Numerical Investigation of Chamber Repressurization

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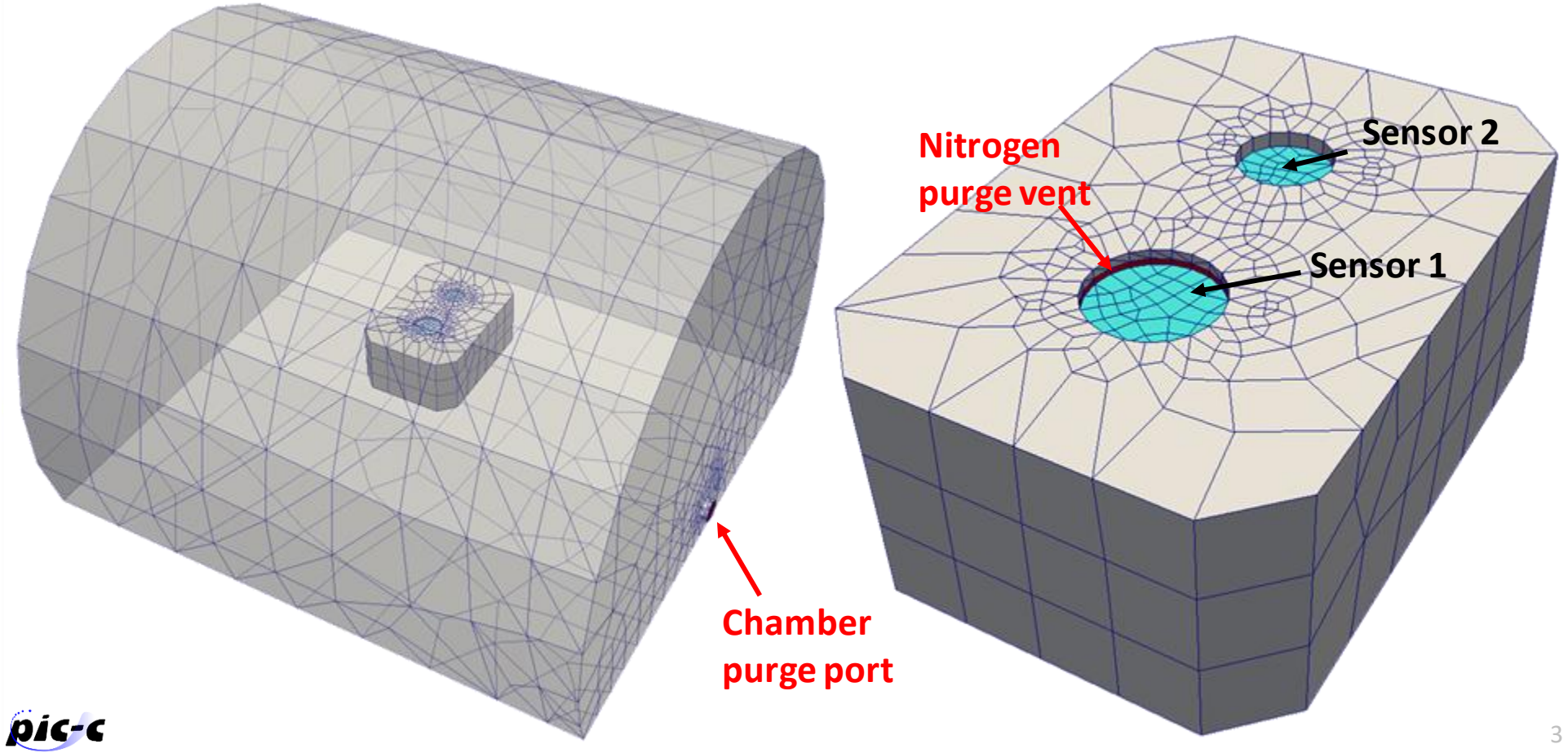
Introduction

- Common difficulty encountered in thermal vacuum testing is deciding how to bring the chamber back to the ambient pressure without adversely affecting the flight hardware
- Instruments usually attached to purge lines and often there is desire to start repress by flowing gas through these lines
- This is expected to create positive pressure gradient in respect to the ambient environment and thus prevent infiltration of external contaminants into the instrument cavity
- On the other hand, thin foils and other fragile components may be damaged if pressure gradient too high
- This work presents a “proof of concept” from a DSMC study to characterize the effect of purge on molecular deposition
- Computing pressure gradients around thin foils is left for future work

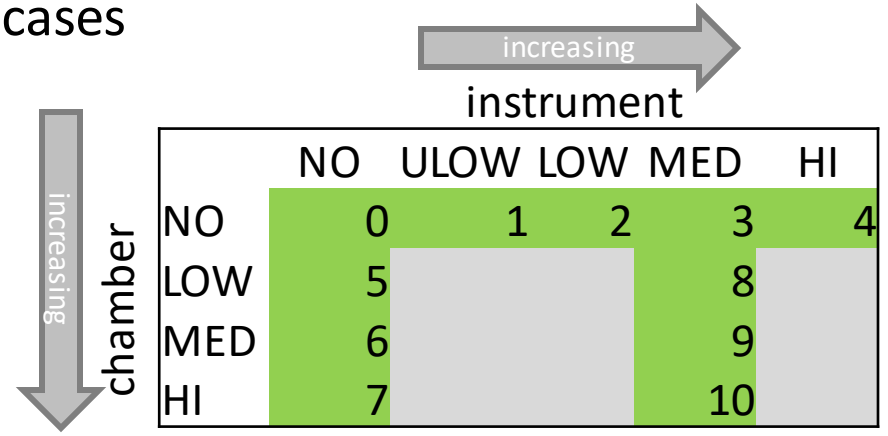
Problem Description

- We consider some hypothetical instrument containing two contamination sensitive sensors and placed in a vacuum chamber
- The instrument is attached to a purge line with nitrogen gas venting around the circumference of the larger sensor
- **Does gas flow from the instrument vent reduce the sensor deposition?**



Parameter Space

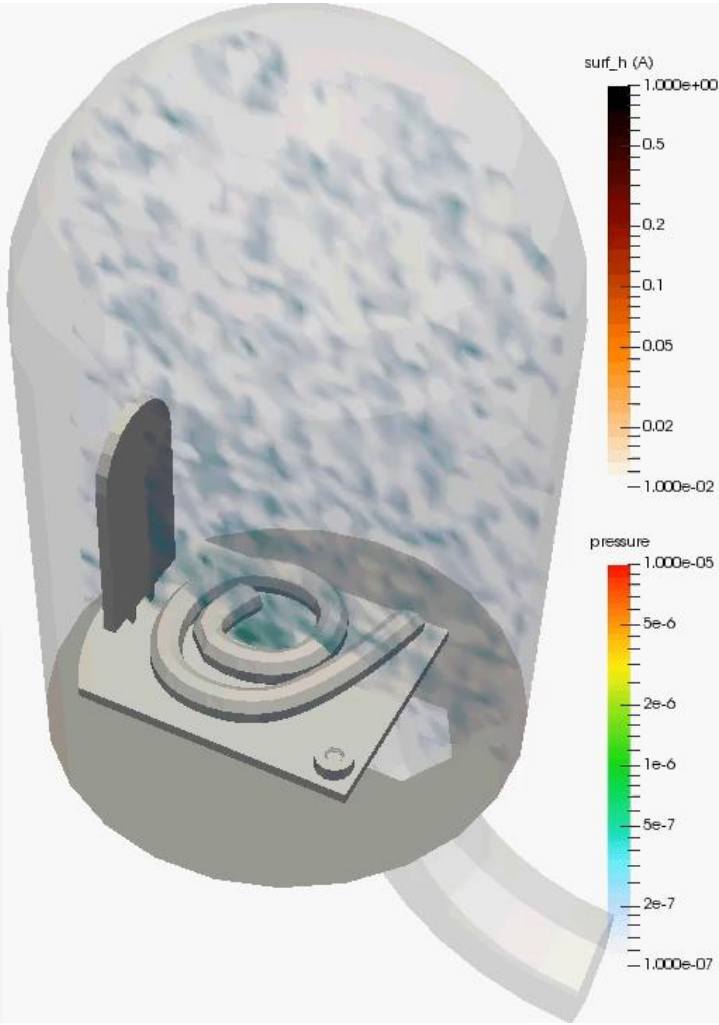
- Simulation started with the chamber filled with a hypothetical 94 amu hydrocarbon at 5×10^{-6} Torr
- Instrument and/or chamber N_2 purge initiated and the simulation ran for 25,000 time steps of 5×10^{-6} (0.125 seconds of real time)
- Sensors set to 100K: 100% sticking of HC, but N_2 does not condense
- Table on right summarizes the test cases
  - NO: no flow
  - ULOW: 0.001 L/min
  - LOW: 0.01 L/min
  - MED: 0.1 L/min
  - HI: 0.2 L/min

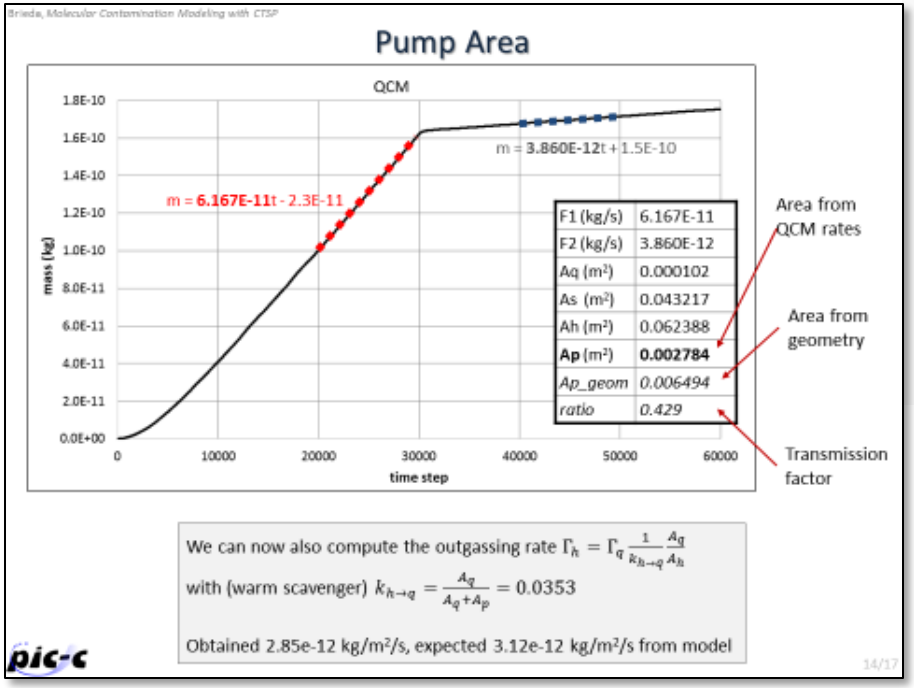


- Cases 0, 1, 2, 3, 4 consider the effect of instrument purge with chamber repressurization line off
- Cases 5-10 then consider the impact of chamber repress line. In cases 5,6,7 the chamber is being repressurized with the instrument purge off.

Simulation Algorithm

- Simulations performed using PIC-C developed CTSP
- Code based on particle approach, concurrently pushes many molecules and/or particulates through small time steps Δt
- Supports aerodynamic, gravitational, electrostatic, forces
- Used on various NASA / AF missions, including GOES-R, MMS, JPSS, Restore, MOMA
- Example on right presented at 30th Rarefied Gas Dynamics conference. Harness outgassing in a bell jar containing a QCM, scavenger activation yields lower pressure and reduced deposition rate on the QCM.





