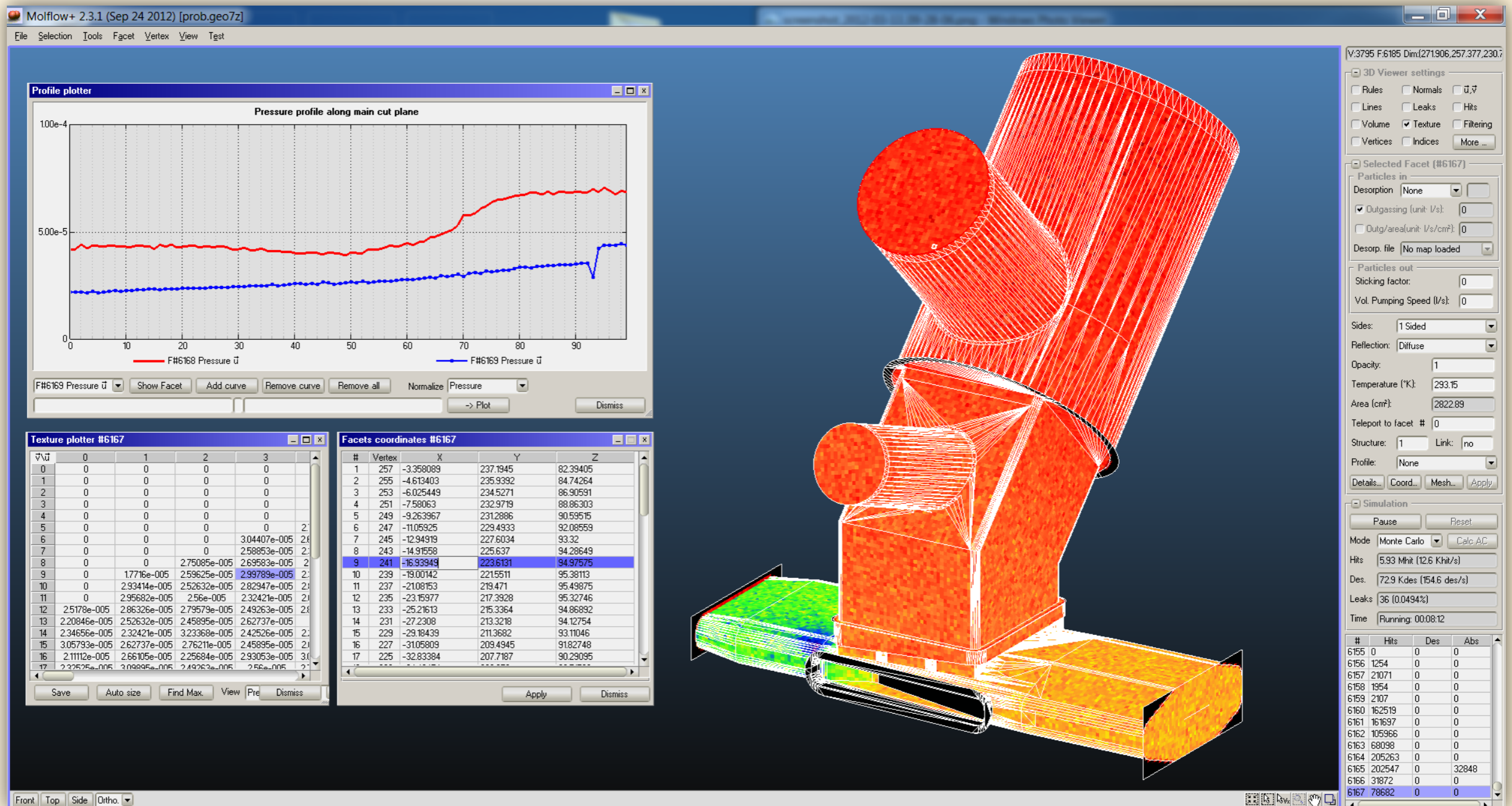


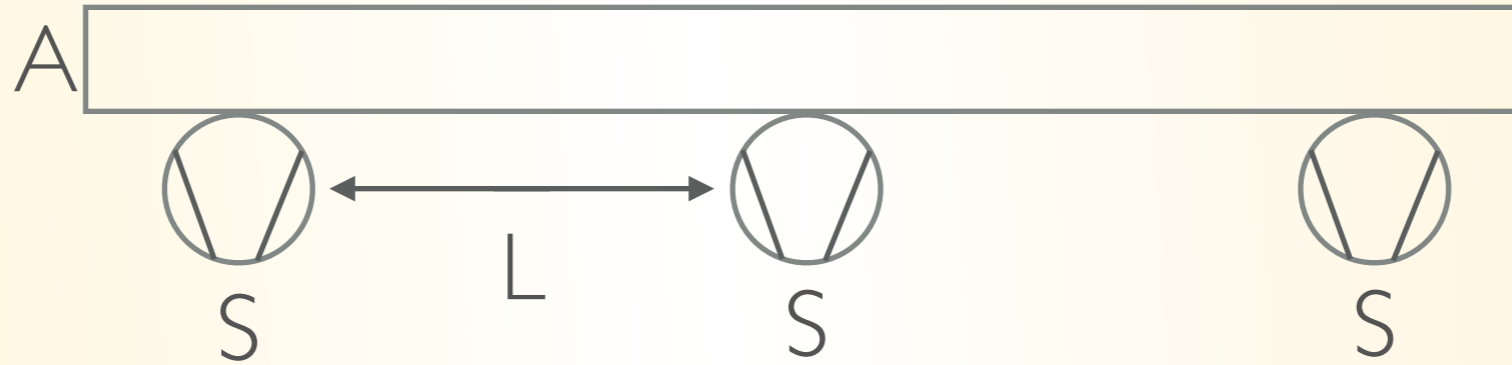
MOLFLOW SEMINAR

Monte Carlo simulation of ultra high vacuum systems

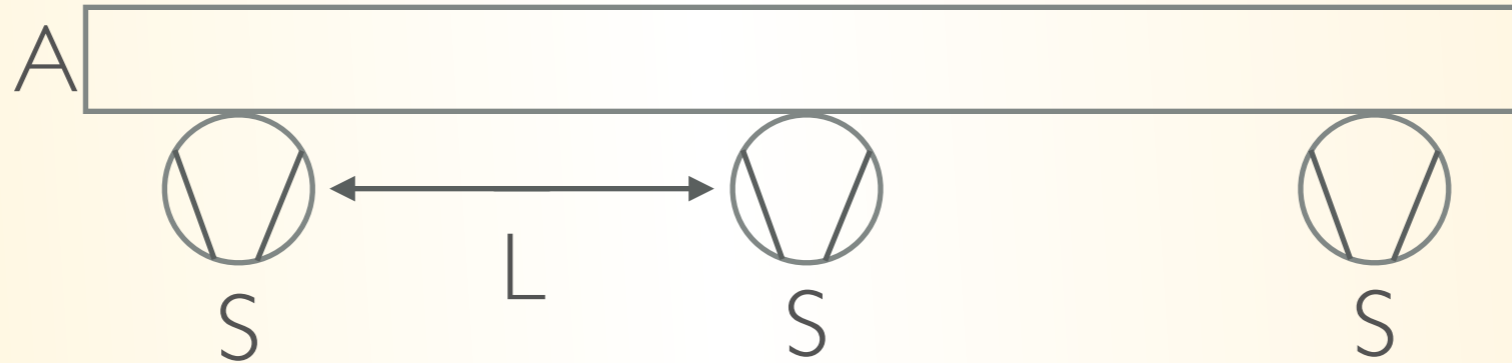


2014.11.26, KEK - Marton Ady

VACUUM CALCULATIONS: ANALYTICAL METHOD



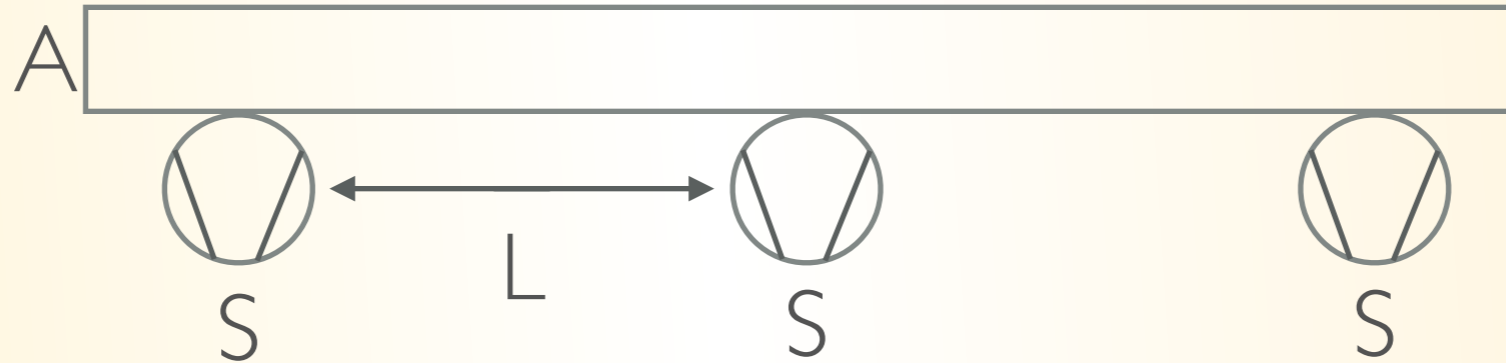
VACUUM CALCULATIONS: ANALYTICAL METHOD



$$P = Q/S$$

$$Q = C^*(p_1 - p_2)$$

VACUUM CALCULATIONS: ANALYTICAL METHOD

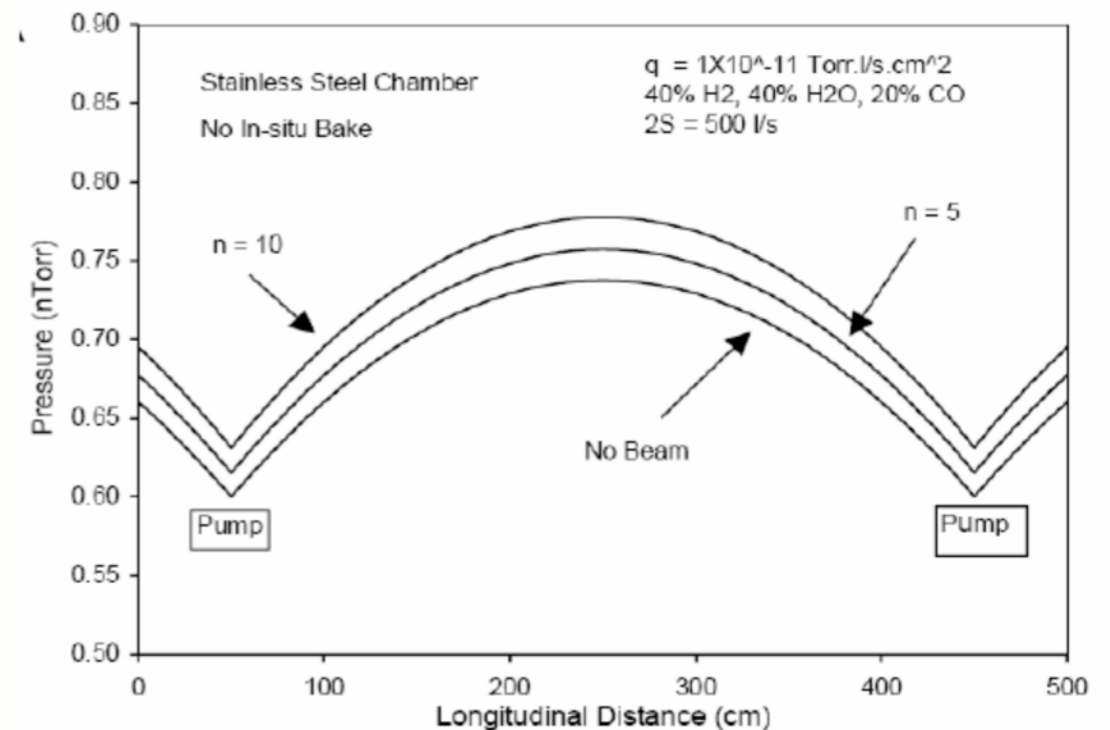
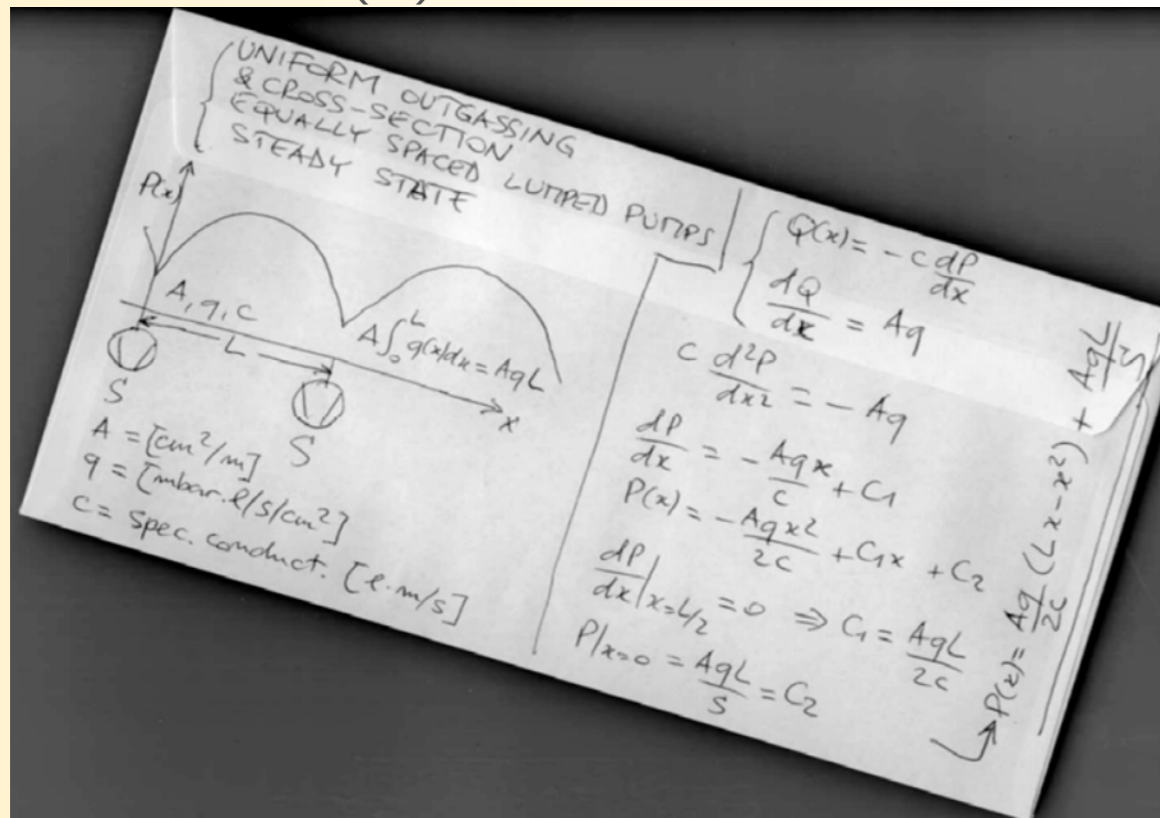


$$P = Q/S$$

$$Q = C * (p_1 - p_2)$$


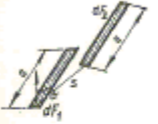
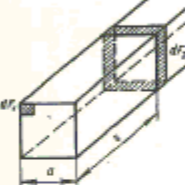
$$Q(x) = -C * dP/dx$$

$$P(x) = Q \left(\frac{L}{S} + \frac{L^2 - x^2}{2C'} \right)$$



DIFFICULTY: CONDUCTANCE

Table 2.2 Equations for calculating the angular coefficients

Geometric structure	Design equation	References
	<p>I. Two infinitesimal elements</p> <p>Two arbitrarily oriented elementary areas</p> $d\varphi_{dF_1-dF_2} = \frac{\cos \alpha_1 \cos \alpha_2}{\pi r^2} dF_2$	[47]
	<p>Two strips of finite length and infinitesimal width with parallel generatrices</p> $d\varphi_{dF_1-dF_2} = \frac{1}{\pi} \cos \alpha \operatorname{arctg} \frac{a}{s} ds$	[47]
	<p>End-face element of a channel with a square cross section, located in a corner, and a channel surface element</p> $d\varphi_{dF_1-dF_2} = \frac{as}{\pi(a^2+s^2)^{3/2}} \left[\operatorname{arctg} \frac{a}{\sqrt{a^2+s^2}} + \operatorname{arctg} \frac{a\sqrt{a^2+s^2}}{s^2+2a^2} \right] ds$	[47]


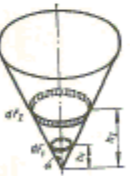


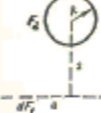
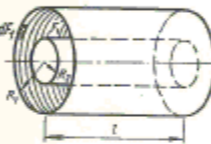
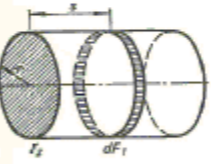
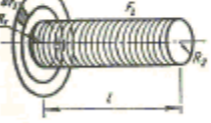
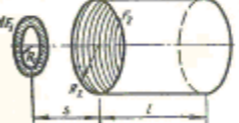
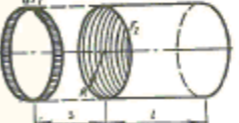
	<p>Two annular elements on the inside surface of a right circular cylinder</p> $d\varphi_{dF_1-dF_2} = \frac{1}{2R} \left[1 - \frac{s(s^2+6R^2)}{(s^2+4R^2)^{3/2}} \right] ds$	[47]
	<p>Two annular elements on the inside surface of a right circular cone</p> $d\varphi_{dF_1-dF_2} = \frac{\cos^2 \alpha}{2h_1 \sin \alpha} \left\{ 1 - h_1 - h_2 \frac{(h_1 - h_2)^2 + 6h_1 h_2 \sin^2 \alpha}{[(h_1 - h_2)^2 + 4h_1 h_2 \sin^2 \alpha]^{3/2}} \right\} dh_2$	[136]
	<p>Two infinitesimal elements on the inside surface of a spherical cavity</p> $d\varphi_{dF_1-dF_2} = \frac{dF_2}{4\pi R^2}$	[137]

Table 2.2 (continued)

