Contamination Transport Simulation Program (CTSP)

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SPIE. OPTICS + PHOTONICS DIGITAL FORUM

Dr. Lubos Brieda
President, Particle in Cell Consulting LLC

Welcome to our virtual booth

We would like to introduce the Contamination Transport Simulation Program (CTSP)

Marc Laugharn
Software Developer and Contamination Analyst

Motivation

- Sensors, components, and processes in the space industry, photonics, and nanoprocessing are frequently highly sensitive to **contamination**
- Despite best practices, it is simply not possible to eliminate all sources of contaminants
- Numerical modeling becomes an extremely valuable tool for predicting end-of-life contamination levels or establishing cleanliness requirements

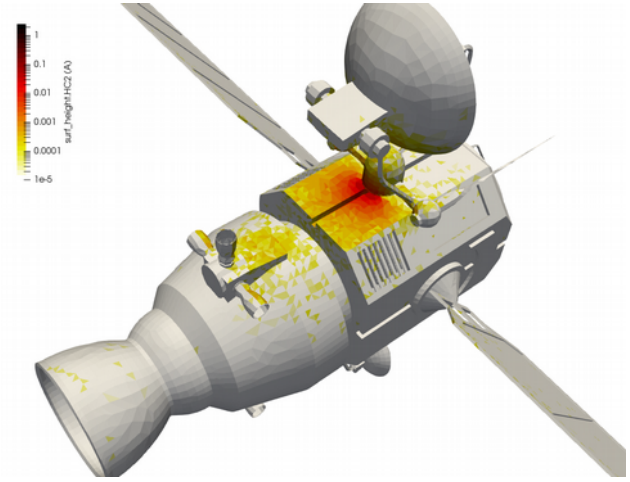
CTSP and PIC-C can help you meet your contamination analysis needs!

With our codes, you can model both **neutral** and **charged** (plasma) gas-surface interactions

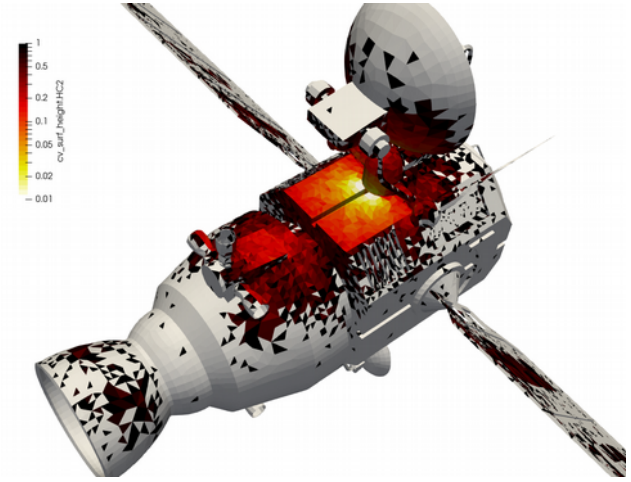
CTSP Overview

- Computer program for simulating transport of **molecular** and/or **particulate** contaminants
- In development since 2015, see *J. Spacecraft & Rockets, 2018* and *SPIE-2020-OP20O-OP311-1*
- Supports complex geometries (as FEM meshes in **.unv**, **.abq**, **.stl**, **.obj** formats or **.tssgm** Thermal Synthesizer System assemblies)
- Implements many contamination-specific sources, including **outgassing**, vent **outflow**, and surface **particulate coverage**
- Utilizes **temperature**-based surface adhesion and outgassing models
- Takes into account ambient environment, including **gravity**, **aerodynamic drag**, and **electrostatic attraction** on particulates, and **inter-molecular collisions** in rarefied gas flows
- Runs serially or in parallel on Microsoft Windows and Ubuntu or CentOS Linux

