Apparatus Schematic Improvements and Vacuum Simulations for Astrochemical Experiments

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Columbia Nevis Labs REU Program, Summer 2025
Savin Group

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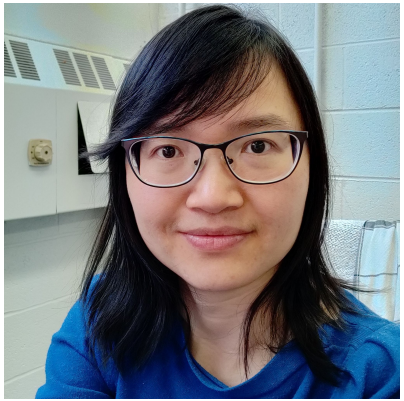


Dr. Caixia Bu
Associate Research Scientist

Savin Group

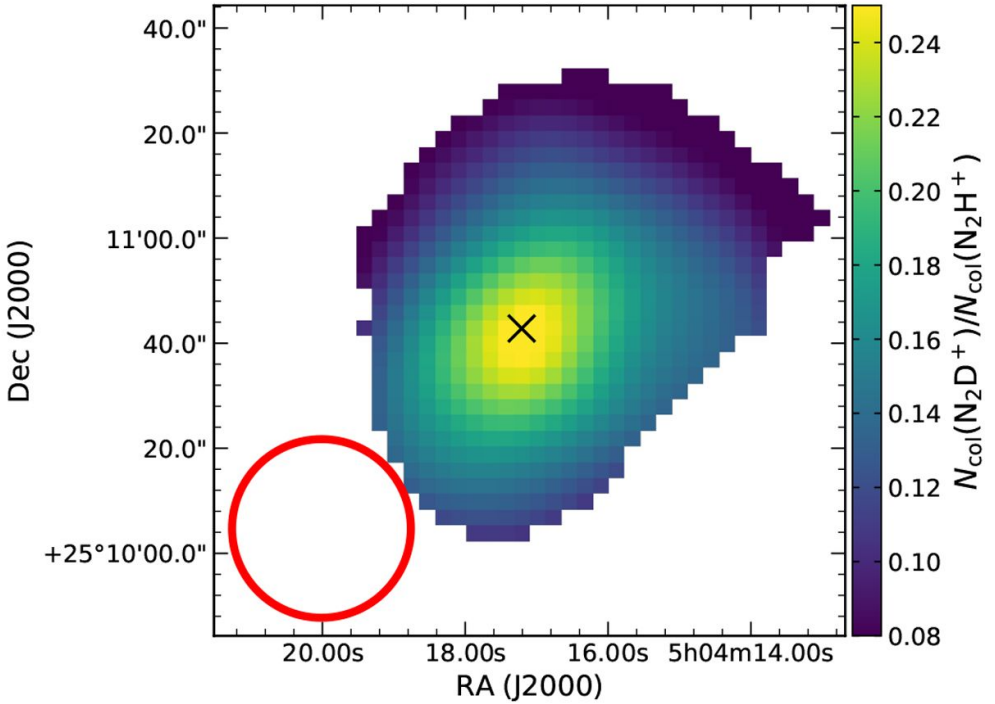
Outline

- **Astrochemical Motivation**
- Project 1: Leak Detection
- Project 2: Apparatus Schematic Updates
- Project 3: Vacuum Simulations
- Summary

$$N_2 + H_3^+ (H_2D^+) \rightarrow N_2H^+ (N_2D^+) + H_2$$

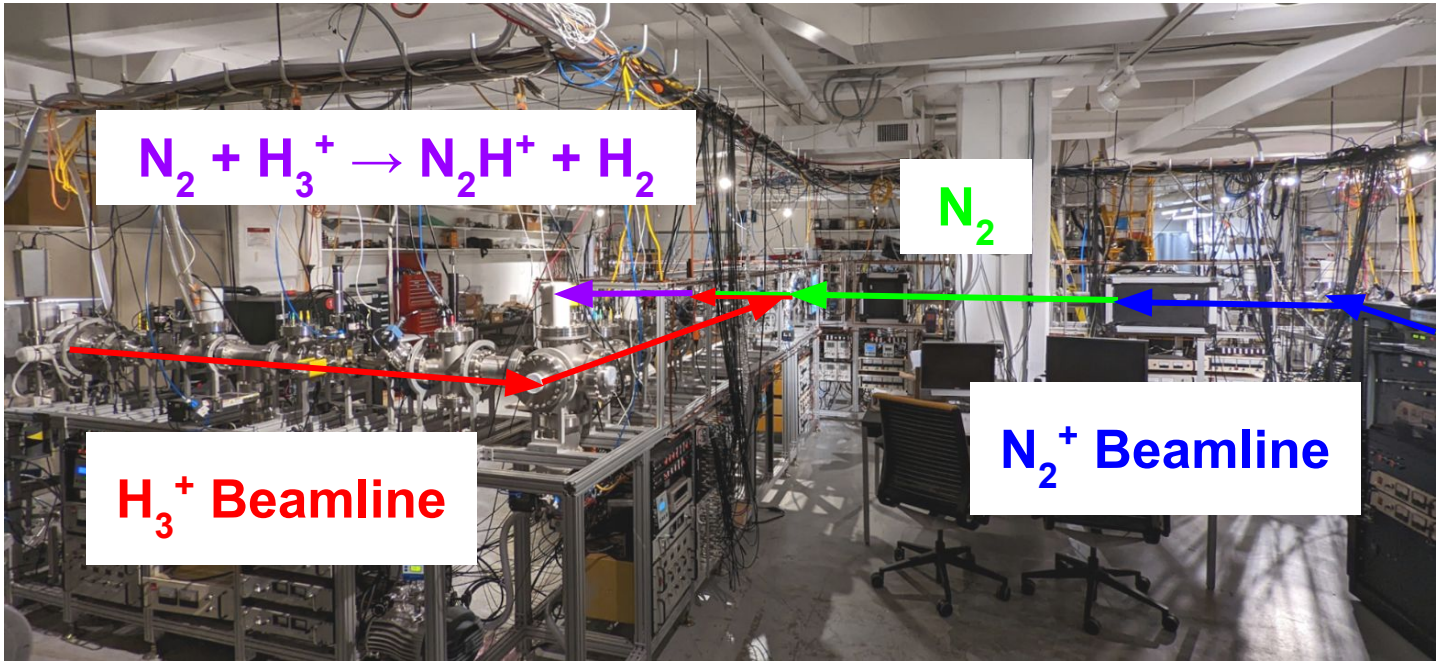
Measuring key reaction rates to improve astrochemical models of prestellar cores

(Redaelli et al. 2019)



Observed N_2H^+ and N_2D^+ in L1544, a prestellar core

Experimental Apparatus



Dual-source merged fast beams apparatus

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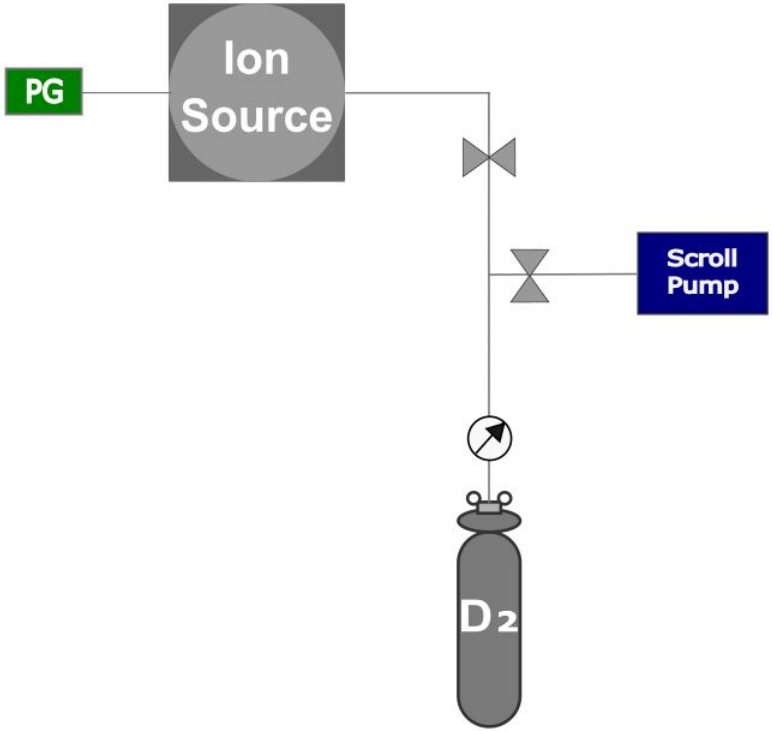
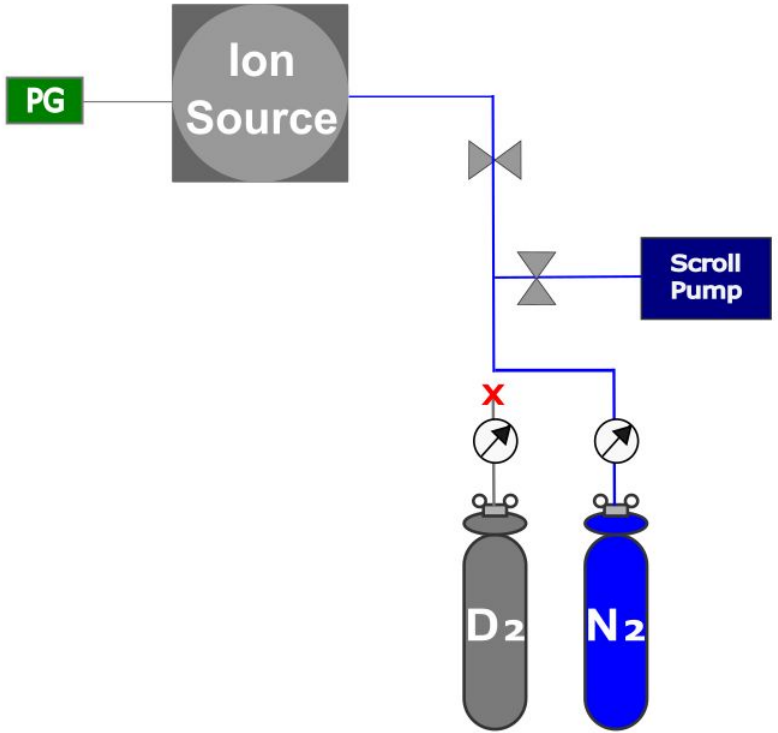
Leak in the Ion Source Gas Line

