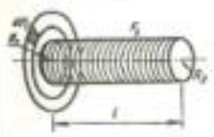
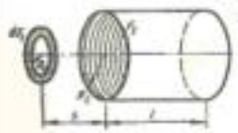
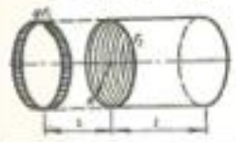


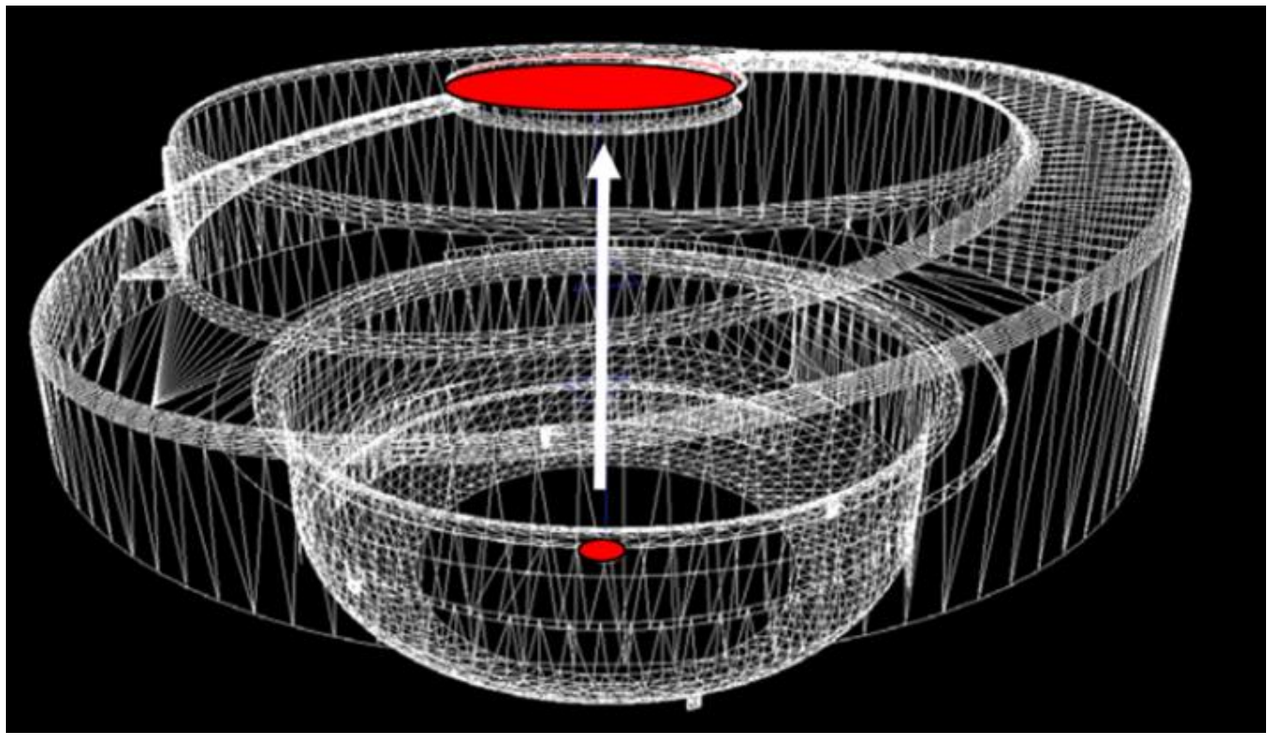
Difficulty: Conductance

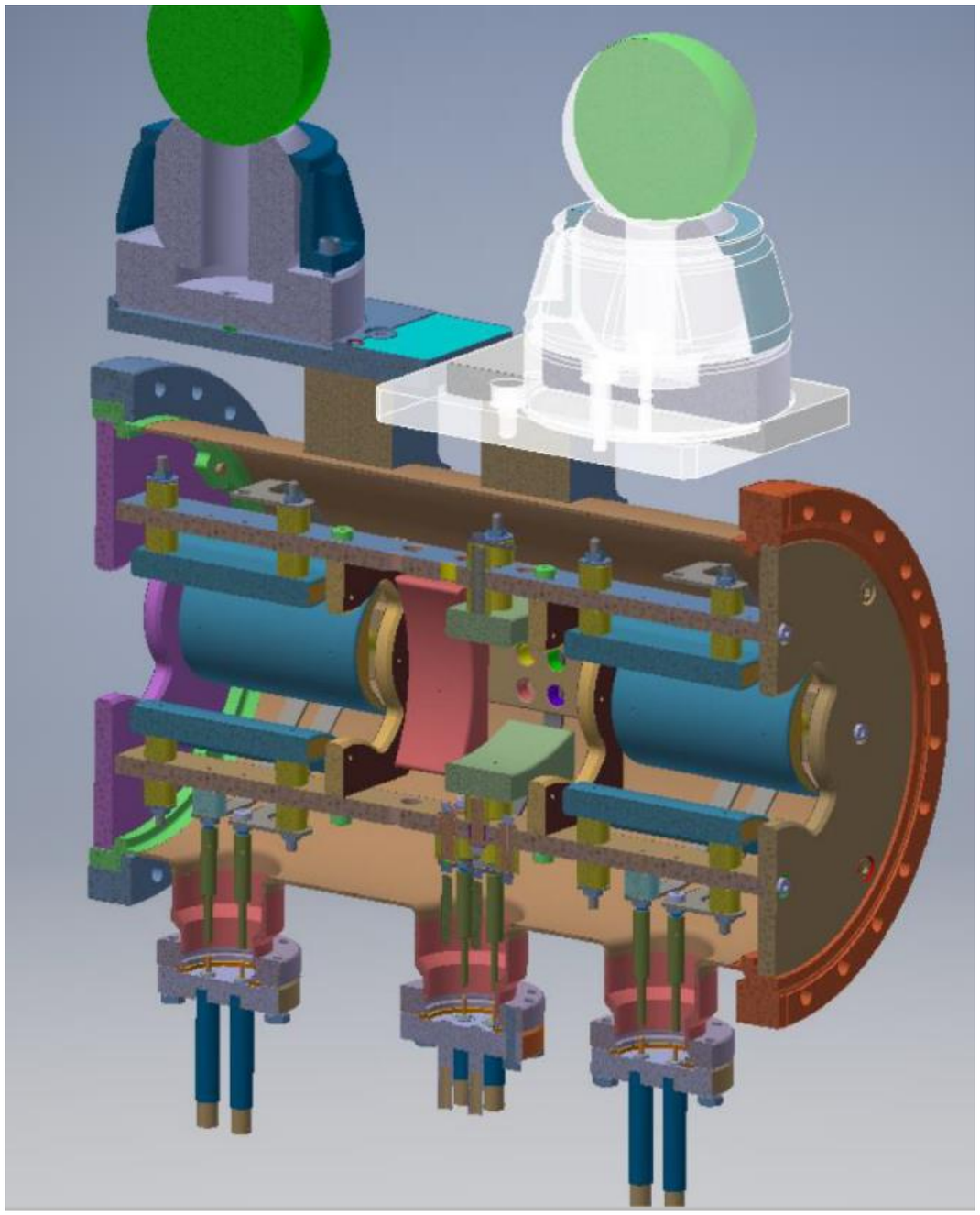
Table 2.2 Equations for calculating the angular coefficients

Geometric structure	Design equation	References
	**I. Two infinitesimal elements** Two arbitrarily oriented elementary areas $d\varphi_{dF_1-dF_2} = \frac{\cos\varepsilon_1 \cos\varepsilon_2}{\pi s^2} dF_2$	[47]
	Two strips of finite length and infinitesimal width with parallel generatrices $d\varphi_{dF_1-dF_2} = \frac{l}{\pi} \cos\alpha \operatorname{arctg} \frac{a}{c} da$	[47]
	End-face element of a channel with a square cross section, located in a corner, and a channel surface element $d\varphi_{dF_1-dF_2} = \frac{ab}{\pi(a^2+a^2)^{1/2}} \left[\operatorname{arctg} \frac{a}{\sqrt{a^2+z^2}} + \operatorname{arctg} \frac{a\sqrt{a^2+z^2}}{z^2+2a^2} \right] dz$	[47]
	Two annular elements on the inside surface of a right circular cylinder $d\varphi_{dF_1-dF_2} = \frac{1}{2R} \left[1 - \frac{z(z^2+4R^2)}{(z^2+4R^2)^{3/2}} \right] dz$	[47]
	Two annular elements on the inside surface of a right circular cone $d\varphi_{dF_1-dF_2} = \frac{\cos^2\alpha}{2h_1 \sin\alpha} \left\{ 1 - |h_1 - h_2| \frac{(h_1-h_2)^2 + 6h_1h_2\sin^2\alpha}{[(h_1-h_2)^2 + 4h_1h_2\sin^2\alpha]^{1/2}} \right\} dh_2$	[136]
	Two infinitesimal elements on the inside surface of a spherical cavity $d\varphi_{dF_1-dF_2} = \frac{dF_2}{4\pi R^2}$	[137]

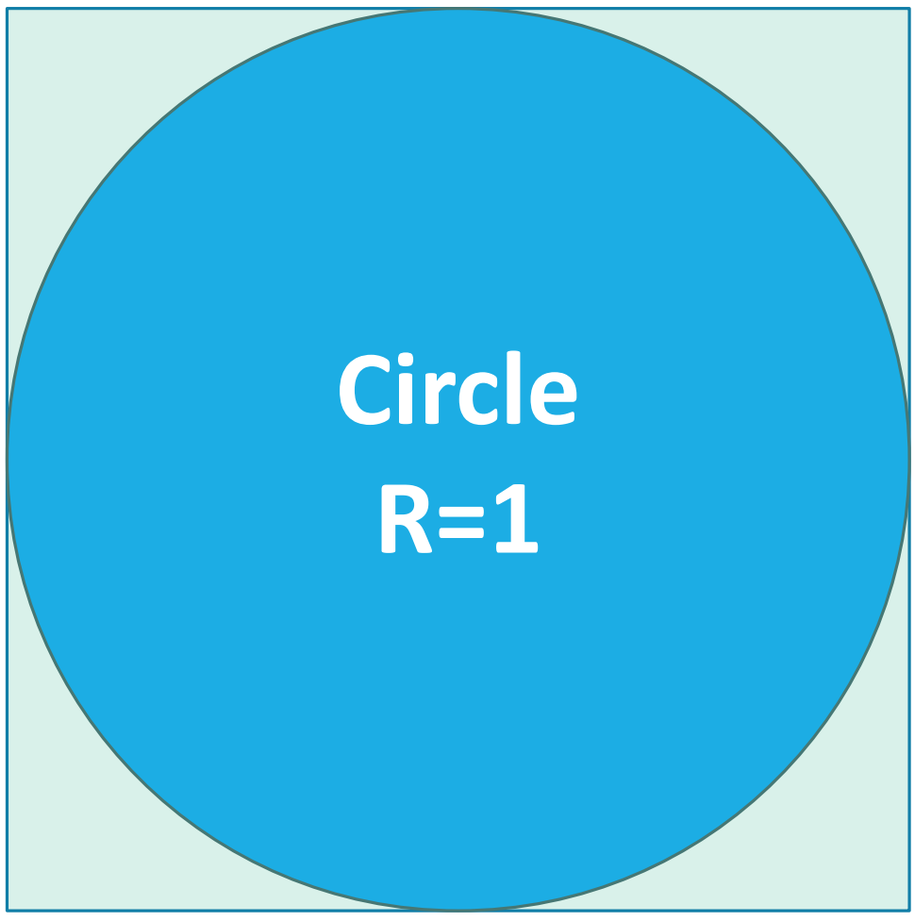
Table 2.2 (continued)