Geometric structure	Design equation	References
	<p>Plane element and ellipse parallel to it</p> $\varphi_{dF_1-F_2} = \frac{ab}{\sqrt{(s^2+a^2)(s^2+b^2)}}$	[47]
	<p>Elementary strip and infinite-length cylinder parallel to it</p> $\varphi_{dF_1-F_2} = \frac{sR}{a^2+s^2}$	[129]
	<p>Element on the inside surface of the outer cylinder and the inside surface of the same cylinder for a system of two coaxial cylinders</p> $\varphi_{dF_1-F_2} = \frac{1}{2} \frac{R_2 + R_1}{4R_1 + \pi R_1} \times \left[\frac{l}{R_2} \operatorname{arctg} \frac{\sqrt{R_1^2 - R_2^2}}{R_2} - \frac{1}{2} \operatorname{arctg} \frac{l^2 - 4(R_1^2 - R_2^2)}{4l\sqrt{R_1^2 - R_2^2}} - \frac{l^2 + 2R_1^2}{R_2\sqrt{l^2 + 4R_1^2}} \times \operatorname{arctg} \frac{\sqrt{(R_1^2 - R_2^2)(l^2 + 4R_1^2)}}{R_2 l} \right]$	[129]
	<p>Annular element on the inside surface of a right circular cylinder and the end face of the cylinder</p> $\varphi_{dF_1-F_2} = \frac{1}{2R} \left[\frac{s^2 + 2R^2}{\sqrt{s^2 + 4R^2}} - s \right]$ <p><i>Handwritten note:</i> $\int dF_2 = dF_2 = \frac{1}{R^2} \left[\frac{s^2 + 2R^2}{\sqrt{s^2 + 4R^2}} - s \right] ds$</p>	[47]
	<p>Element of a plane ring and outside surface of a right circular cylinder</p> $\varphi_{dF_1-F_2} = \frac{1}{\pi} \left[\frac{1}{2} \arccos \frac{R_2}{R_1} + \operatorname{arctg} \frac{R_2}{\sqrt{R_1^2 - R_2^2}} - \frac{l^2 + R_1^2 - R_2^2}{A} \times \operatorname{arctg} \frac{A \operatorname{tg} [(1/2) \arccos (R_2/R_1)]}{l^2 + R_1^2 + R_2^2 - 2R_1 R_2} \right]$ $A = \sqrt{(l^2 + R_1^2 + R_2^2)^2 - 4R_1^2 R_2^2}$	[137]
	<p>Plane annular element and inside surface of a cylinder</p> $\varphi_{dF_1-F_2} = \frac{1}{2} \left[\frac{(l+s)^2 + R_1^2 - R_2^2}{\sqrt{[(l+s)^2 + R_1^2 + R_2^2]^2 - 4R_1^2 R_2^2}} - \frac{s^2 + R_1^2 - R_2^2}{\sqrt{(s^2 + R_1^2 + R_2^2)^2 - 4R_1^2 R_2^2}} \right]$	[126]
	<p>Annular cylindrical element and inside surface of a cylinder</p> $\varphi_{dF_1-F_2} = \frac{1}{2R} \left[1 + \frac{s^2 + 2R^2}{\sqrt{s^2 + 4R^2}} - \frac{(l+s)^2 + 2R^2}{\sqrt{(l+s)^2 + 4R^2}} \right]$	[126]

DIFFICULTY: CONDUCTANCE

Table 2.2 Equations for calculating the angular coefficients

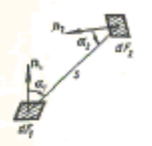

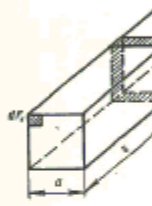
Geometric structure	Design equation	References
	<p>I. Two infinitesimal elements</p> <p>Two arbitrarily oriented elementary areas</p> $d\varphi_{dF_1-dF_2} = \frac{\cos \alpha_1 \cos \alpha_2}{\pi s^2} dF_2$	[47]
	<p>Two strips of finite length and infinitesimal width with parallel generatrices</p> $d\varphi_{dF_1-dF_2} = \frac{1}{\pi} \cos \alpha \operatorname{arctg} \frac{a}{s} dx$	[47]
	<p>End-face element of a channel with a square cross section, located in a corner, and a channel surface element</p> $d\varphi_{dF_1-dF_2} = \frac{as}{\pi(a^2+s^2)^{3/2}} \left[\operatorname{arctg} \frac{a}{\sqrt{a^2+s^2}} + \operatorname{arctg} \frac{a\sqrt{a^2+s^2}}{s^2+2a^2} \right] ds$	[47]

Table 2.2 (continued)



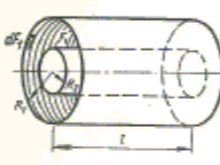
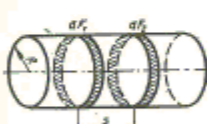
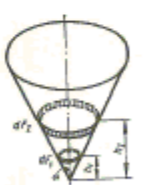


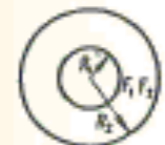
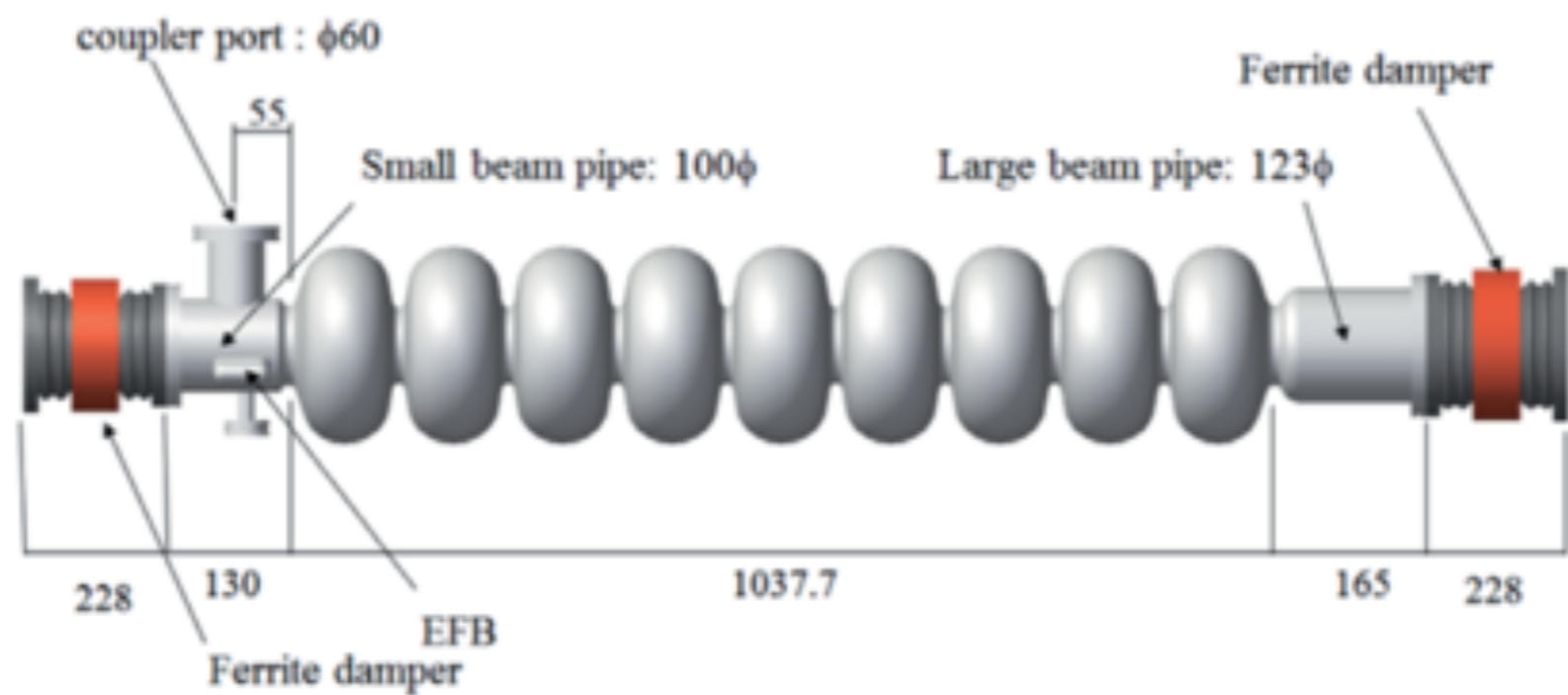
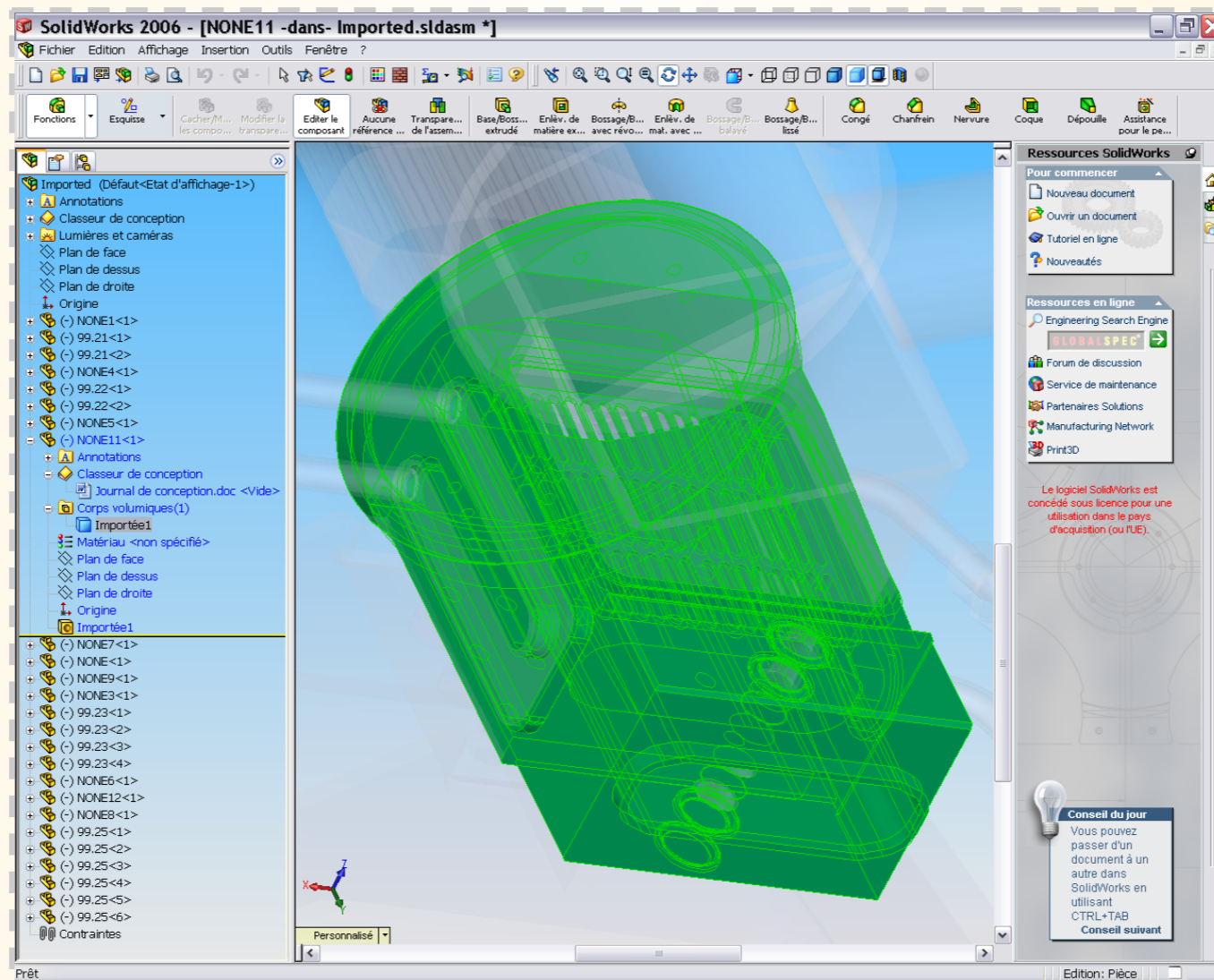
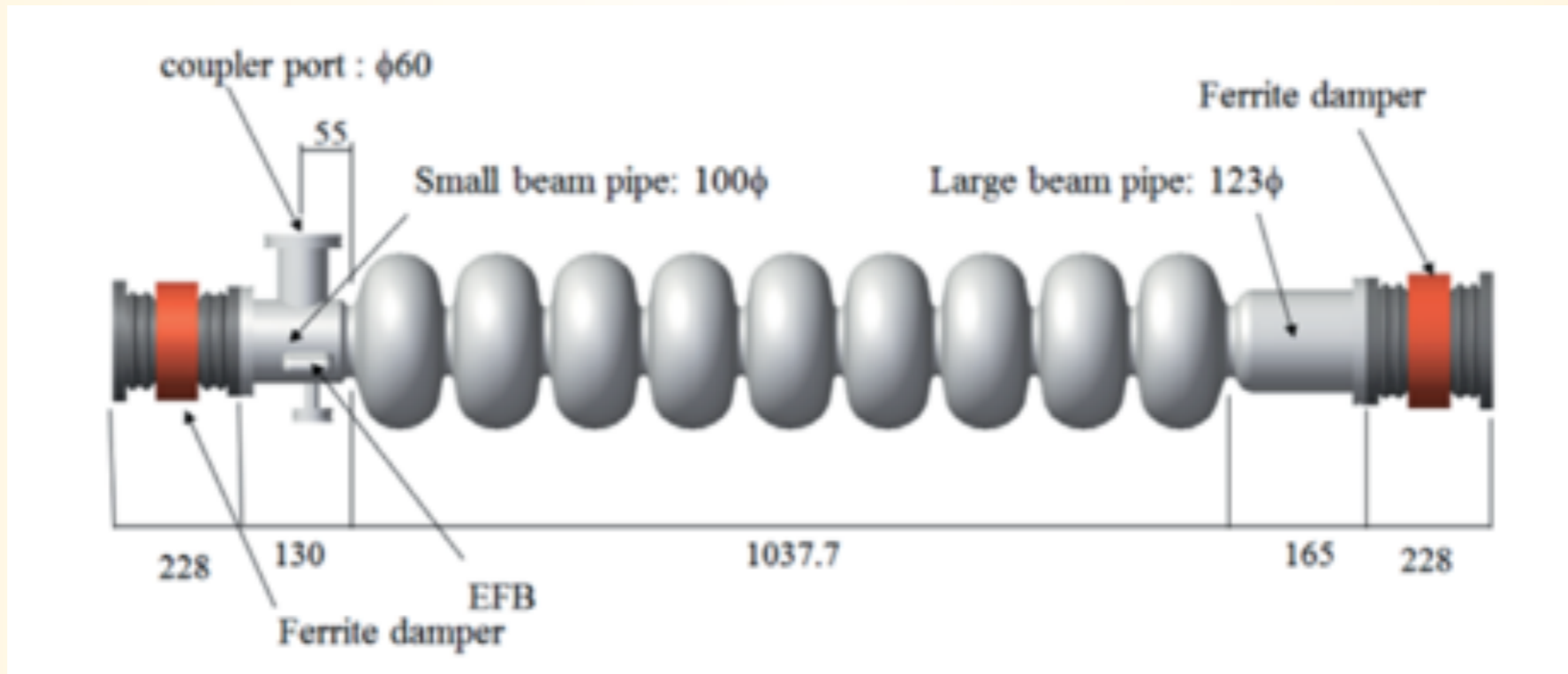
Geometric structure	Design equation	References
	<p>Plane element and ellipse parallel to it</p> $\varphi_{dF_1-F_2} = \frac{ab}{\sqrt{(s^2+a^2)(s^2+b^2)}}$	[47]
	<p>Elementary strip and infinite-length cylinder parallel to it</p> $\varphi_{dF_1-F_2} = \frac{2R}{a^2+s^2}$	[129]
	<p>Element on the inside surface of the outer cylinder and the inside surface of the same cylinder for a system of two coaxial cylinders</p> $\varphi_{dF_1-F_2} = \frac{1}{2} \frac{R_2 + R_1}{4R_1 + \pi R_1} \times \left[\frac{l}{R_2} \operatorname{arctg} \frac{\sqrt{R_1^2 - R_2^2}}{R_2} - \frac{1}{2} \operatorname{arctg} \frac{l^2 - 4(R_1^2 - R_2^2)}{4l\sqrt{R_1^2 - R_2^2}} - \frac{l^2 + 2R_1^2}{R_2\sqrt{l^2 + 4R_1^2}} \times \operatorname{arctg} \frac{\sqrt{(R_1^2 - R_2^2)(l^2 + 4R_1^2)}}{R_2 l} \right]$	[129]

Table 2.2 (continued)

Geometric structure	Design equation	References
	<p>Two coaxial cylinders</p> $\varphi_{21} = \frac{R_1}{R_2} - \frac{R_1}{\pi R_2} \left\{ \operatorname{arccos} \frac{B}{A} - \frac{1}{2lR_2} \left[\sqrt{(A+2R_1^2)^2 - 4R_1^2 R_2^2} \right. \right. \\ \left. \left. \times \operatorname{arccos} \frac{R_1 B}{R_2 A} + B \operatorname{arcsin} \frac{R_1}{R_2} - \frac{\pi A}{2} \right] \right\}$ <p>$A = l^2 + R_2^2 - R_1^2; B = l^2 - R_2^2 + R_1^2;$</p>	[103]
	<p>Two annular elements</p> $d\varphi_{dF_1-dF_2} = \frac{\cos \alpha}{2h_1}$	[137]
	<p>Two infinitesimal elements</p> $d\varphi_{dF_1-dF_2} = \frac{dF_1}{4\pi h}$	[126]
	<p>Inside surface and end-faces of a truncated cone</p> $\varphi_{21} = \frac{\sqrt{(h^2 + R_1^2 + R_2^2)^2 - 4R_1^2 R_2^2} - (h^2 - R_1^2 + R_2^2)}{2(R_1 + R_2)\sqrt{h^2 + (R_1 - R_2)^2}}$ $\varphi_{22} = 1 - \frac{\sqrt{(h^2 + R_1^2 + R_2^2)^2 - 4R_1^2 R_2^2} - h^2}{(R_1 + R_2)\sqrt{h^2 + (R_1 - R_2)^2}}$	[136]
	<p>Two coaxial cylinders of infinite length</p> $\varphi_{12} = 1; \varphi_{21} = \frac{R_1}{R_2}; \varphi_{22} = 1 - \frac{R_1}{R_2}$	[47]