Rarefied Gas

- CTSP originally developed to tackle free-molecular problems
- Gas flows can be divided into three regimes by Knudsen number, $Kn = \frac{\lambda}{L}$
- $\lambda = 1/(\sigma n)$ is the mean free path, the average distance molecule travels between collisions. σ is the collision cross-section and n is gas density. L is some characteristic problem dimension, such as vacuum chamber diameter.
- If $\lambda \ll L$ ($Kn \ll 1$, n high), molecules much more likely to collide with each other than with chamber walls. Gas is in **continuum**, and can be modeled using fluid approaches such as CFD.
- On other hand, if $\lambda \gg L$ ($Kn \gg 1$, n low), molecules much more likely to collide with chamber walls before colliding with each other. Gas is in **free molecular** state. This is the typical scenario encountered in contamination modeling.
- Finally, if $\lambda \approx L$ ($Kn \approx 1$), collisions happen, but not sufficiently often to assume continuum. Rarefied gas and kinetic simulation codes need to be utilized. This is the case encountered in the initial stages of chamber repressurization.
- Some regions (near the purge inlet) may be in continuum, while at least briefly, regions far from inlet may be in free molecular flow

DSMC

- Rarefied gases can be modeled using technique known as Direct Simulation Monte Carlo (DSMC)
  - G. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows,* Oxford Science Publications,1994.
  - Computational domain discretized into a computational mesh. Can use uniform Cartesian cells, or (better) adaptive collision cells that grow with local density.
  - "Grid-free" DSMC (based on octree) also demonstrated by Olson and Christlieb.
  - Gas represented by simulation macroparticles, not numerically feasible to model all real molecules
  - At each time step, particles grouped into cell and in each cell number of collision pairs to check for collisions computed from

$$(N_C)_{a,b} = \frac{(N_a/\Delta V) N_b \Delta t (\sigma_t c_r)_{max}}{P_{a,b} + (W_b/W_a) P_{b,a}} \qquad \begin{aligned} P_{a,b} &= \max(W_b/W_a, 1) \\ P_{b,a} &= \max(W_b/W_a, 1) \end{aligned}$$

  - This is a modification of Bird's No Time Counter scheme for gases with non-equal macroparticle weights per *Boyd I., 1996.* For each, relative probability computed from

$$P = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}}$$

  - This value compared to a random number. If $P > R_1$, elastic collision used to computed new velocities. Post-collision velocities changed if $P_{a,b} \left| P_{b,a} > R_2 \right| R_3$

Cross-section and validation

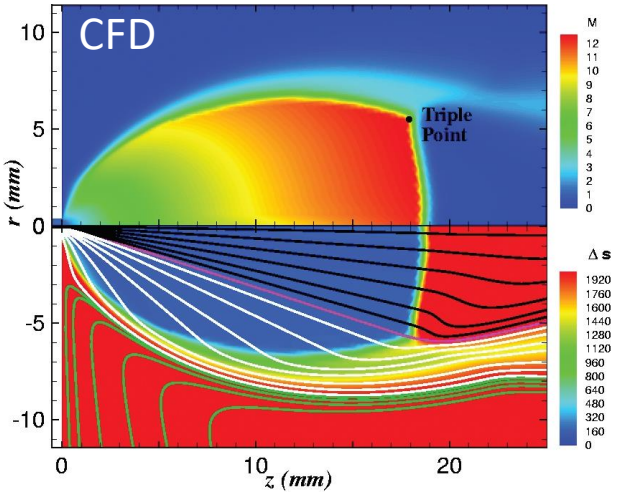
- Bird's Variable Hard Sphere (VHS) model captures the observation that molecules don't interact like hard sphere billiard balls, instead their apparent molecular diameter (and hence cross-section) scale with relative velocity.
- Collision cross-section obtained from $\sigma_T = \pi d_{a,b}^2$ where

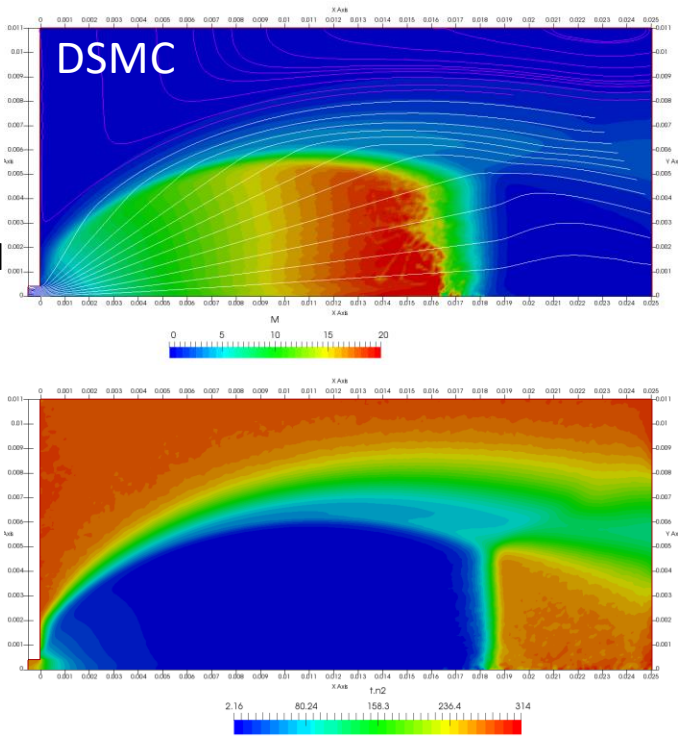
$$d_{a,b} = \left(d_{ref}\right)_{a,b} \sqrt{\frac{\left[\left(2k\left(T_{ref}\right)_{a,b}\right)/\left(m_r c_r^2\right)\right]^{\omega_{a,b}-0.5}}{\Gamma\left(5/2-\omega_{a,b}\right)}}$$

- Bird provides reference values for molecular diameter d_{ref} and viscosity index ω for commonly used gases (like N2).
  $\left(d_{ref}\right)_{a,b} = 0.5(d_{ref,a} + d_{ref,b})$
- Assumed that $d_{ref,HC} = 2d_{ref,N2}$, $\omega_{HC} = \omega_{N2}$
- Only modeled N2:HC momentum transfer collisions, N2:N2 ignored

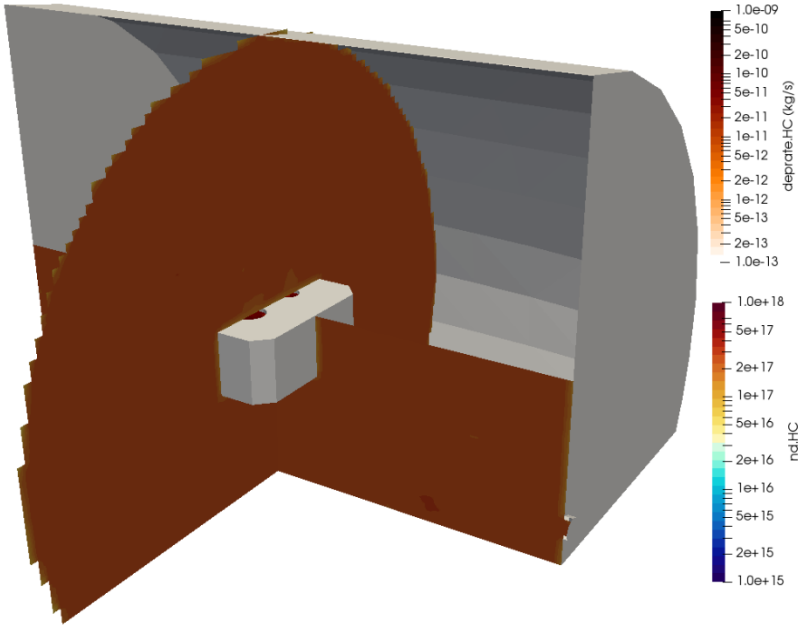
DSMC now implemented in CTSP, can use the code on rarefied gas problems

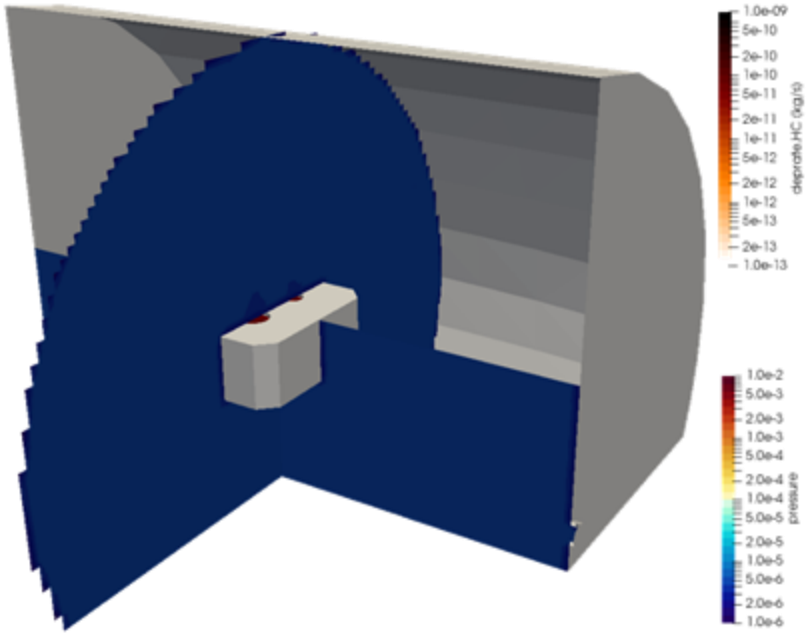
Validation: replicated setup from *Jugroot, 2004*, in which authors used CFD to model atmospheric gas expanding to a low pressure tank. Authors noted that $Kn \sim 1$ but stated that CFD still valid. DSMC produces similar profile, including the triple point and Mach disc, maximum Mach M=15, while CFD predicts M=12.