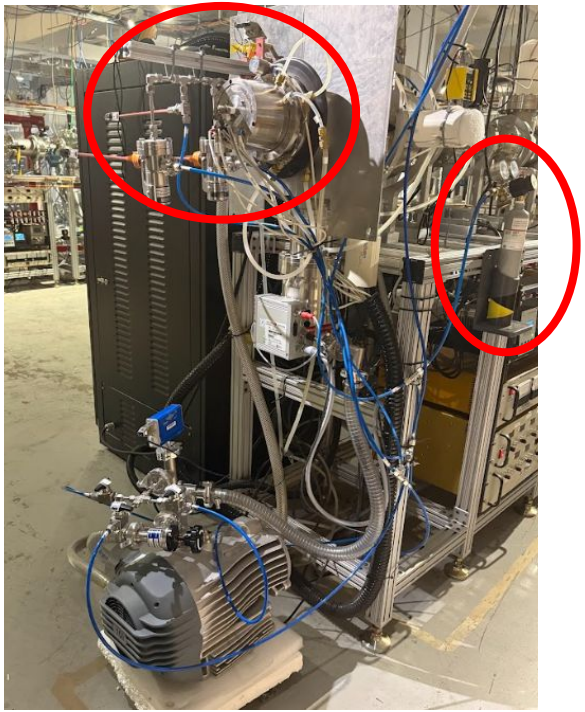
The Deuterium gas cylinder provides the gas for the ion source

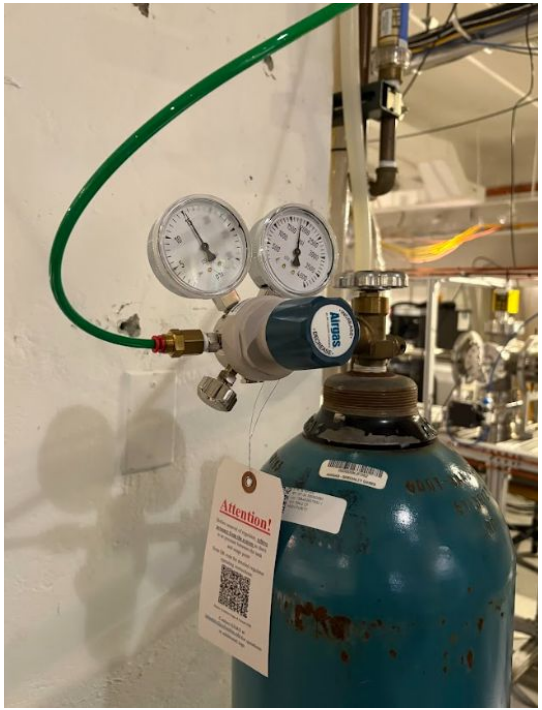
Searching for a Leak in the Ion Source Gas Line





Searching for a Leak in the Ion Source Gas Line





Leak Detection Methods

Sherlock leak detection liquid

Leak Detection Methods

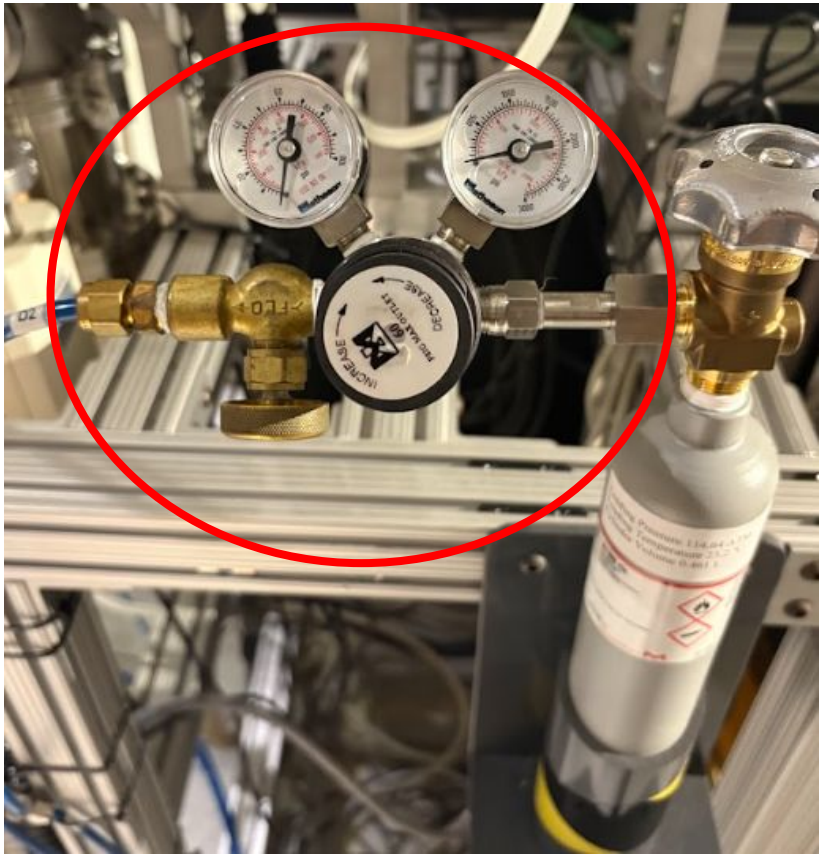
Ion source pressure gauge

This is a measure of the gas pressure in the source before we put gas into the source, we added gas until the pressure rose to 1 * 10^{-5} Torr.

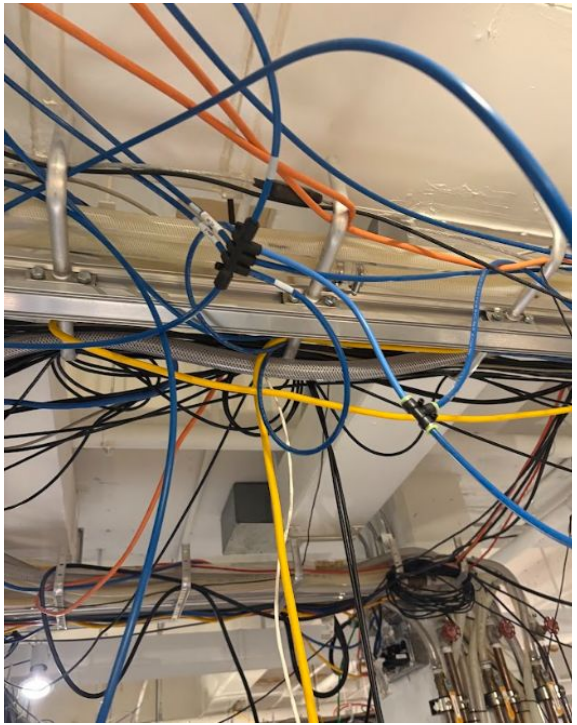
Since the pressure remained constant, we could conclude that the leak was not at any of the connections after the deuterium tank

Conclusion for Leak in the Ion Source Gas Line

Our results indicate that the ion source gas leak came from somewhere in the Deuterium gas regulator and connections

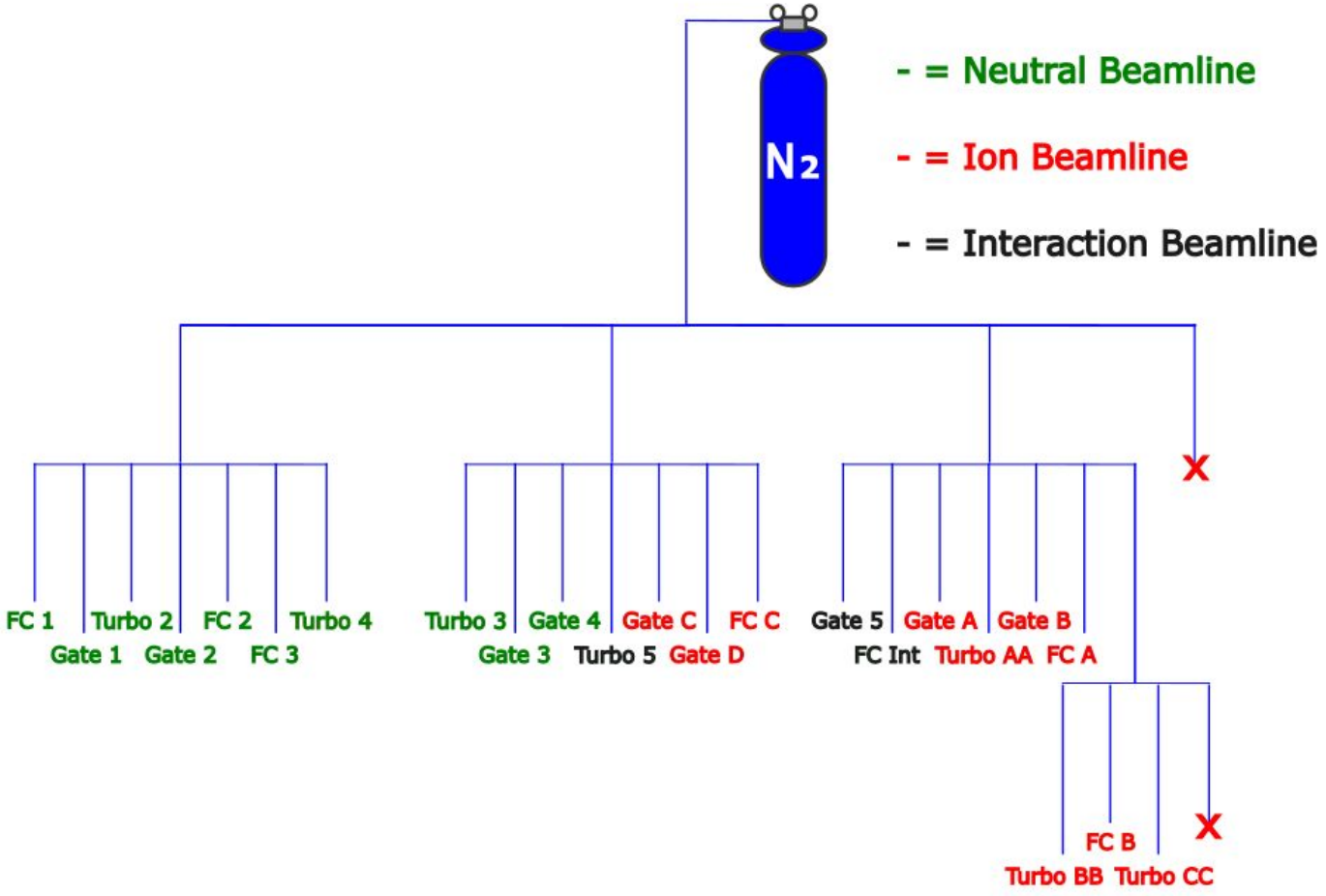


Searching for Leak in Instrument Operation Gas line



The Nitrogen gas cylinder produces gas to operate different parts on the apparatus, like the Faraday cups and gate valves