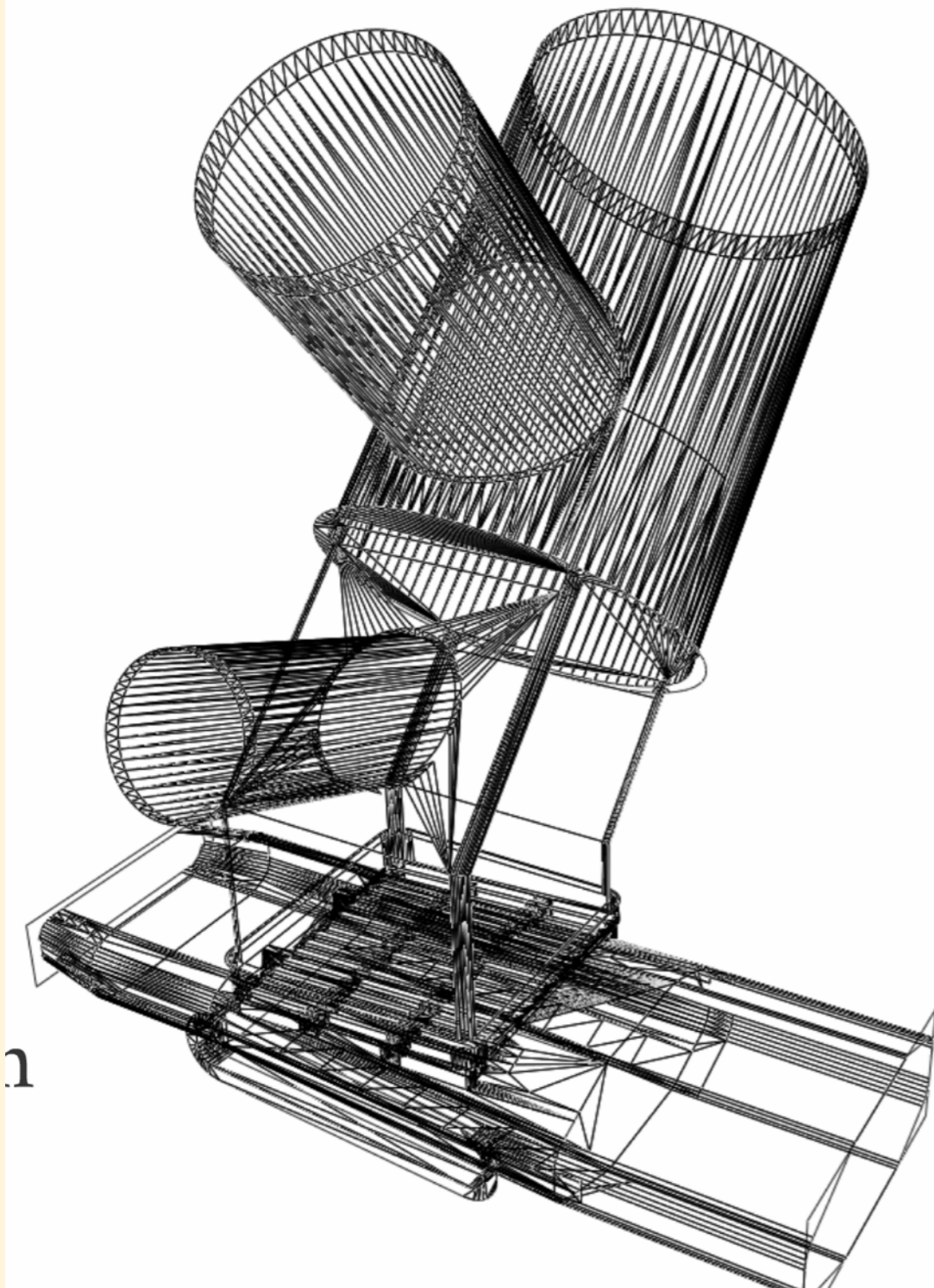
to end face
 $\left. \begin{matrix} [103] \\ \frac{+2R^2}{l^2+4R^2} - 5 \end{matrix} \right\} \Delta S$





MC SIMULATIONS

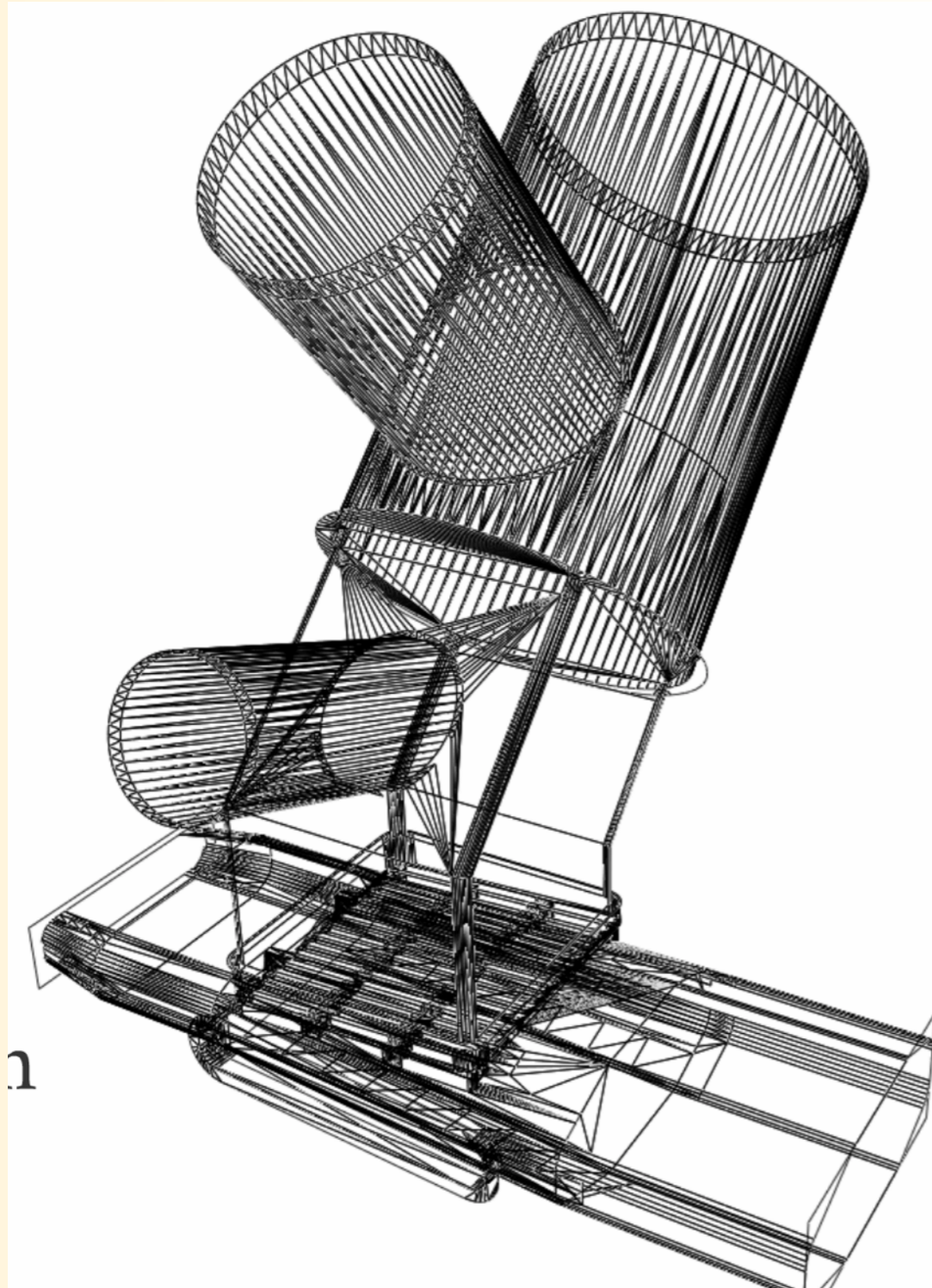
Geometry: polygons



MC SIMULATIONS

Geometry: polygons

Gas input:



$$pV=NkT$$

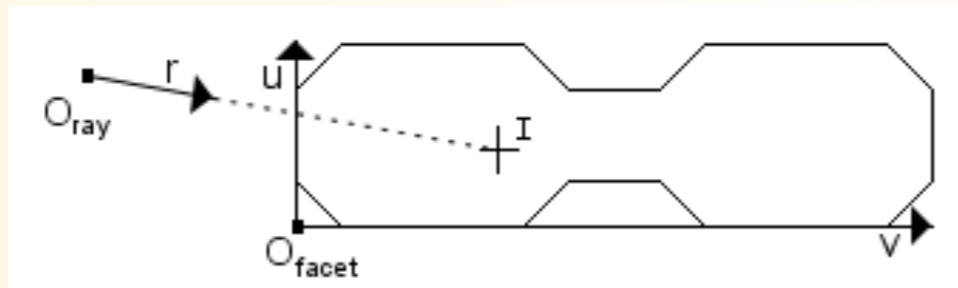
$$1 \text{ Pa} \cdot \text{m}^3/\text{s} = 2.4 \cdot 10^{20} \text{ molecules/s}$$

Virtual / Physical particle ratio

Ray tracing

Ray-plane intersection:

- Use Cramer's rule to find I coordinates.
- $\vec{w} = \vec{u} \wedge \vec{v}$ is **pre-calculated once** for each facet.
- Faster to solve I_u and I_v first (best elimination method than solving distance I_r first).



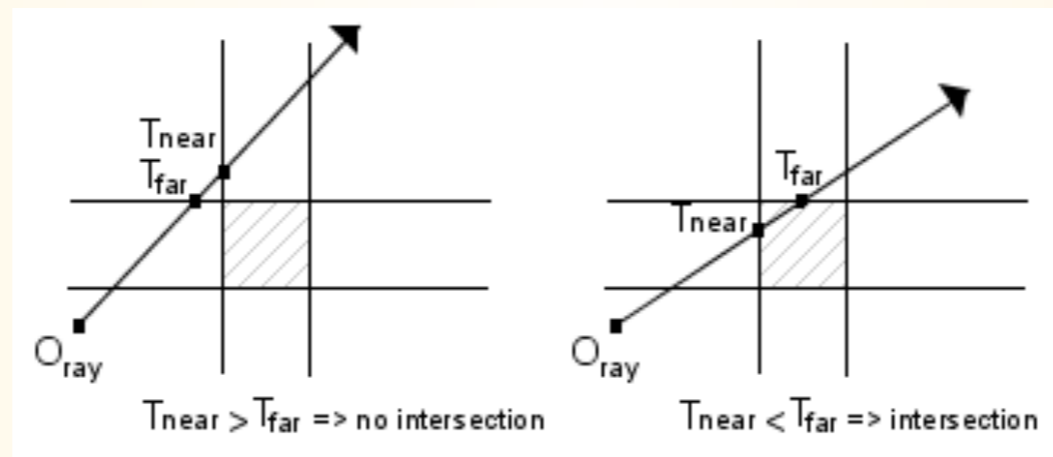
$$I_u = \frac{(\vec{O}_{fr} \wedge \vec{v}) \cdot \vec{r}}{\vec{w} \cdot \vec{r}} \in [0,1]$$

$$I_v = \frac{(\vec{u} \wedge \vec{O}_{fr}) \cdot \vec{r}}{\vec{w} \cdot \vec{r}} \in [0,1]$$

$$I_r = -\frac{\vec{w} \cdot \vec{O}_{fr}}{\vec{w} \cdot \vec{r}} > 0$$

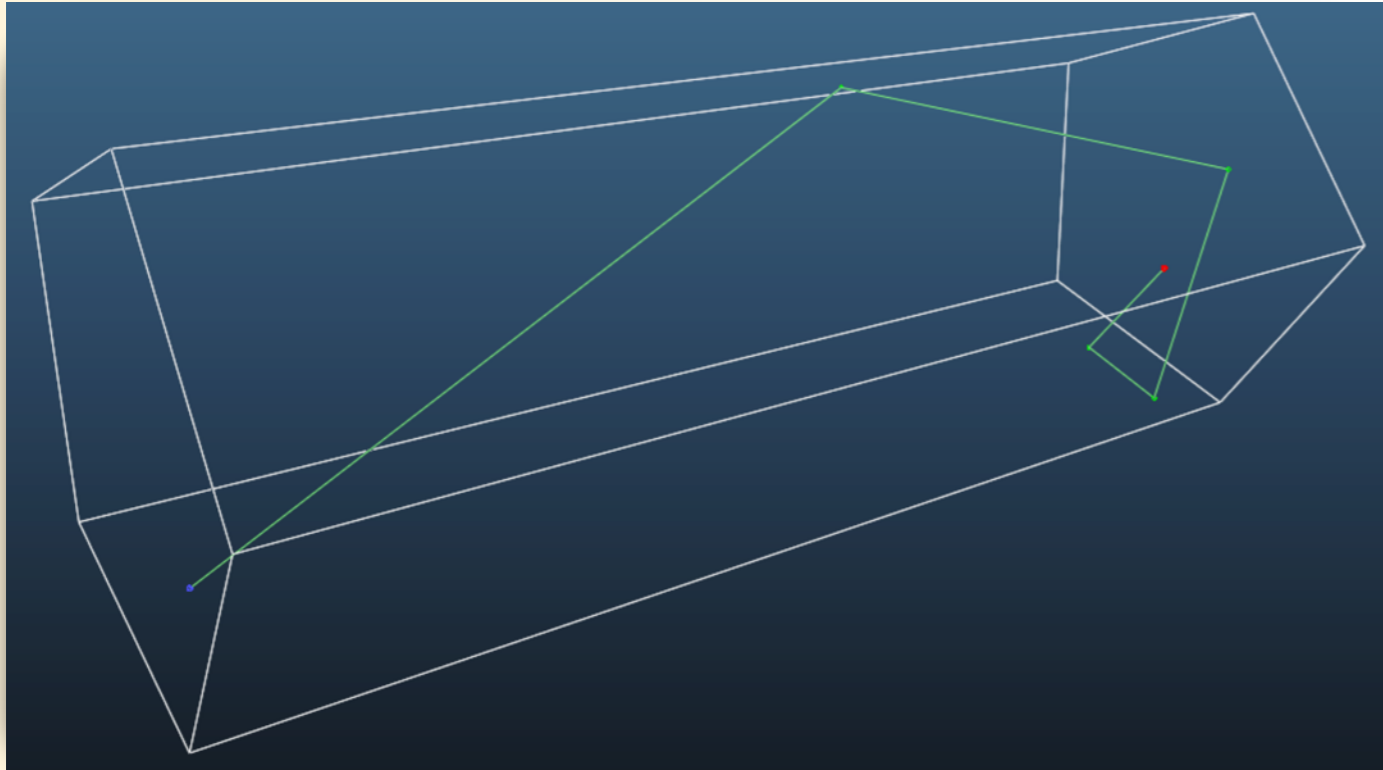
AABB Tree optimisation:

- Use of “**Axis Aligned Bounding Box**” tree structure to speed collision detection
- Box/ray intersection performed using the “**slabs method**”

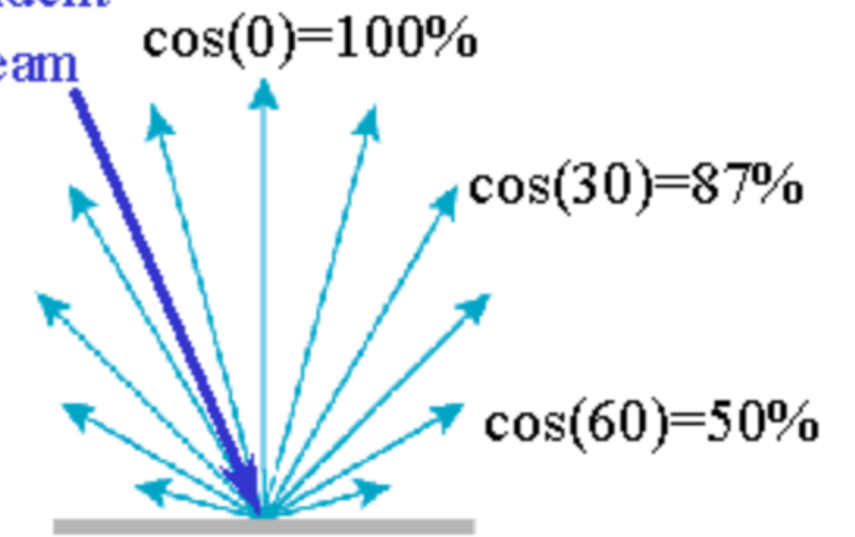


- Minimum of **8 facets per box** and maximum **tree depth of 5** (using “**best axis**” method for **AABB tree balancing**)
- Result: **more than 5 times faster** for complex geometries