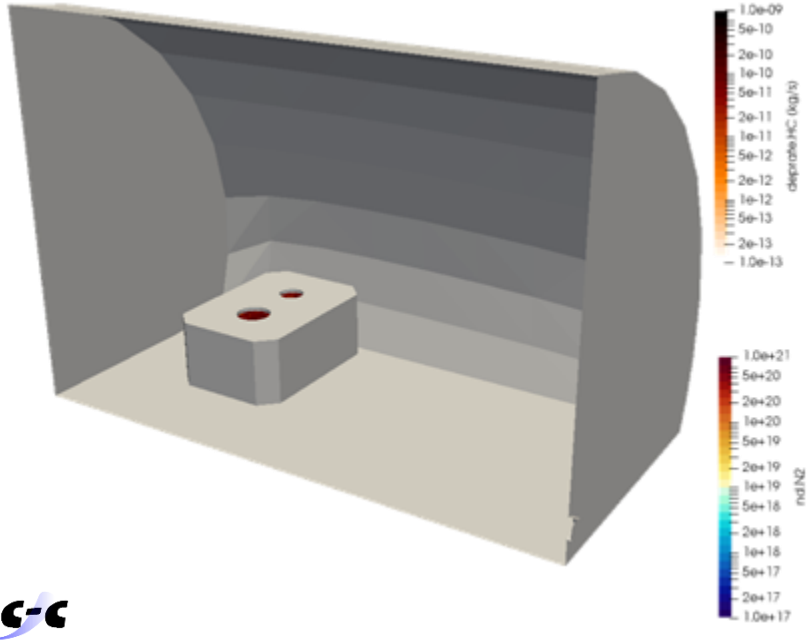


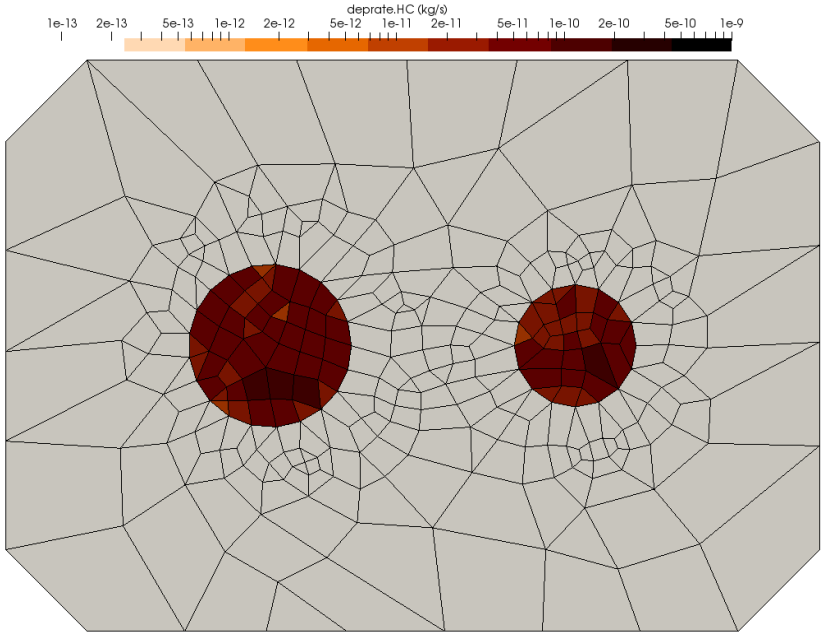


Case 0: instrument NO, chamber NO

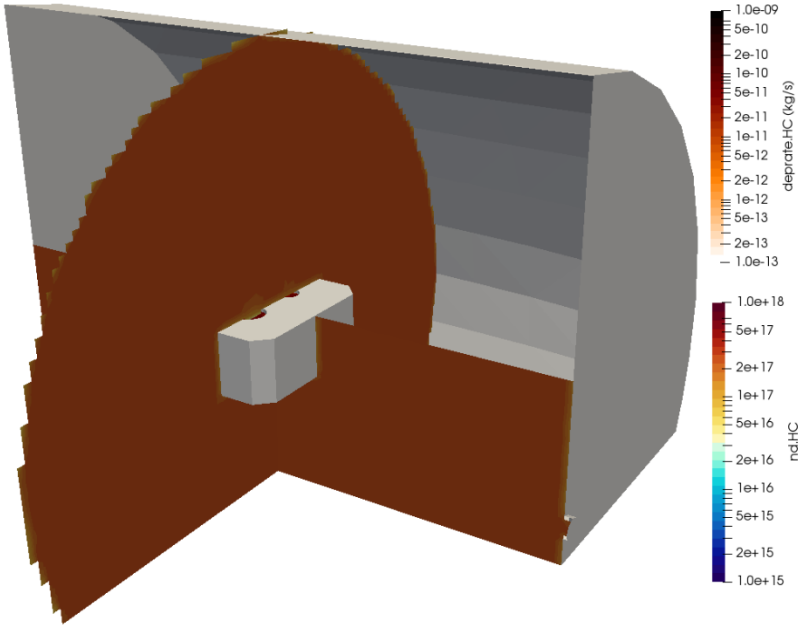


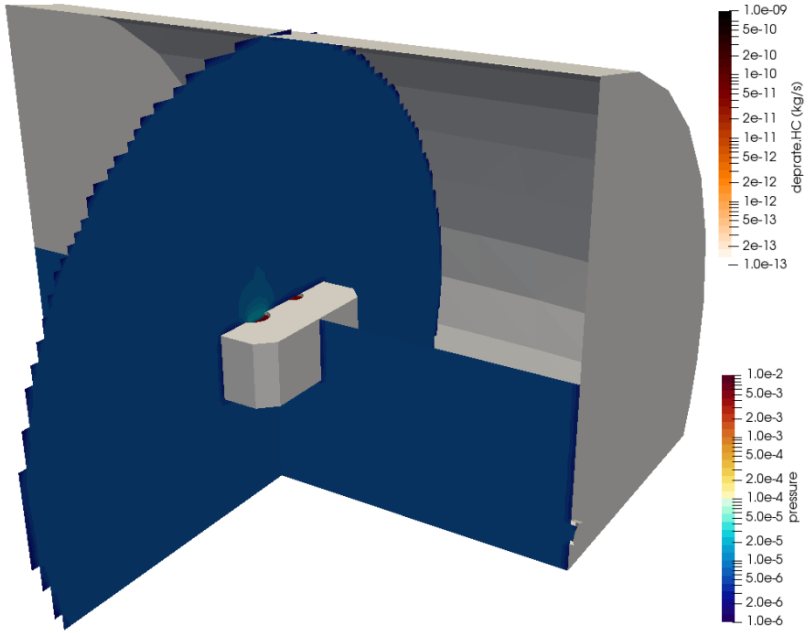


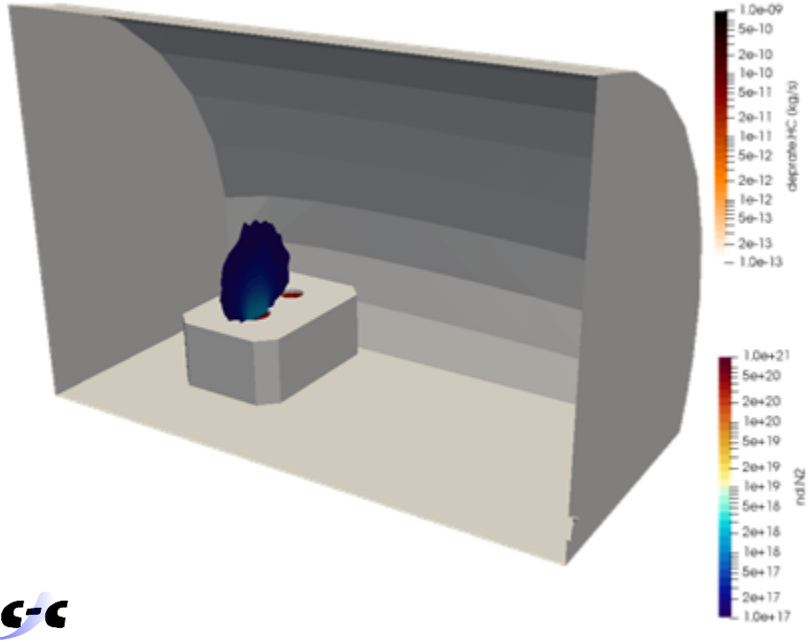


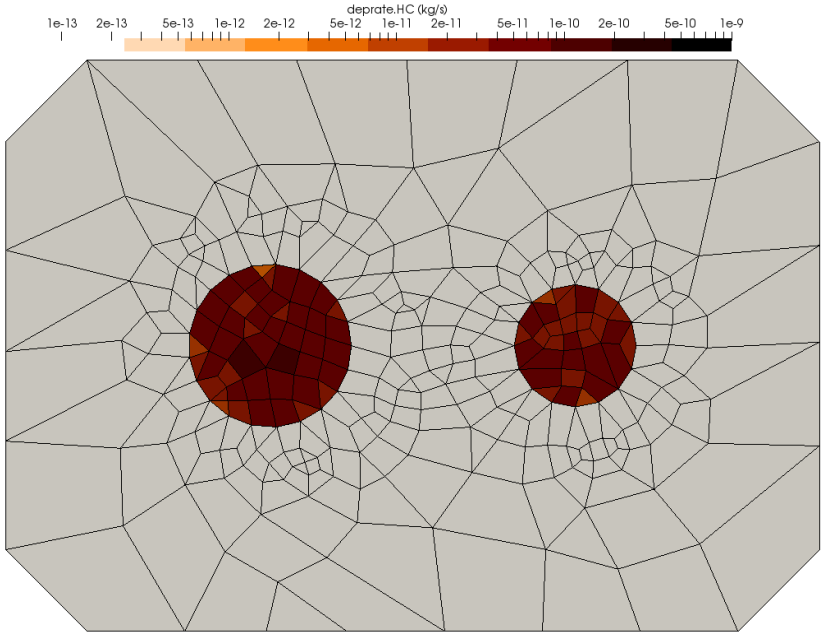


Case 1: instrument ULOW, chamber NO

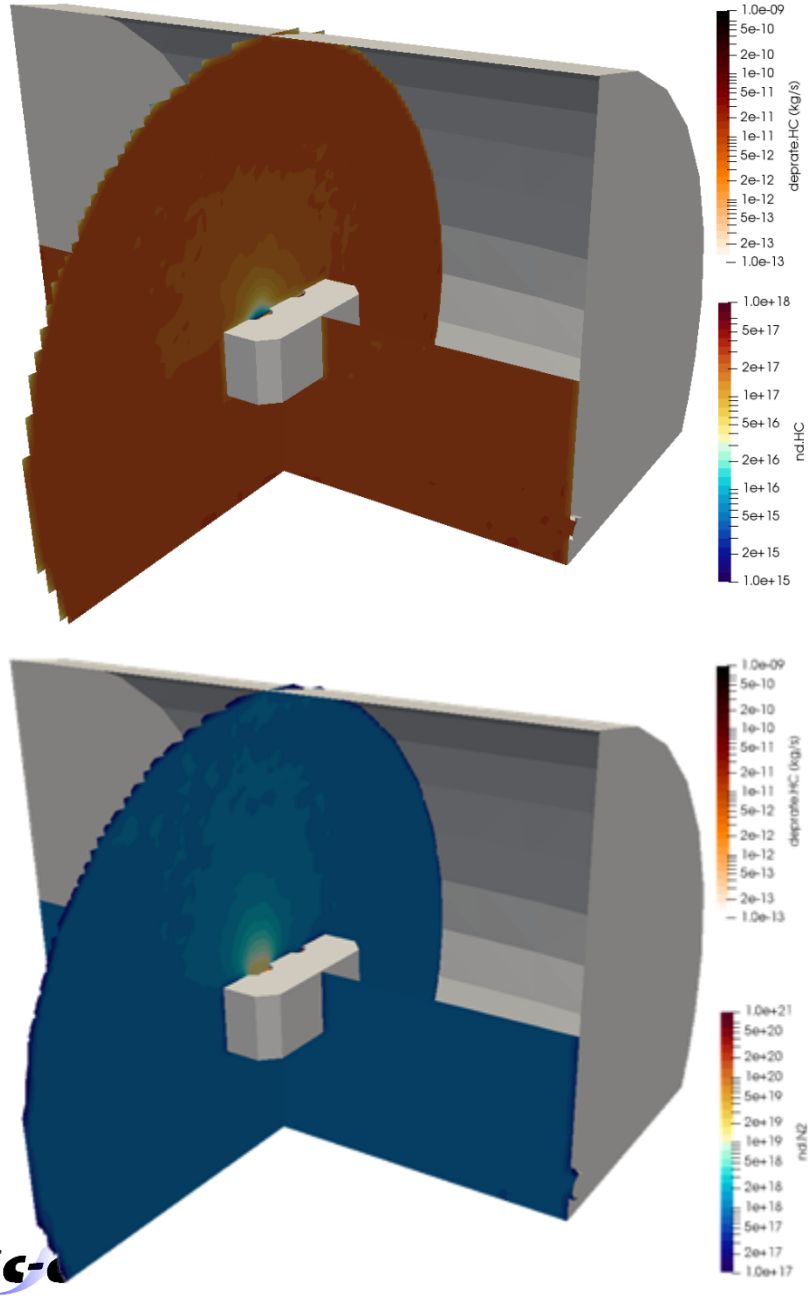




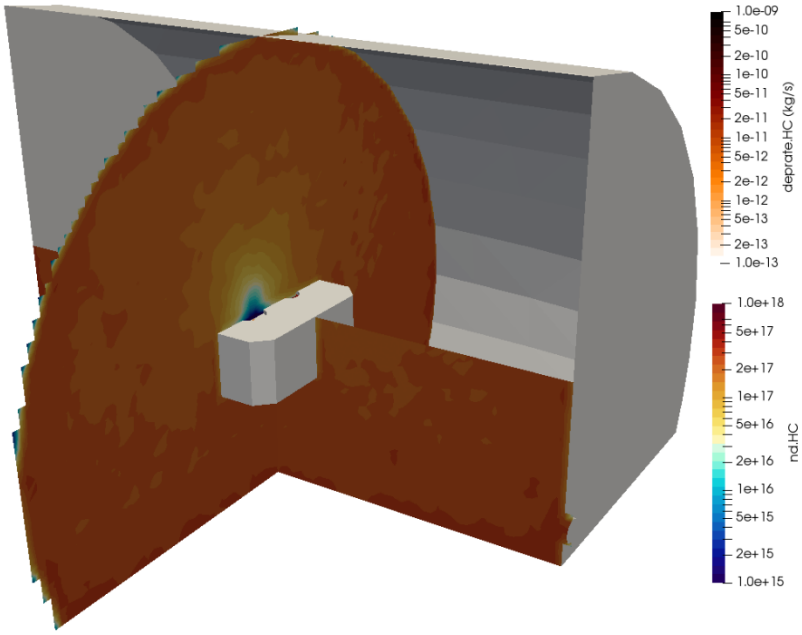


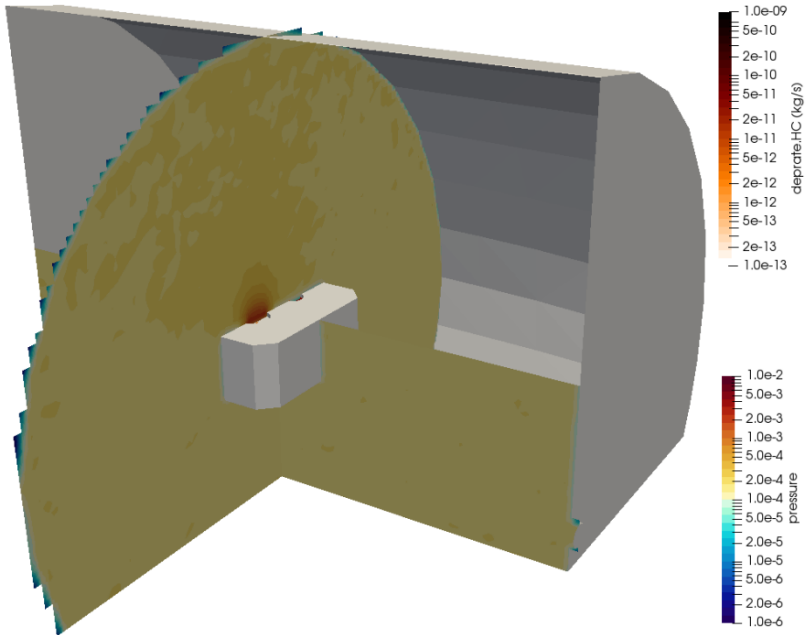


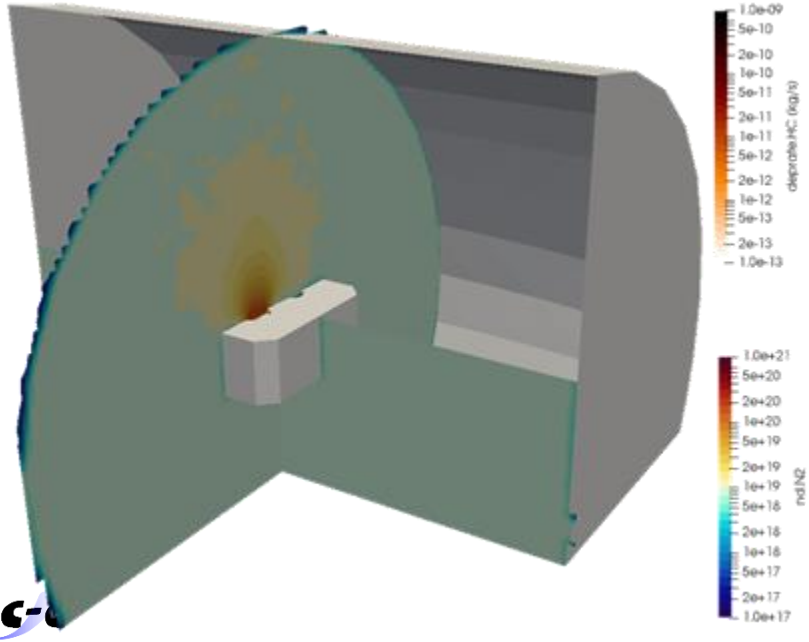
Case 2: instrument LOW, chamber NO