Troubleshooting Instrument Operation Gas Line Leak



Leak Detection Methods

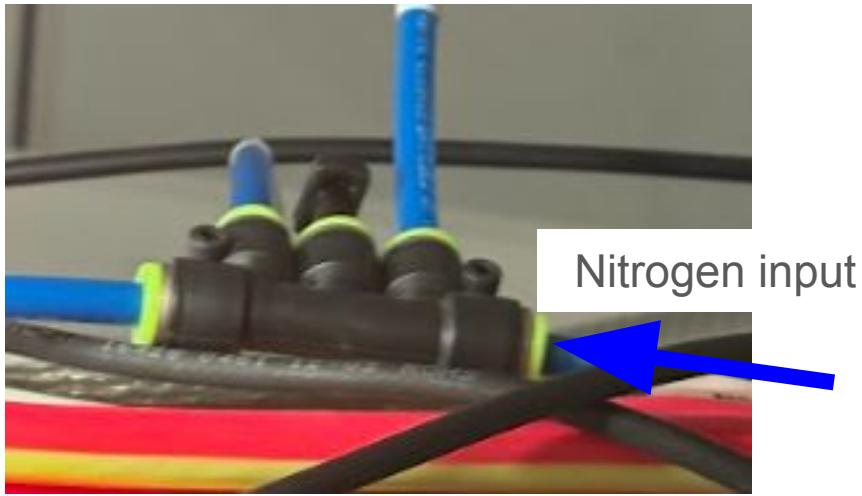
This is a measure of the gas pressure before the gas was in the instrument operation line. We did each test at 15 psi.

We saw that each connector was running out of gas relatively quickly,

Nitrogen gas regulator

Troubleshooting the Leak in Instrument Operation Gas Line

Since all four connectors ran out of gas at the same time, the gas leak could be from the main connector or in the following gas sections



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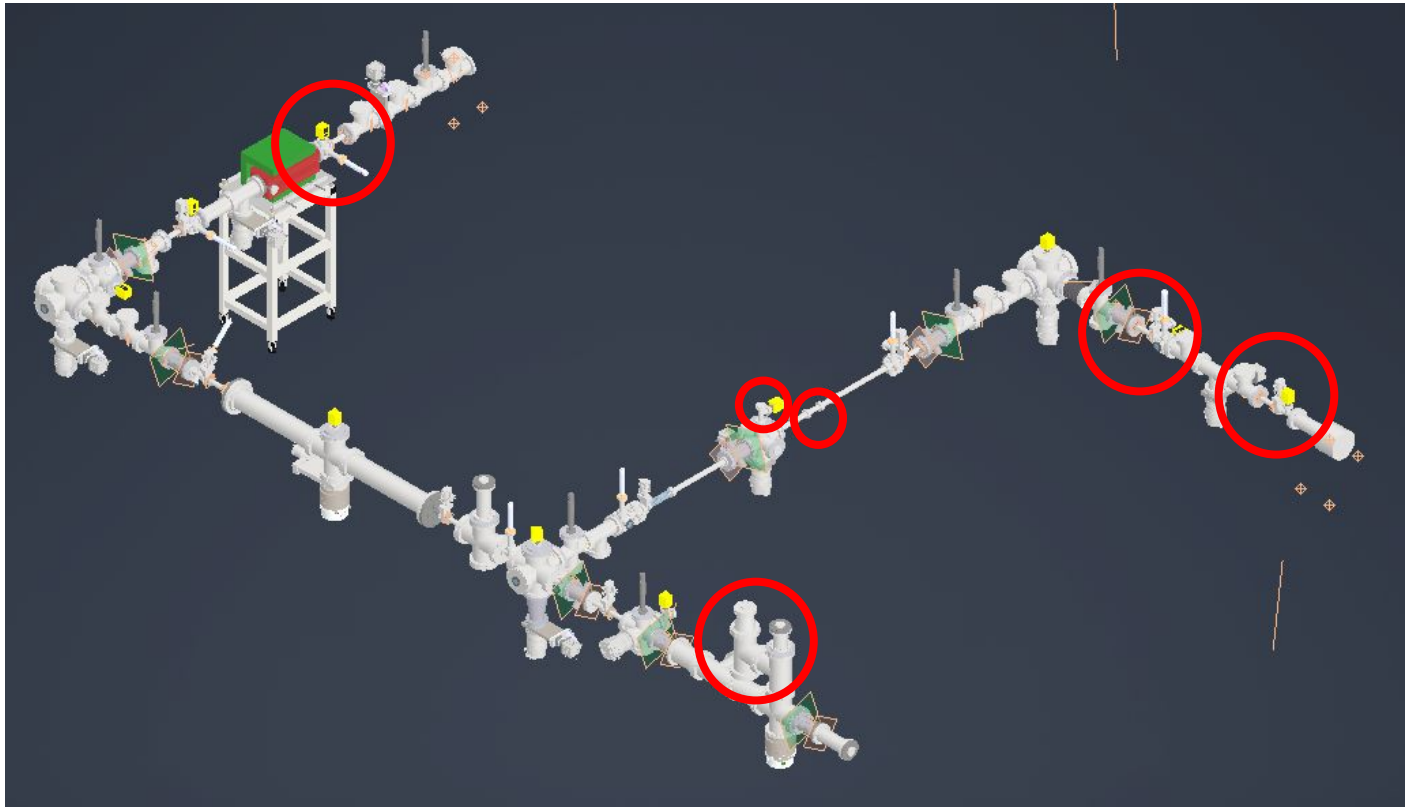
Apparatus Schematic Update

- A 3D Computer Automated Design (CAD) software used for product design, simulation, and visualization
- Allows precise modeling of parts, assemblies, and mechanical components
- Commonly used in engineering and manufacturing industries
- Helps create accurate technical drawings for prototyping

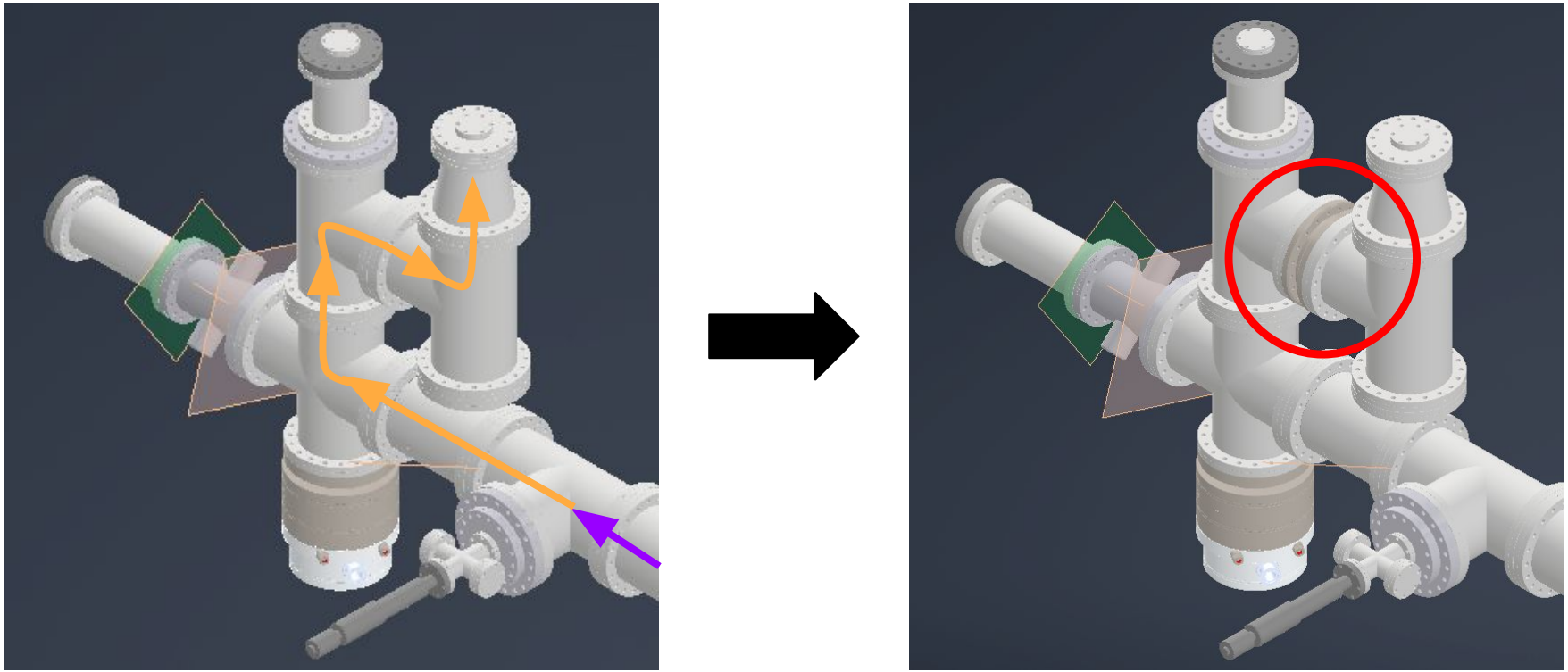
https://www.autodesk.com/products/inventor/overview