Reflection

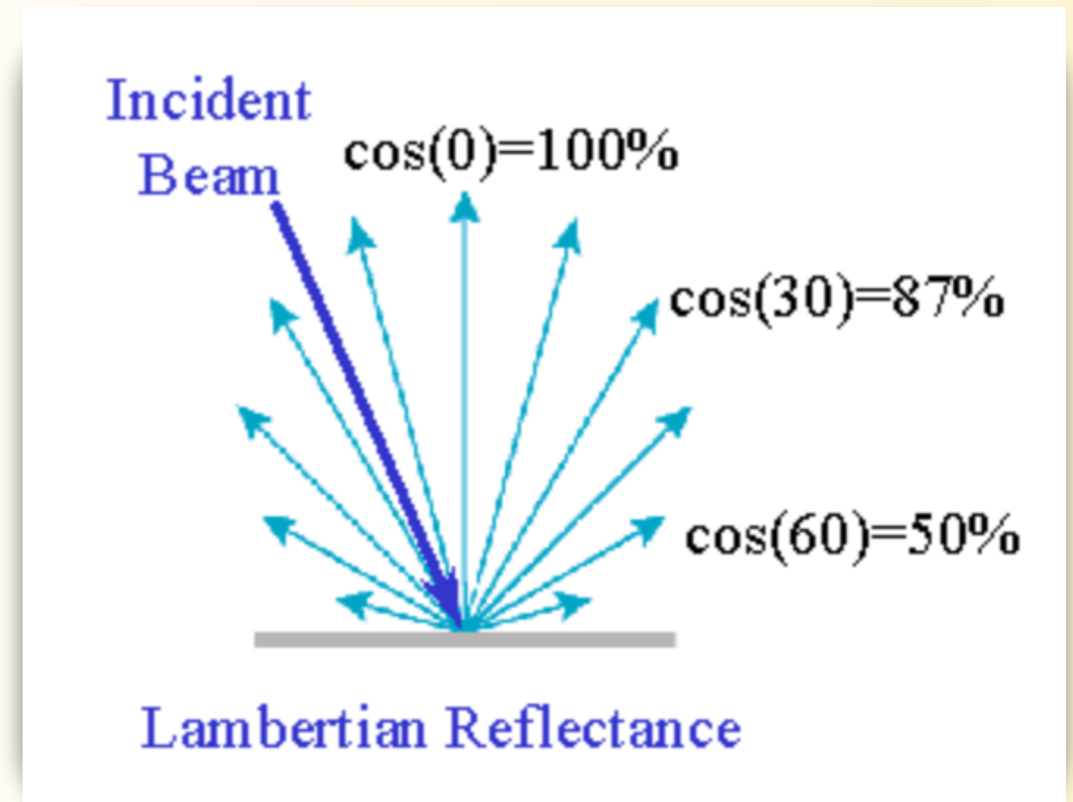
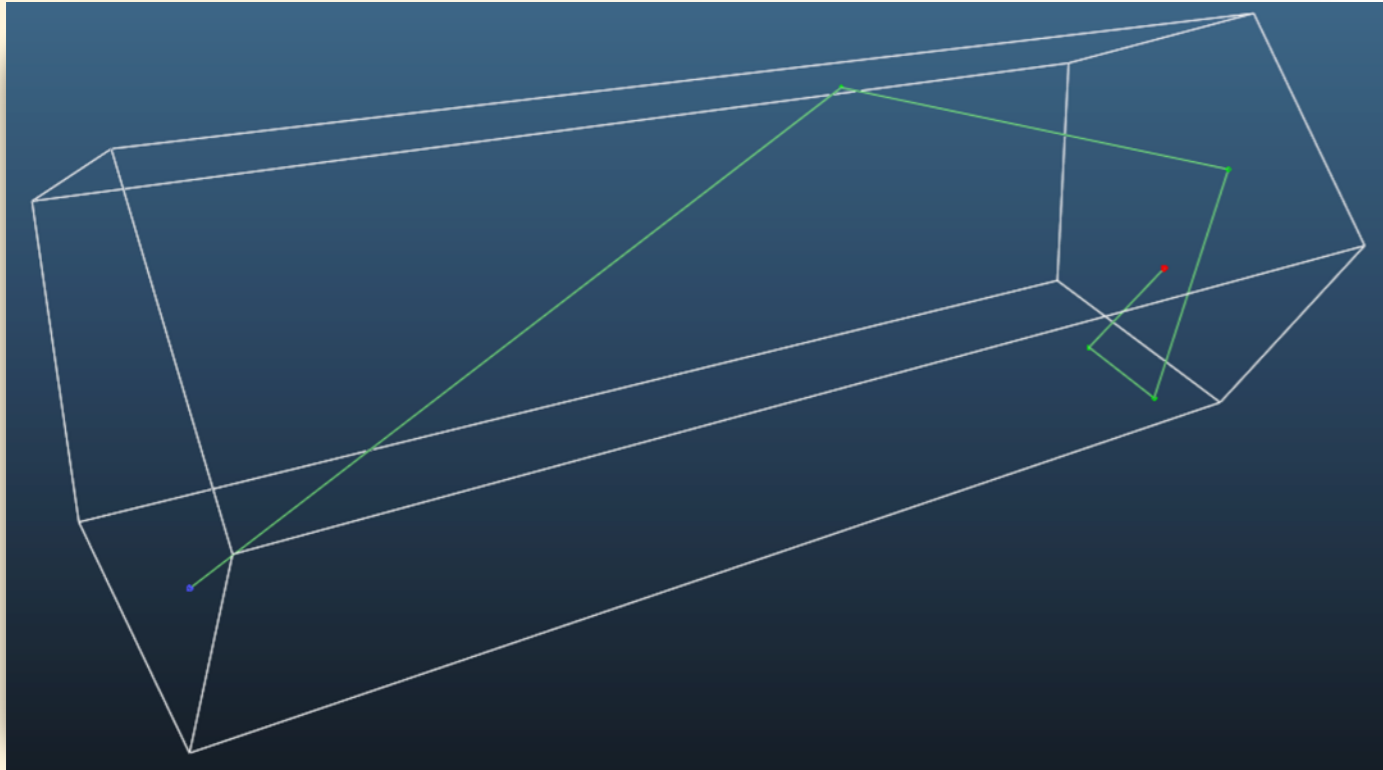


Incident
Beam



Lambertian Reflectance

Reflection

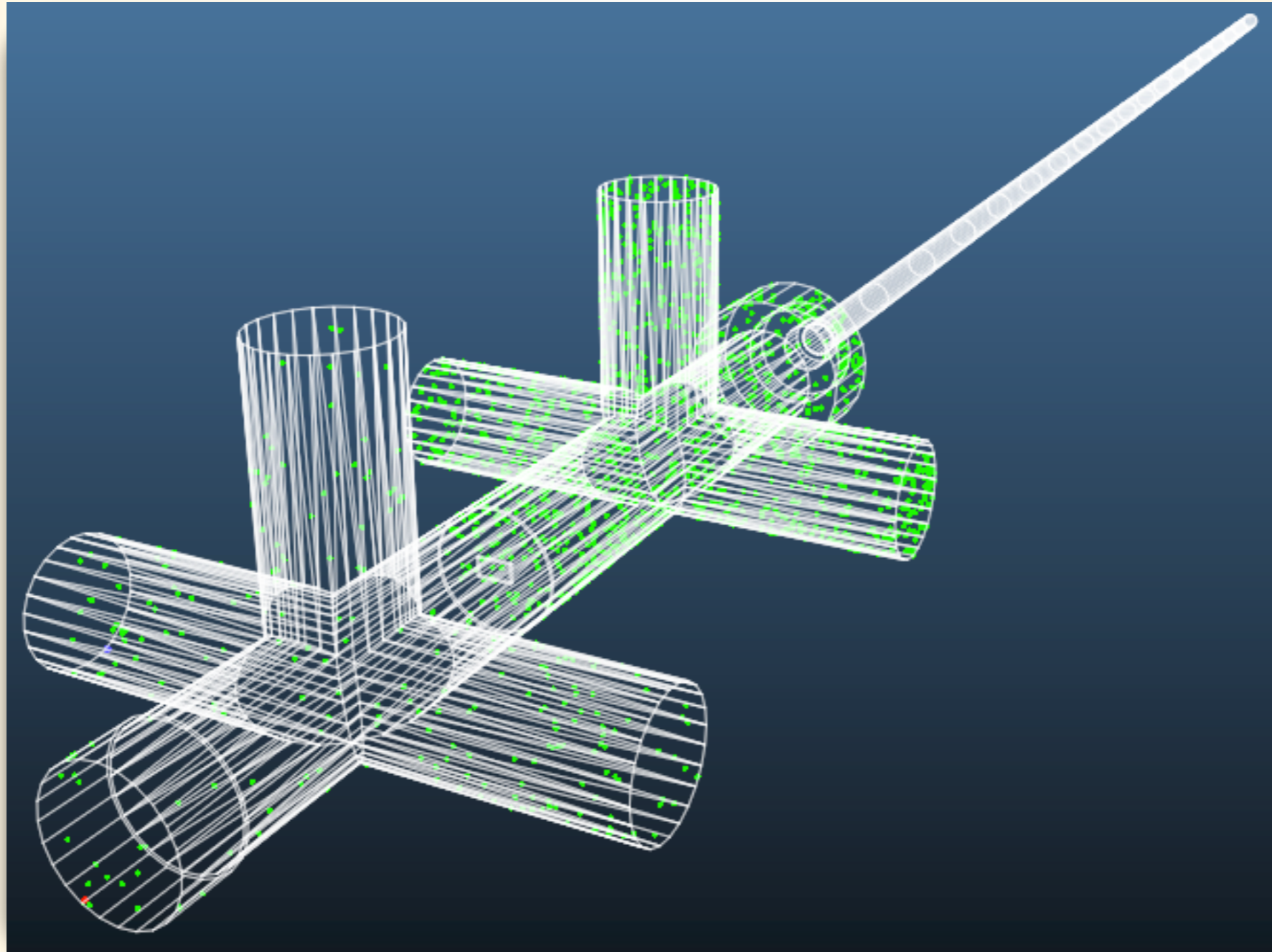


Pumping / absorption

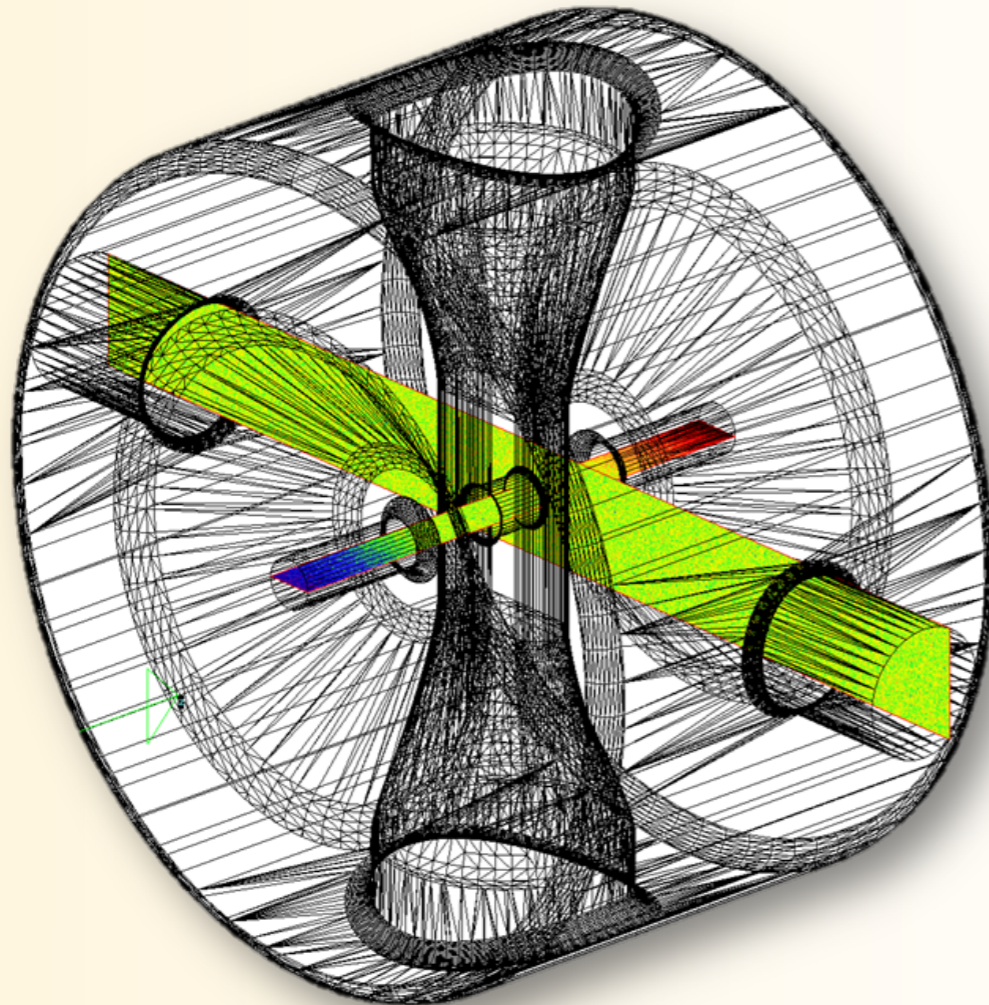


$$S \text{ [m}^3\text{/s]} = \text{sticking [0..1]} * 1/4 * A \text{ [m}^2\text{]} * v_{\text{avg}} \text{ [m/s]}$$

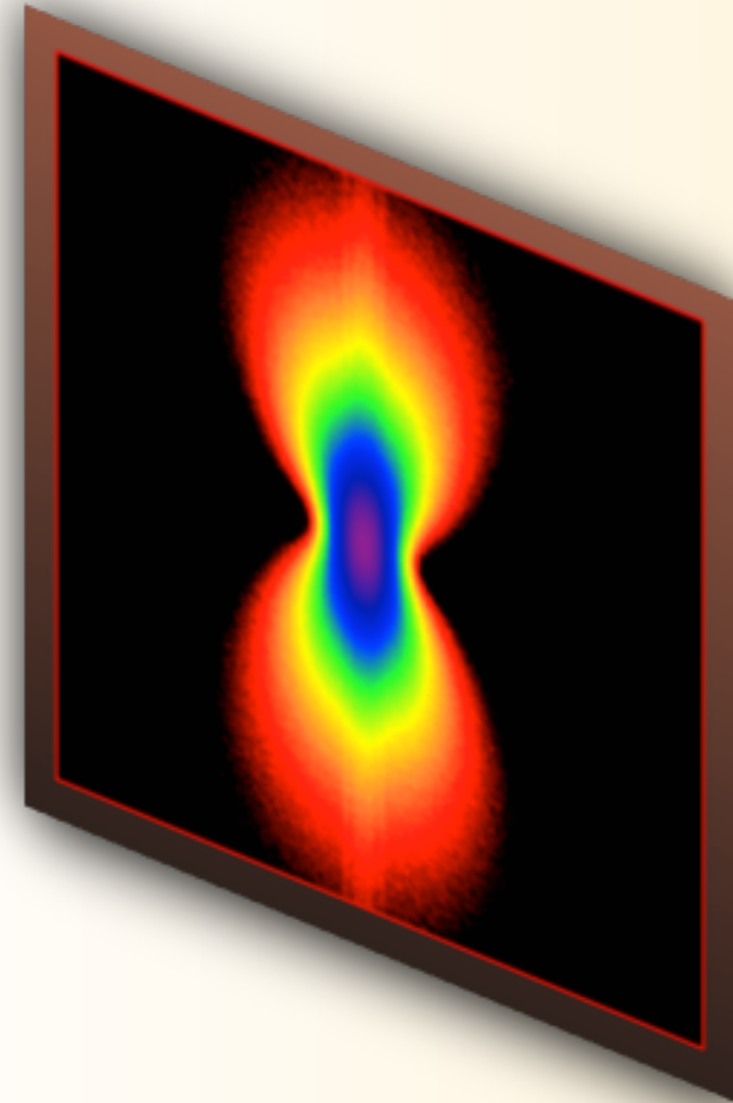
Collecting statistics



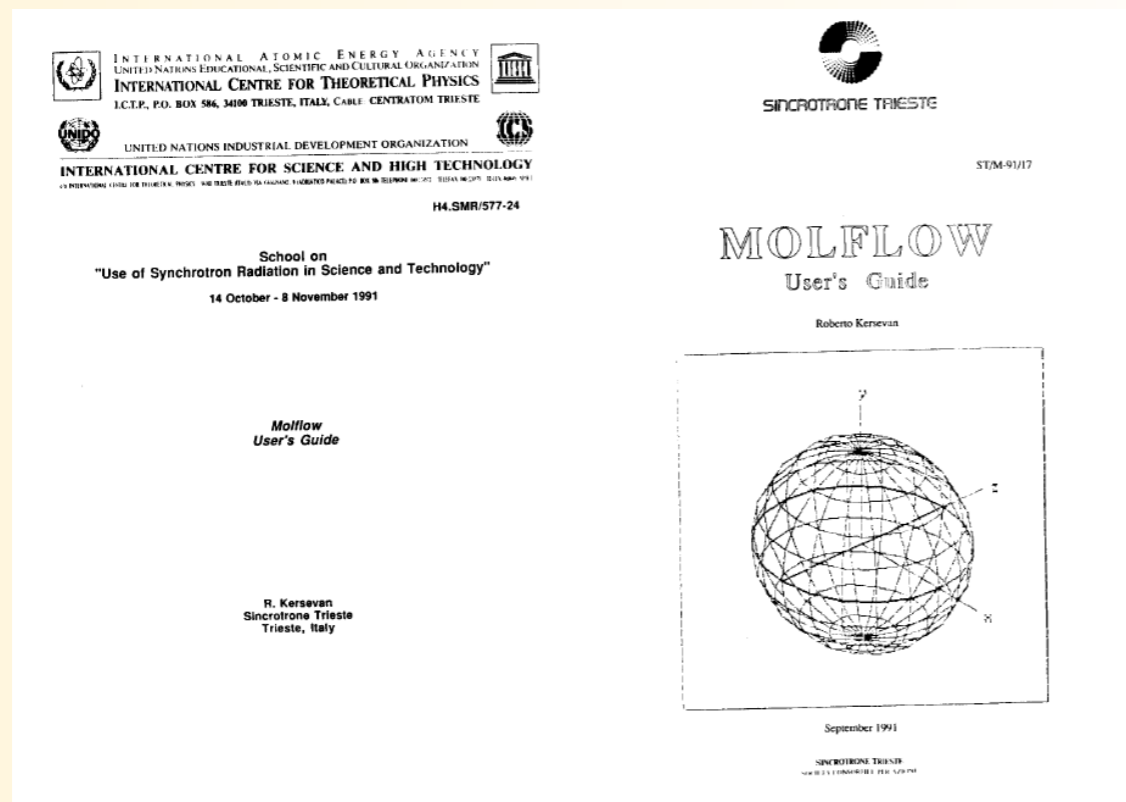
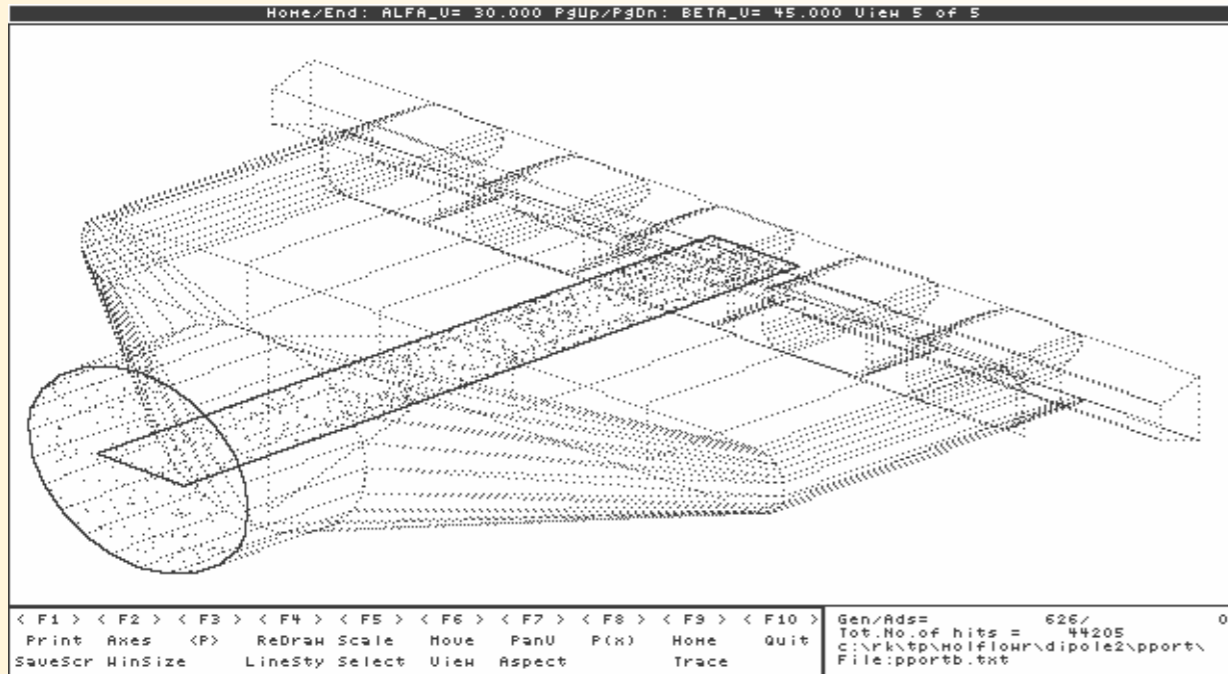
MolFlow