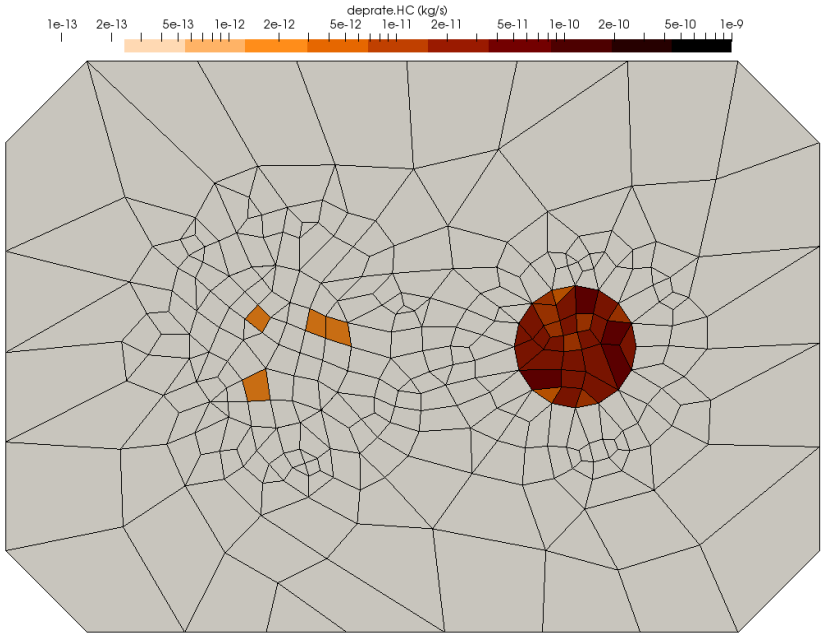


Case 3: instrument MED, chamber NO

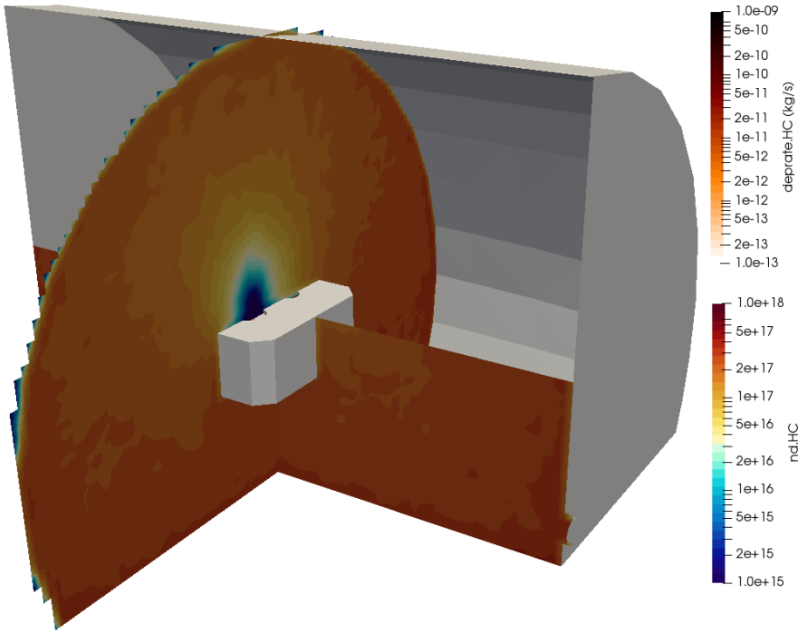


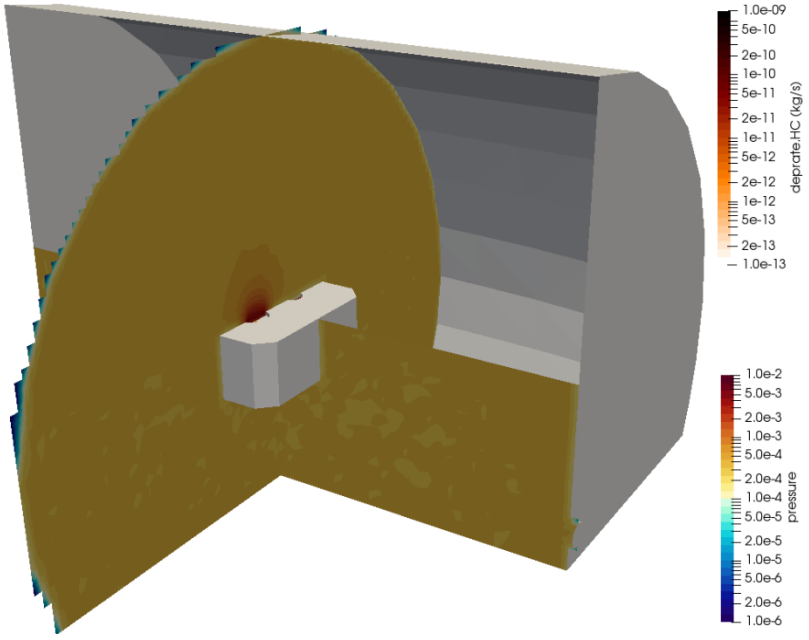


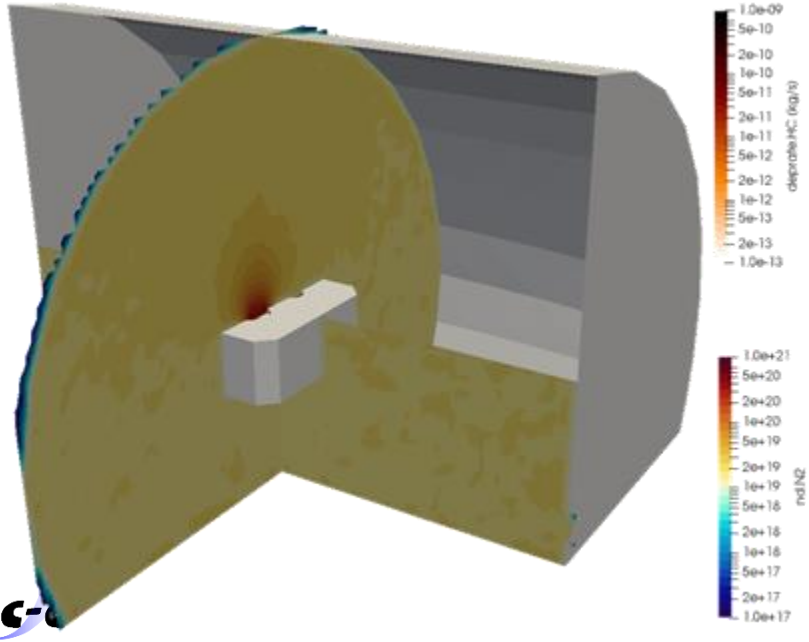


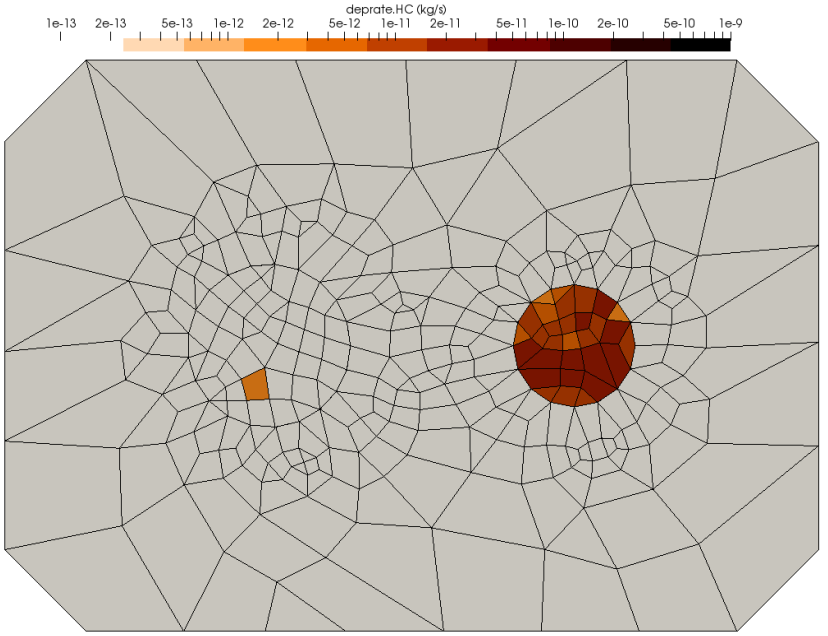


Case 4: instrument HI, chamber NO

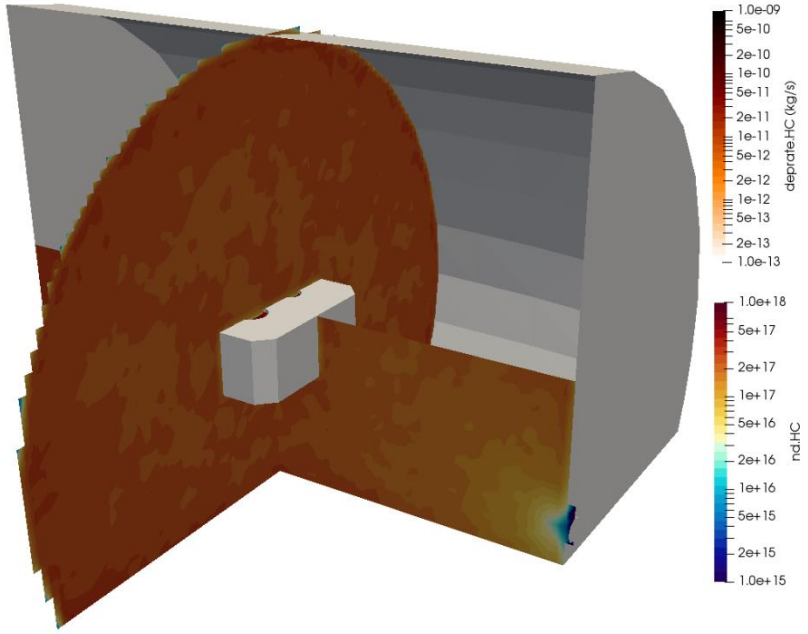


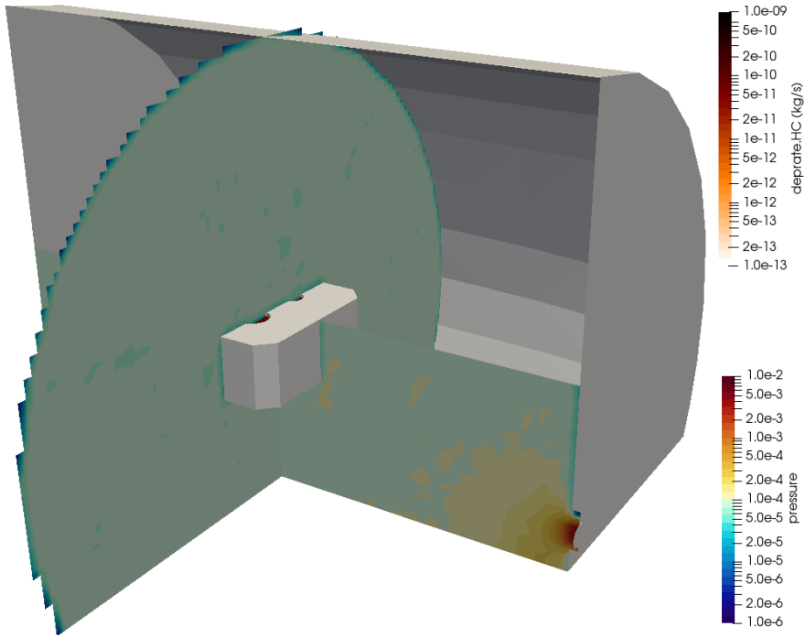


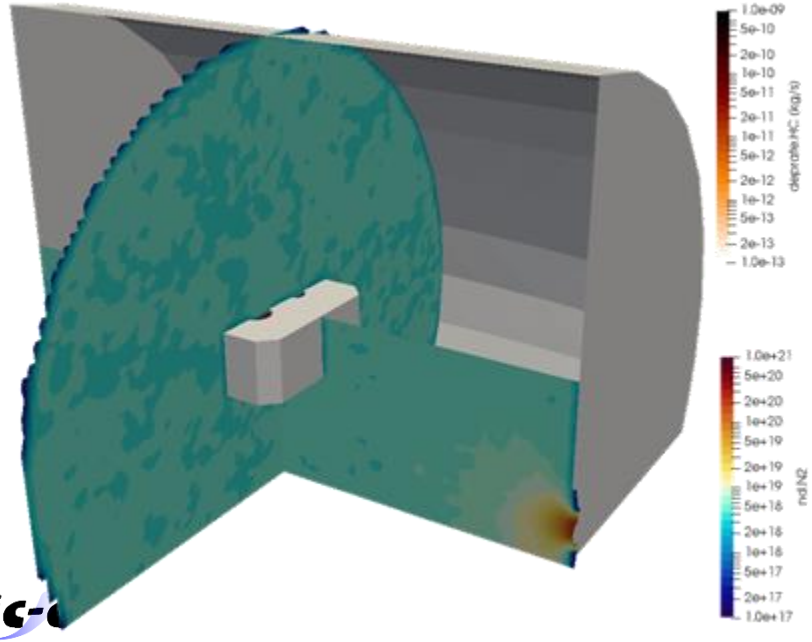


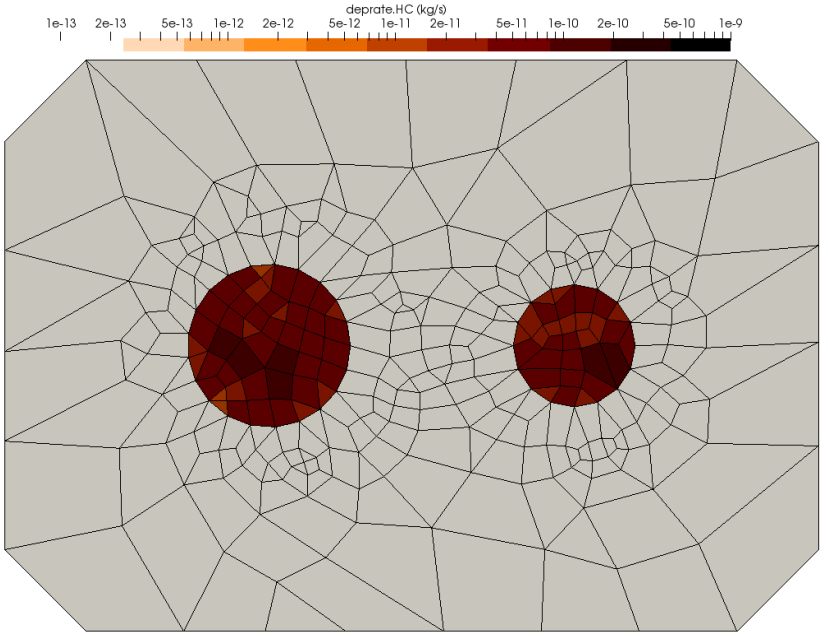


Case 5: instrument NO, chamber LOW

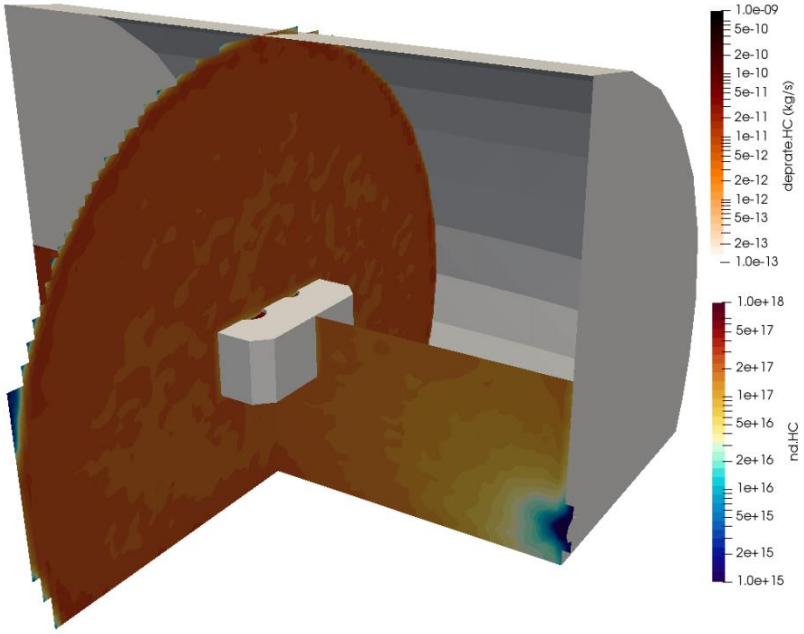