Geometric structure	Design equation	References
	Plane element and ellipse parallel to it $\varphi_{dF_1-F_2} = \frac{ab}{\sqrt{(c^2+a^2)(c^2+b^2)}}$	[47]
	Elementary strip and infinite-length cylinder parallel to it $\varphi_{dF_1-F_2} = \frac{\pi R}{a^2+c^2}$	[128]
	Element on the inside surface of the outer cylinder and the inside surface of the same cylinder for a system of two coaxial cylinders $\varphi_{dF_1-F_2} = \frac{1}{2} - \frac{R_2}{4R_1} + \frac{R_2}{\pi R_1}$ $\times \left[\frac{l}{R_2} \operatorname{arctg} \frac{\sqrt{R_1^2-R_2^2}}{R_2} - \frac{1}{2} \operatorname{arctg} \frac{l^2-4(R_1^2-R_2^2)}{4l\sqrt{R_1^2-R_2^2}} - \frac{l^2+2R_2^2}{R_2\sqrt{l^2+4R_1^2}} \right.$ $\left. + \operatorname{arctg} \frac{\sqrt{(R_1^2-R_2^2)(l^2+4R_1^2)}}{R_2 l} \right]$	[129]
	Annular element on the inside surface of a right circular cylinder and the end face of the cylinder $\varphi_{dF_1-F_2} = \frac{1}{2R} \left[\frac{z^2+2R^2}{\sqrt{z^2+4R^2}} - z \right]$	[47]
	Element of a plane ring and outside surface of a right circular cylinder $\varphi_{dF_1-F_2} = \frac{1}{\pi} \left[\frac{1}{2} \arccos \frac{R_2}{R_1} + \operatorname{arctg} \frac{R_2}{\sqrt{R_1^2-R_2^2}} - \frac{l^2+R_1^2-R_2^2}{A} \right.$ $\left. + \operatorname{arctg} \frac{A \operatorname{tg}[(1/2)\arccos(R_2/R_1)]}{l^2+R_1^2+R_2^2-2R_1R_2} \right],$ $A = \sqrt{(l^2+R_1^2+R_2^2)^2 - 4R_1^2R_2^2}$	[137]
	Plane annular element and inside surface of a cylinder $\varphi_{dF_1-F_2} = \frac{1}{2} \left[\frac{(l+z)^2+R_2^2-R_1^2}{\sqrt{(l+z)^2+R_2^2+R_1^2)^2-4R_2^2R_1^2}} \right.$ $\left. - \frac{z^2+R_2^2-R_1^2}{\sqrt{(z^2+R_2^2+R_1^2)^2-4R_2^2R_1^2}} \right]$	[126]
	Annular cylindrical element and inside surface of a cylinder $\varphi_{dF_1-F_2} = \frac{1}{2R} \left[1 + \frac{z^2+2R^2}{\sqrt{z^2+4R^2}} - \frac{(l+z)^2+2R^2}{\sqrt{(l+z)^2+4R^2}} \right]$	[126]





The idea: Monte Carlo method



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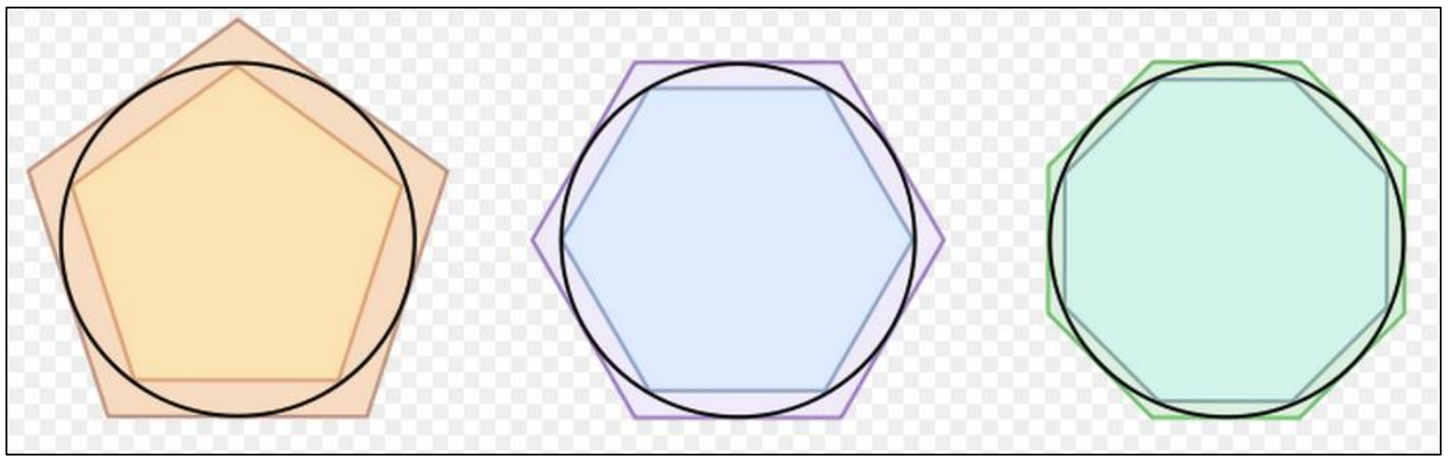
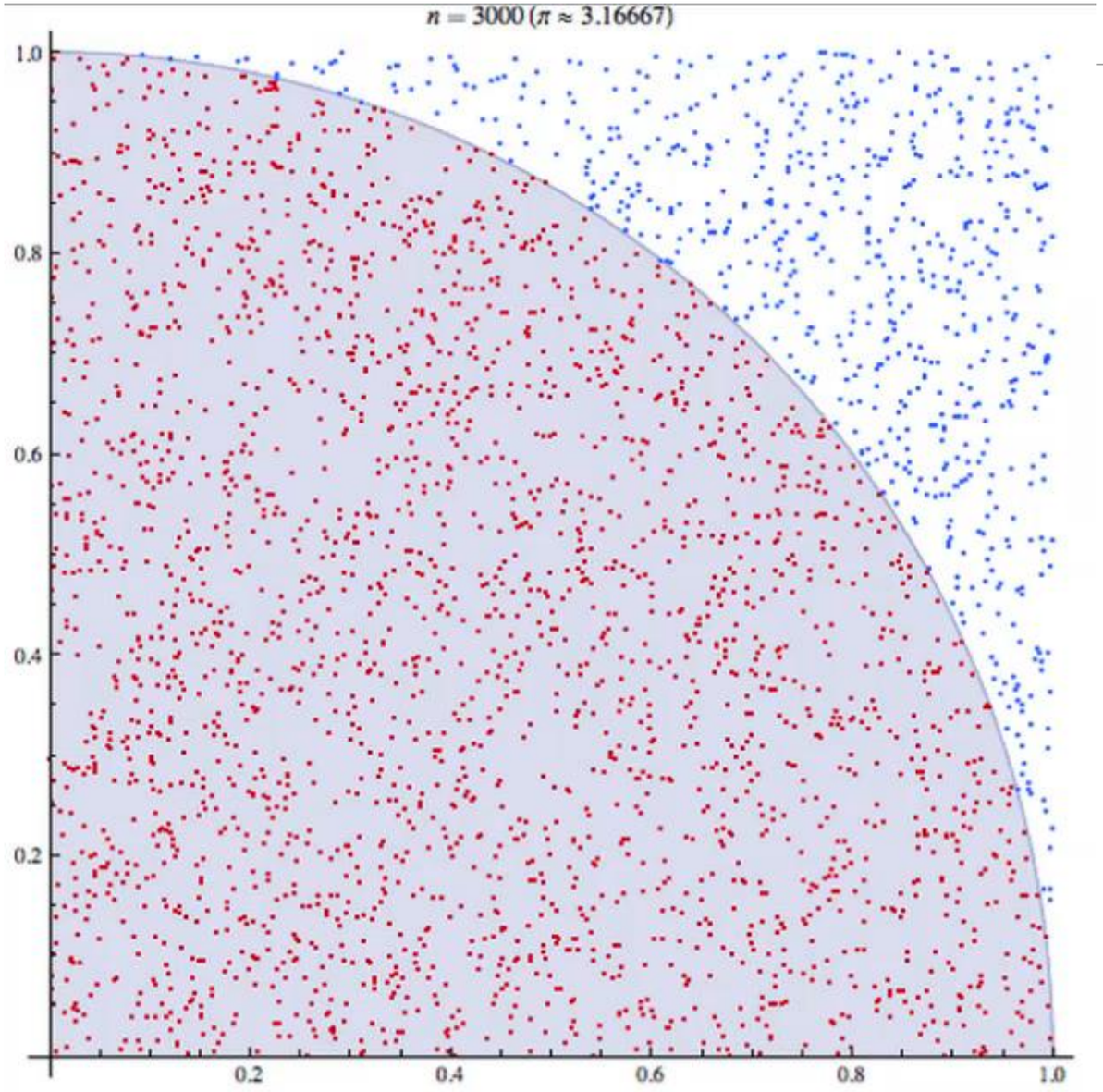


$$\pi = \cfrac{4}{1+\cfrac{1^2}{2+\cfrac{3^2}{2+\cfrac{5^2}{2+\cfrac{7^2}{2+\cfrac{9^2}{2+\ddots}}}}}}$$