SynRad

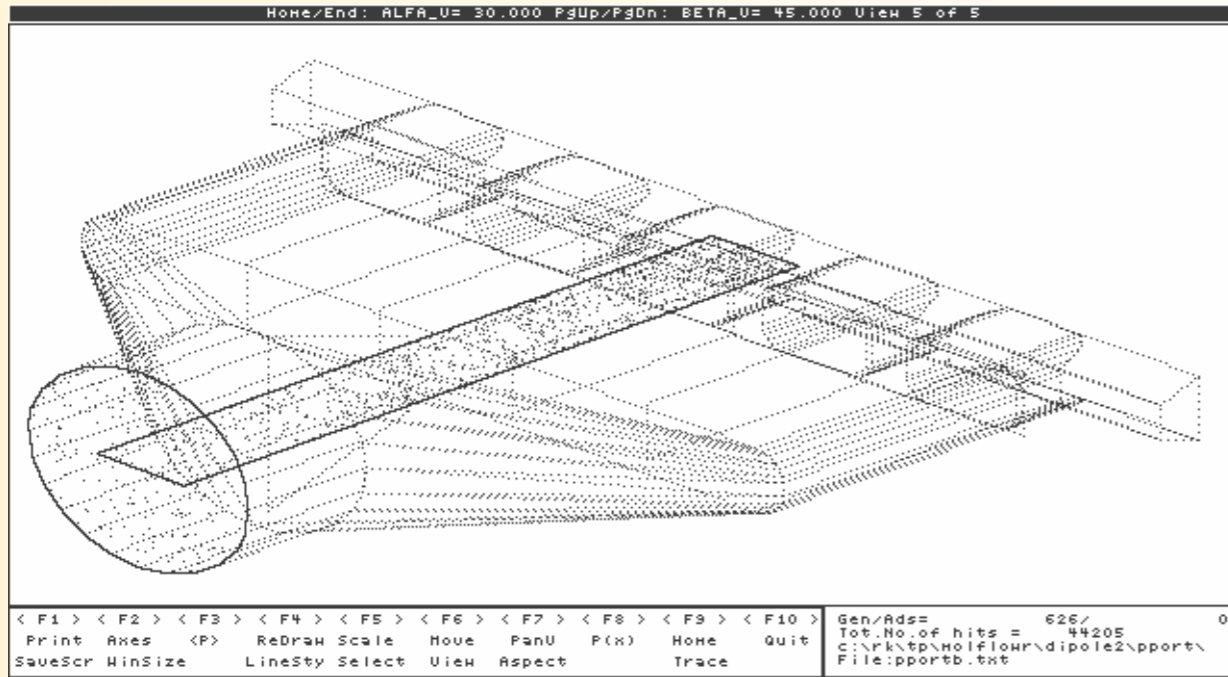


Molflow (1990)

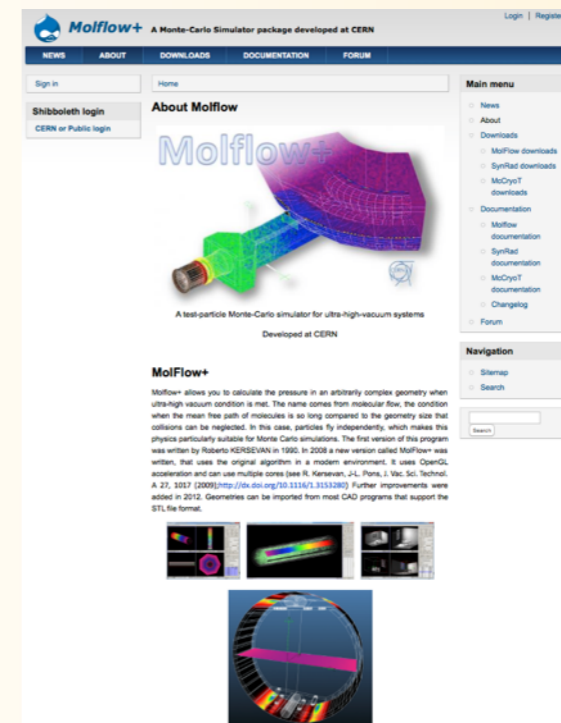
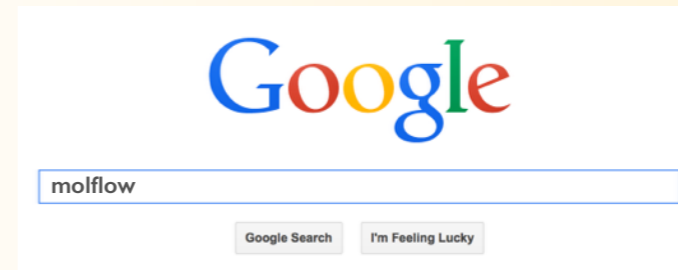
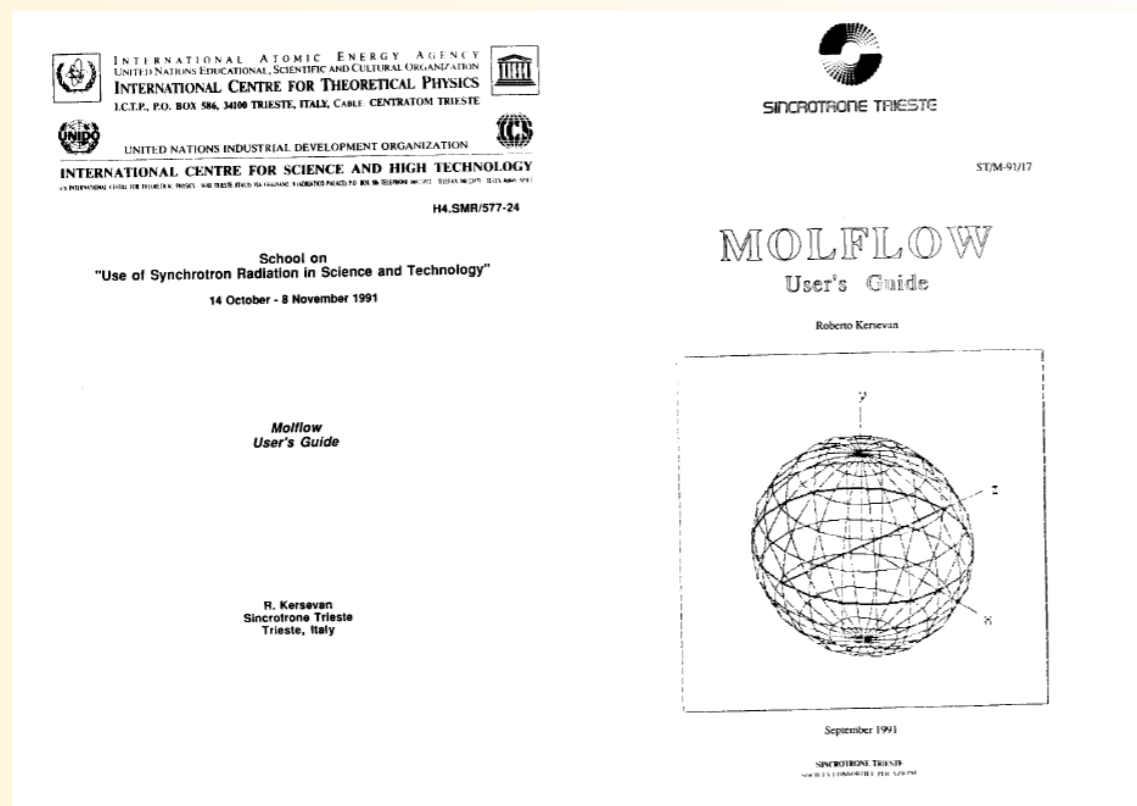
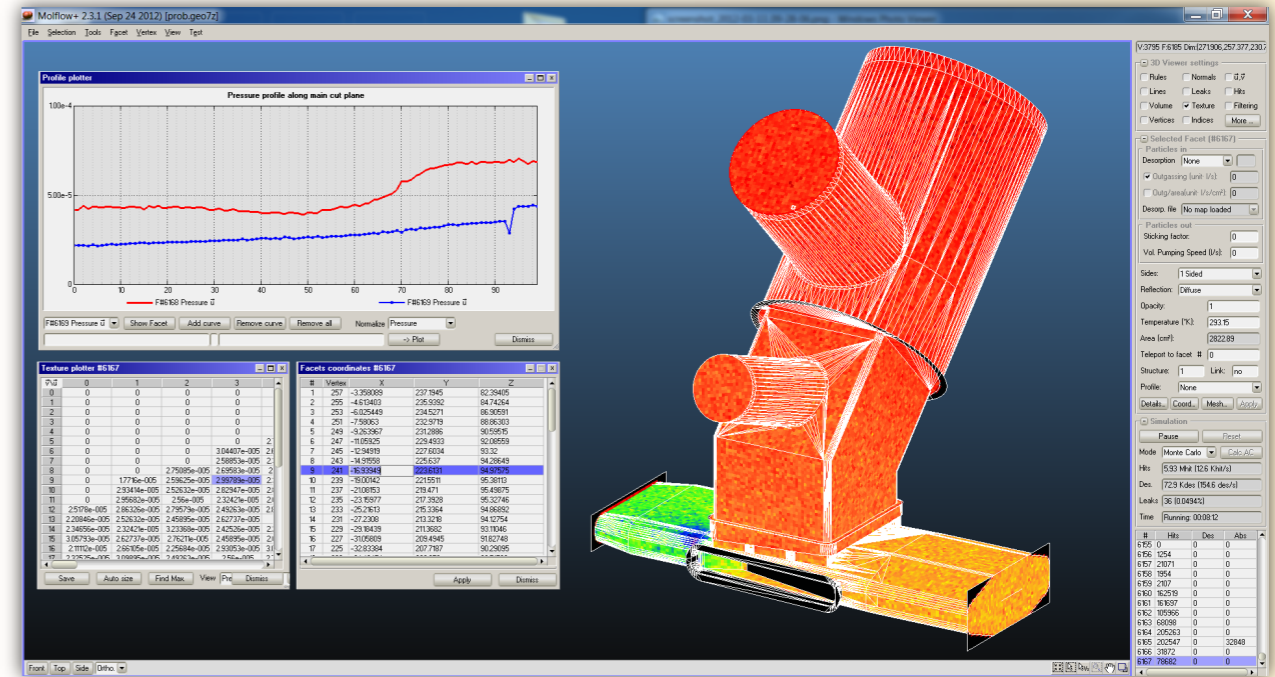


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Molflow (1990)



Molflow+ (2008-)

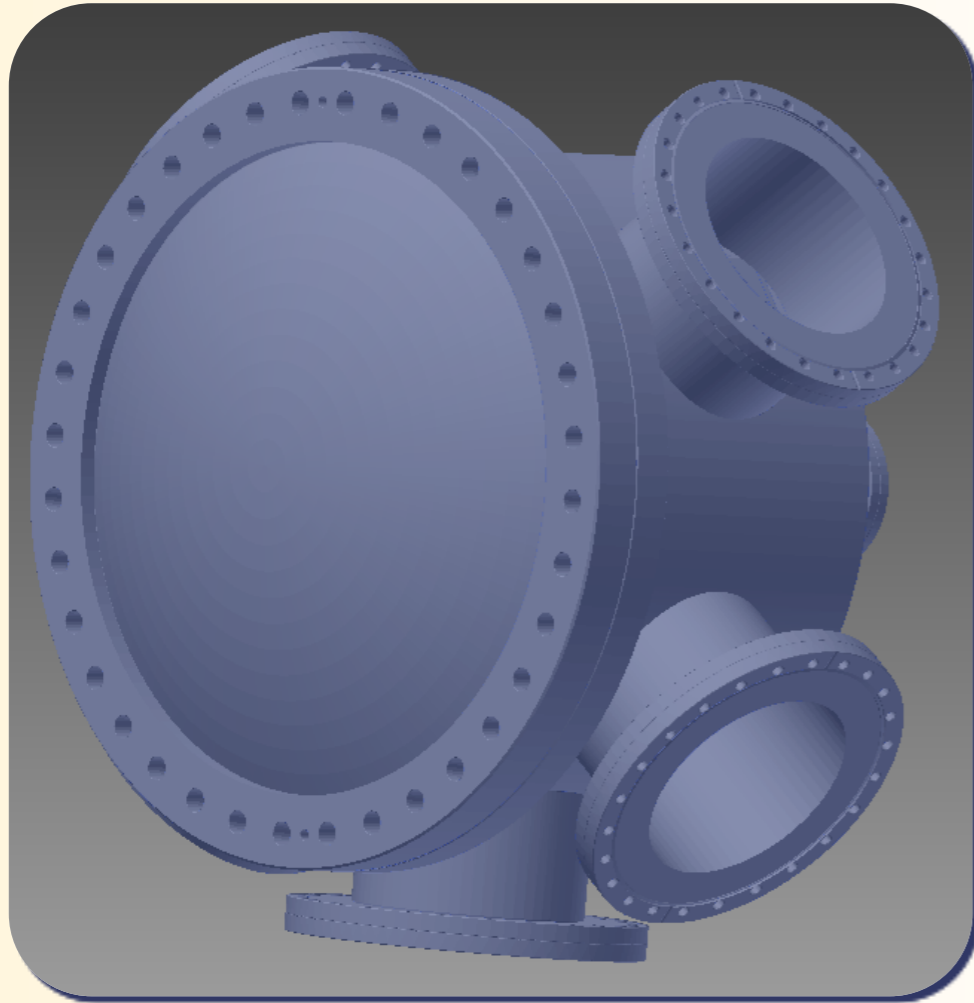


Roberto Kersevan

WORKING WITH MOLFLOW

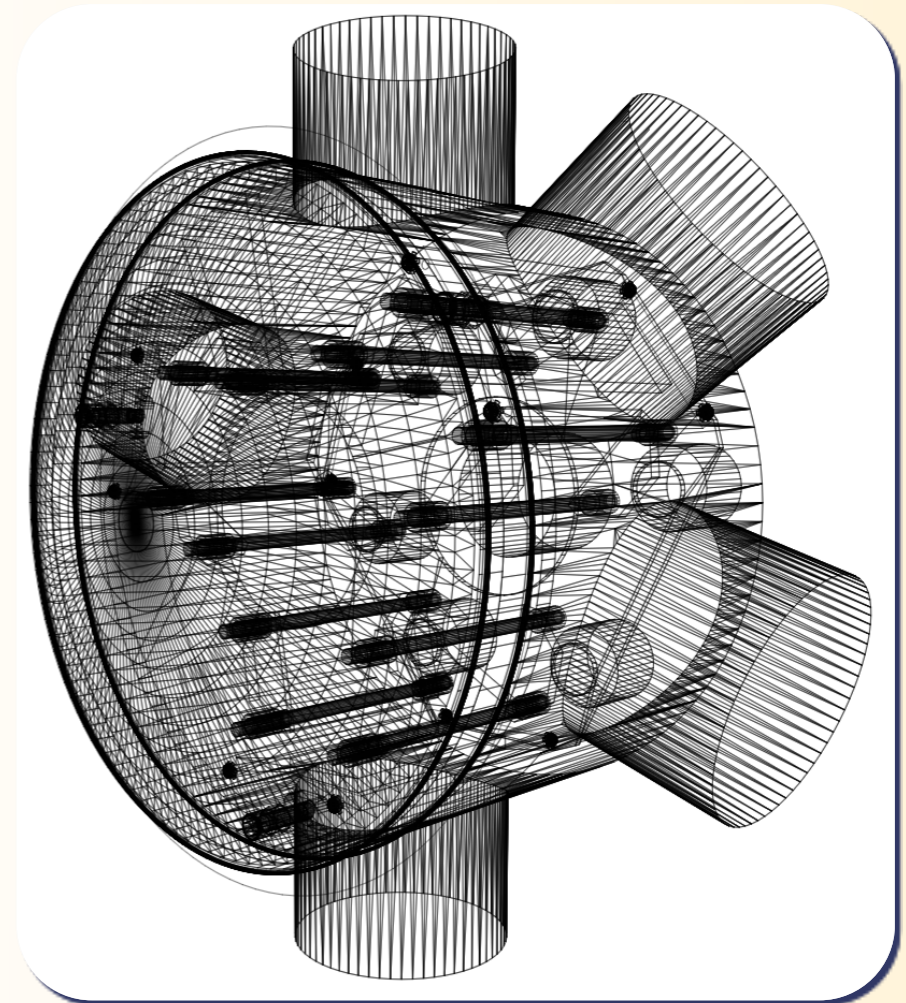
Step 1: creating geometry

CAD



STL format

Molflow+



WORKING WITH MOLFLOW

Step 2: adding physics

The screenshot displays the Molflow+ 2.4.0.2 software interface. The main window is divided into four quadrants showing different views of a 3D model of a chamber with several ports. The top-left view is a wireframe mesh, the top-right is a solid gray model, the bottom-left is a wireframe mesh with blue arrows indicating particle paths, and the bottom-right is a solid gray model with a red circle highlighting a specific facet.