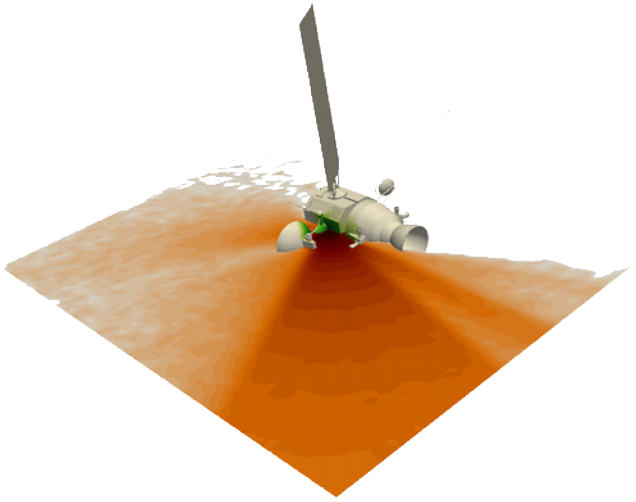
"Hello World" Example



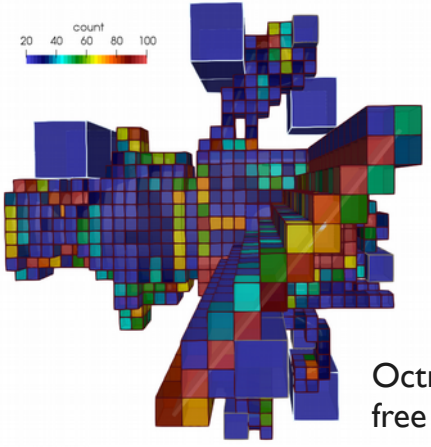
contaminant surface layer height



coefficient of variation (normalized std. dev.) from a 48-CPU run

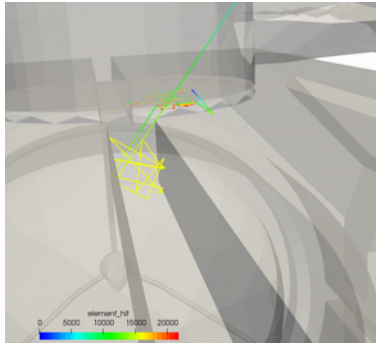


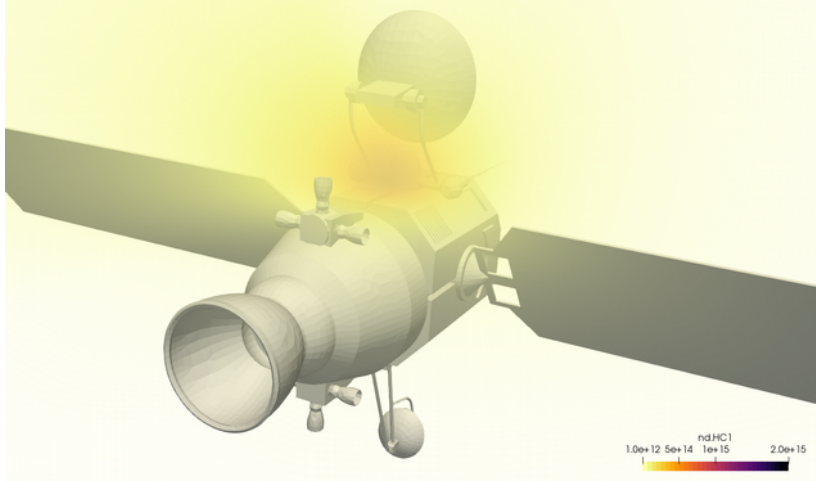
contaminant plume density as a slice (above) and volume rendering (below)