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801}\sum_{k=0}^{\infty}\frac{(4k)!(1103+26390k)}{(k!)^4 396^{4k}}$$

$$\frac{2}{\pi} = \frac{\sqrt{2}}{2}\cdot\frac{\sqrt{2+\sqrt{2}}}{2}\cdot\frac{\sqrt{2+\sqrt{2+\sqrt{2}}}}{2}\cdots$$

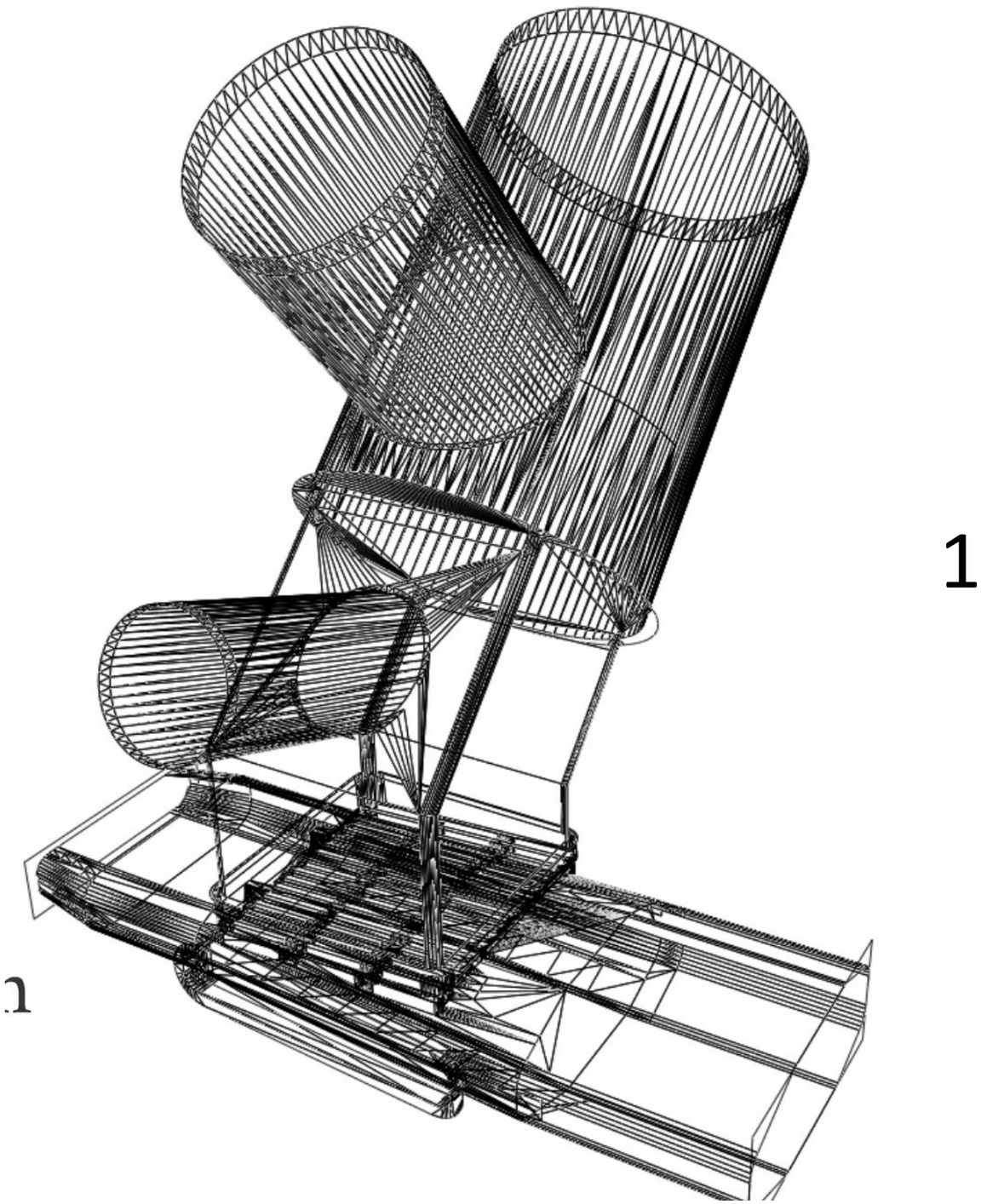
Monte Carlo



$$\frac{\text{points inside}}{\text{all points}} \sim \frac{\text{circle area}}{\text{square area}} = \frac{\pi}{4}$$

Monte Carlo simulations

Geometry: polygons



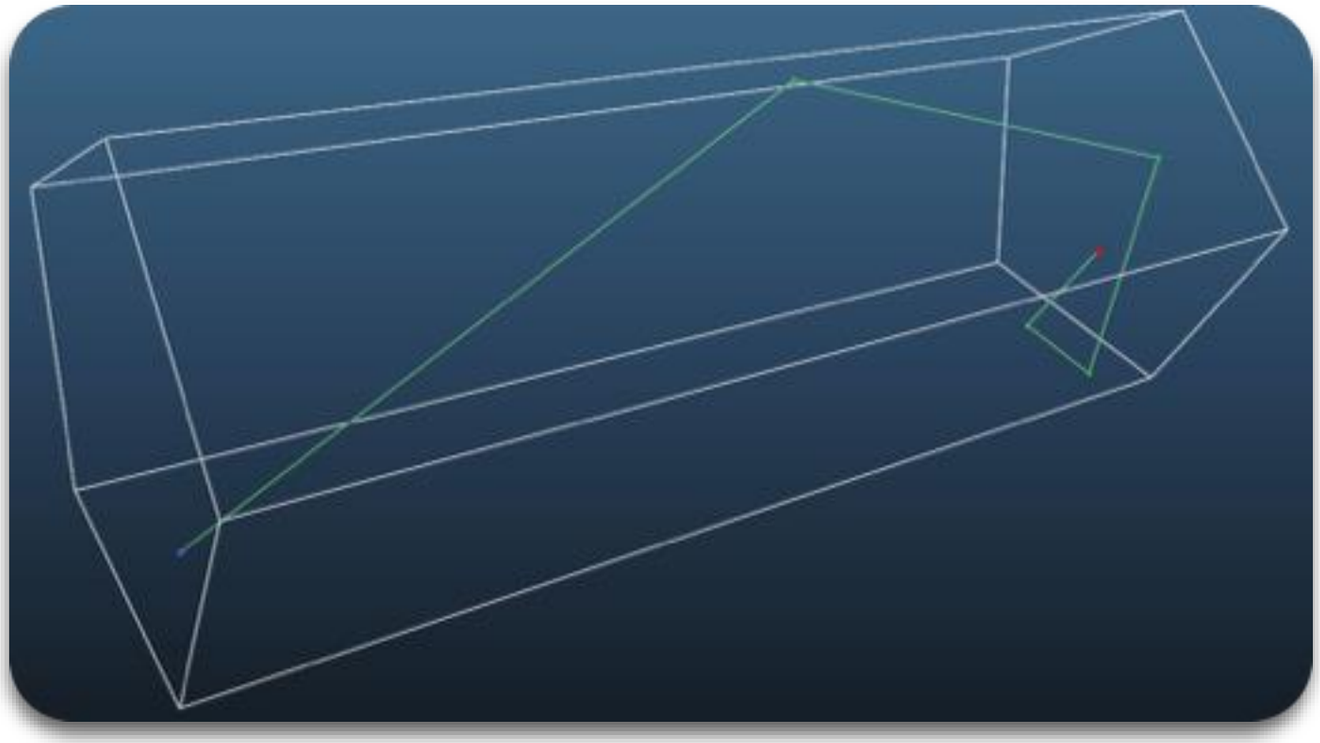
Gas input:

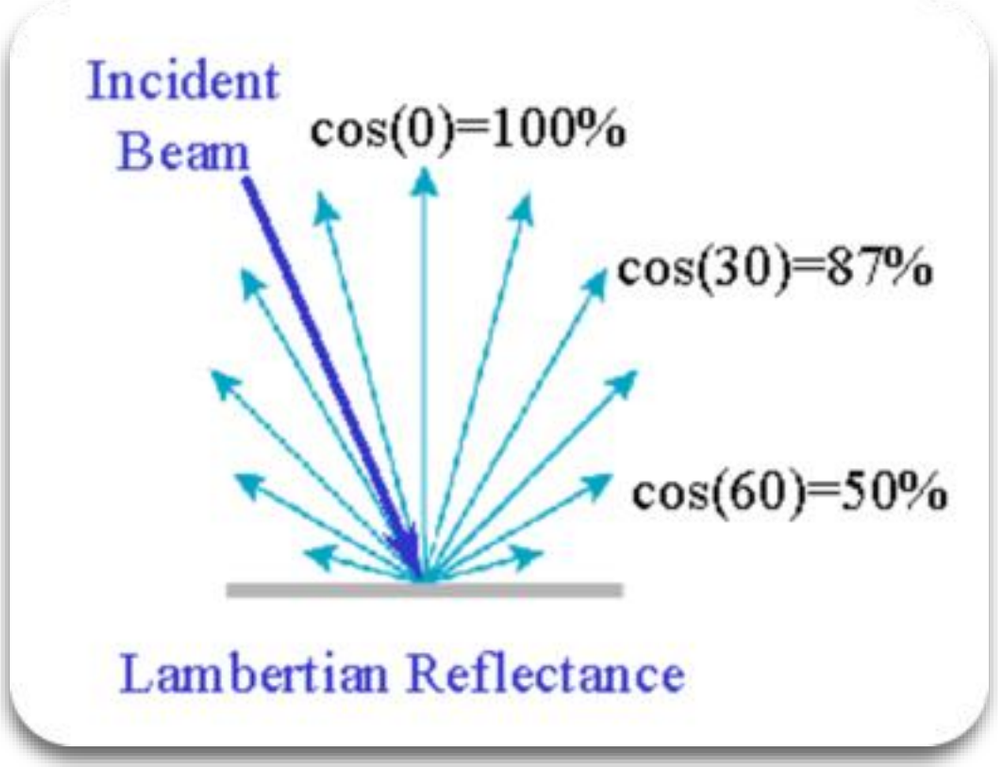
$$pV=NkT$$

1 Pa*m^3/s = 2.4*10^{20} molecules/s

Virtual / Physical particle ratio

Reflection

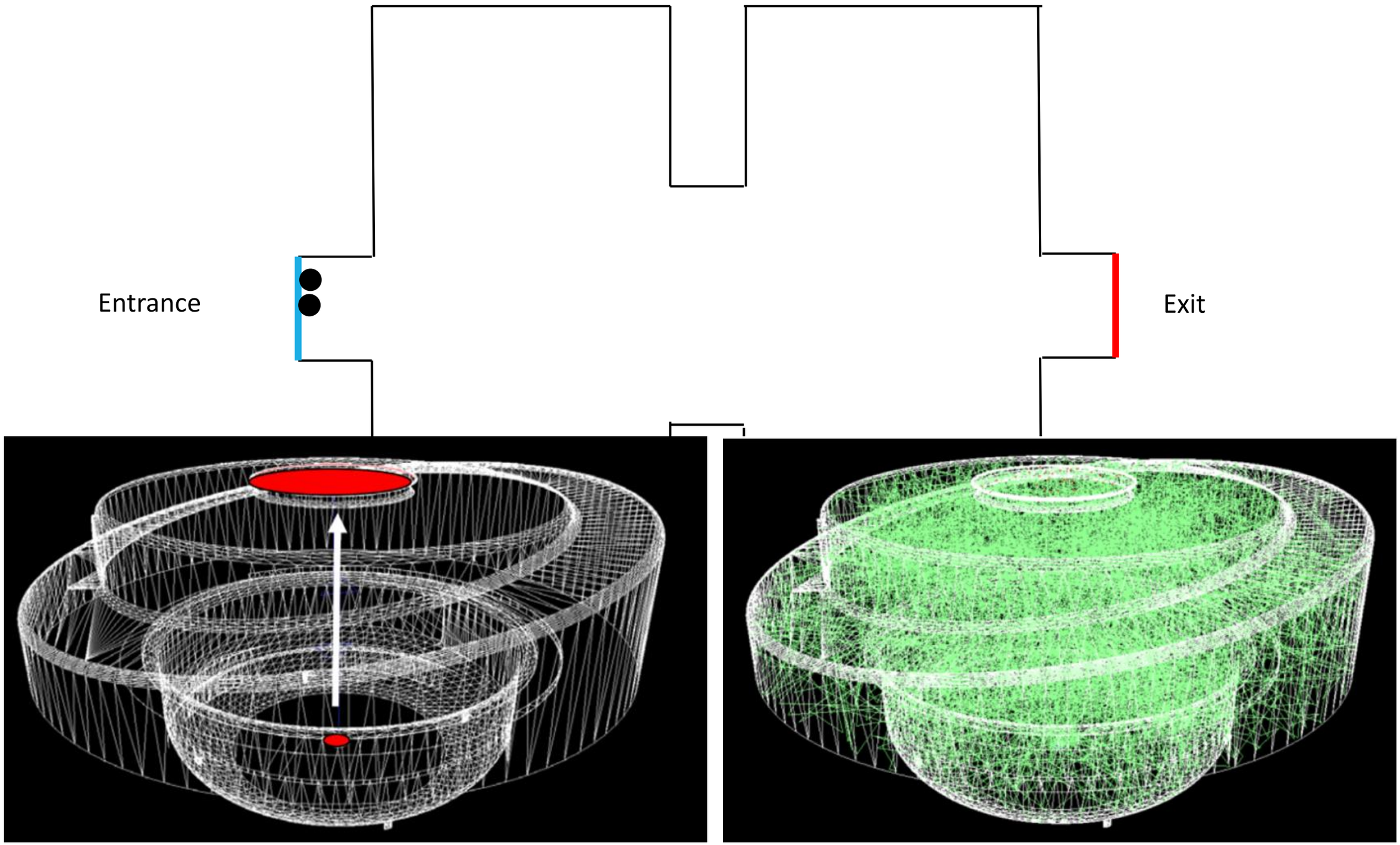




Pumping / absorption

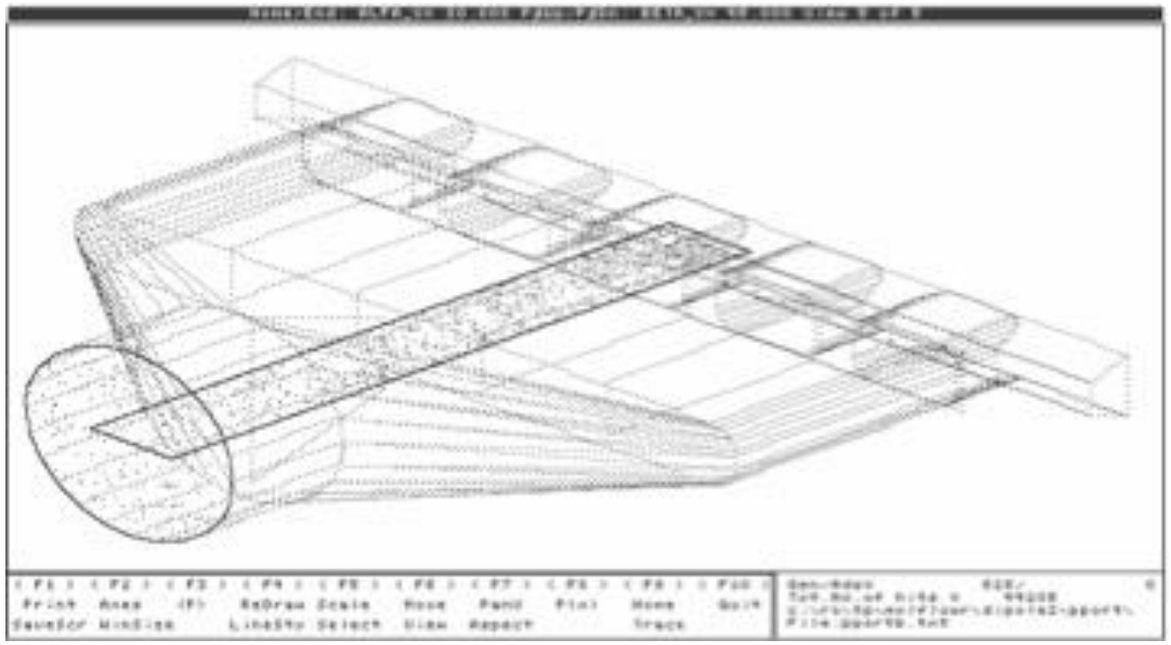
$$S\ [m^3/s] = sticking\ [0..1] * 1/4 * A\ [m^2] * v_{avg}\ [m/s]$$

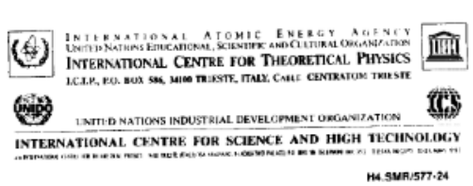
Monte Carlo



Molflow (1990)

Roberto Kersevan





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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
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UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION

INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

H4.SMR/577-24

School on
"Use of Synchrotron Radiation in Science and Technology"

14 October - 8 November 1991

Molflow
User's Guide

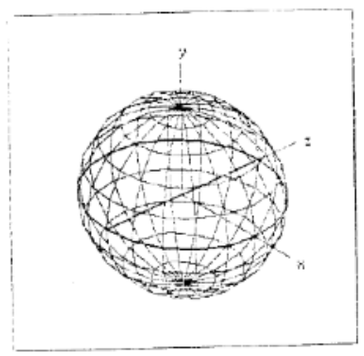
R. Kersevan
Sincrotrone Trieste
Trieste, Italy

SINCROTRONE TRIESTE

ST/M-91/17

MOLFLOW
User's Guide

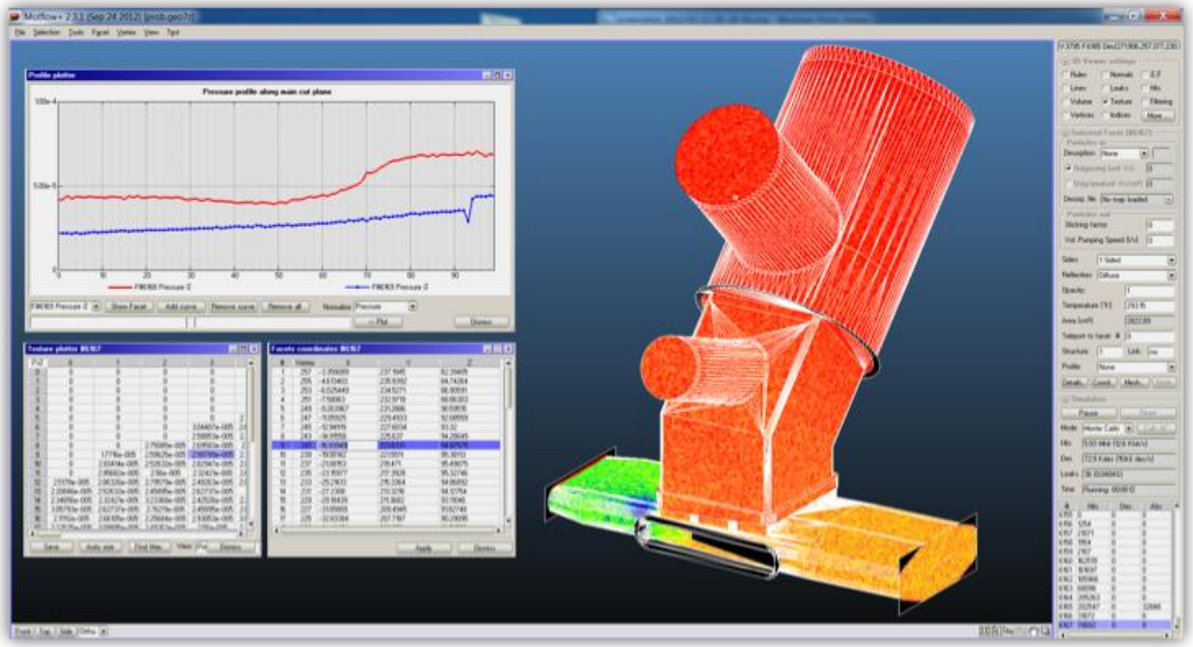
Roberto Kersevan



September 1991

SINCROTRONE TRIESTE

Molflow+ (2008-)



Molflow+

A Monte-Carlo Simulator package developed at CERN

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About Molflow

A test-particle Monte-Carlo simulator for ultra-high-vacuum systems

Developed at CERN

MolFlow+

Molflow+ allows you to calculate the pressure in an arbitrarily complex geometry when ultra-high vacuum condition is met. The name comes from *molecular 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. In 2008 a new version called MolFlow+ was written, that uses the original algorithm in a modern environment. It uses OpenGL acceleration and can use multiple cores (see R. Kersevan, J-L. Pons, J. Vac. Sci. Technol. A 27, 1017 (2009)[http://dx.doi.org/10.1116/1.3153280) Further improvements were added in 2012. Geometries can be imported from most CAD programs that support the STL file format.

