Mesh-Free Contamination Transport Modeling using CAD Geometries

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2023 NASA Goddard Contamination Control, Materials, and Planetary Protection Workshop

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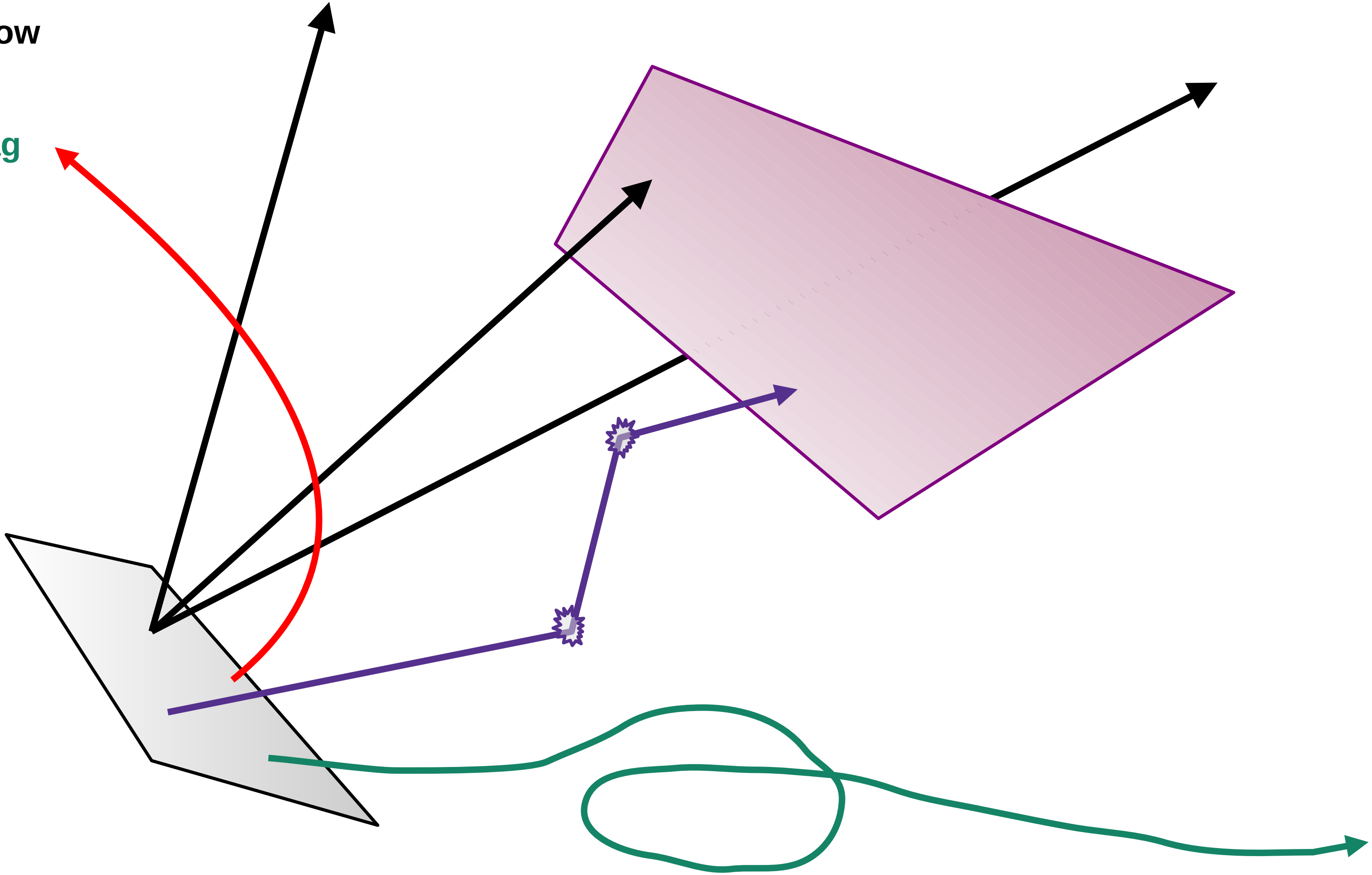
Betsy Pugel was the Task Manager.

Contamination modeling conceptually very simple:

Determine how much material deposits on surfaces of interest due to outgassing and particulation on other surfaces

Transport Mechanisms

- free-molecular flow
- electric fields
- collisions
- aerodynamic drag



Contamination Transport Modelling

- Contaminant build up on some element "e" can be described mathematically as

$$\Gamma_{e,net} = \sum_{j}^{n_{el}} k_{je}\Gamma_{i,out} - \Gamma_{e,out} \quad ; j \neq e$$

  - where k_{ie} is the **view factor** between from some source element "j"

- Various numerical tools available to calculate view factors

- Monte-Carlo methods use some form of ray tracing (for free-molecular flow) or particle pushing (to account for forces or collisions):