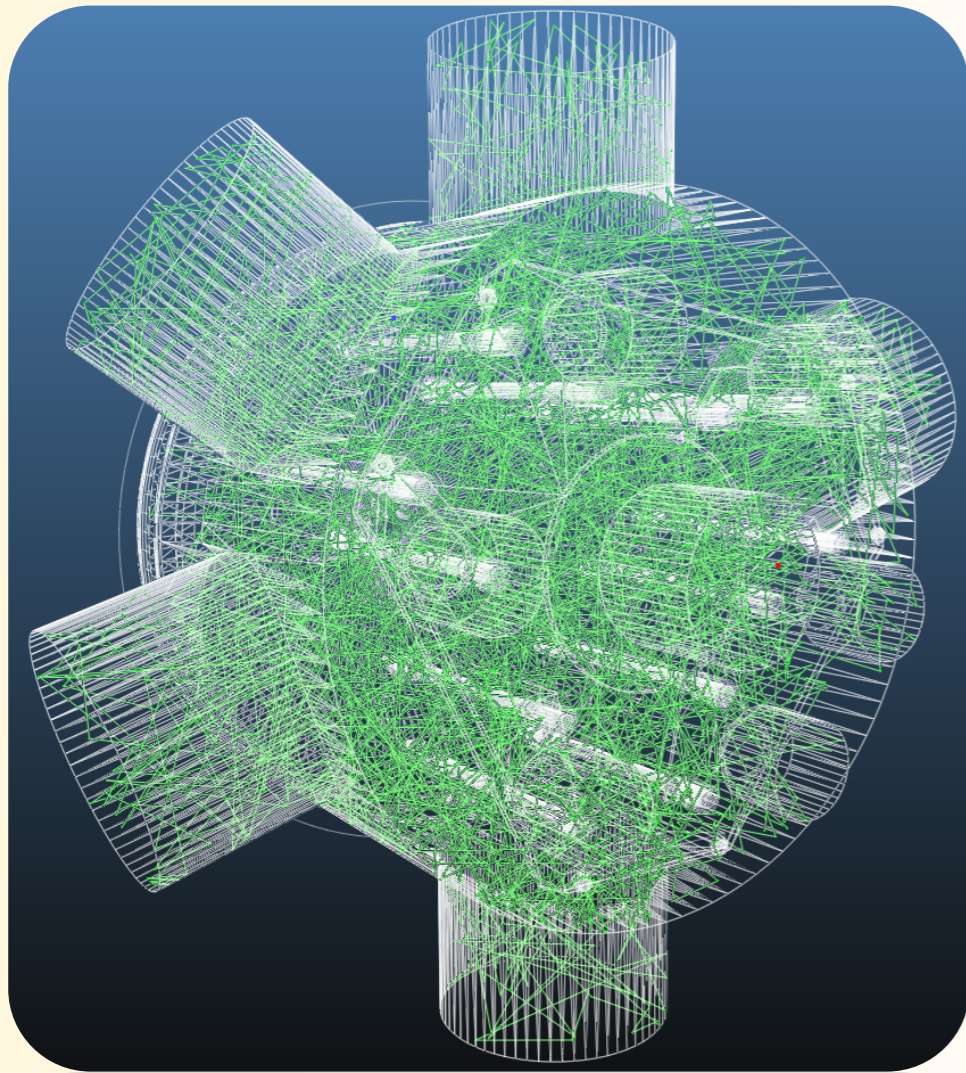
The software window title is "Molflow+ 2.4.0.2 (Jun 5 2013) [ion switch collapsedMODrkHITgt0.geo]". The menu bar includes "File", "Selection", "Tools", "Facet", "Vertex", "View", "Time", and "Test".

The right-hand panel contains the following settings:

- 3D Viewer settings:**
 - Rules
 - Normals
 - \vec{u}, \vec{v}
 - Lines
 - Leaks
 - Hits
 - Volume
 - Texture
 - Filtering
 - Vertices
 - Indices
 - More ...
- Selected Facet (7 selected):**
 - Particles in:
 - Description: Cosine
 - Outgassing (unit: l/s): 2.67598
 - Outg/area (unit: l/s/cm²): 1.333e-C
 - Desorp. file: No map loaded
 - Particles out:
 - Sticking factor: 0
 - Vol. Pumping Speed (l/s): ...
 - Sides: 1 Sided
 - Reflection: Diffuse
 - Opacity: 1
 - Temperature (*K): 293.15
 - Sum Area (cm²): 1065.84
 - Teleport to facet #: 0
 - Structure: 1 Link: no
 - Profile: None
 - Buttons: Details... Coord... Mesh... Apply
- Simulation:**
 - Buttons: Resume, Reset
 - Mode: Monte Carlo Calc AC
 - Hits: 38.7 Khit (0.0 hit/s)
 - Des.: 44 des (0.0 des/s)
 - Q_tot (mbar^l/s): 2.826e-008

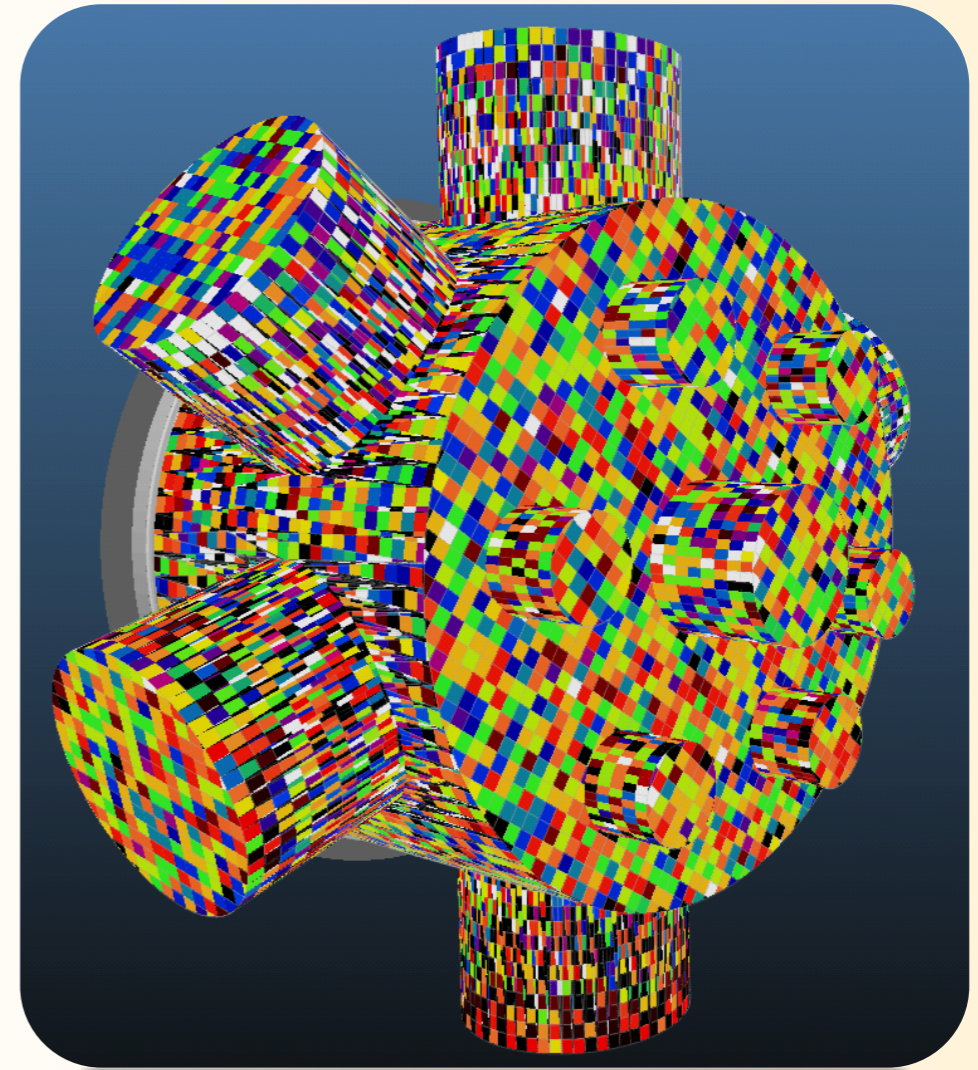
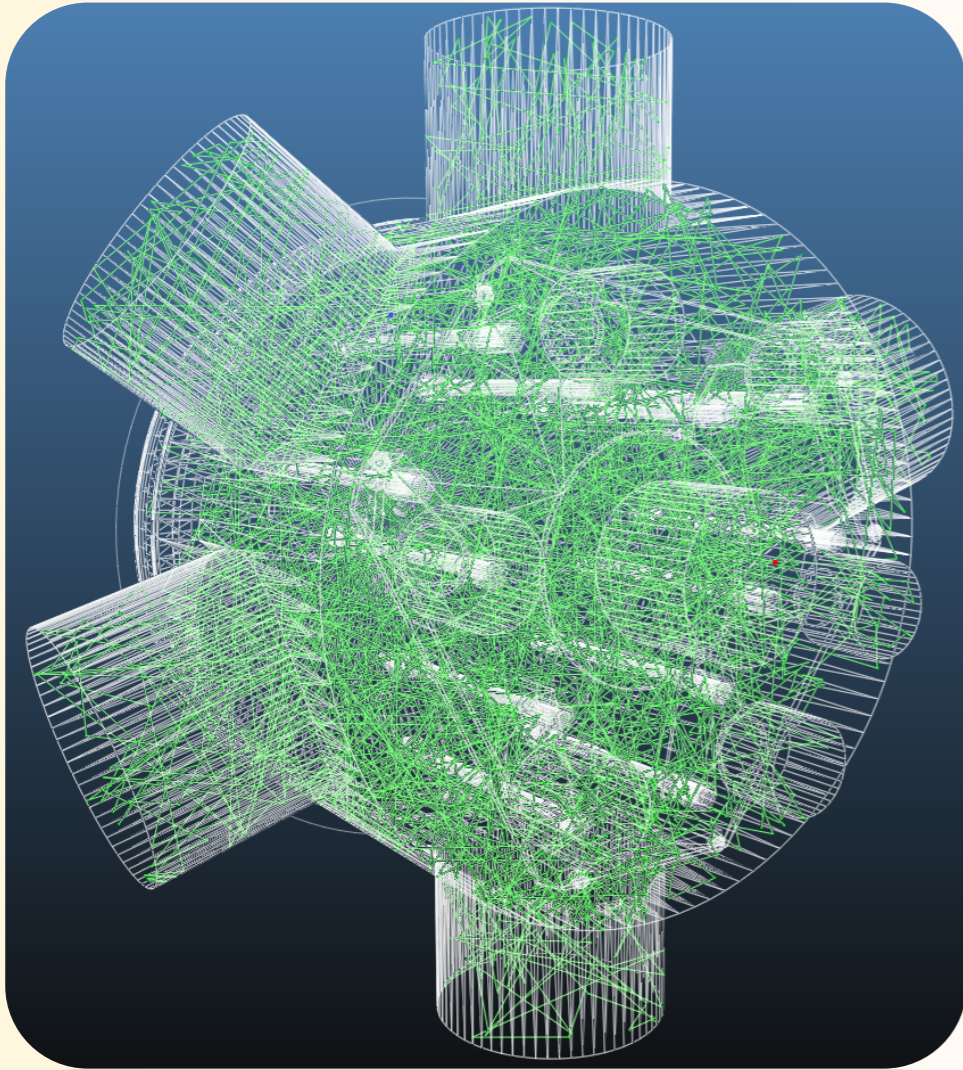
WORKING WITH MOLFLOW

Step 3: simulation and results



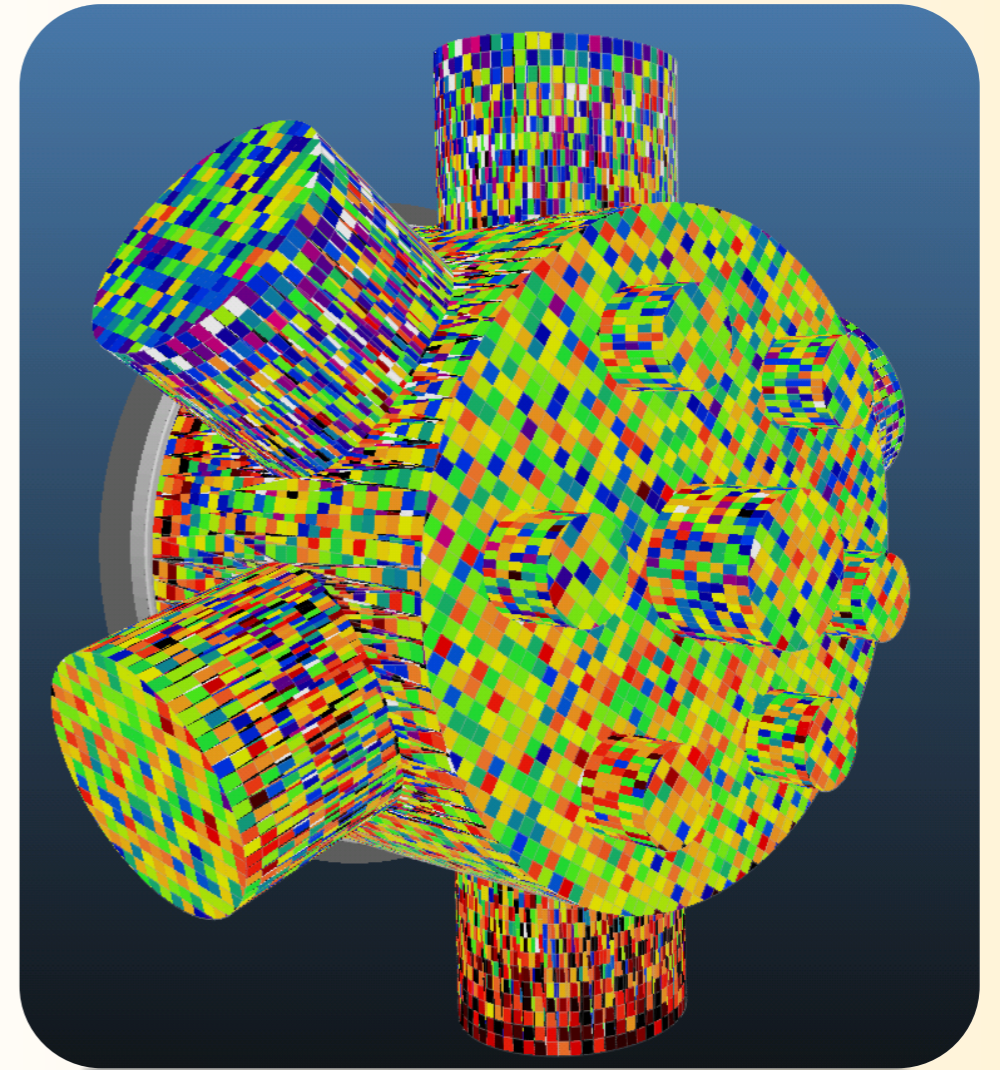
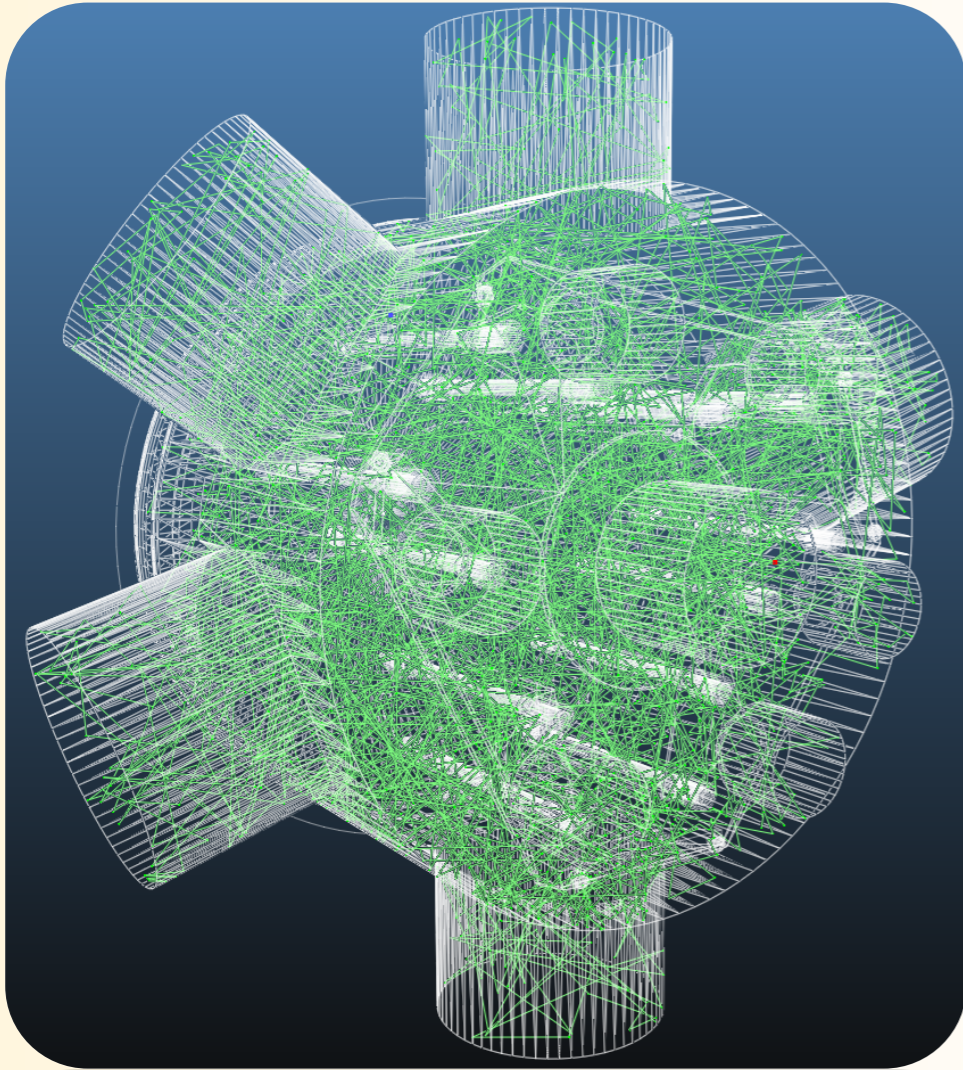
WORKING WITH MOLFLOW