Apparatus Updates



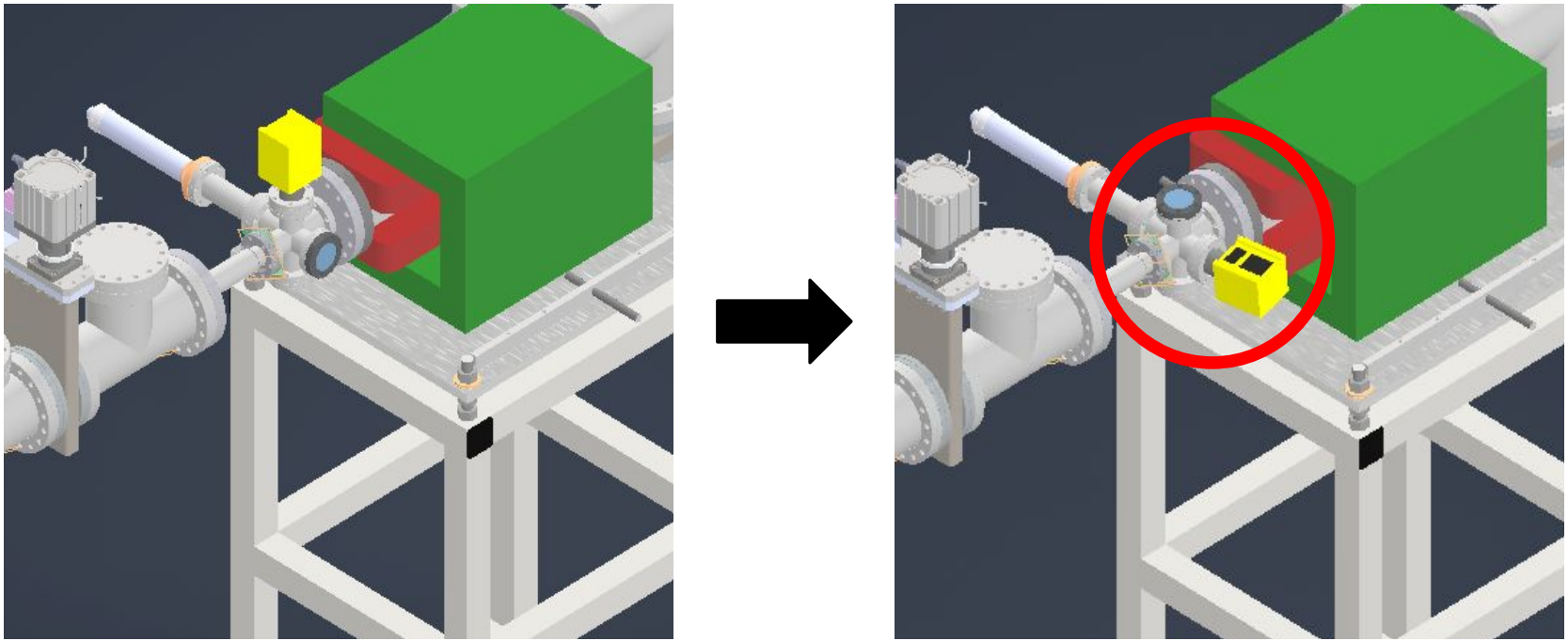
Old version in Inventor

Updates



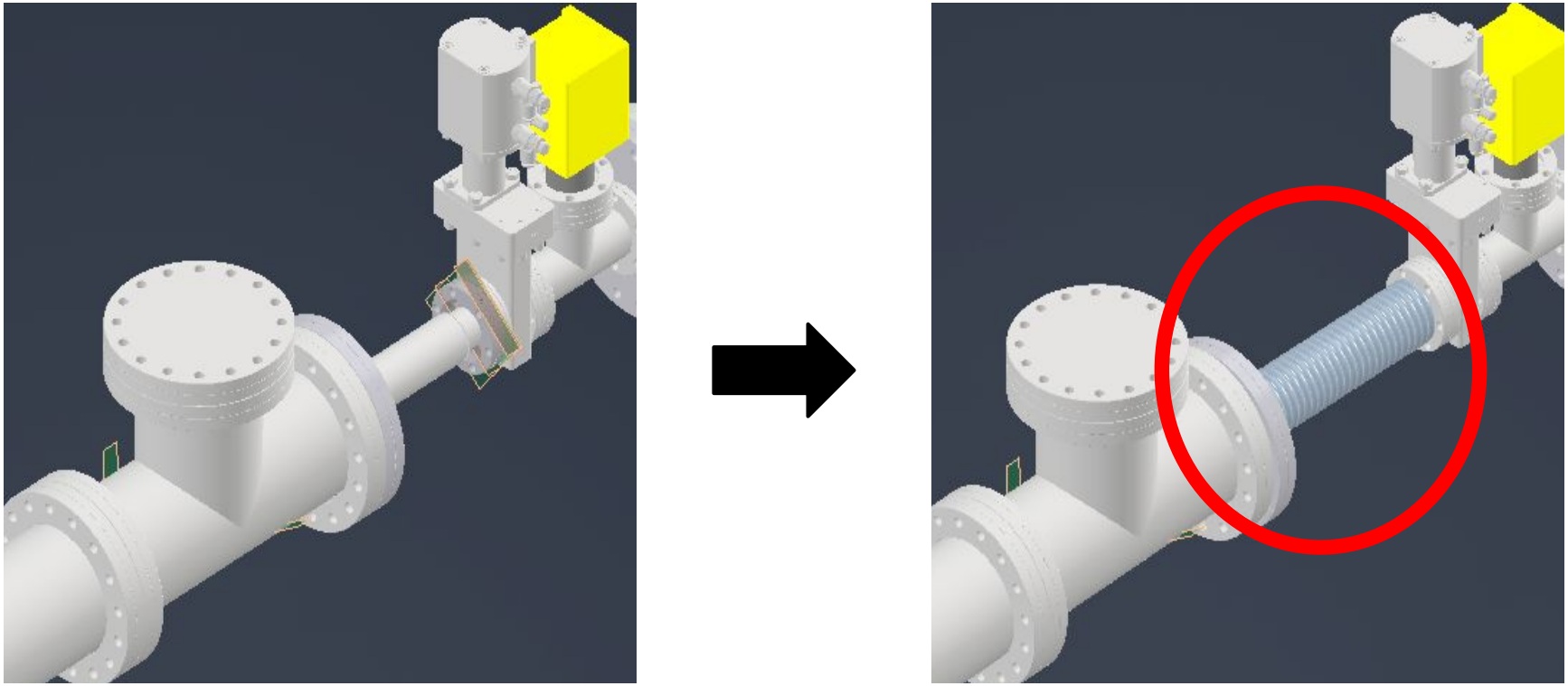
Extender added to final analyzer

Updates



Example of rotating orientations

Updates