Octree used for mesh-free particle tracing

Single particle trace

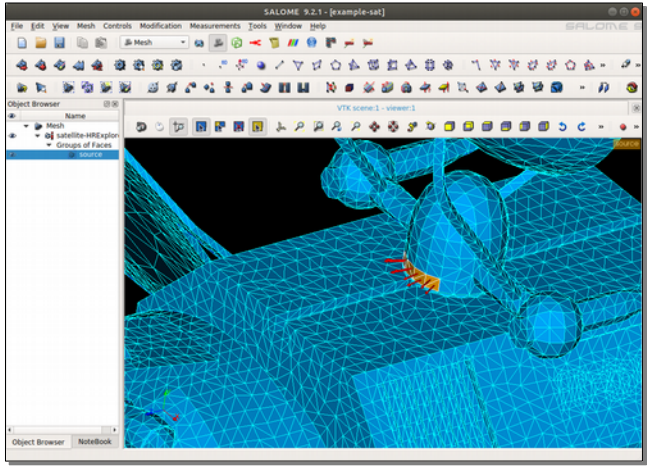




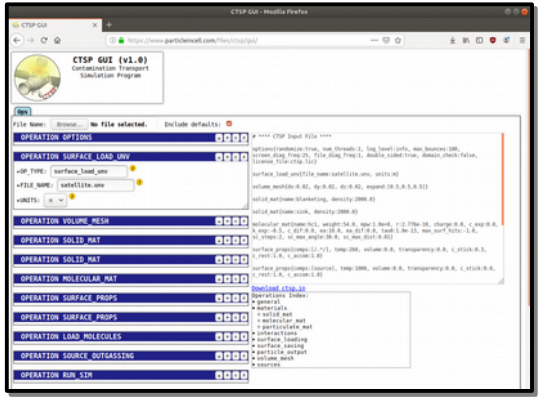
Satellite model from grabcad.com/library/satellite-11, meshed in Pointwise

Using CTSP

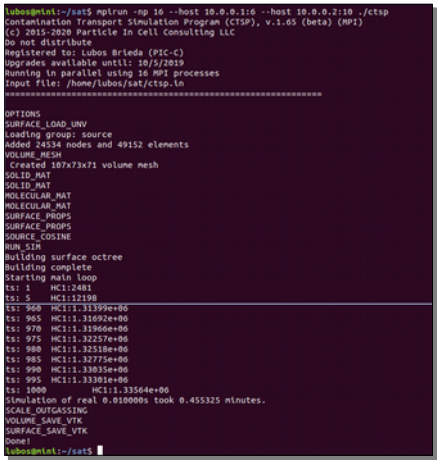
(1) Surface Mesh Preparation
CAD model is meshed or TSS model is reviewed for correctness (such as normal vector orientation). We also assign element **component groups** to specify surface properties and mass generation sources



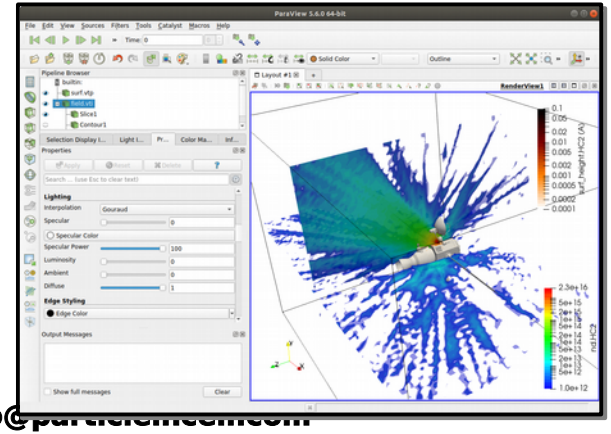
(2) Generate Input Files
Use our web-based HTML **GUI** to generate the simulation input file. Alternatively, an existing file can be modified in a text editor.