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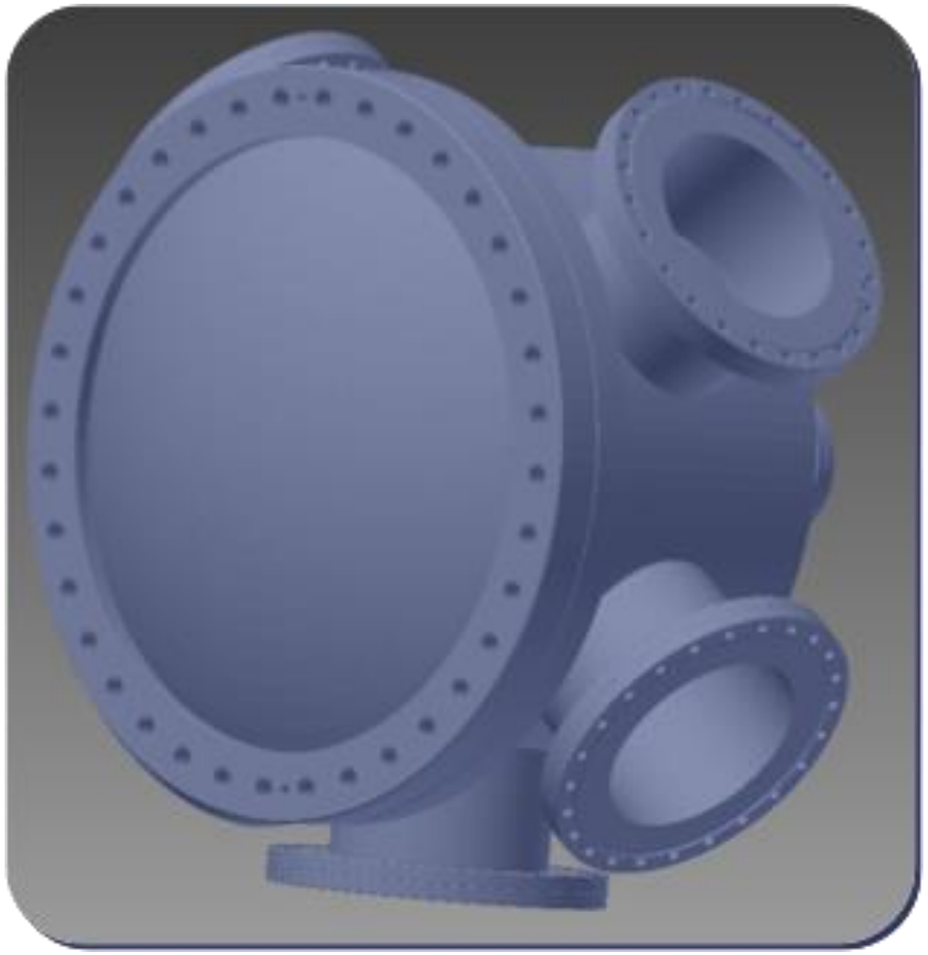
WORKING WITH MOLFLOW