Added flex bellows

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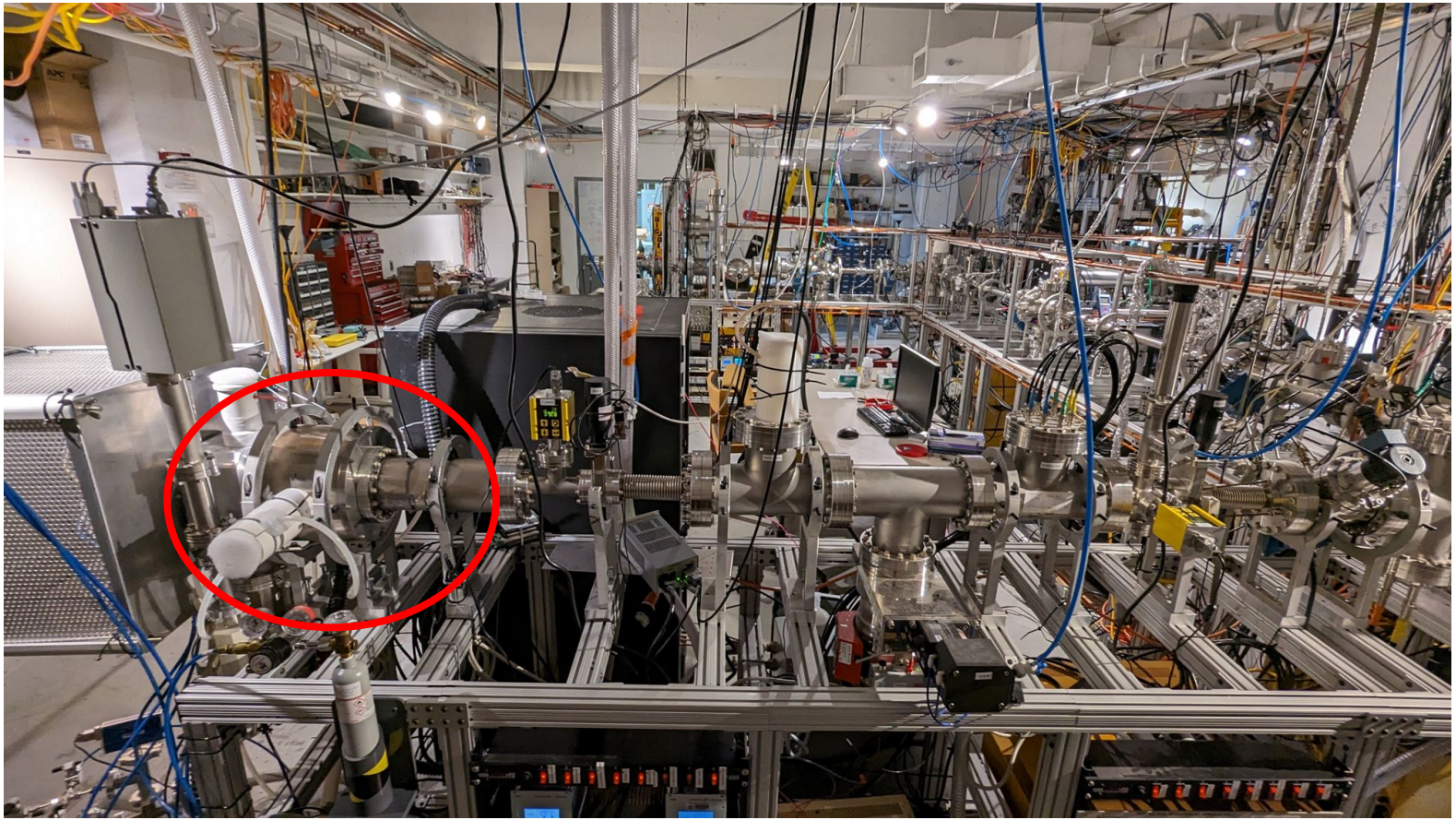
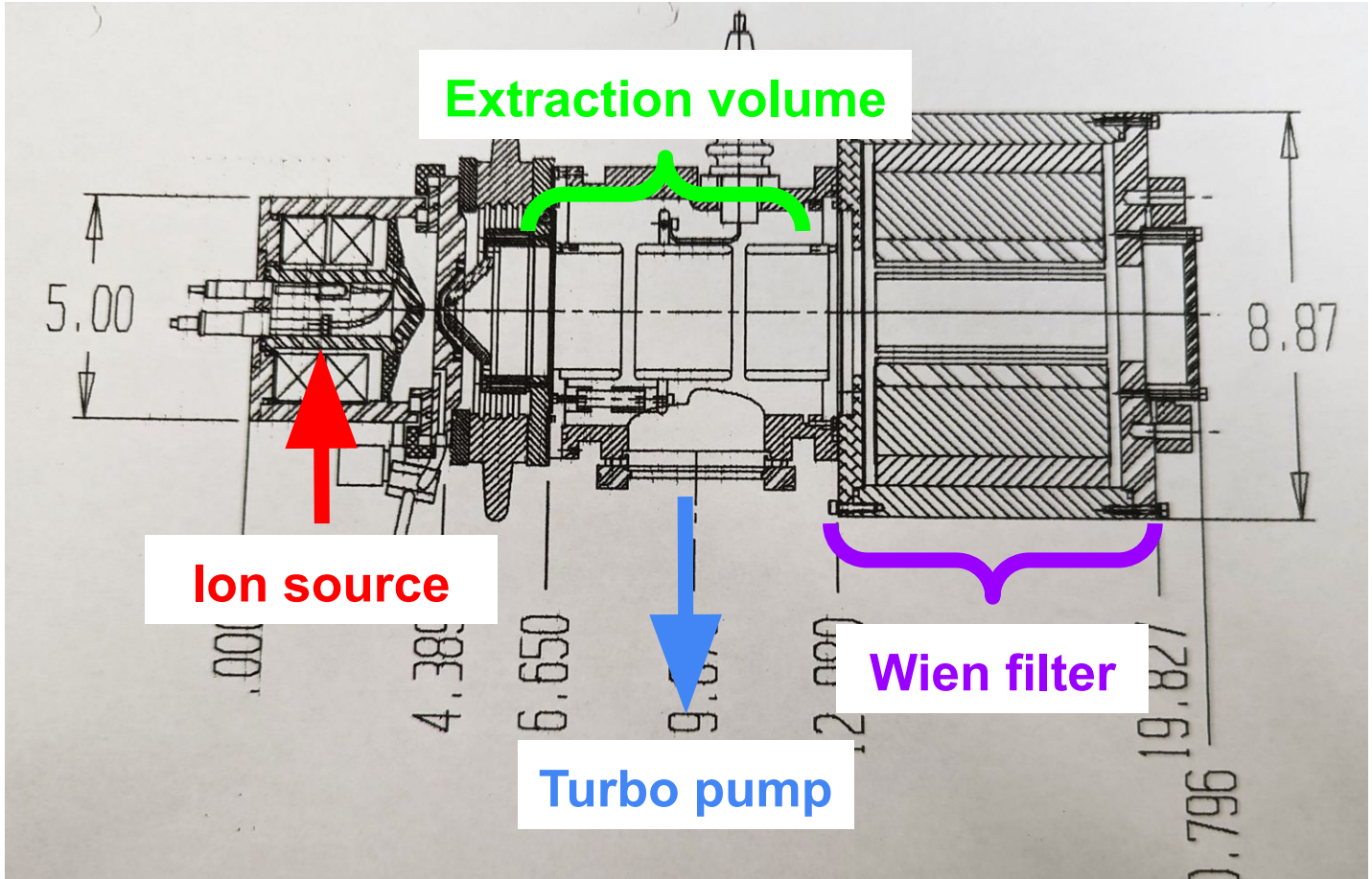
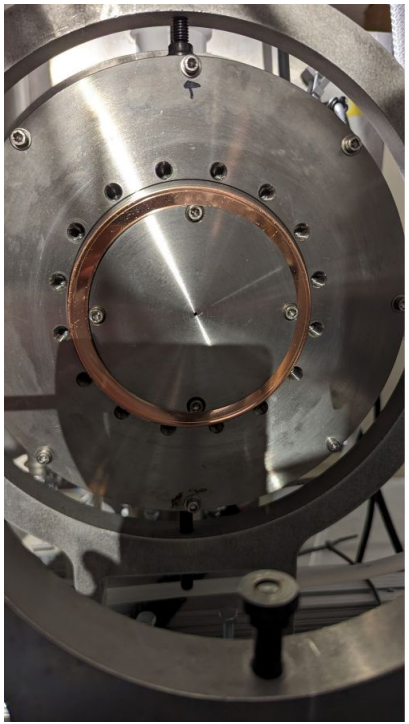
Simulating Pressure in the Apparatus