(3) Run the Simulation
CTSP is run serially or using MPI on Windows or Linux

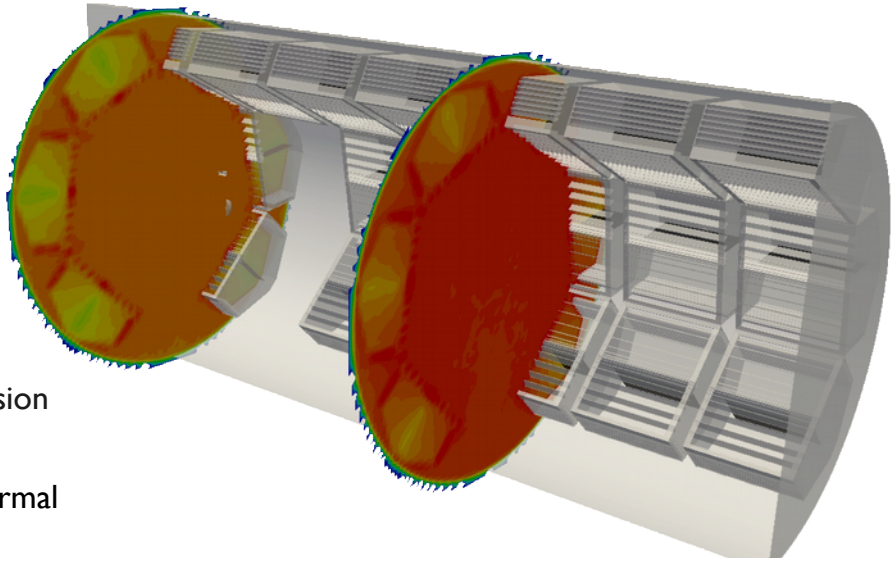


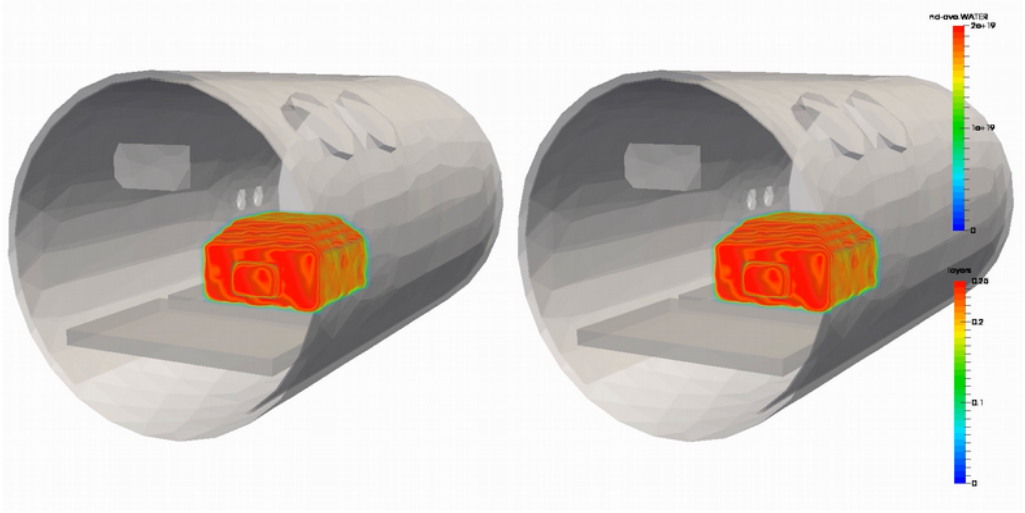
(4) Analyze Results
CTSP surface and volume data is saved in VTK (Paraview) or Tecplot formats. CTSP also outputs xy time data and surface histograms.