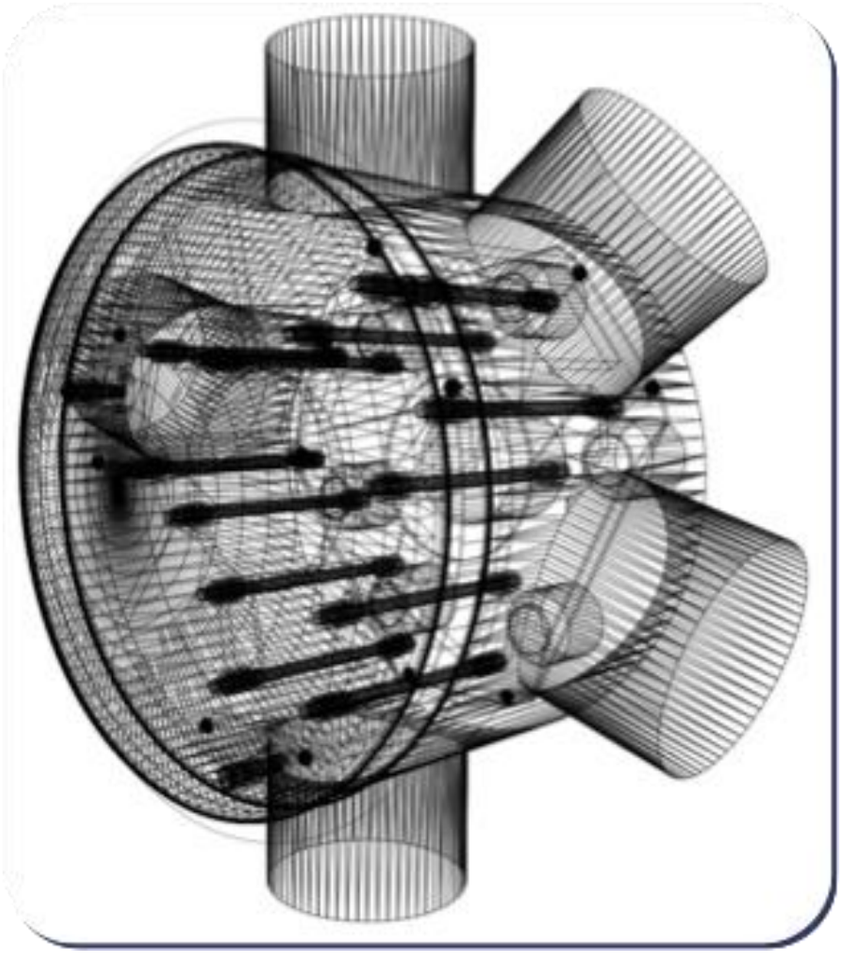
Step 1: creating geometry

CAD

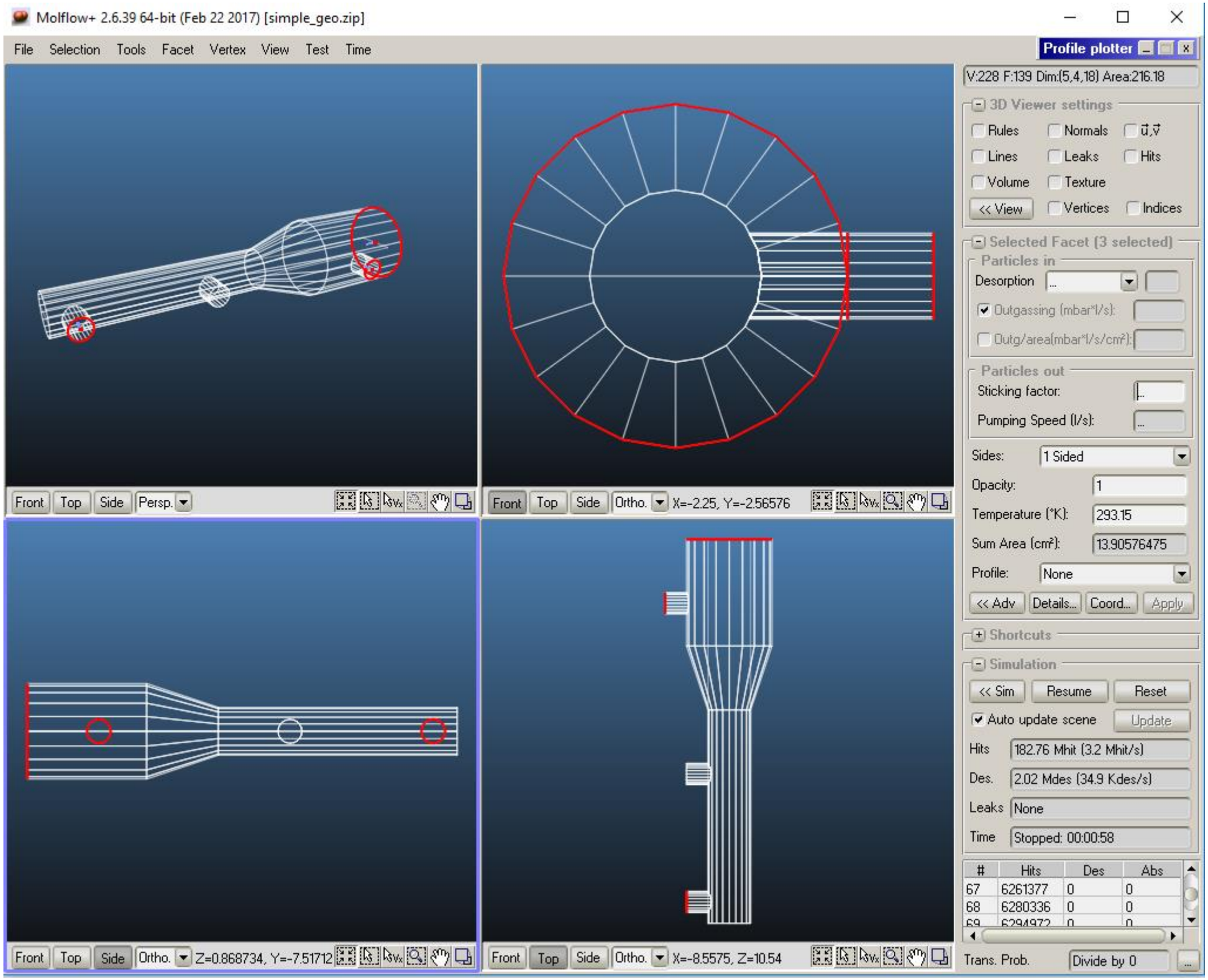


STL format

Molflow+

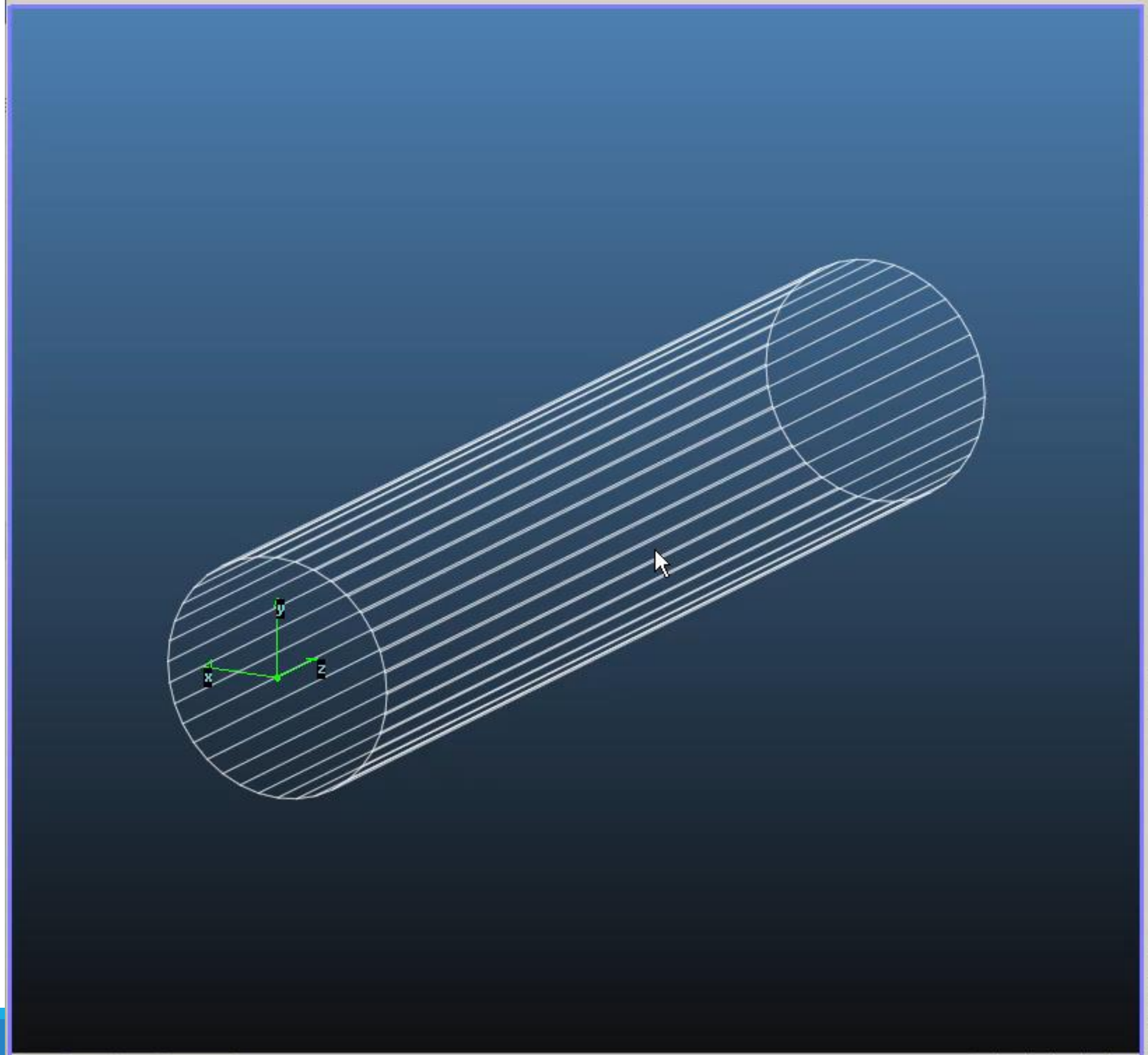


Step 2: adding physics



Molflow+ 2.8.6 (Mar 29 2022) []

File Selection Tools Facet Vertex View Test Time About



Front Top Side Ortho.

V:72 F:38 Dim:(2,2,10) Area:69.0035

3D Viewer settings

Rules Normals u⃗,v⃗
Lines Leaks Hits
Volume Texture FacetIDs
<< View Indices VertexIDs

Selected Facet (none)

Particles in

Desorption
Outgassing (mbar*l/s):
Outg/area(mbar*l/s/cm²):

Particles out

Sticking factor:
Pumping Speed (l/s):

Sides:
Opacity:
Temperature (°K):
Sum Area (cm²):
Profile:

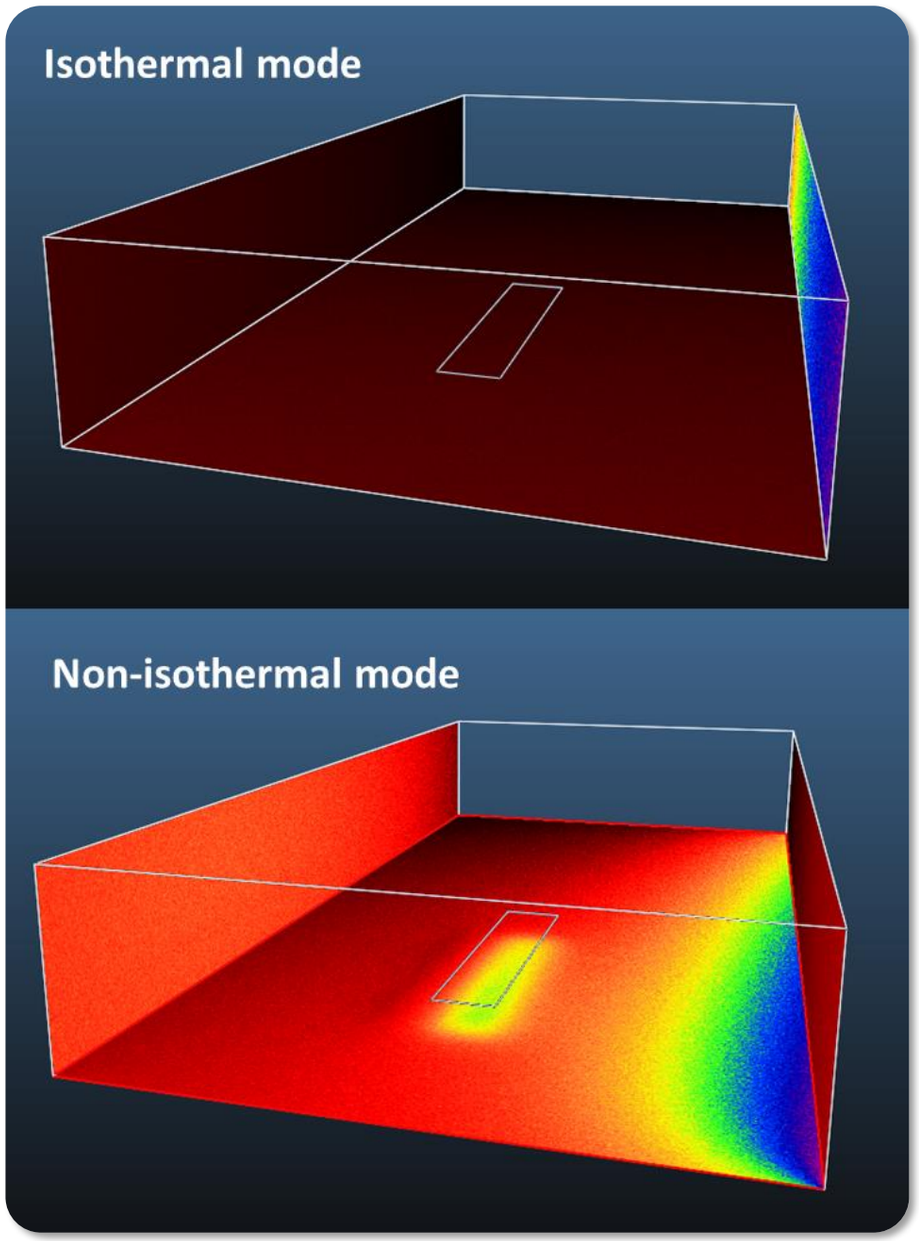
<< Adv Details... Coord. Apply

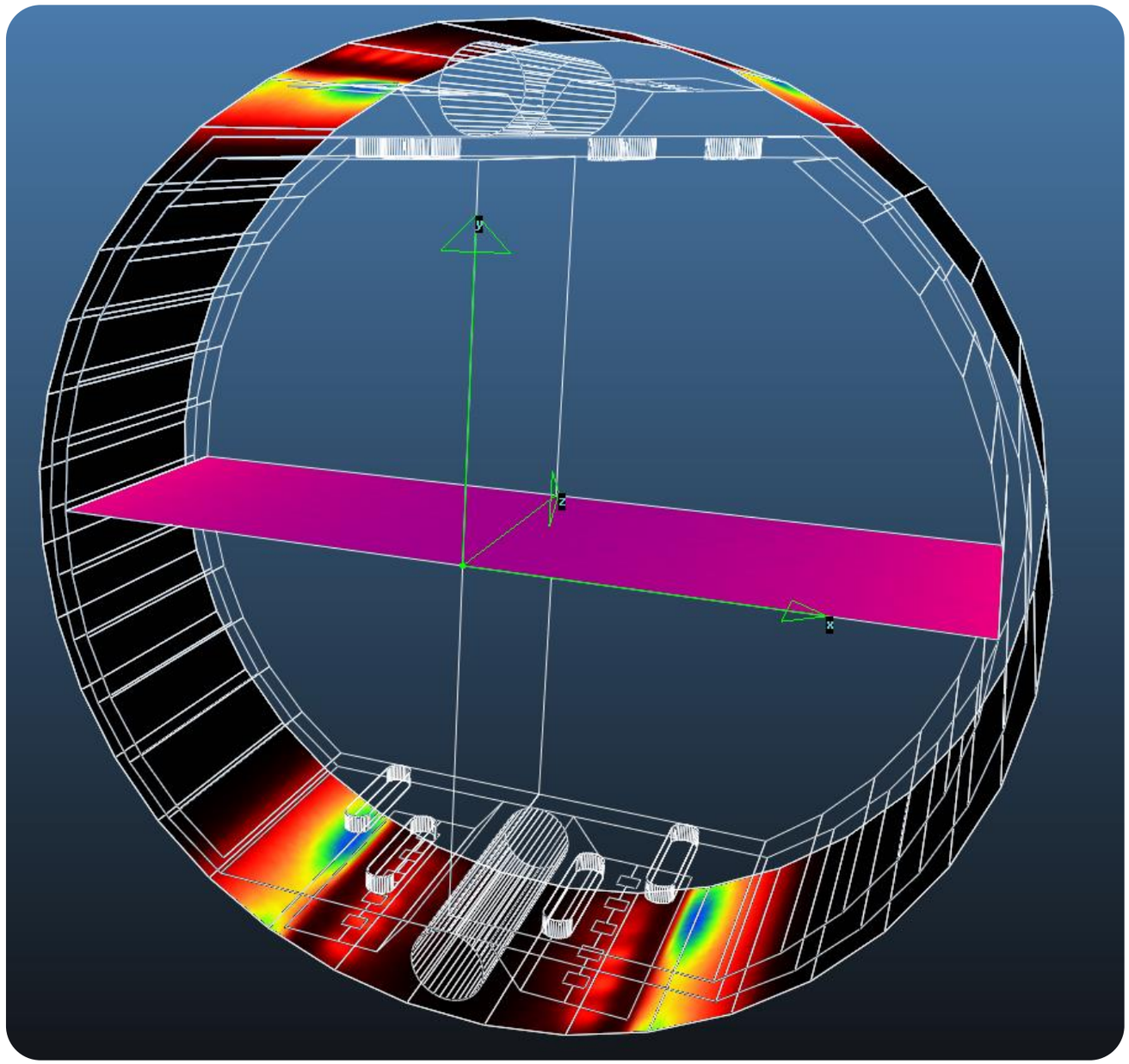
Shortcuts

Simulation

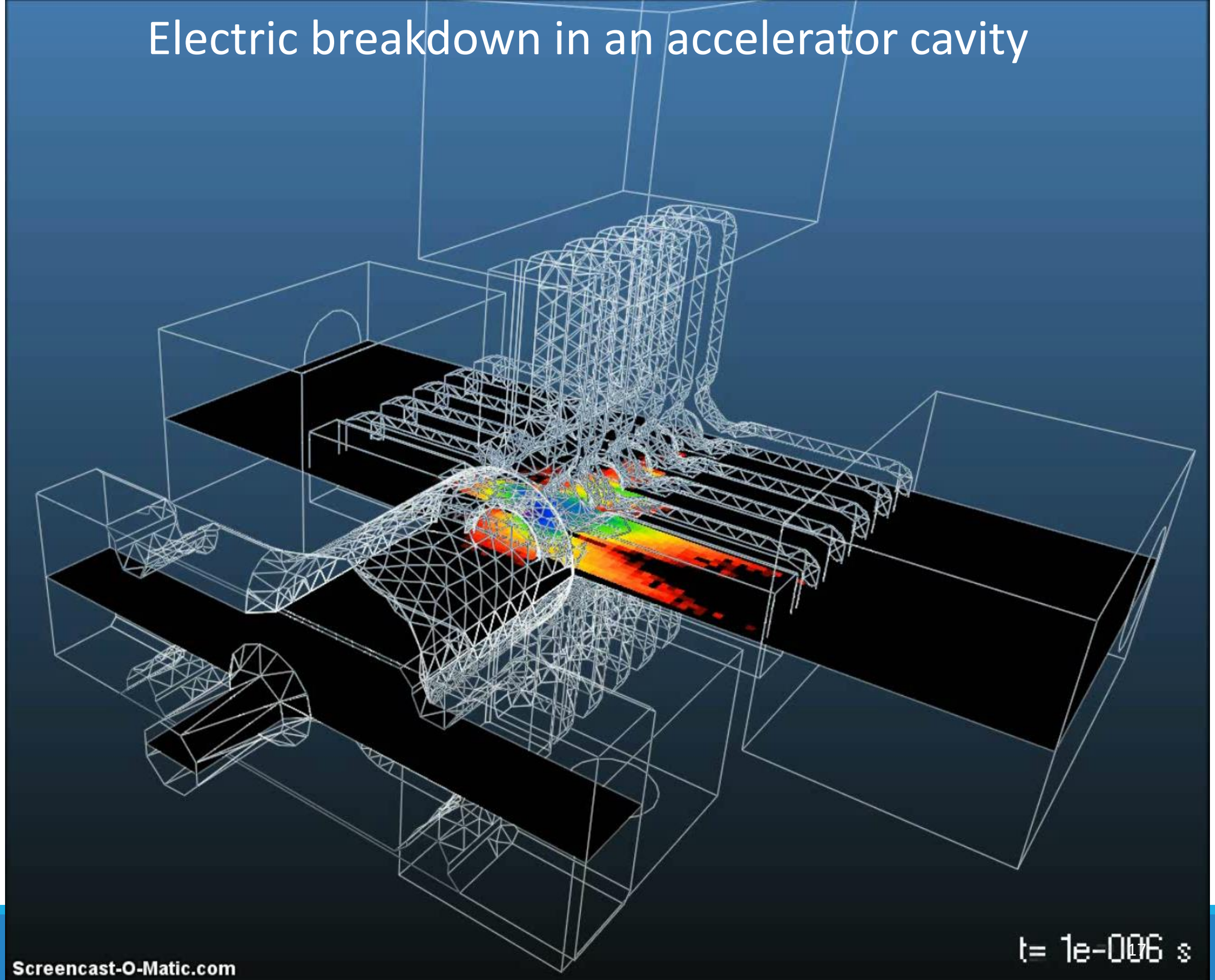
<< Sim Begin Reset
Auto update scene Update
Hits 0 hit (0.0 hit/s)
Des. 0 des (0.0 des/s)
Leaks None
Time Stopped: 00:00:00