Simulating Pressure in the Apparatus

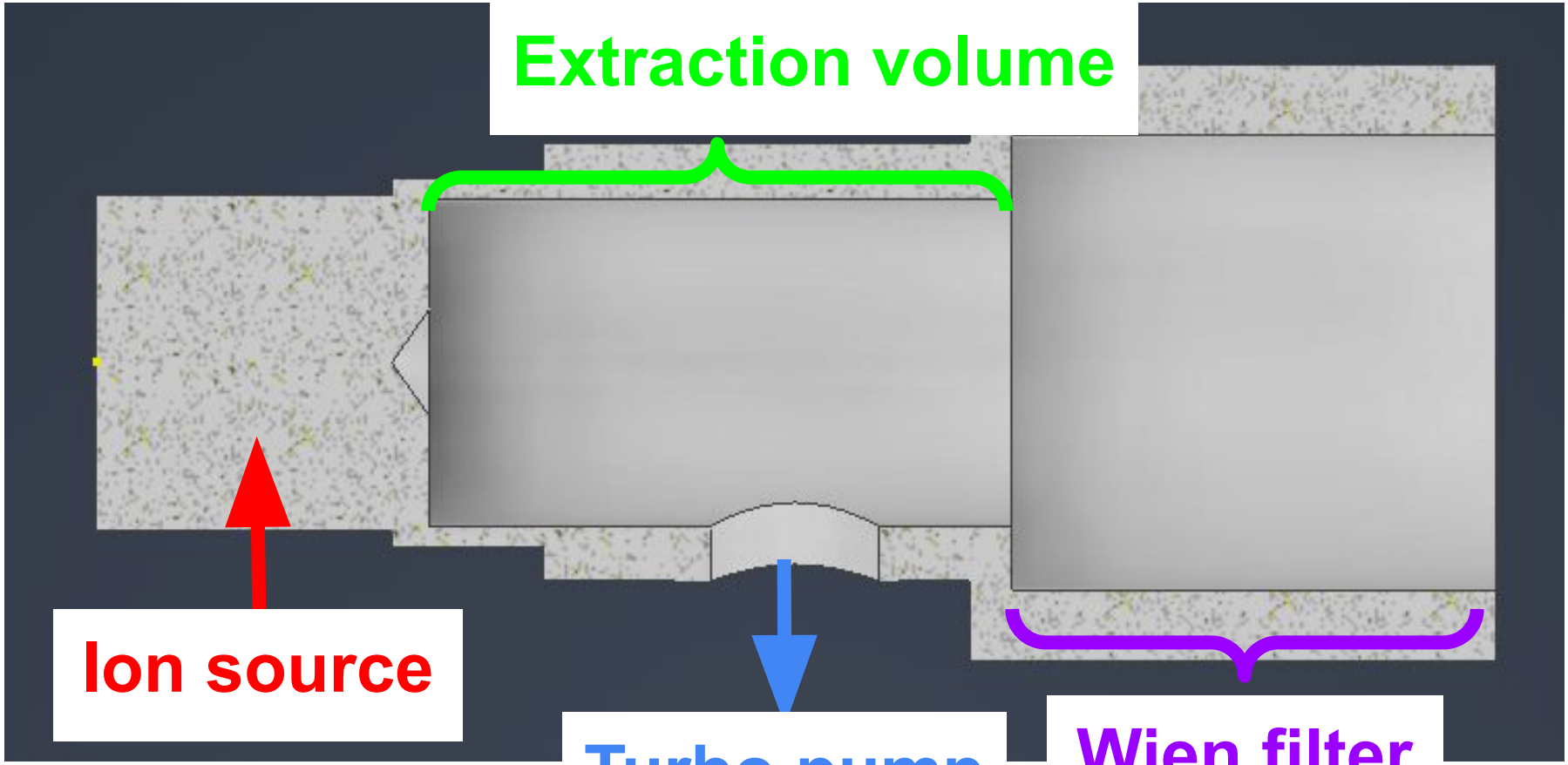


Investigating Pumping Efficiency

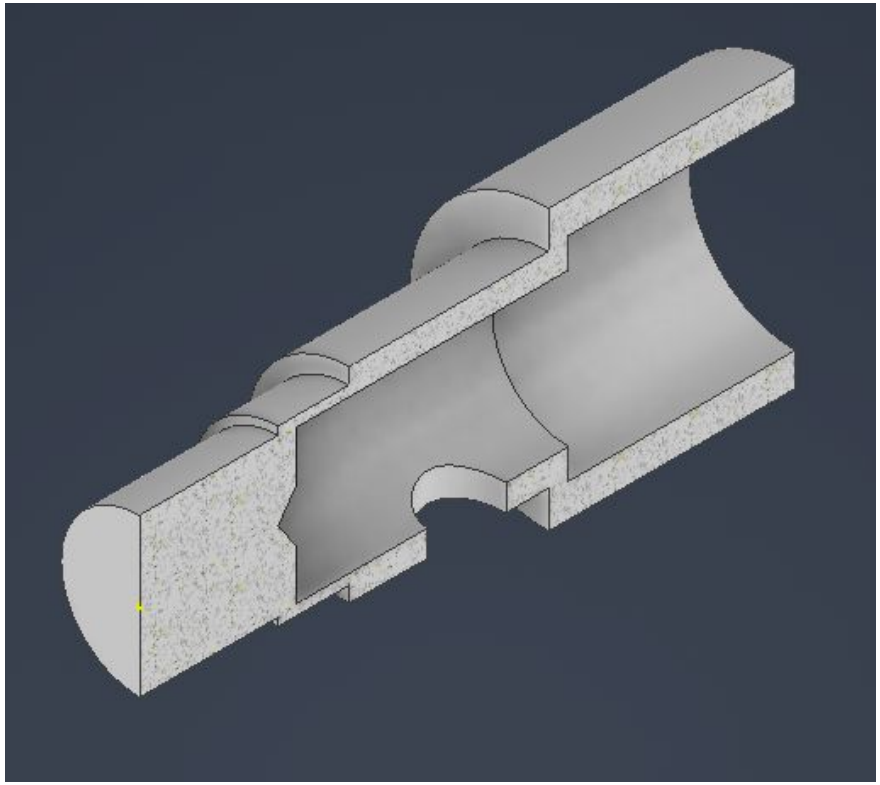


The exit aperture of the Wien filter was updated

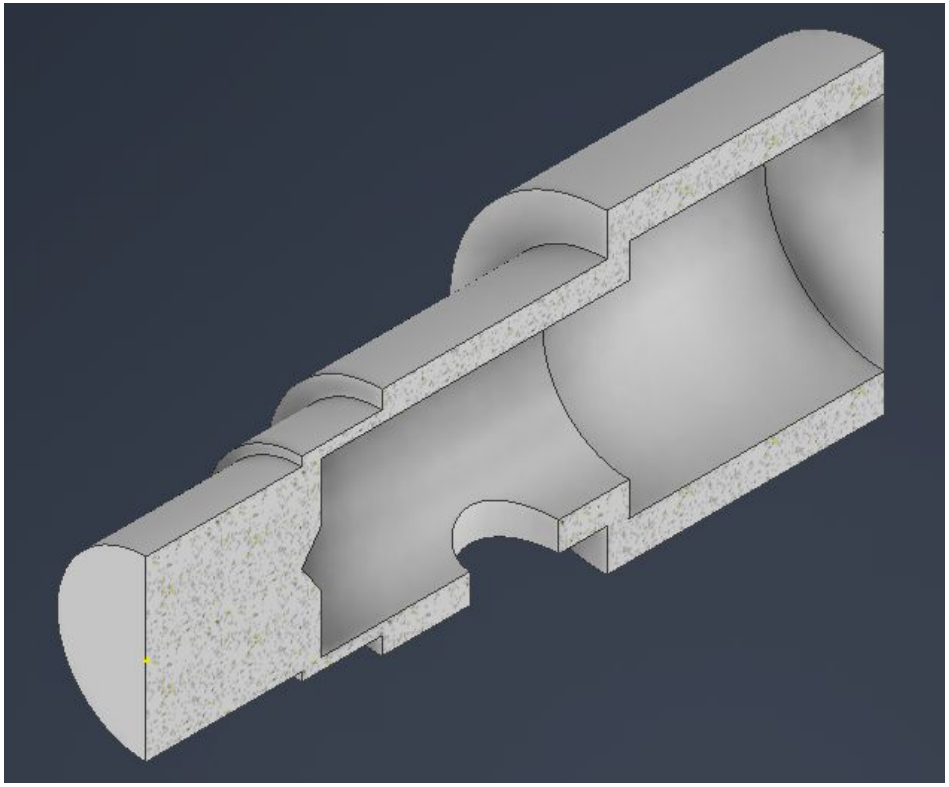
Simulating Pressure in the Apparatus



Simulating Pressure in the Apparatus



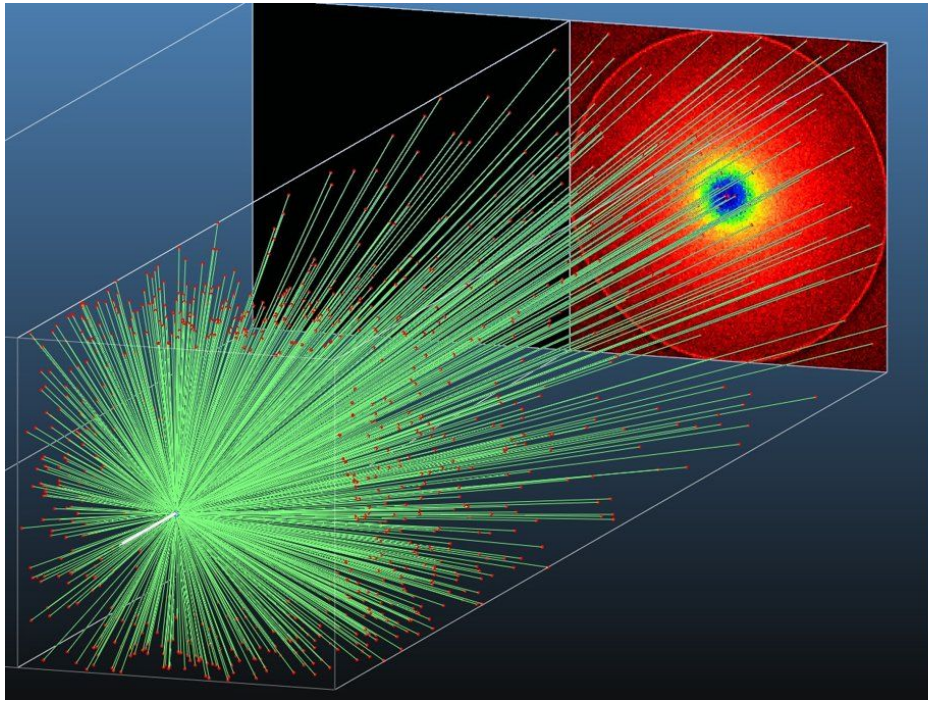
Open exit aperture



Closed exit aperture

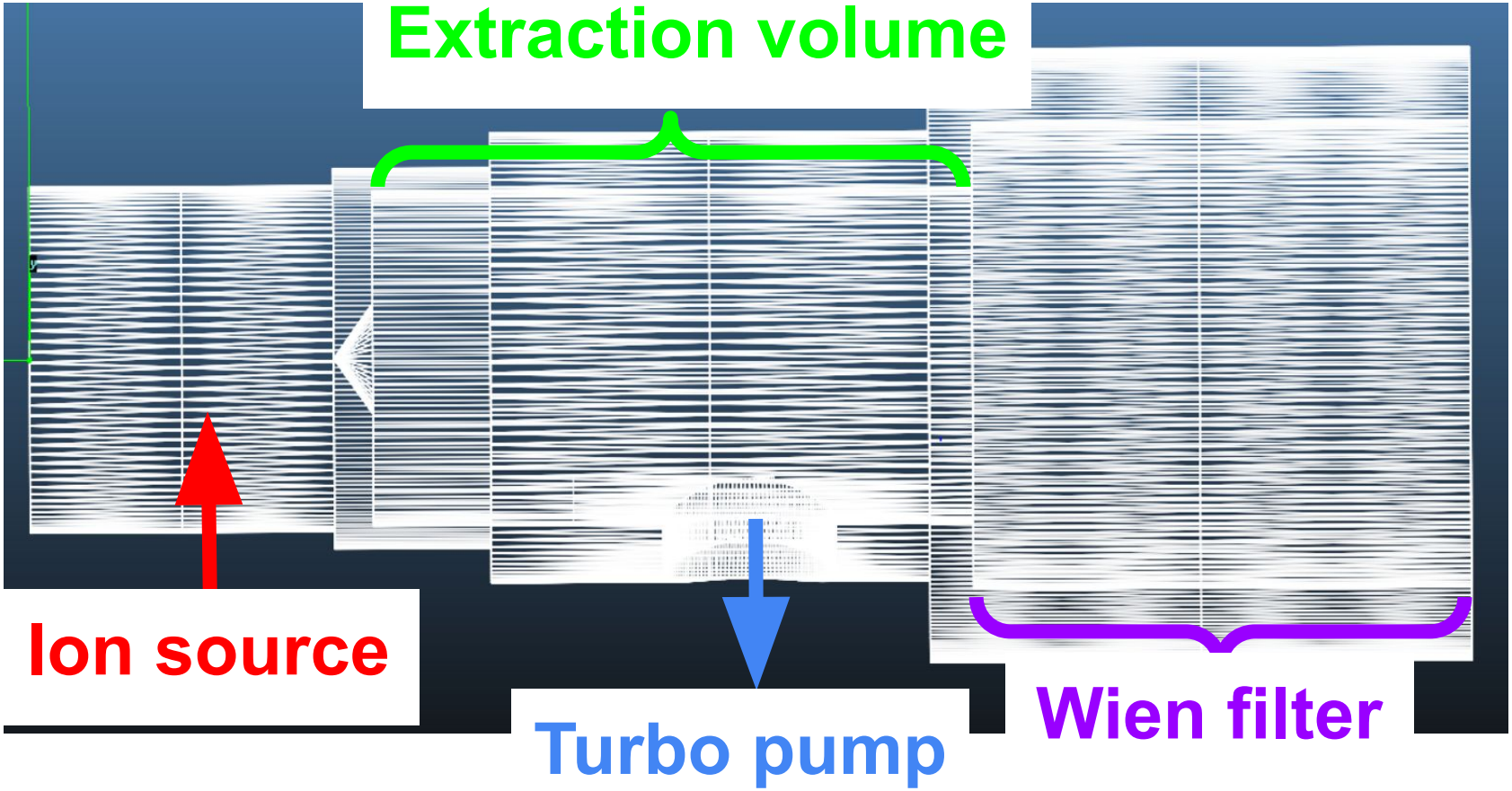
MolFlow+

- Simulates how gas flows in ultra-high vacuum system
- Uses Monte Carlo simulations to model the movement of gas molecules
- Tracks particle collisions with walls
- Allows estimations of local pressure and pumping efficiency