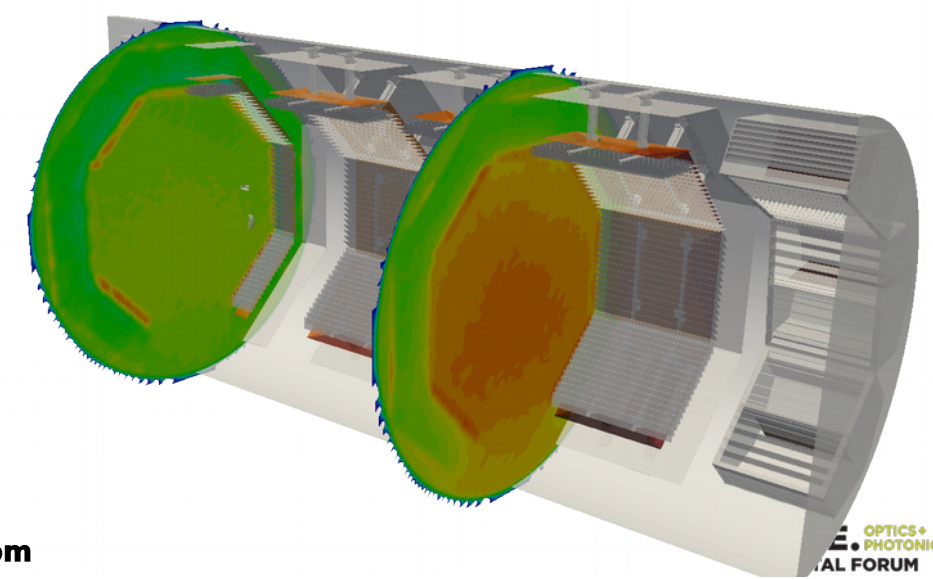


Vacuum Chamber Modeling

- Aerospace Corp interested in refurbishing chamber used for electric propulsion testing
  - Considered adding more pumps or a custom cold shroud
  - CTSP simulations performed to estimate resulting pressure with an EP thruster operating
  - See: Spektor, R., et.al, "Analytical Pumping Speed Models for Electric Propulsion Vacuum Facilities", *Space Propulsion Conference*, Seville, Spain, 2018
- Video below shows the effect of surface temperature on pressure in a generic thermal vacuum chamber

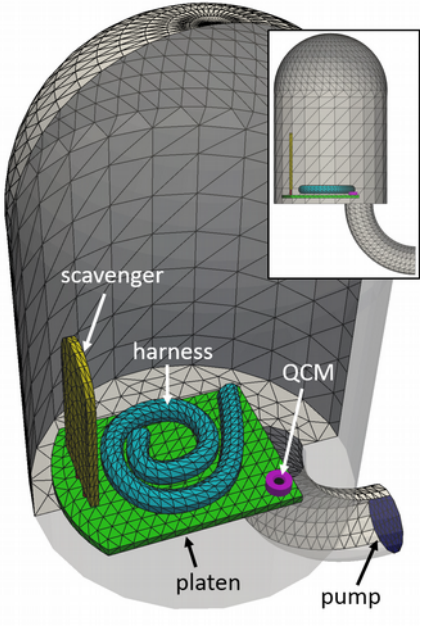


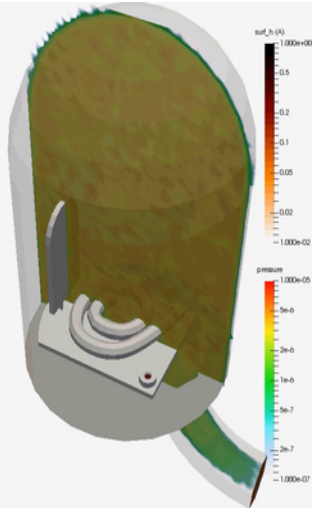


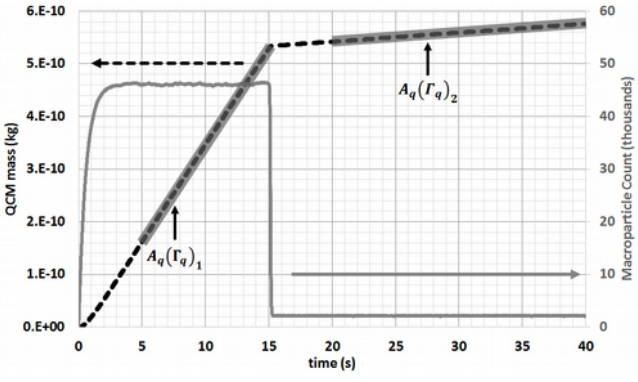


Effective Pump Area

- Numerical experiment simulating using a QCM to obtain outgassing rate
- This correlation requires knowing the **view factor**, obtained from effective pump area
- Can be estimated by comparing deposition rate **without** and **with** a scavenger plate of known dimensions
  - Single simulation with scavenger temperature changing rapidly at a specified time point
- Good agreement with source input rate