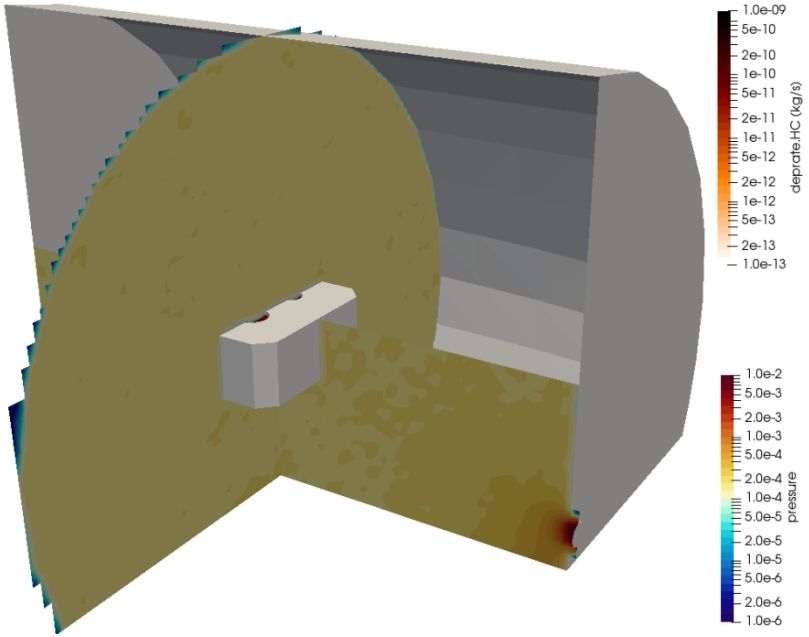


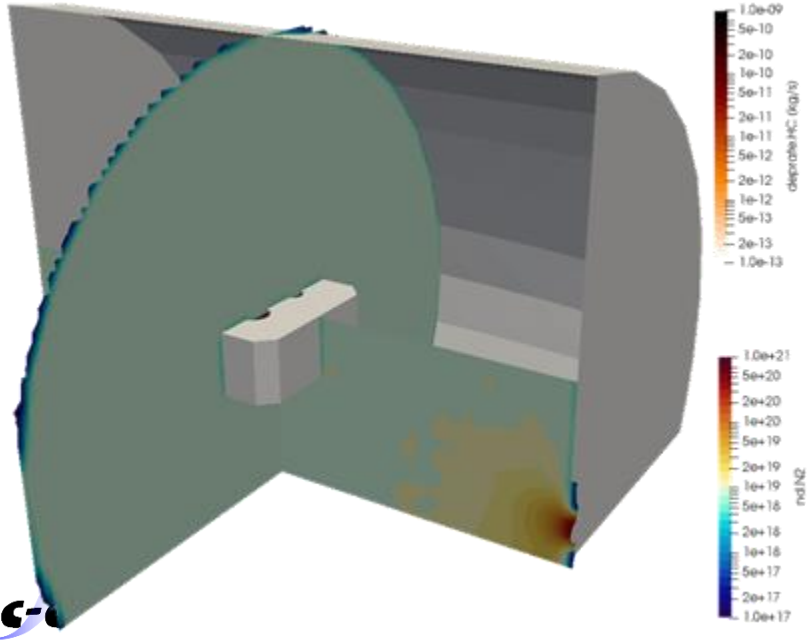


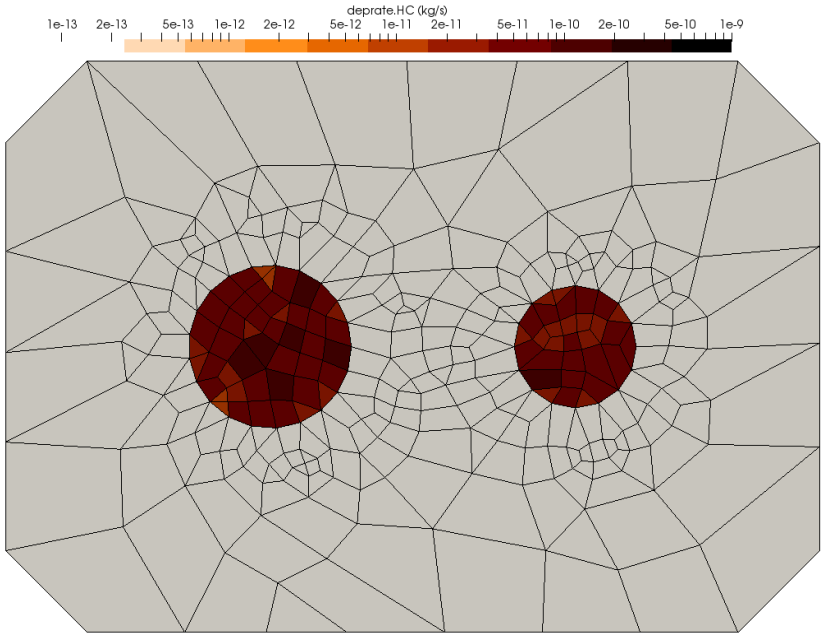


Case 6: instrument NO, chamber MED

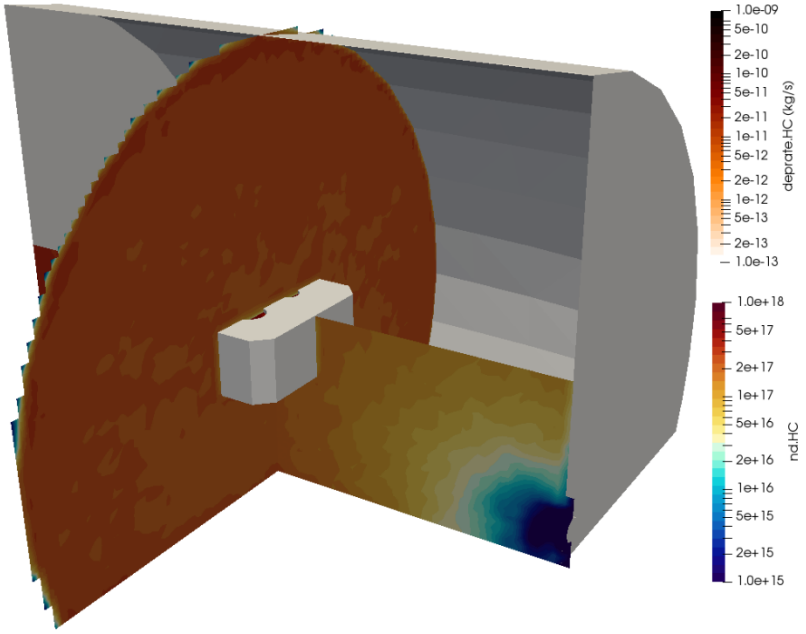


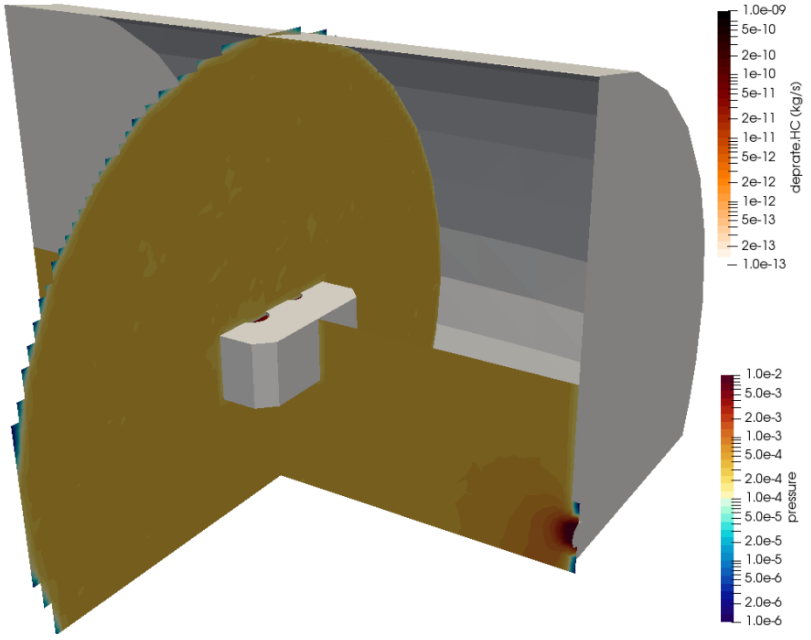


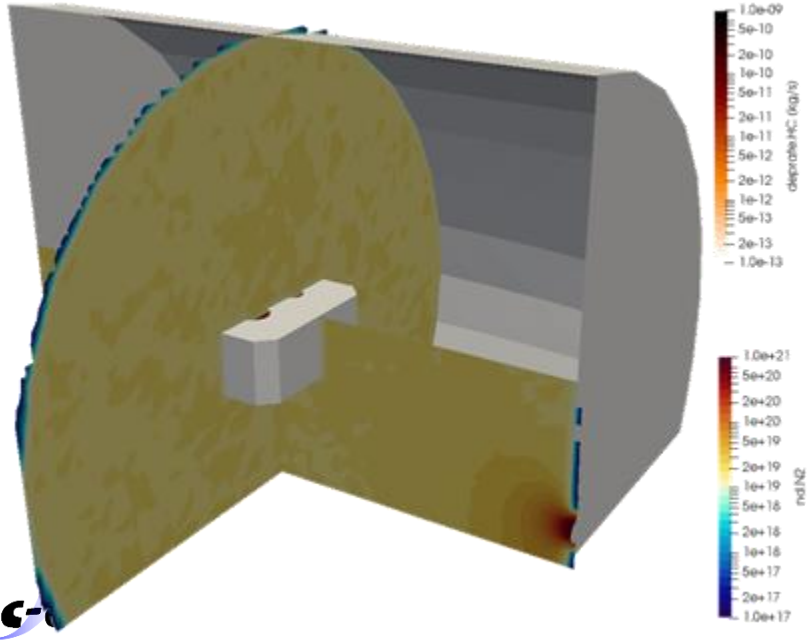


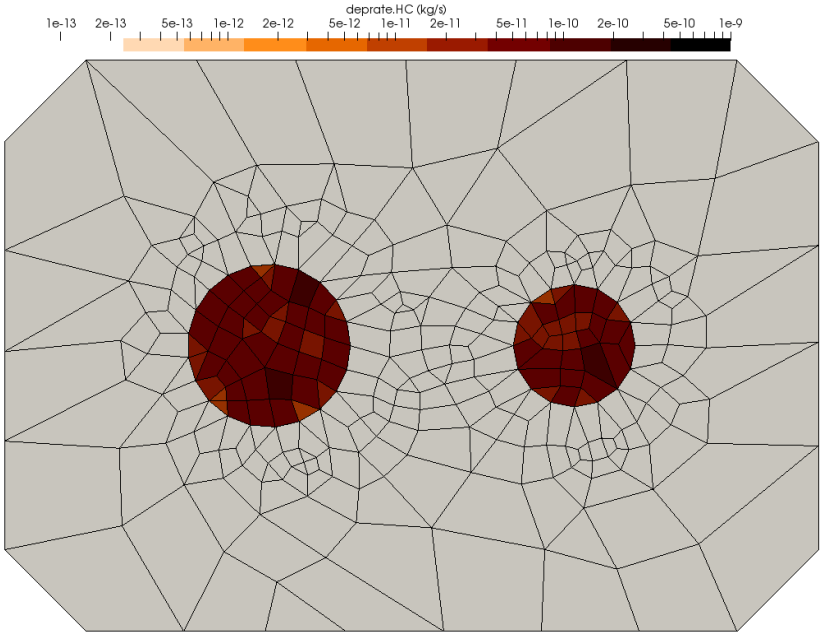


Case 7: instrument NO, chamber HI

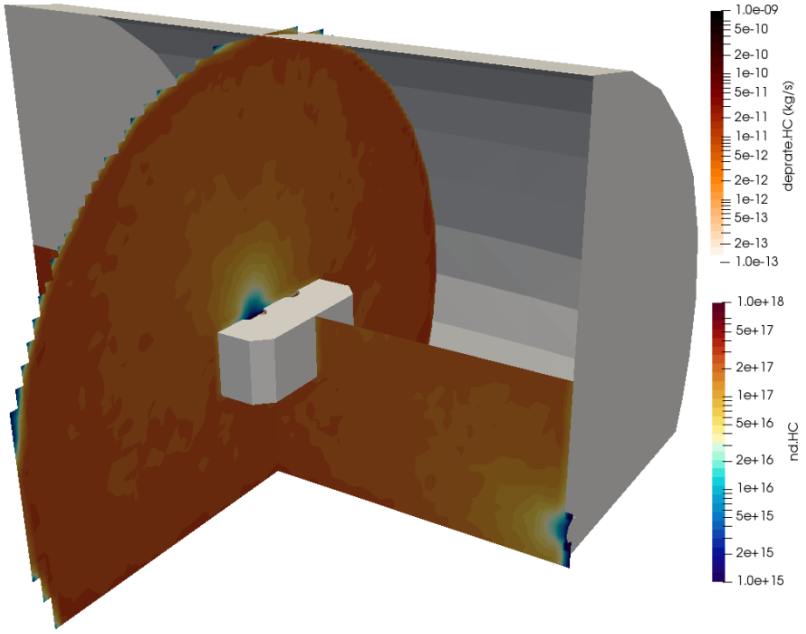


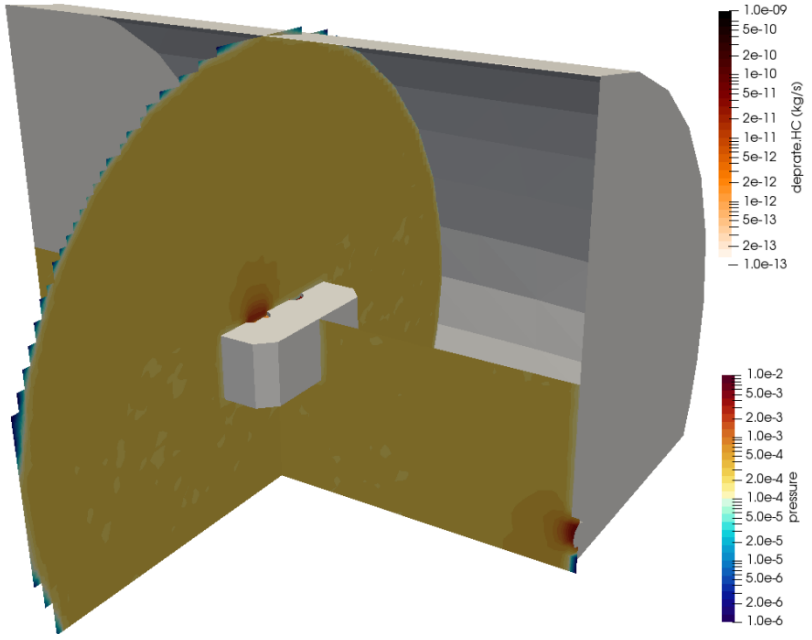


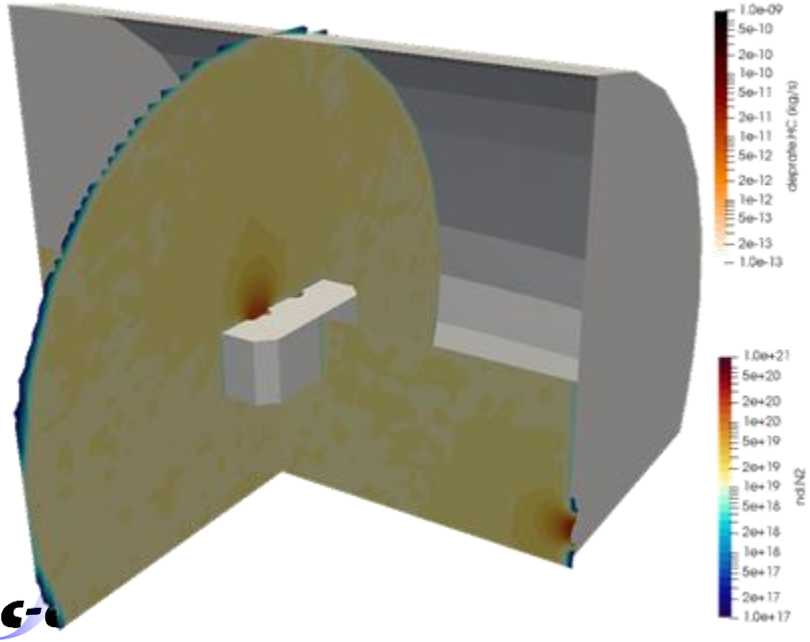


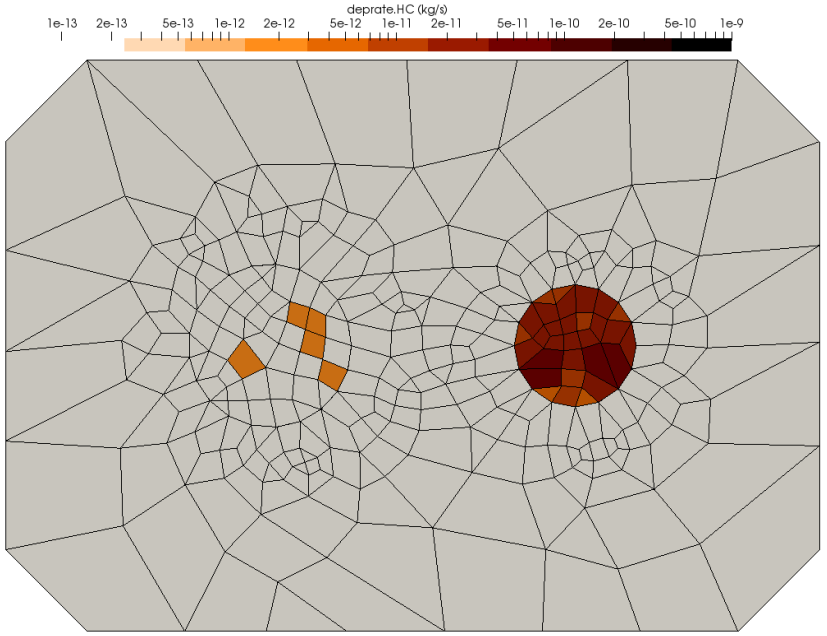


Case 8: instrument MED, chamber LOW