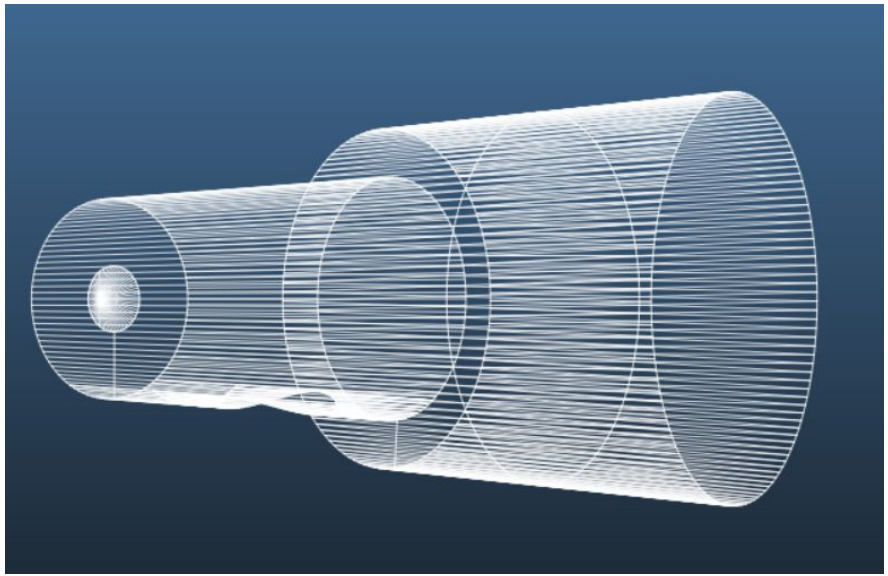


https://molflow.docs.cern.ch/guide/molflow/general/getting_started/

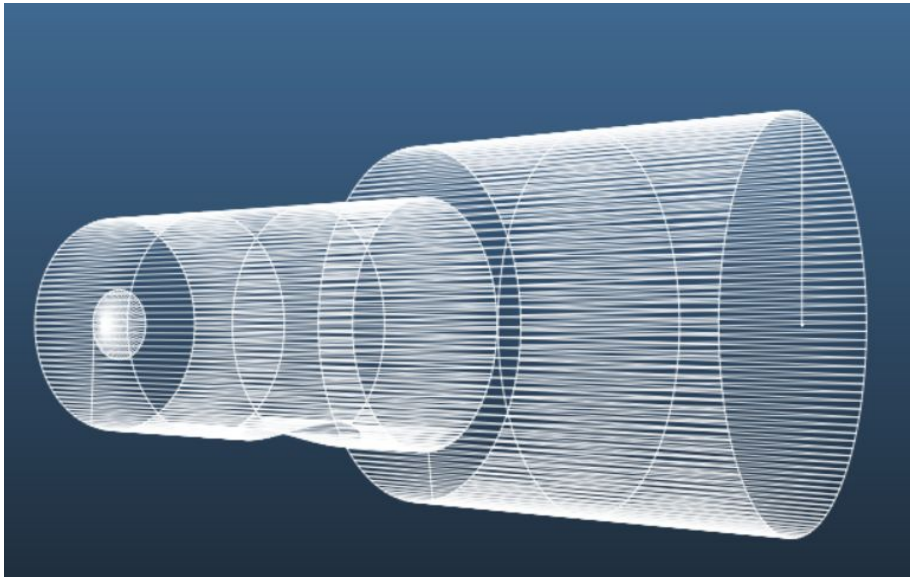
Imported from Inventor to Molflow+



Simulating in Molflow+

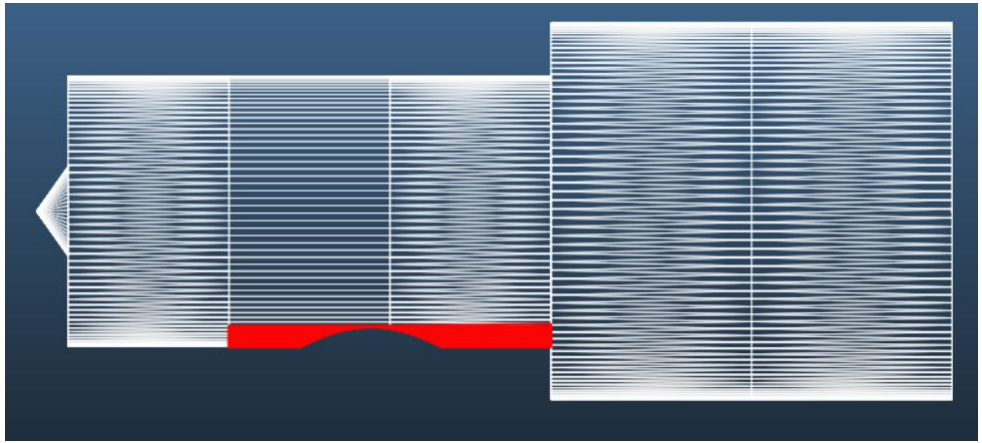


Inner walls with open aperture



Inner walls with closed aperture

Running Simulations in Molflow+



- The gas is coming from the ion source (leftmost triangle)
- The gas is going to the turbo pump (highlighted in red)

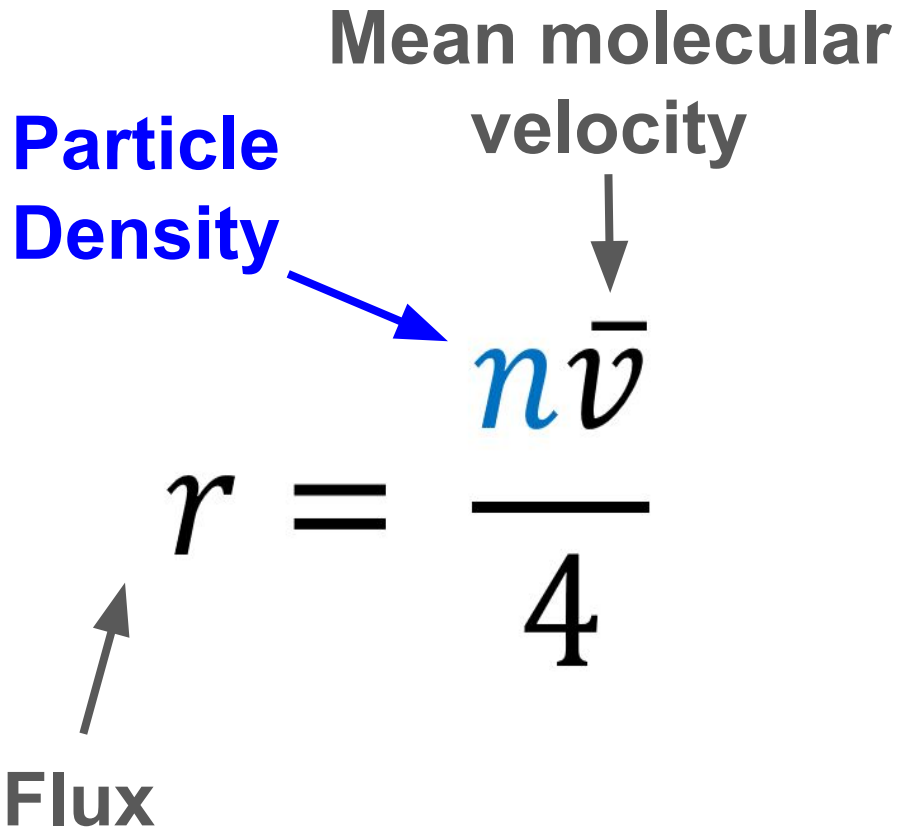
Flux Values from Molflow+

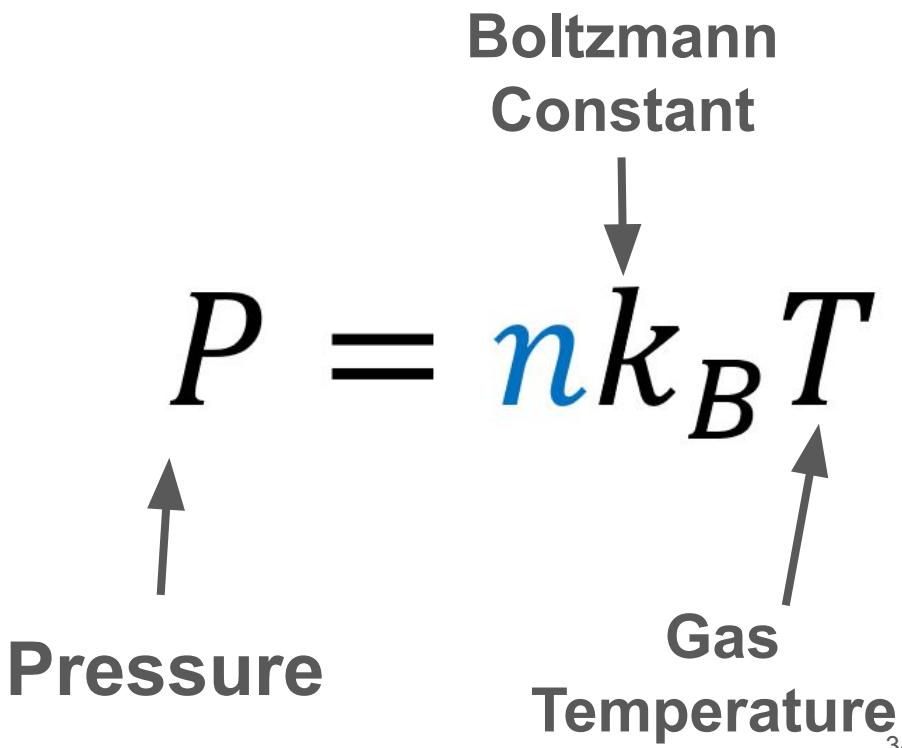
Flux: The flow/movement of the H_2 particles

Flux of the open aperture extraction volume:
$1.9 * 10^{16}$ molecules/cm^2/second

Flux of the closed aperture extraction volume:
$5.7 * 10^{16}$ molecules/cm^2/second

Converting Flux to Pressure





Converting Flux to Pressure

$$P = \frac{4k_B T}{\bar{v}} * r$$

$k_B = 1.38 * 10^{-23}$ J/K

Estimated Values:
T = 300 K (room temperature)
$\bar{v} \sim 1.49 * 10^5$ cm/s

Pressure Calculations

Pressure for open aperture exit:

$8.3 * 10^{-10}$ Torr

Pressure for closed aperture exit:

$4.2 * 10^{-9}$ Torr

Open aperture has a lower pressure than the closed aperture by a factor of 0.2.

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Results

Leak Detection

- Identified and helped resolve two gas leaks.

Apparatus Schematic Update

- Created an accurate 3D CAD model of the apparatus.

Vacuum Simulations

- Used Molflow+ to simulate the effect of geometry and pump configuration on vacuum performance.

What I learned

- Practical skills
  - Gas line leak diagnostics
  - CAD modeling for experimental design
  - Vacuum simulations with Molflow+
- Broader impact
  - Gained hands-on understanding about how a slight change in a physical system can affect experimental results

Acknowledgement

- This material is based upon work supported by the National Science Foundation under Grant No. PHY-2349438
- Thank you to Georgia Karagiorgi, Reshmi Mukherjee, Amy Garwood, Grace Ho, Asia Latt, Ashley Delphia, and the Nevis community for their help and guidance

Thank you!