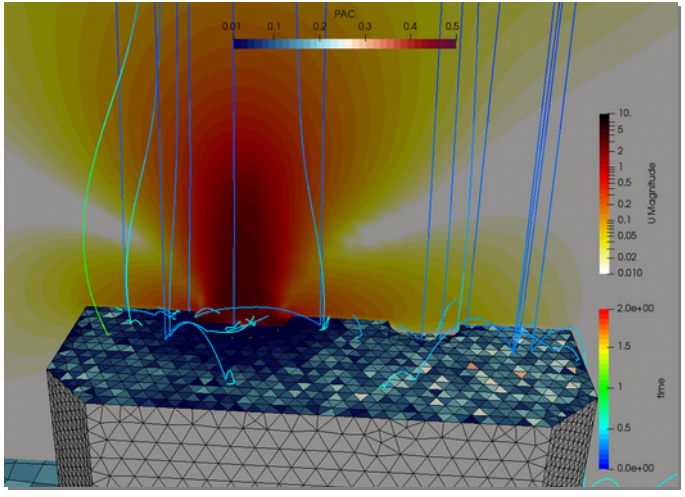


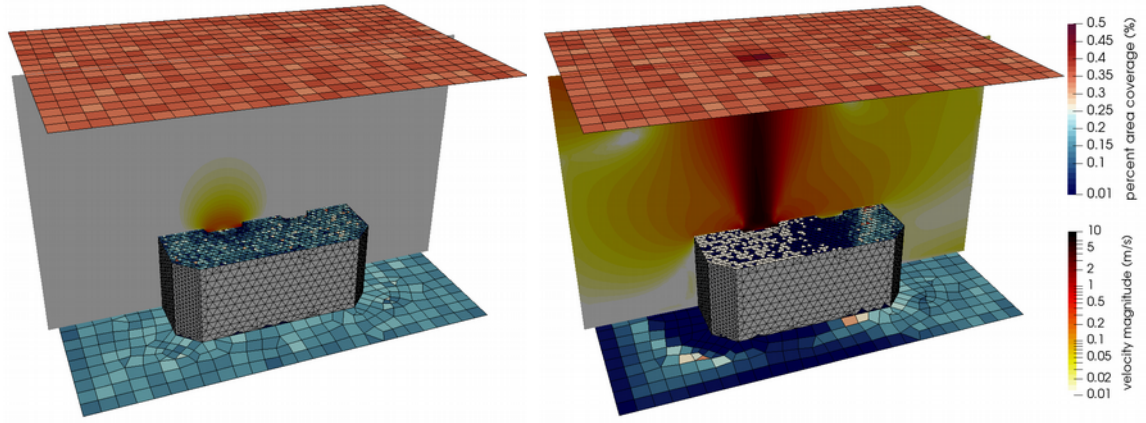


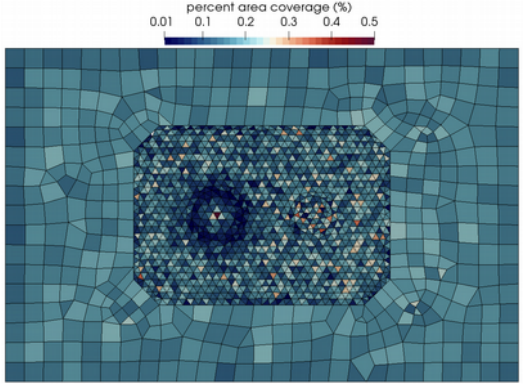
More detail: Brieda, L., *J. Spacecraft & Rockets*, 2018, https://doi.org/10.2514/1.A34158

Particulate Fallout

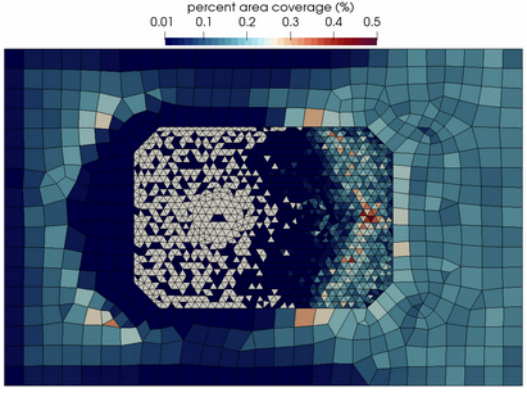
- Another example from *JSR, 2018*
- Gaseous purge used to prevent fallout of dust particulates onto a detector
- Plots compare results with **low** and **high** purge flow rate