#	Hits	Des	Abs
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0

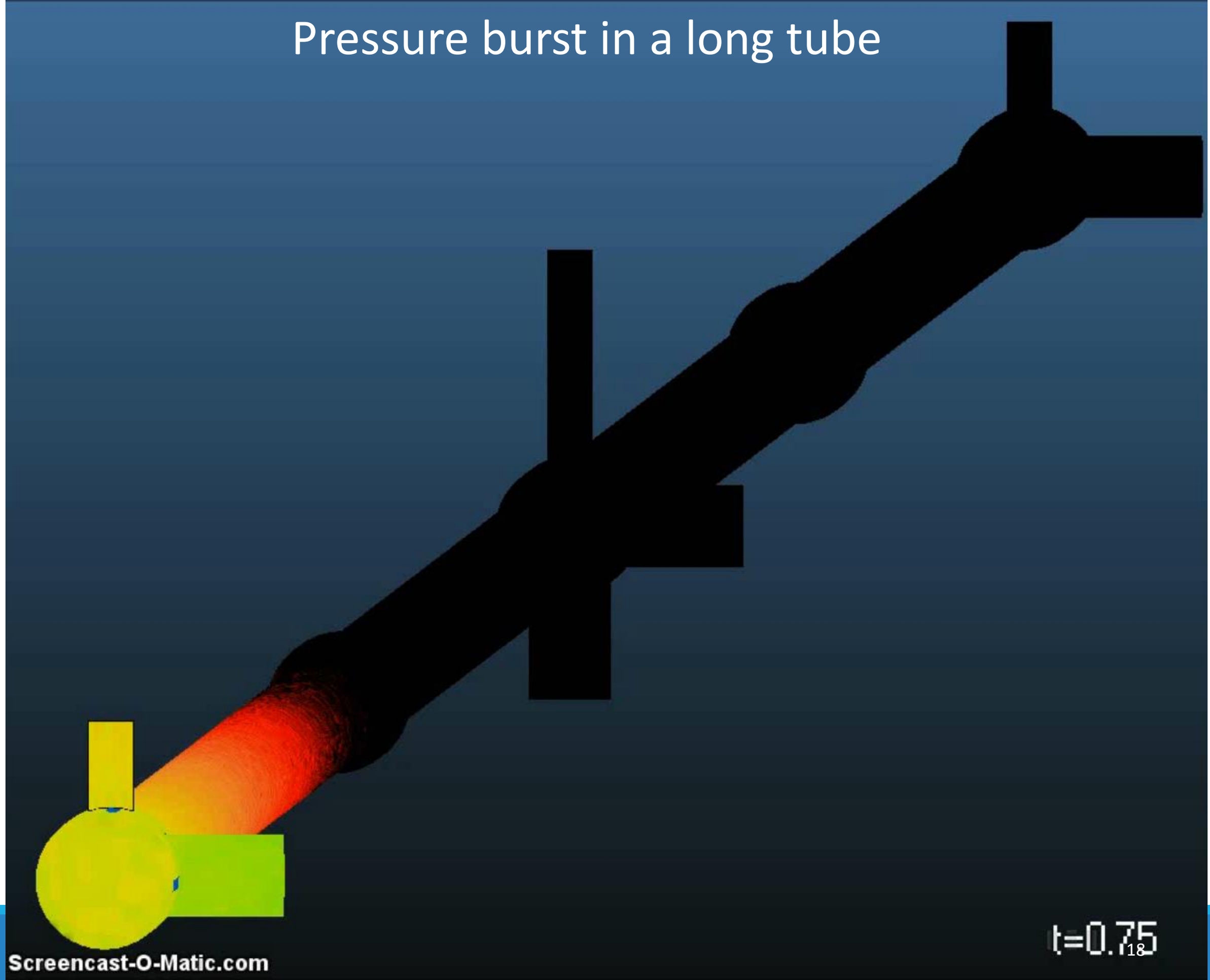

Isothermal mode
Non-isothermal mode



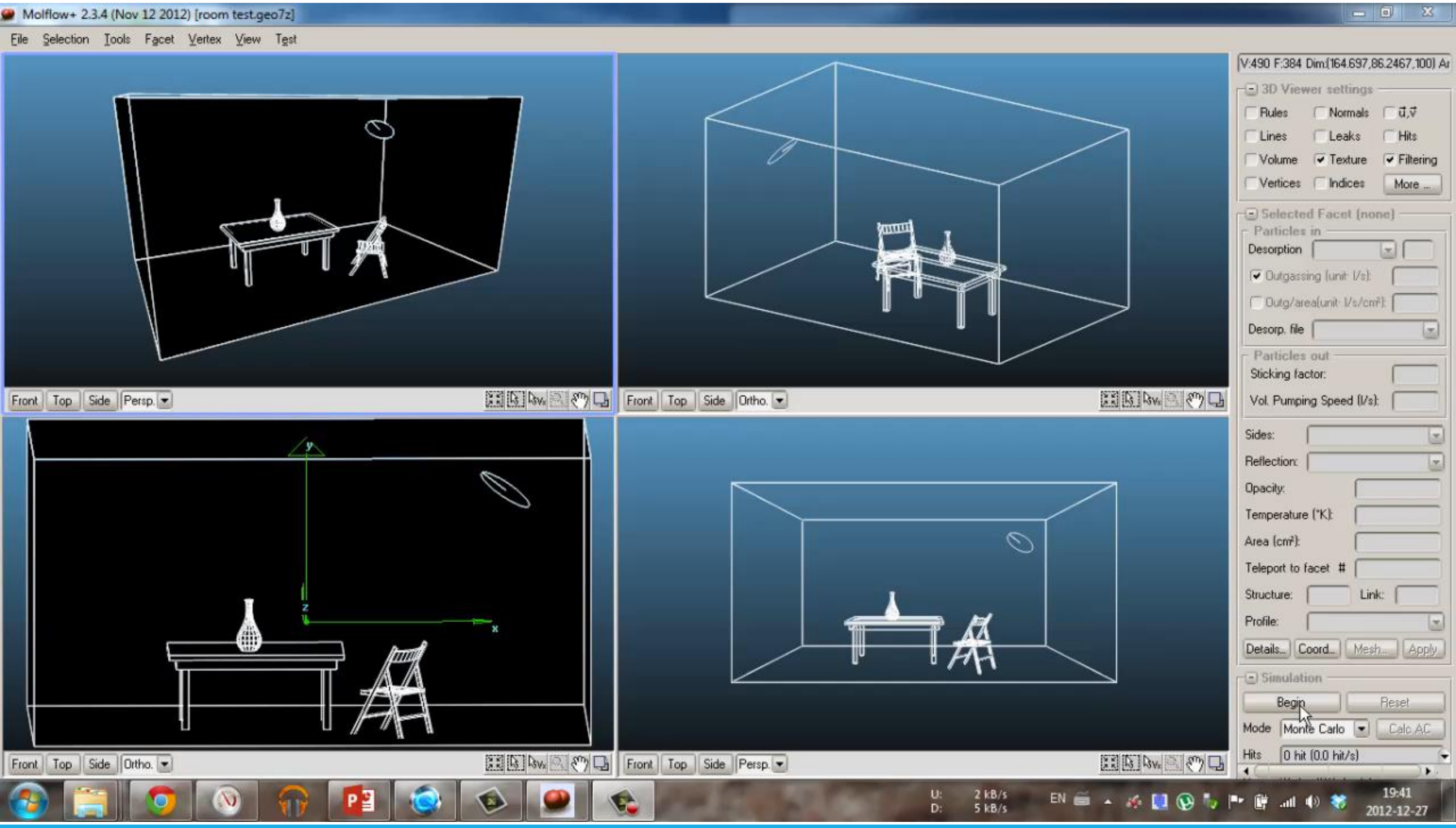
Electric breakdown in an accelerator cavity



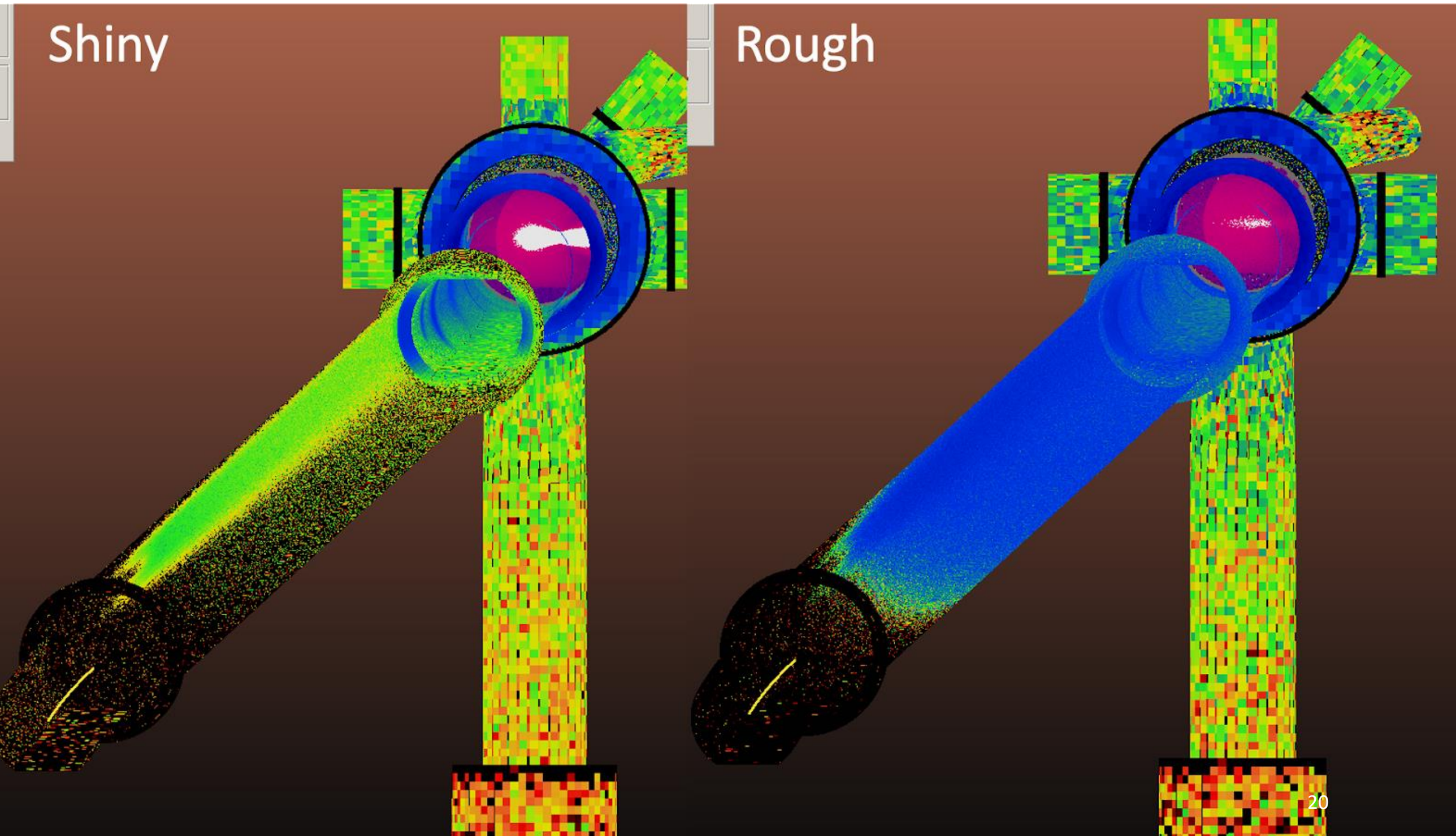
Pressure burst in a long tube

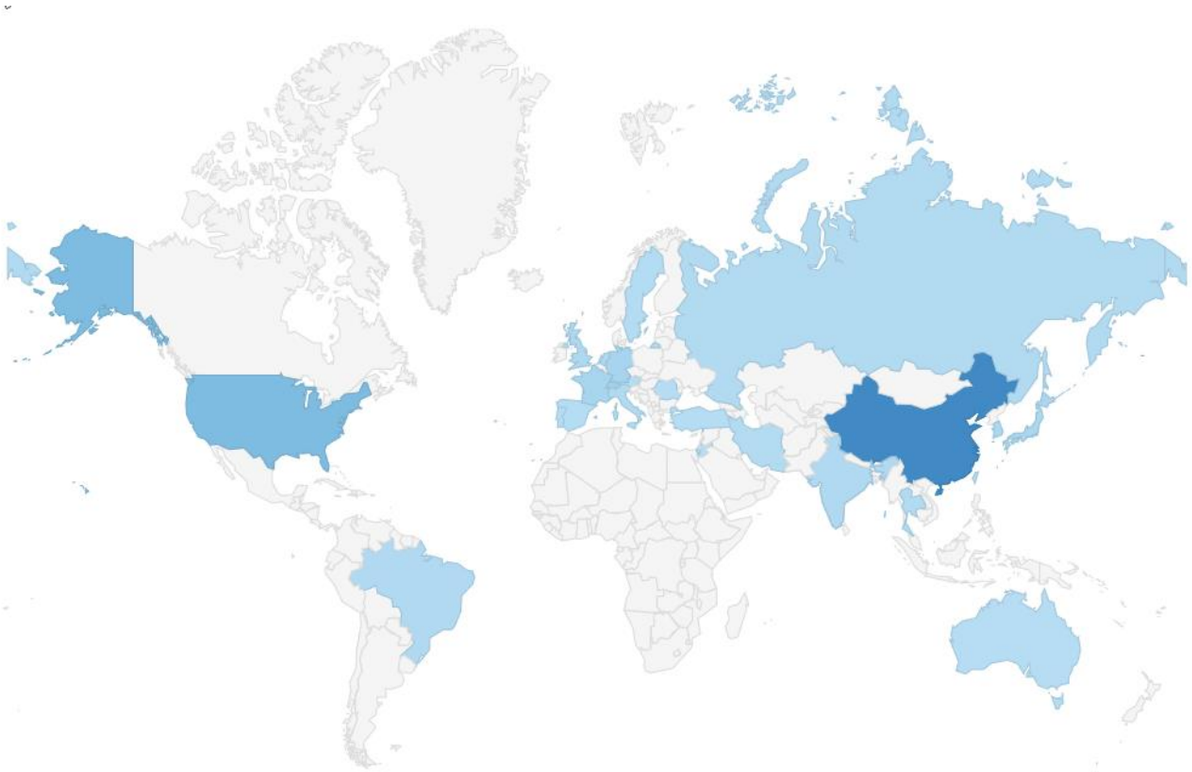


Simulation of light



Synrad+:
Synchrotron radiation simulations





Country	Acquisition		
	Users	New Users	Sessions
	4,983 % of Total: 100.00% (4,983)	4,908 % of Total: 100.12% (4,902)	9,107 % of Total: 100.00% (9,107)
1. China	**2,575** (50.98%)	2,551 (51.98%)	3,508 (38.52%)
2. United States	**702** (13.90%)	684 (13.94%)	1,067 (11.72%)
3. Germany	**215** (4.26%)	209 (4.26%)	513 (5.63%)
4. Japan	**205** (4.06%)	192 (3.91%)	590 (6.48%)
5. Switzerland	**194** (3.84%)	172 (3.50%)	641 (7.04%)
6. South Korea	**173** (3.43%)	170 (3.46%)	334 (3.67%)
7. France	**136** (2.69%)	121 (2.47%)	447 (4.91%)
8. Iran	**111** (2.20%)	112 (2.28%)	157 (1.72%)
9. Russia	**79** (1.56%)	73 (1.49%)	201 (2.21%)
10. India	**77** (1.52%)	73 (1.49%)	222 (2.44%)

https://molflow.web.cern.ch/

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Instructions	Instructions	Debian Instructions[1] Fedora Instructions[2]

Introduction to Monte Carlo simulations

If you're new to these Monte Carlo tools, this presentation is a good overview of the special physics at very low pressures, how it's related to Monte Carlo simulations, and how Molflow actually works.

- Short explanation of the high vacuum physics
- The Monte Carlo method
- History of Molflow and Synrad
- Typical Molflow workflow