Step 3: simulation and results



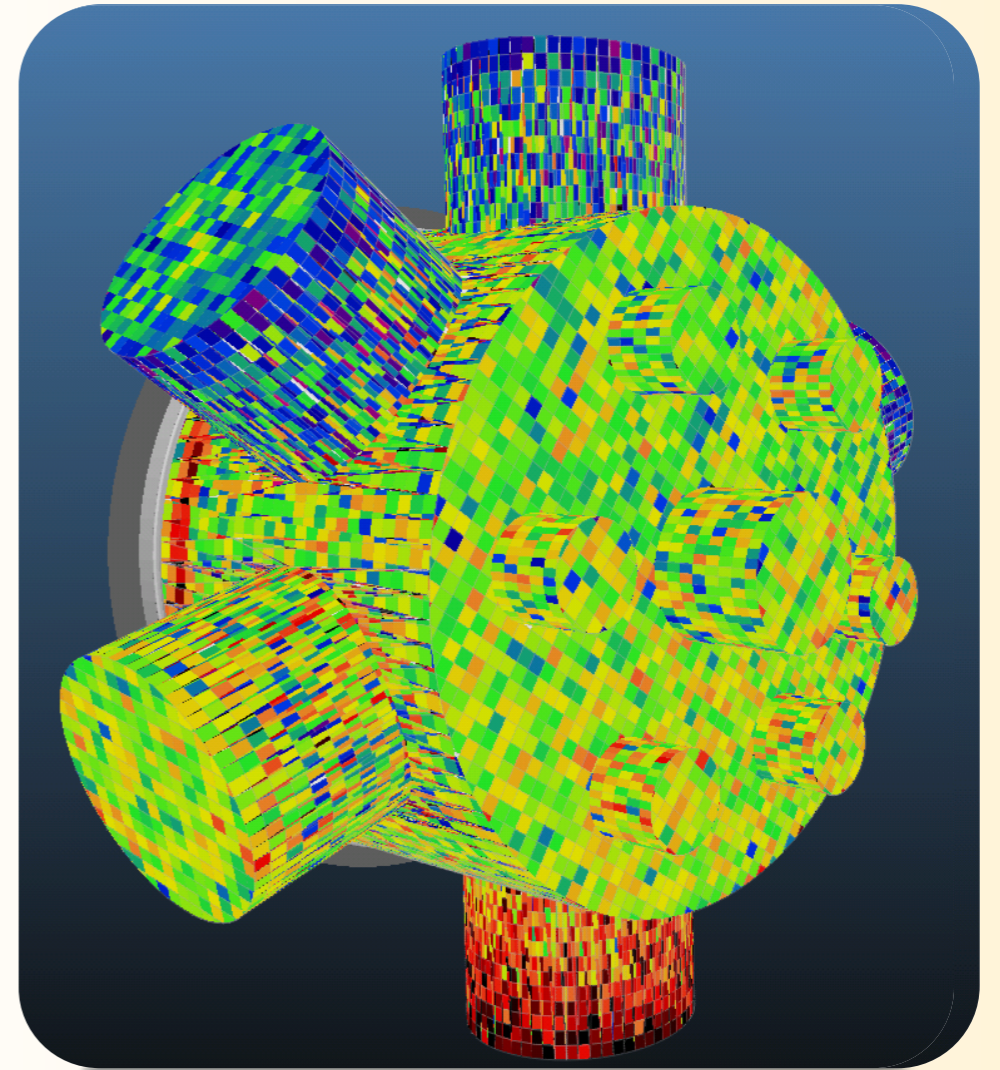
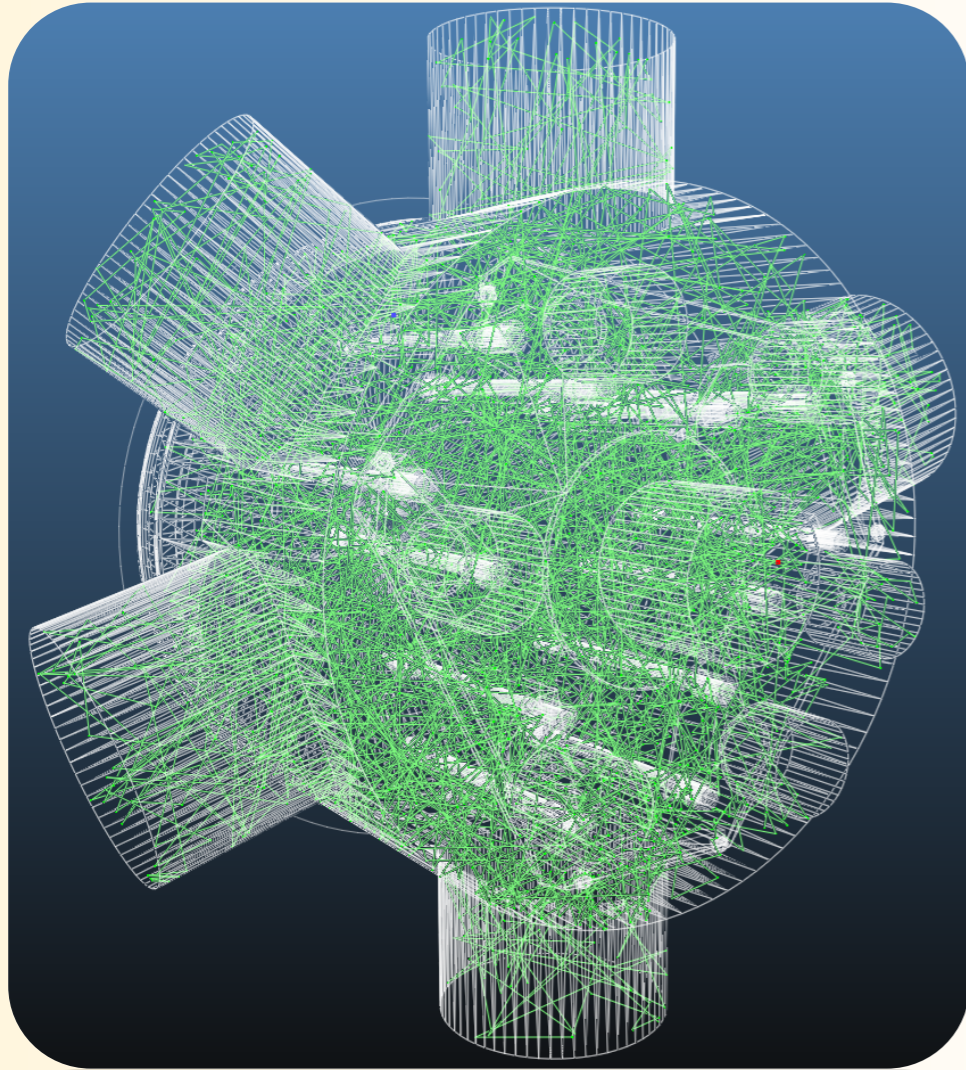
WORKING WITH MOLFLOW

Step 3: simulation and results



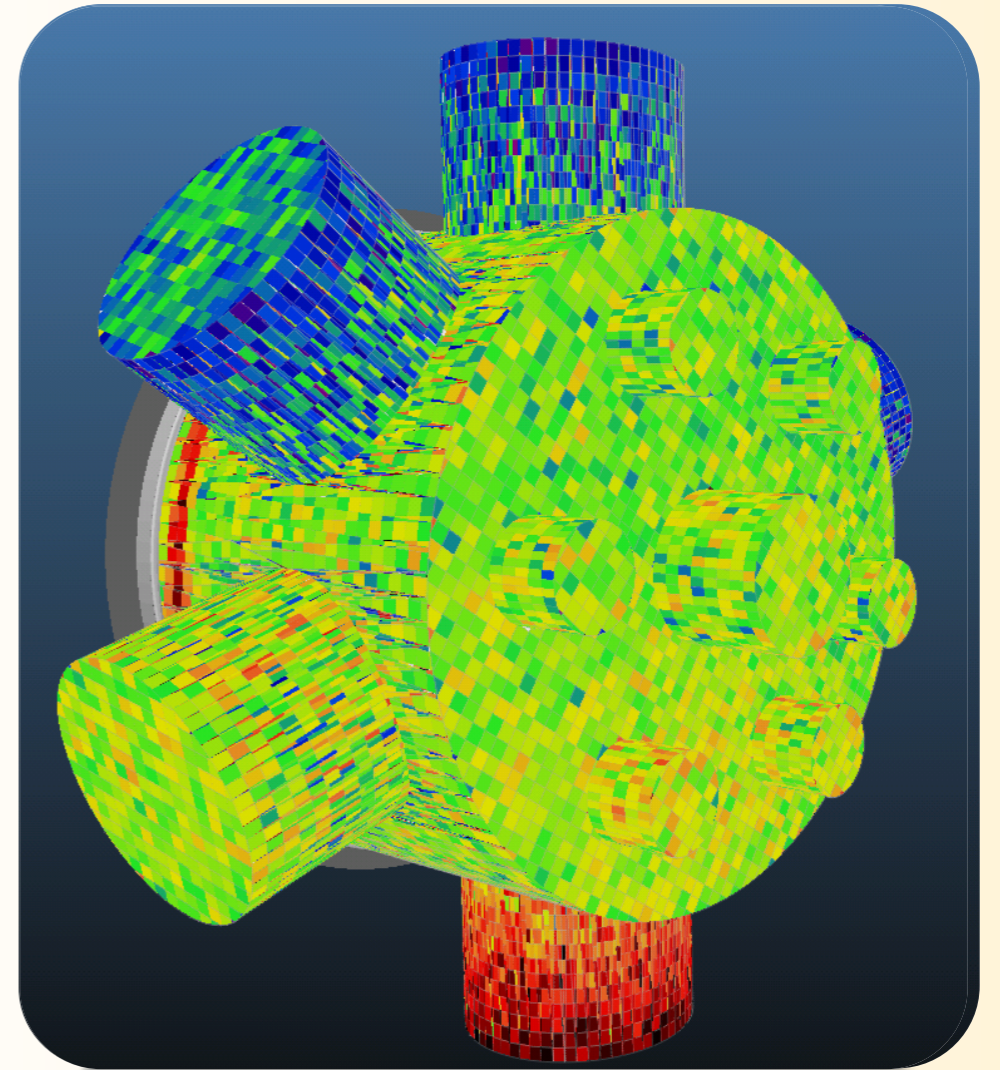
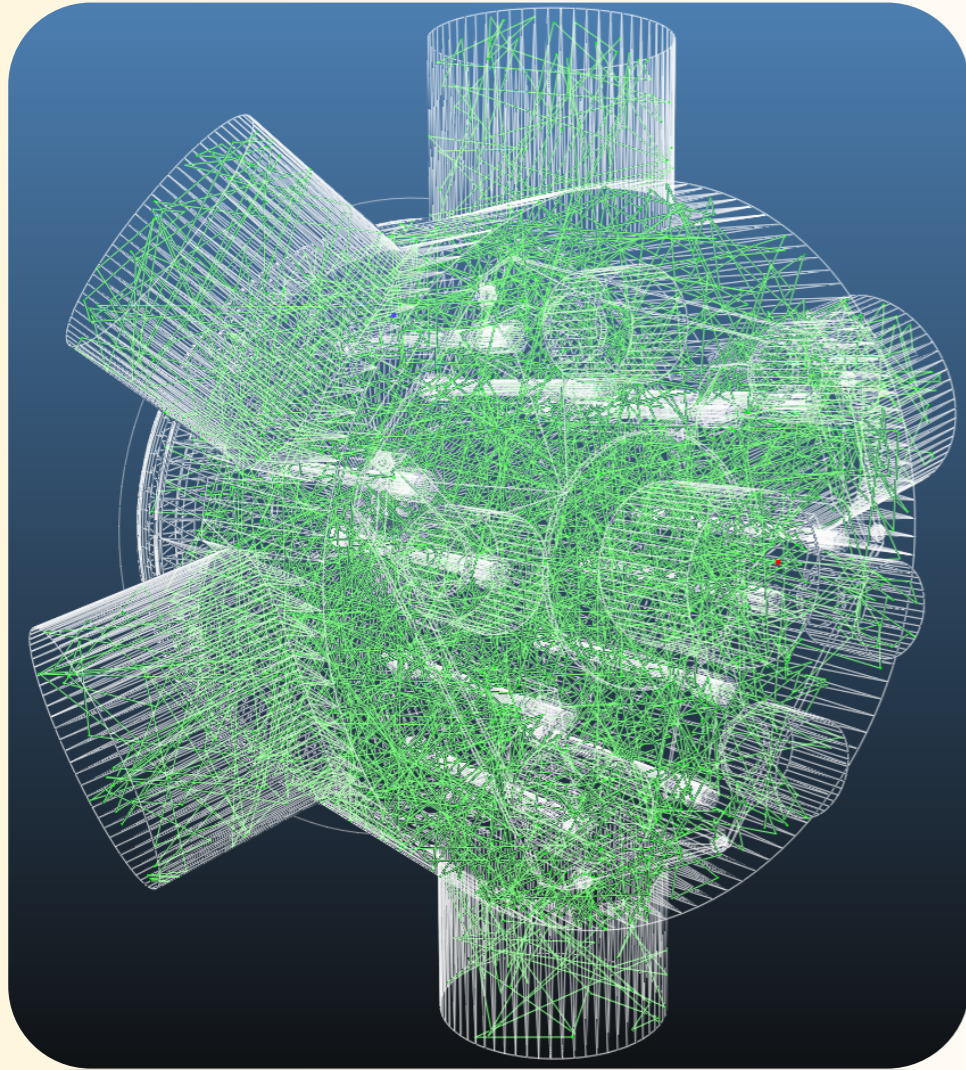
WORKING WITH MOLFLOW

Step 3: simulation and results



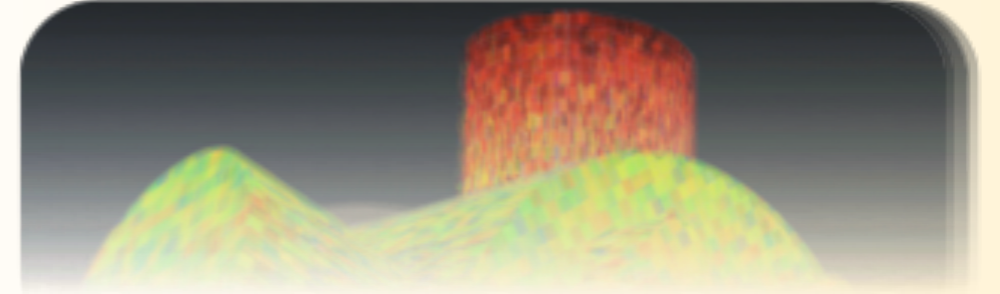
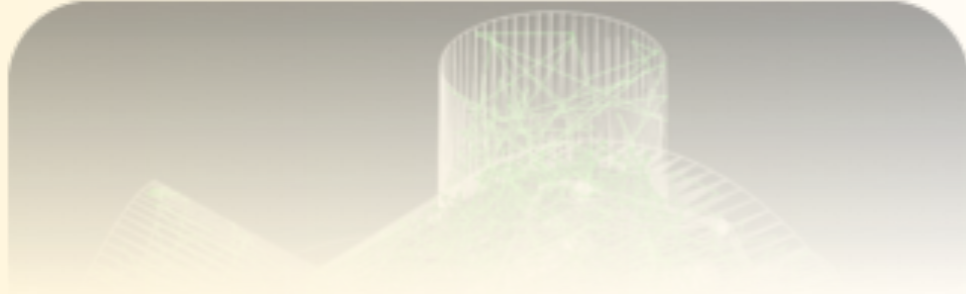
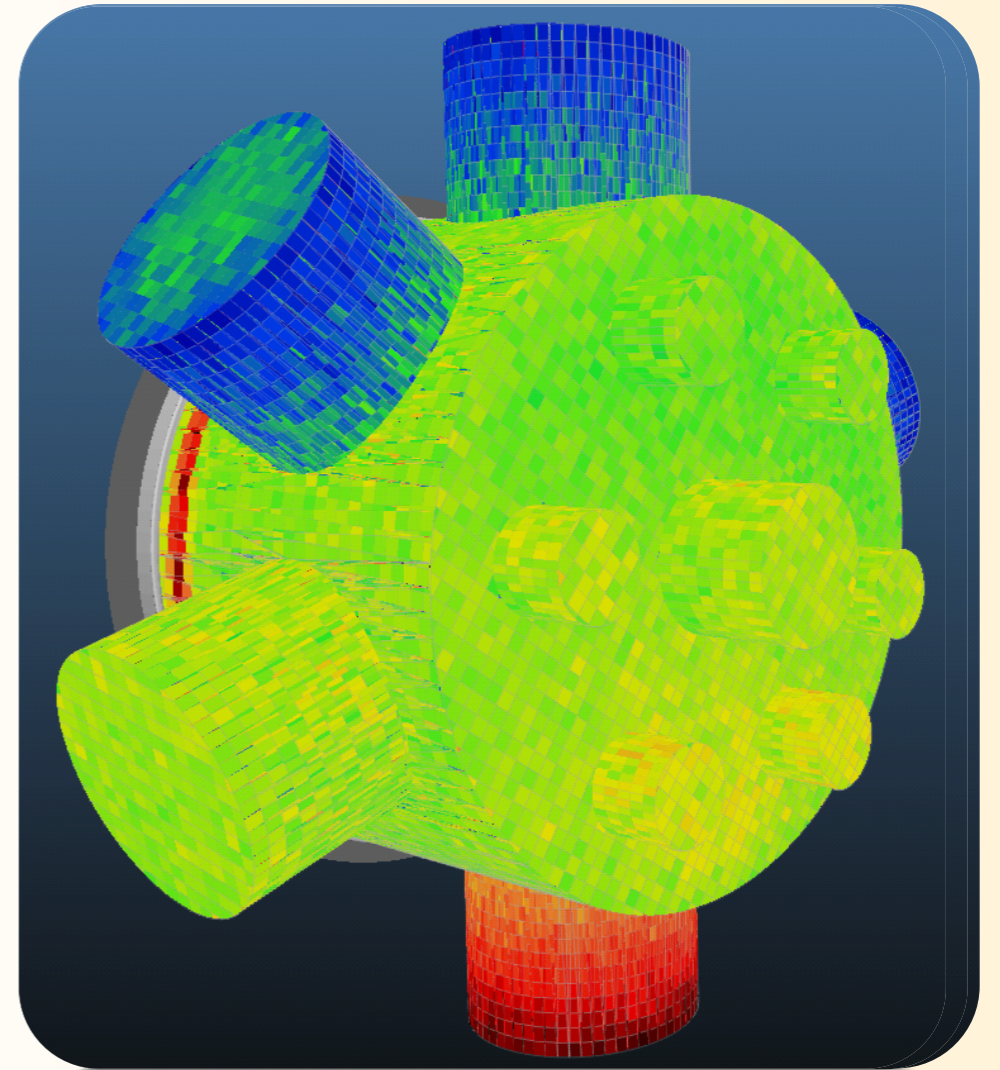
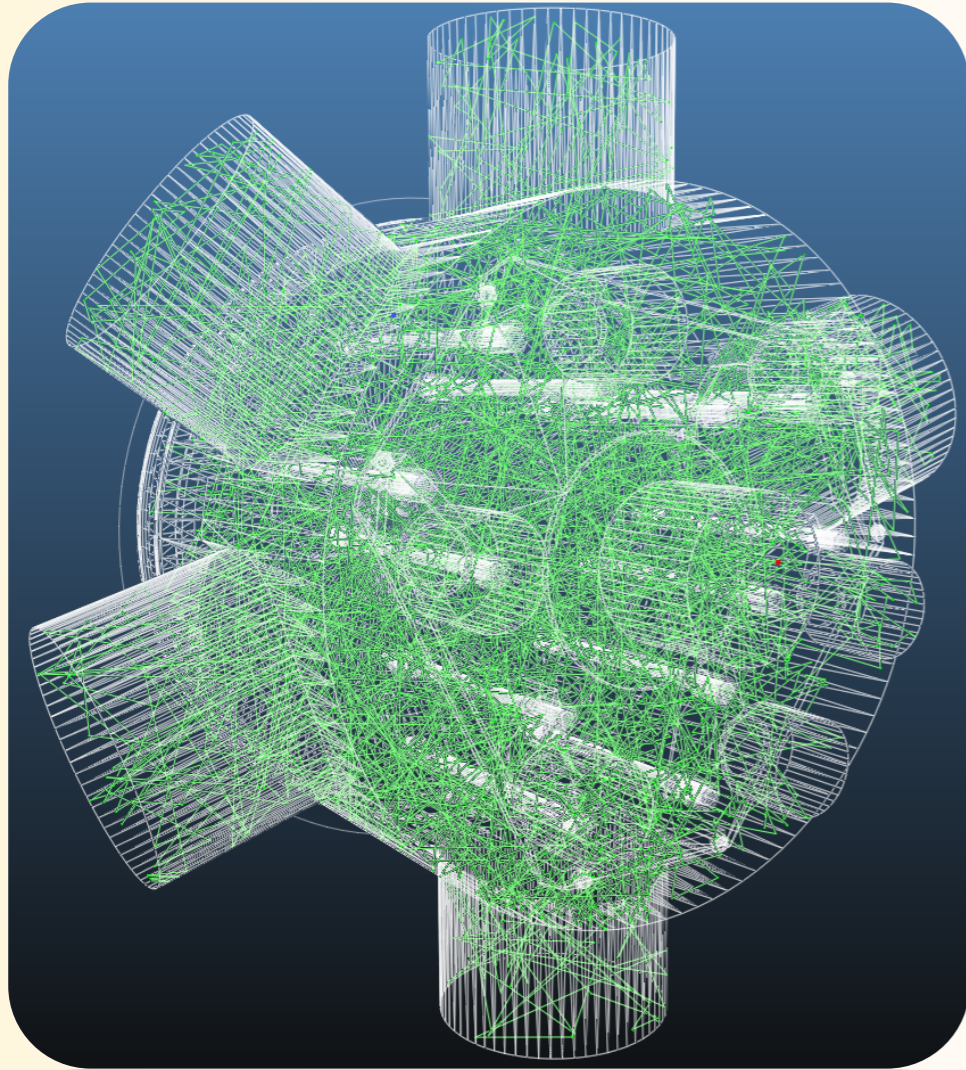
WORKING WITH MOLFLOW