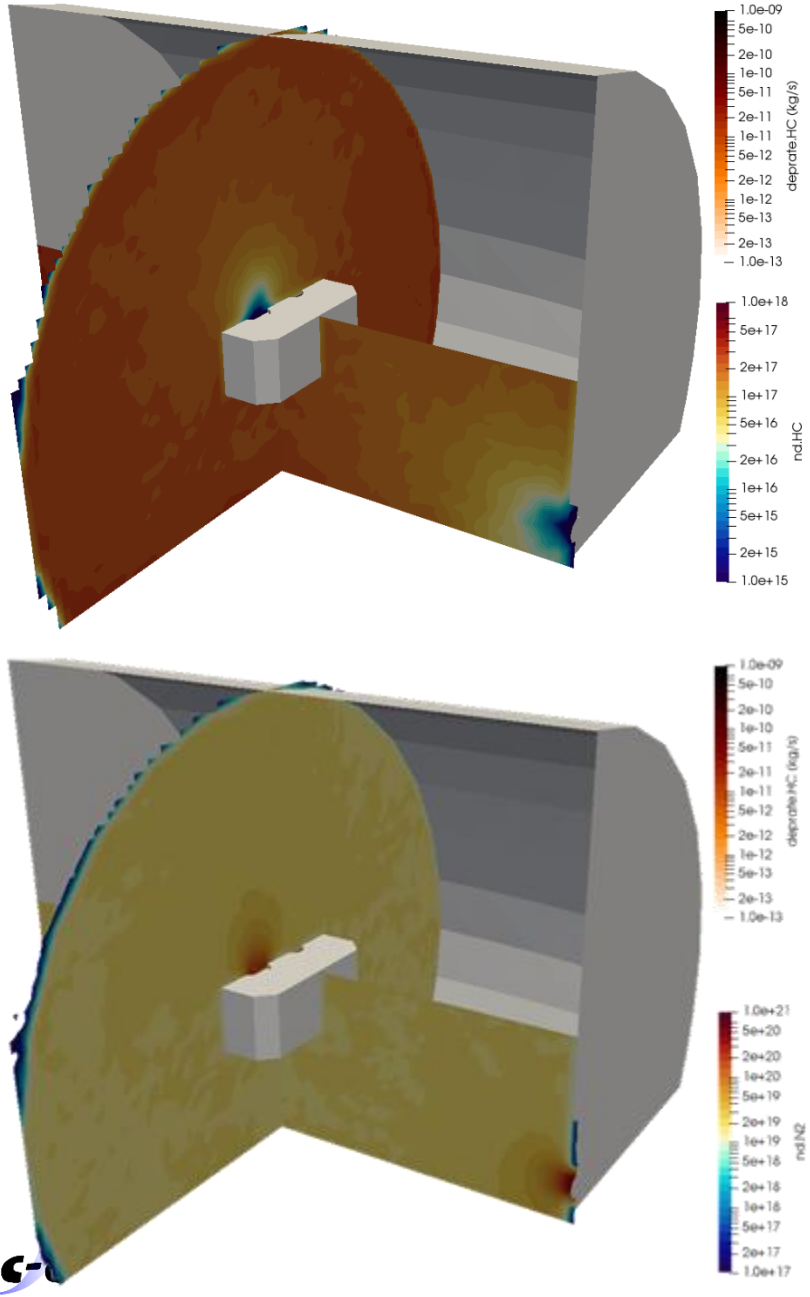




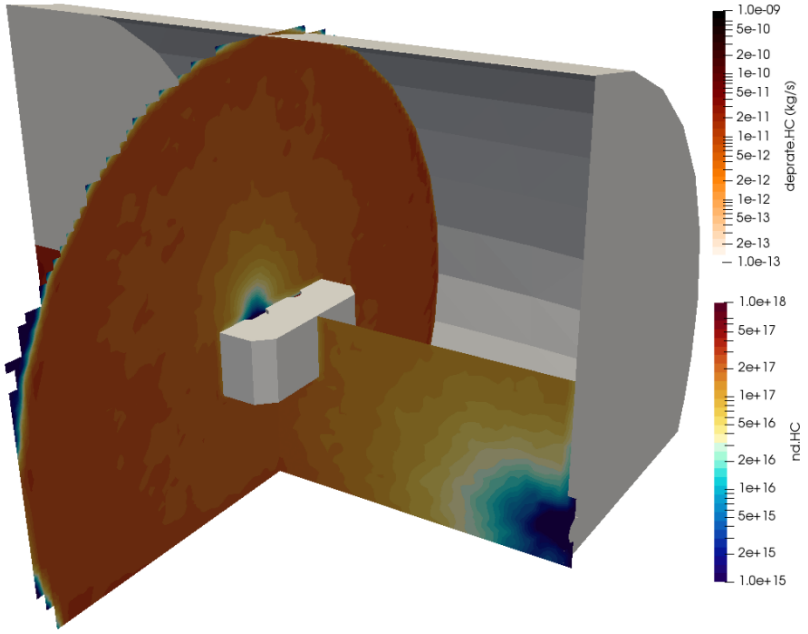


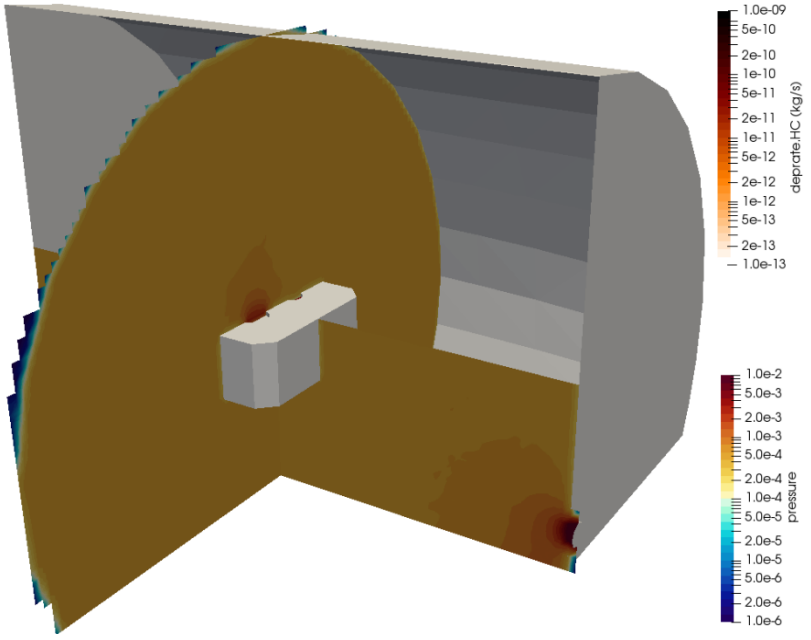


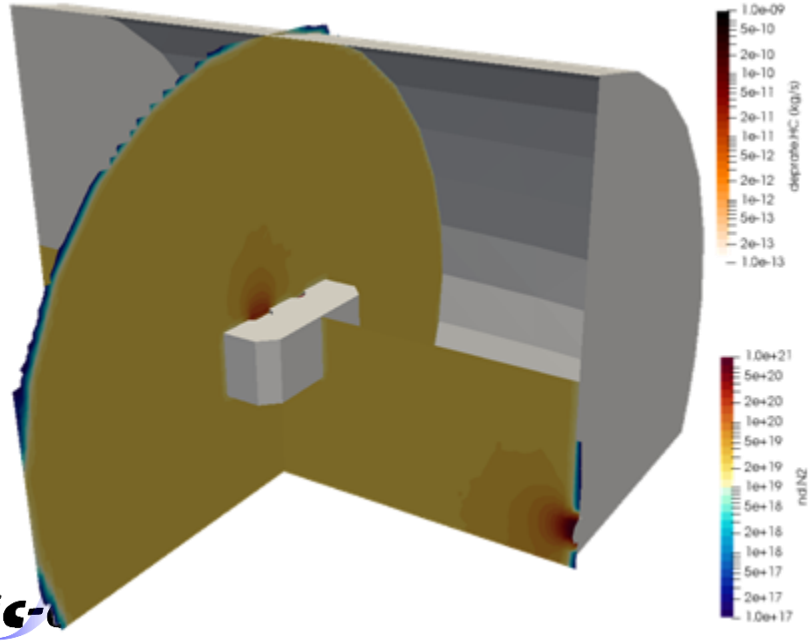
Case 9: instrument MED, chamber MED

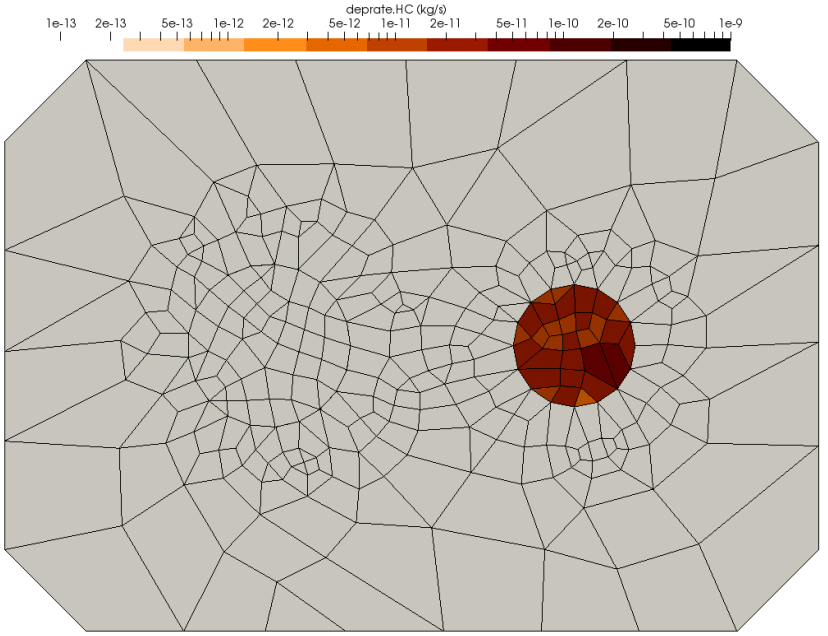


Case 10: instrument MED, chamber HI









Results

- Averaged deposition rate on the two sensors summarized below

$$k = \frac{\sum_e k_e A_e}{\sum_e A_e}$$

- Observations:
  - Deposition on sensor 1 decreases as instrument purge flow increases, ~1500x reduction at the highest flow rate
  - Chamber purge flow rate does not seem to have a strong impact, but could be a numerical artifact due to ignoring N2:N2 collisions
  - Purge plume from sensor 1 also shields sensor 2, deposition rate reduced ~3x

Sensor 1 raw

chamber \ instrument	NO	ULOW	LOW	MED	HI
NO	5.6E-11	5.3E-11	1.6E-12	1.2E-13	3.9E-14
LOW	5.7E-11			1.6E-13	
MED	6.1E-11			3.7E-14	
HI	5.3E-11			0	

Sensor 1 normalized

chamber \ instrument	NO	ULOW	LOW	MED	HI
NO	1.0000	0.9439	0.0280	0.0021	0.0007
LOW	1.0099			0.0029	
MED	1.0826			0.0007	
HI	0.9374			0.0000	