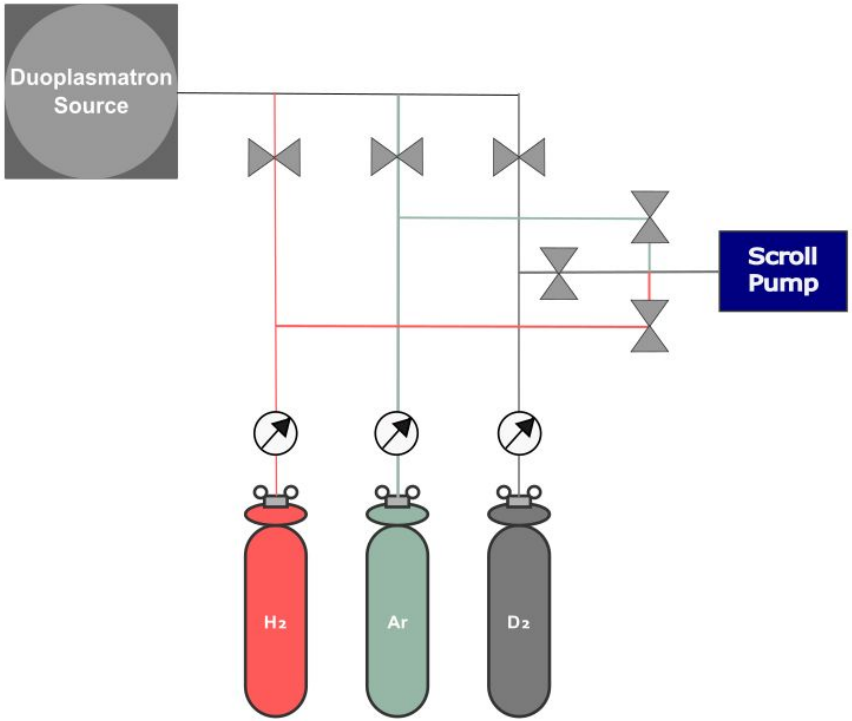
Any questions?

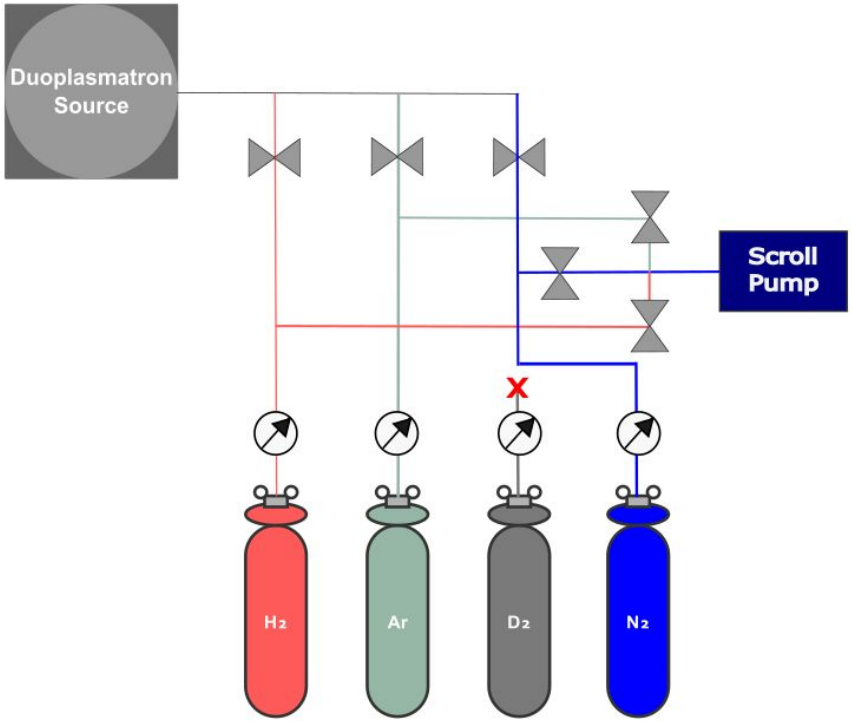
Extra slides

Mean Velocity Calculations

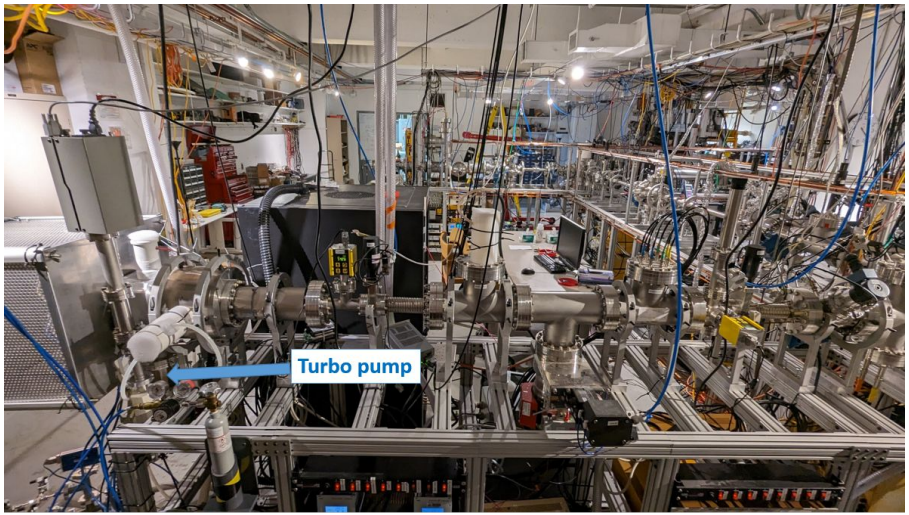
$$\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}$$

Searching for a Leak in the Ion Source Gas Line



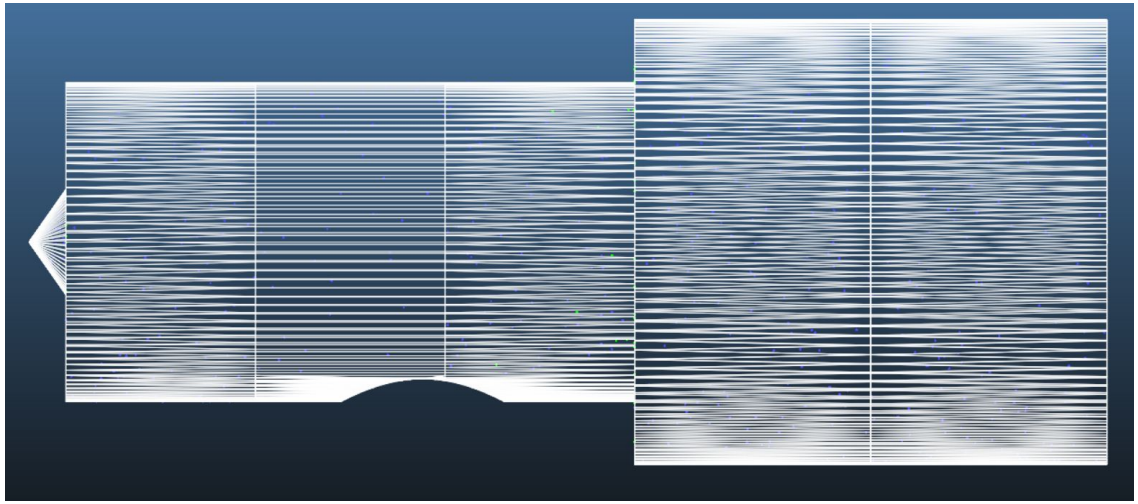


Future Work

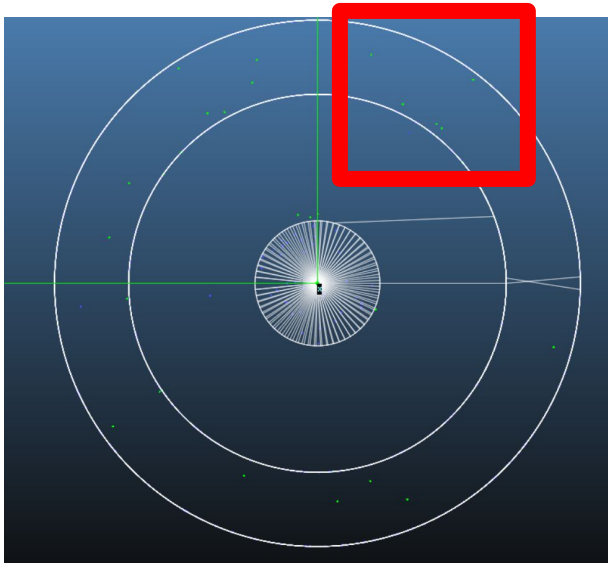


- Running simulations with updated geometry for more parts of the apparatus
- Compare pressure profiles to experimental pressure gauge readings to validate the simulation

Closed Exit Aperture in Molflow+

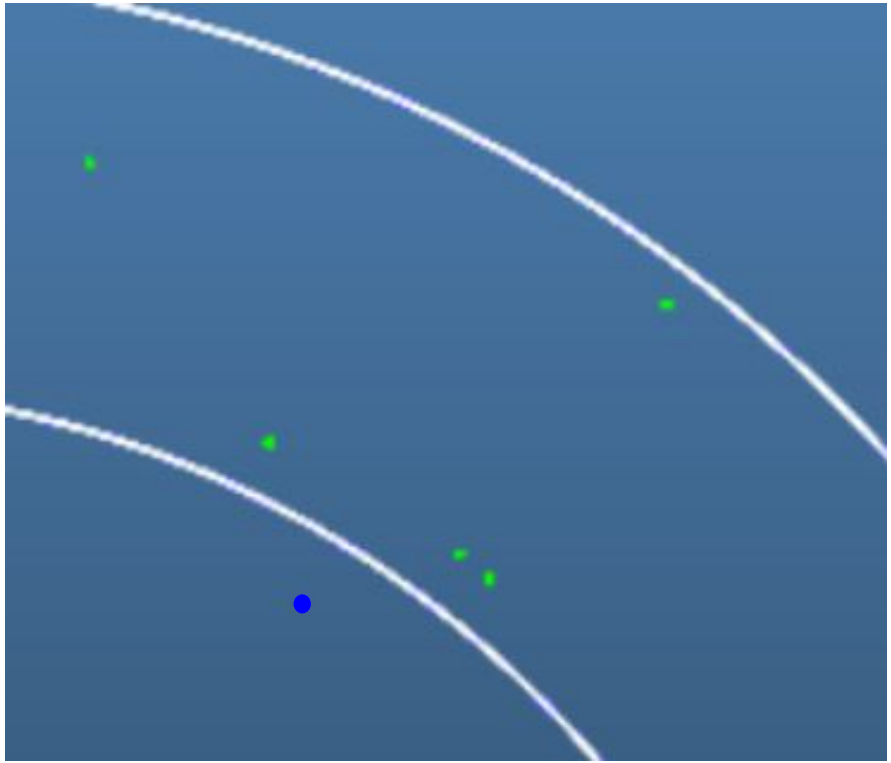


Closed exit aperture side view after simulation



Closed exit aperture front view after simulation

Closed Exit Aperture in Molflow+



Hits on apparatus wall

Searching for Leak in Instrument Operation Gas line