Step 3: simulation and results



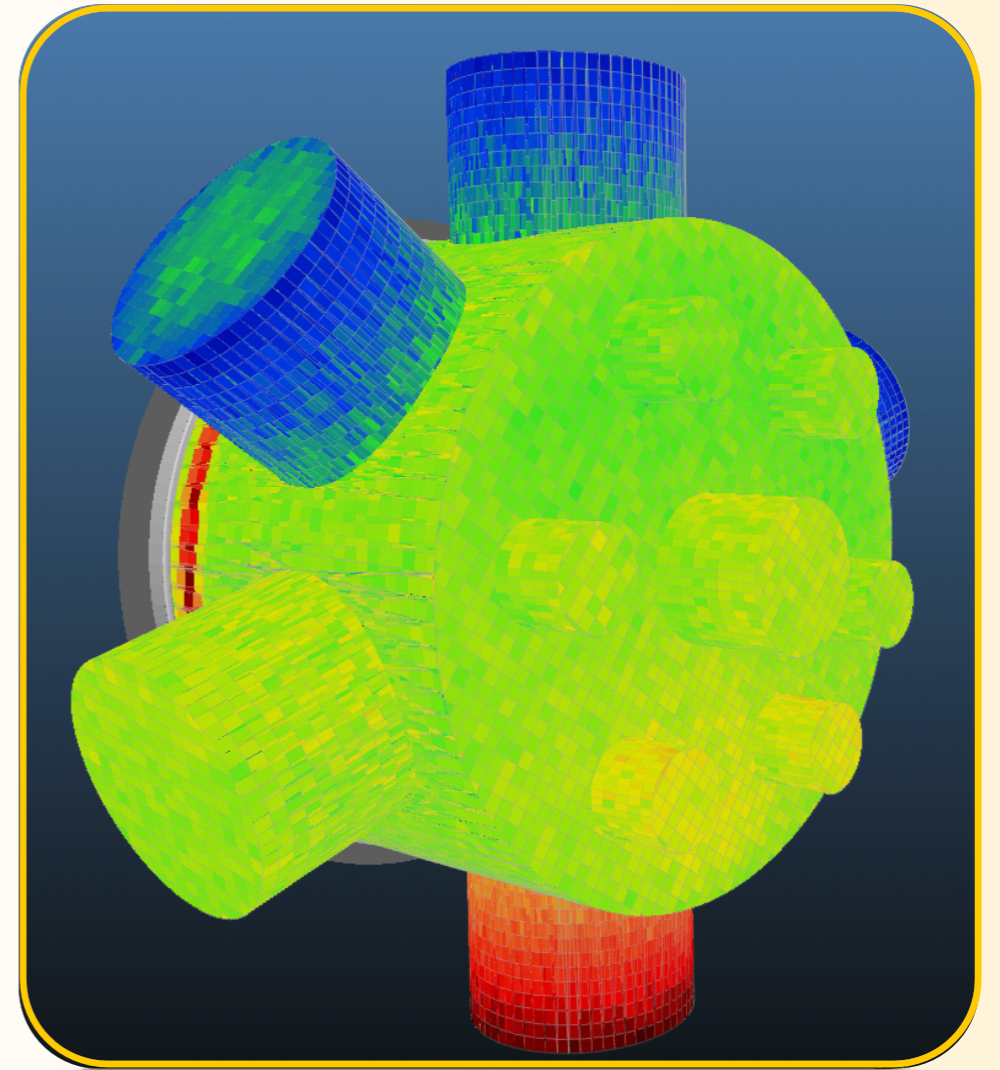
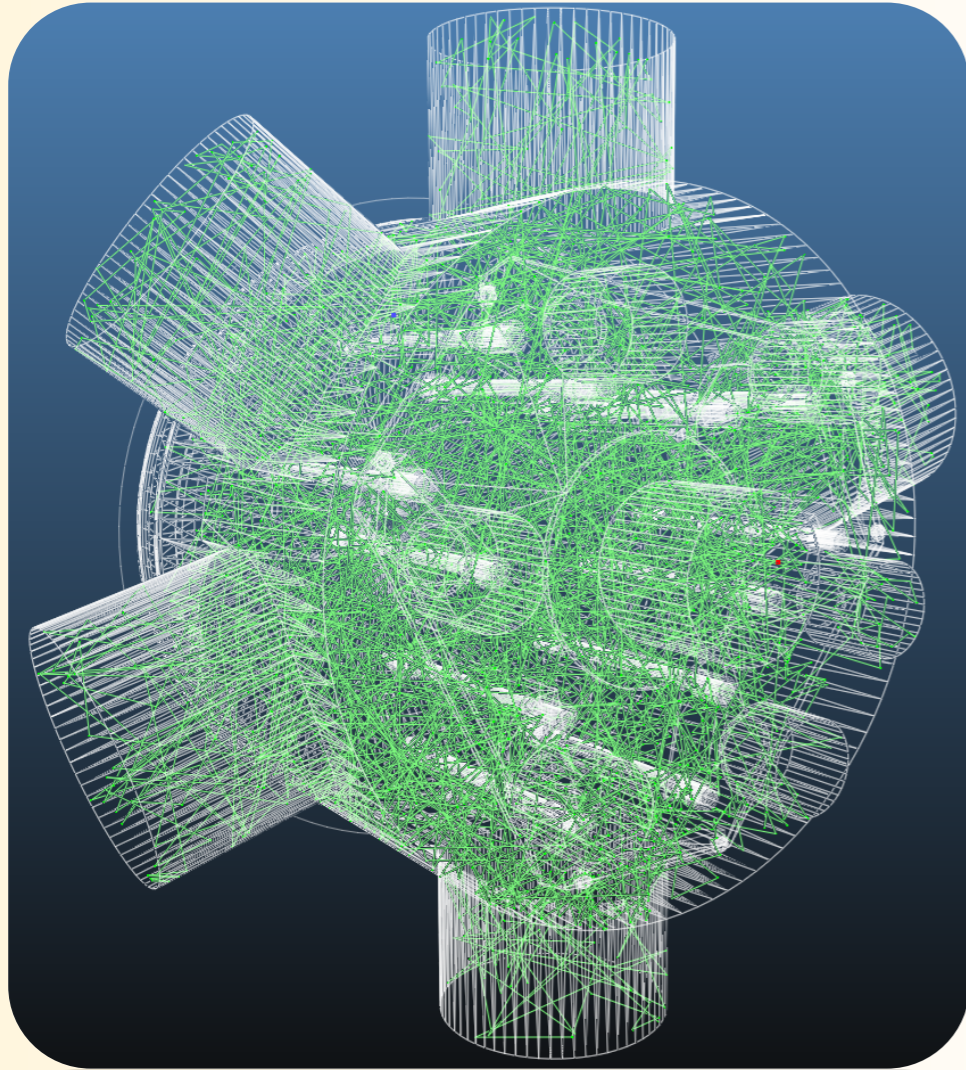
WORKING WITH MOLFLOW

Step 3: simulation and results



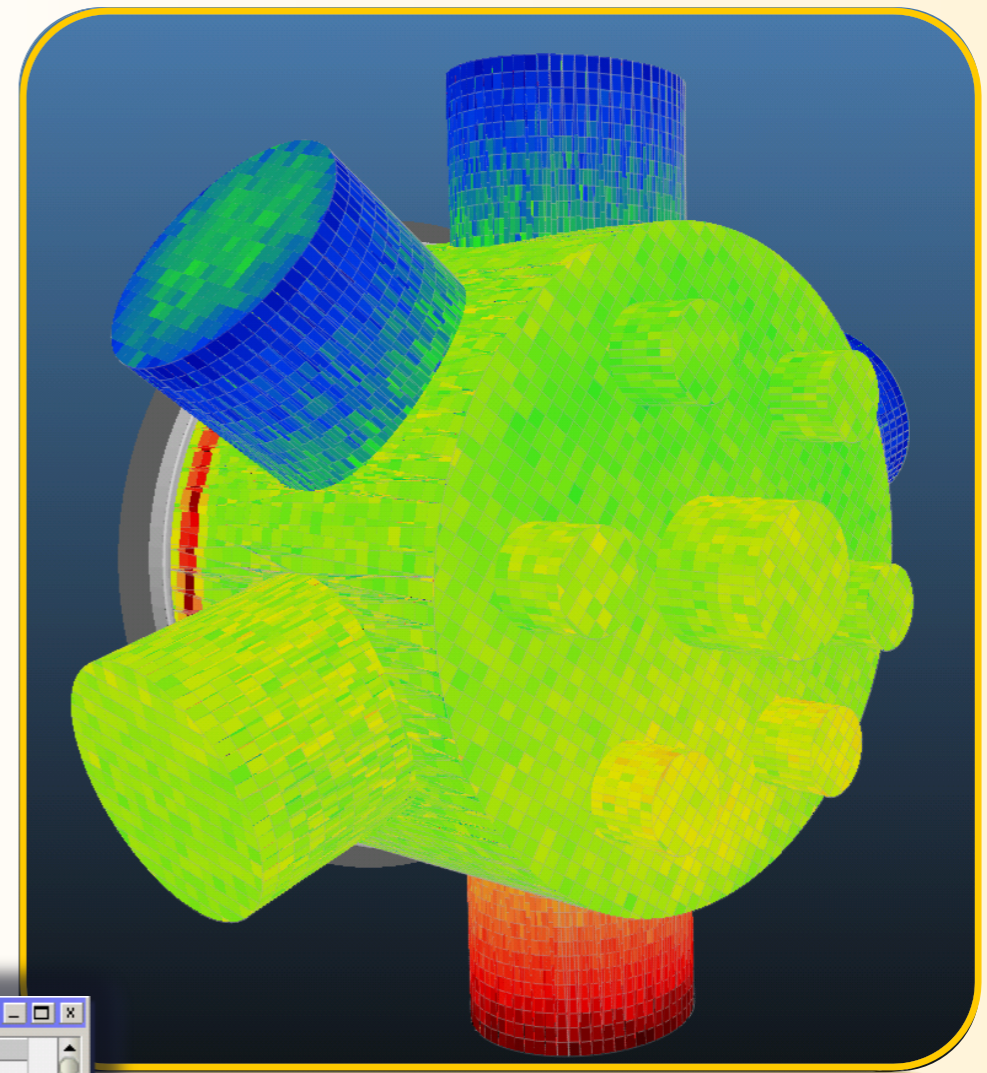
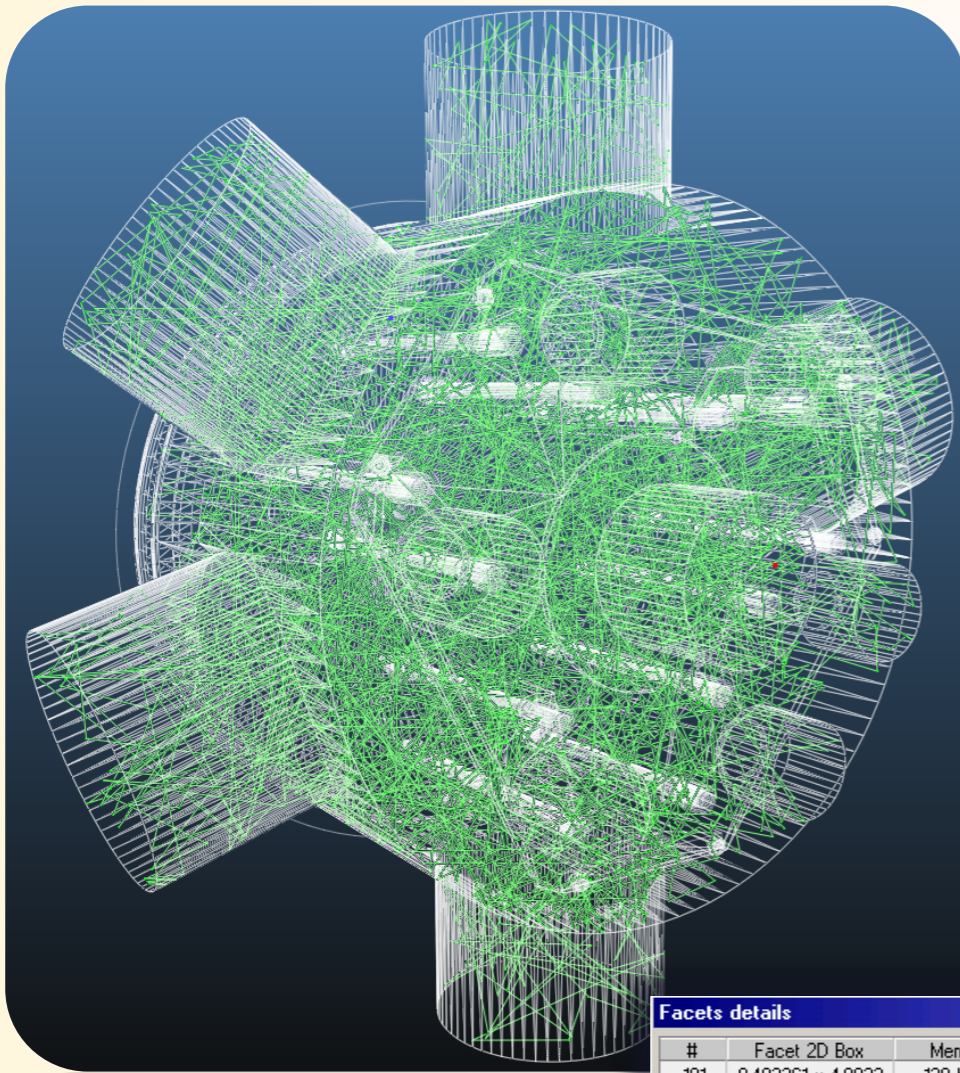
WORKING WITH MOLFLOW

Step 3: simulation and results



WORKING WITH MOLFLOW

Step 3: simulation and results



Facets details

#	Facet 2D Box	Memory	Avg.Pressure	Hits	Abs.
191	0.482261 x 4.8832	120 bytes	0.000248315	7184	71
192	0.482265 x 4.8832	120 bytes	0.000256782	7429	58
193	0.482258 x 4.8832	120 bytes	0.000256302	7415	63
891	10.2182 x 0.772336	264 bytes	0.000346459	16795	168
892	0.388214 x 10.2143	264 bytes	0.000319372	7779	82
893	0.824425 x 10.2085	264 bytes	0.00032376	7968	81
894	10.2381 x 0.77258	264 bytes	0.00035035	17022	187
895	10.2544 x 0.395235	264 bytes	0.000322635	8032	76
896	10.2926 x 0.396098	264 bytes	0.000326687	8181	73
897	0.773009 x 10.2827	264 bytes	0.000344624	16826	179
898	10.3694 x 0.397868	264 bytes	0.000318957	8083	86
899	10.31 x 0.400227	264 bytes	0.000325846	8241	94
900	10.3626 x 0.772692	264 bytes	0.000346192	17027	175
901	10.4055 x 0.399778	264 bytes	0.000318173	8130	65

Show column

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.

Check All Uncheck All Update Dismiss