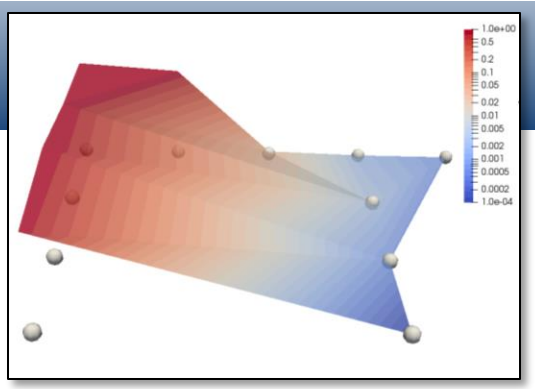
Sensor 2 raw

chamber \ instrument	NO	ULOW	LOW	MED	HI
NO	4.4E-11	4.3E-11	3.1E-11	2.5E-11	1.6E-11
LOW	5.3E-11			2.8E-11	
MED	5.0E-11			2.6E-11	
HI	4.8E-11			2.4E-11	

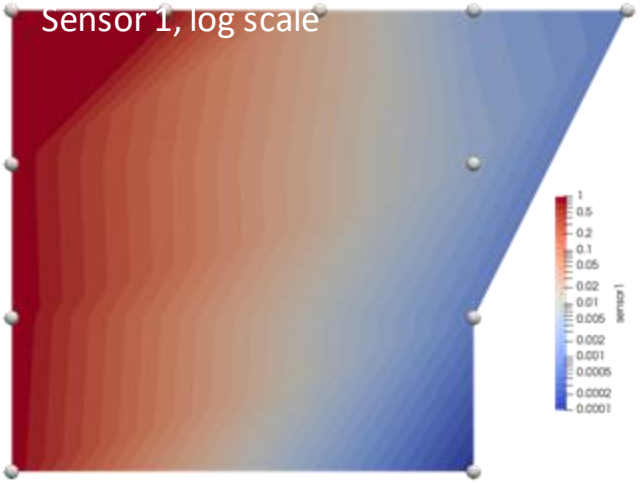
Sensor 2 normalized

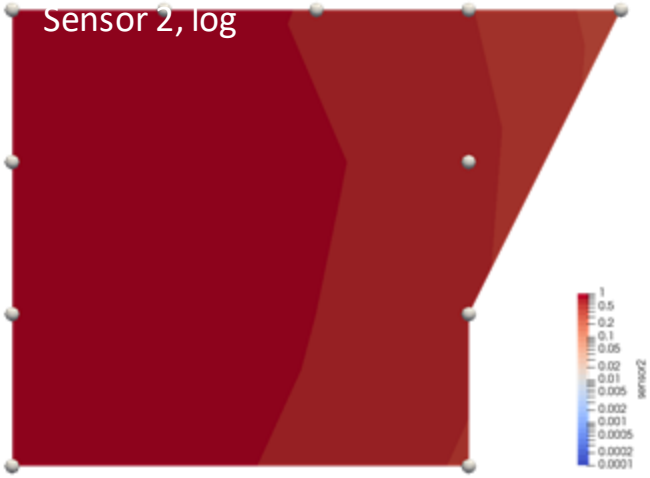
chamber \ instrument	NO	ULOW	LOW	MED	HI
NO	1.0000	0.9785	0.7142	0.5714	0.3724
LOW	1.2013			0.6320	
MED	1.1516			0.6046	
HI	1.0877			0.5441	

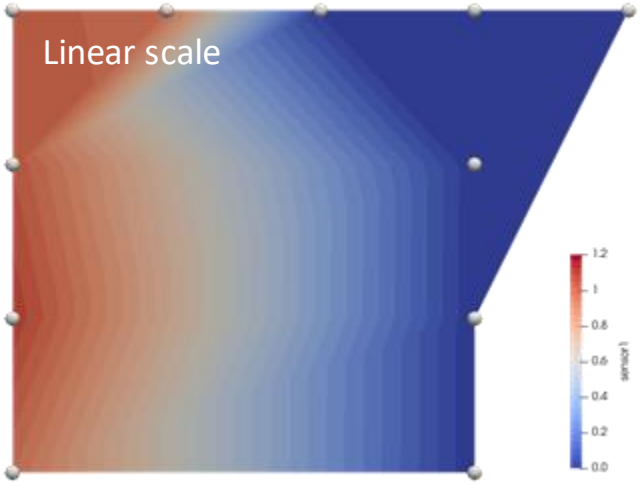
Results

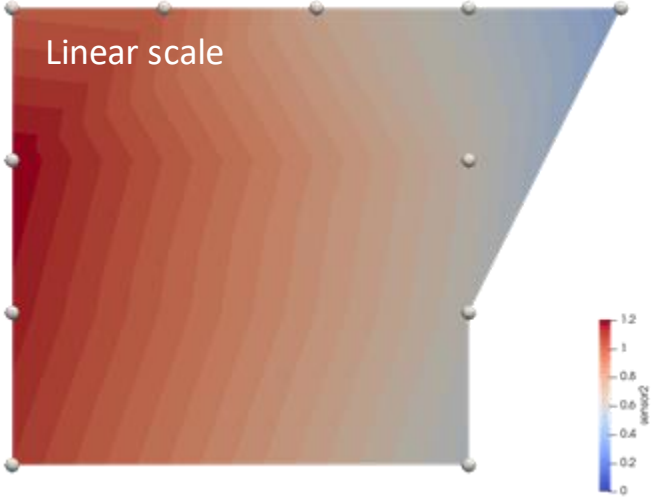


- Data from previous chart visualized graphically
  - Response to instrument purge flow easily seen
  - Similarly, can see lack of dependence on chamber flow (but perhaps numerical artifact!)



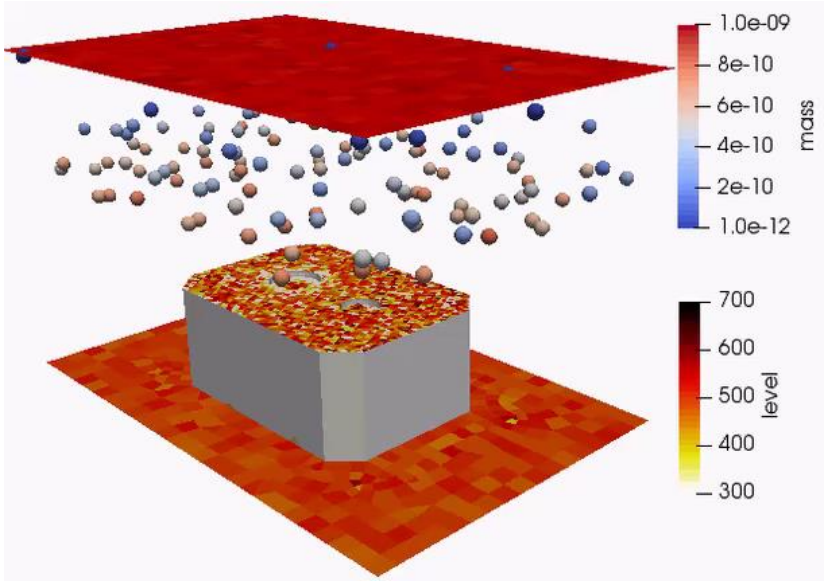


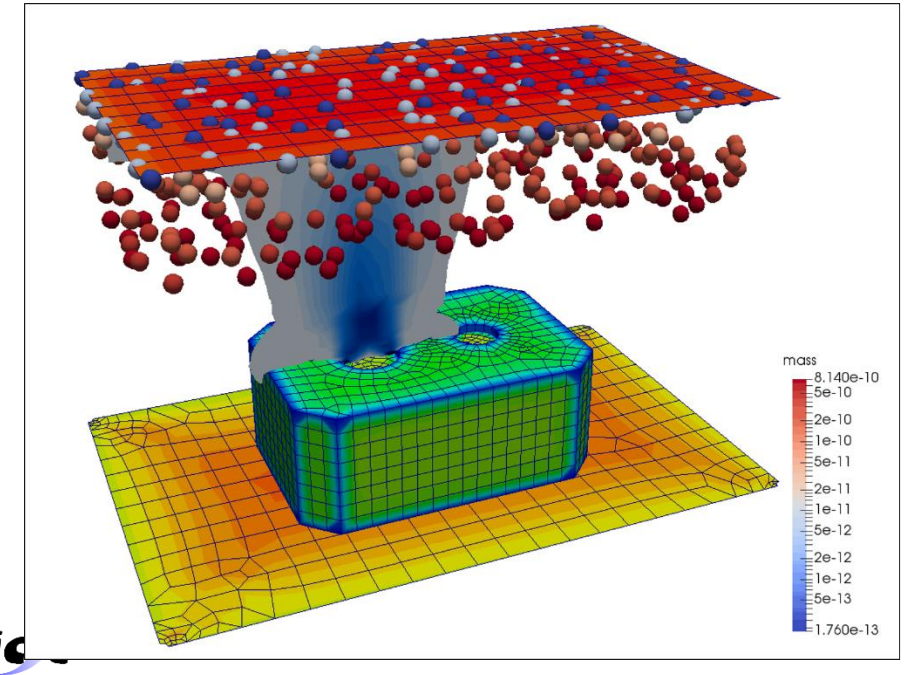


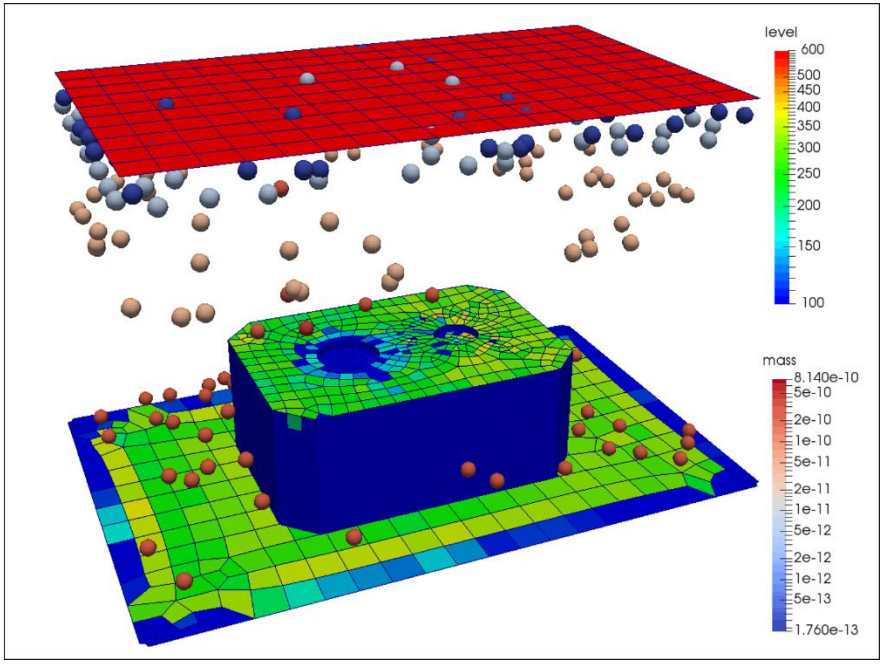


Bonus: effect on particulates

- Also started modeling purge effect on particulates
- OpenFOAM used to compute gas flow
- Particles of various sizes launched from a top shelf. Velocities update by considering aerodynamic drag and gravity
- Heavy particles rapidly settle out, but light particles remains suspended and are turned away from the sensor.







Conclusion

- This talked presented preliminary “proof of concept” results from a study to characterize the effect of purge
  - Purge appears to be useful in preventing infiltration of molecular contaminants and smaller particulates
  - Also observed a “good neighbor” effect, with purge on sensor 1 reducing infiltration to sensor 2
- Future work
  - Effect (if any) of N2:N2 and HC:HC collisions needs to be investigated
  - Include a more detailed instrument model containing thin foils and use DSMC to compute forces
  - Run simulation for longer real time. DSMC becomes computationally expensive at high densities so modeling repress all the way to ambient likely not feasible with DSMC alone.
- For more information:
  - Email: lubos.brieda@particleincell.com
  - Code: https://www.particleincell.com/ctsp (let me know if interested, US only)
  - Paper: to be submitted shortly