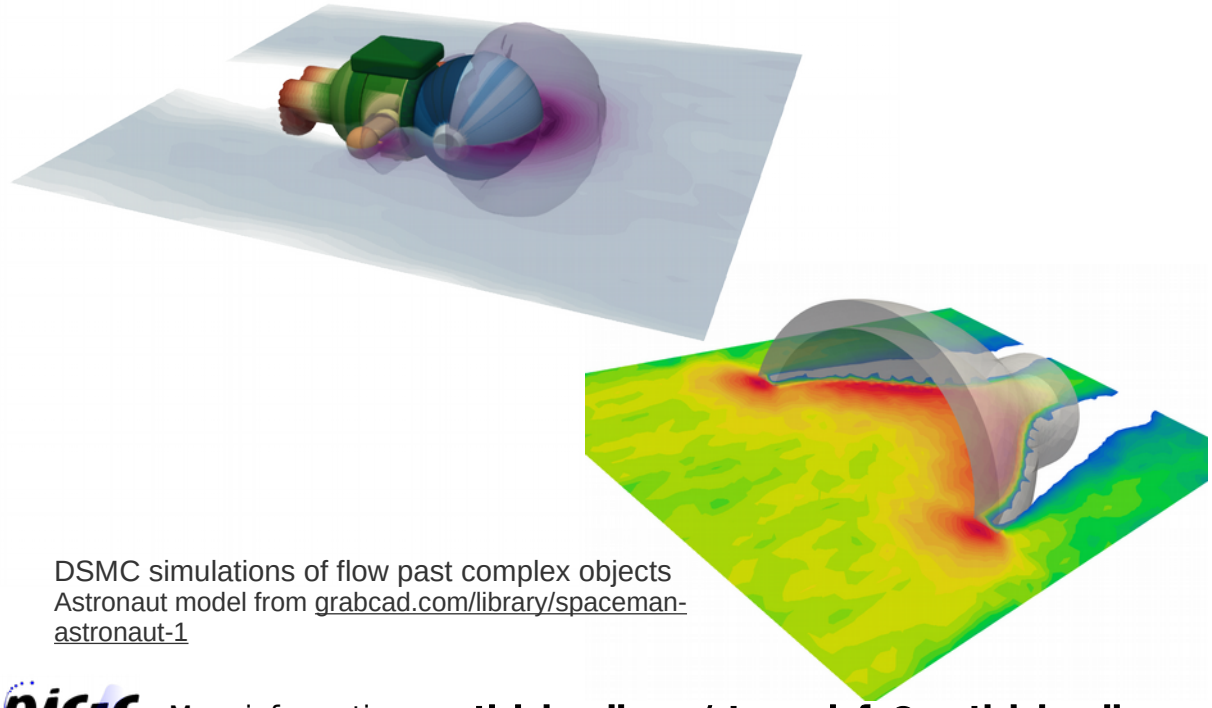
low purge flow



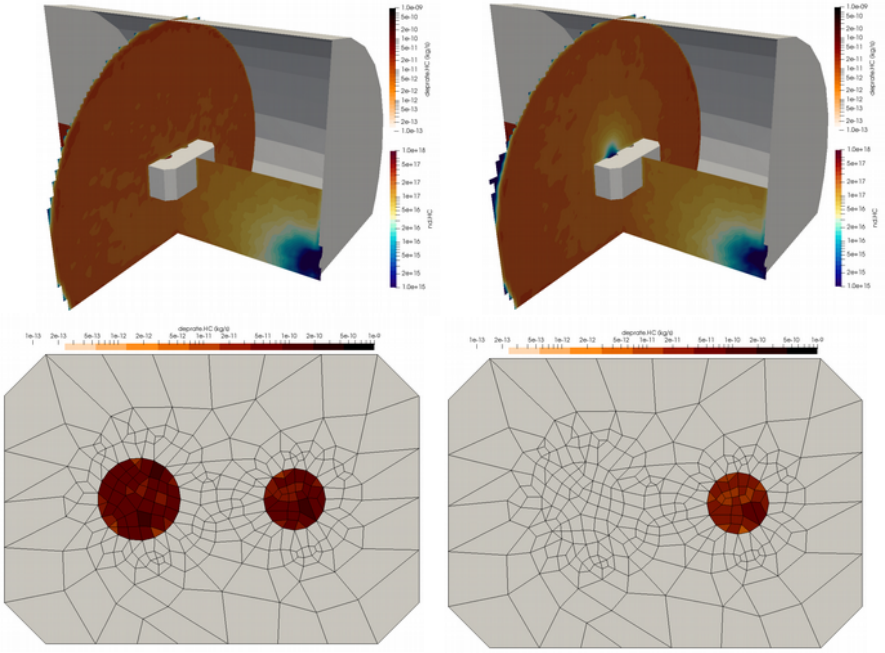
high purge flow

Rarefied Flows

- CTSP also implements the Direct Simulation Monte Carlo (DSMC) method to simulate flow regimes in which inter-molecular collisions cannot be ignored
  - These include vacuum chamber repressurization, or initial cavity venting after exposure to vacuum



DSMC simulations of flow past complex objects
Astronaut model from grabcad.com/library/spaceman-astronaut-1

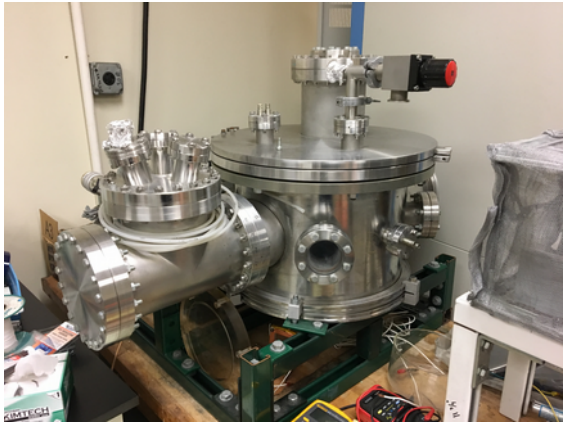


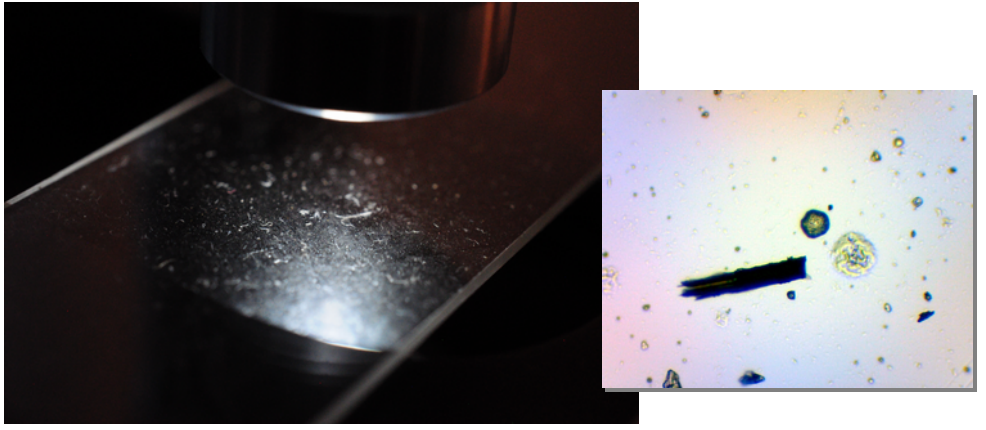
Effect of instrument purge during chamber repressurization

Experimental Validation

- In early stages of experimental validation
  - Collaboration with USC and NASA/GSFC
  - Objective is to simulate molecular transport and QCM deposition in a small vacuum chamber and to characterize particulate fallout under various ambient conditions

Contact us if open to collaboration





Next Steps

Want to get started with CTSP?

Do you need simulating a rarefied gas or plasma system?

- Visit our website: **particleincell.com/ctsp**
- Contact us at **info@particleincell.com**

Free trial license available!