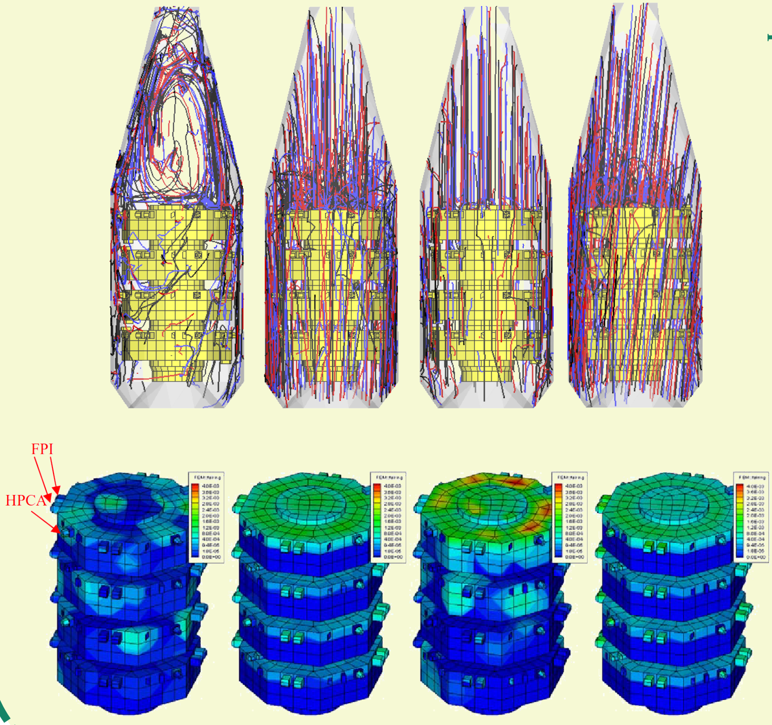
```
for k in num time steps:

    for e in surfaces:
        generate particles on surface e

    for p in particles:
        integrate velocity of particle p through dt
        integrate position of particle p through dt
        check for surface impact (deposit / bounce off)

    apply collisions
```

Successfully Deployed in Support of NASA Missions

Analysis of Particulate Contamination During Launch of MMS Mission

Lubos Brieda, Alexander Barrie
Millennium Engineering and Integration, Arlington, VA

David Hughes, Therese Errigo
NASA Goddard Space Flight Center, Greenbelt, MD

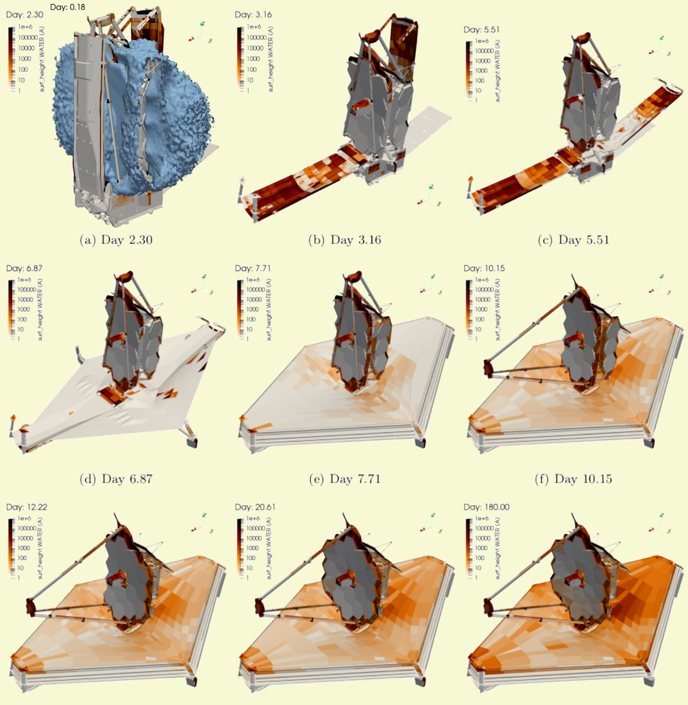


SPIE Optics & Photonics 2010

Numerical study of water ice and molecular contamination build up during JWST deployment

Lubos Brieda[a], Marc Laugharn[a], Michael Woronowicz[b], Kelly Henderson-Nelson[b], Christopher May[c], Eve Wooldridge[d]

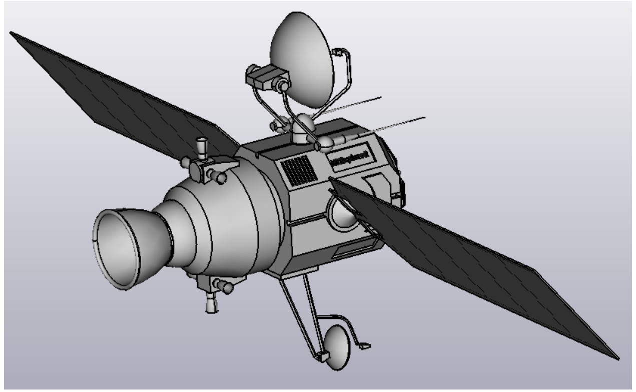
[a]Particle in Cell Consulting LLC, Westlake Village, CA 91362, USA
[b]KBR Inc., Fulton, MD 20759, USA
[c]MAZE Engineering Solutions, Inc., Marshall, VA 20115
[d]NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA



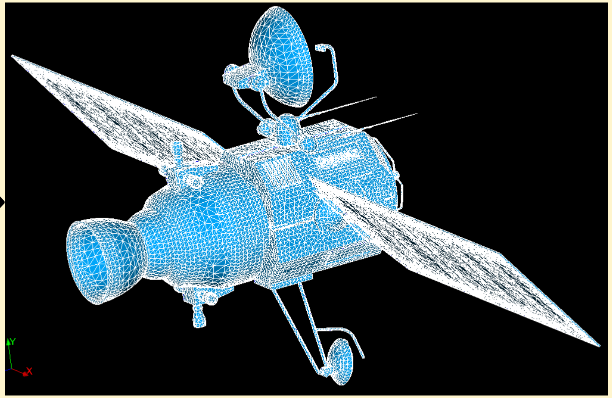
(a) Day 2.30 (b) Day 3.16 (c) Day 5.51
(d) Day 6.87 (e) Day 7.71 (f) Day 10.15
(g) Day 12.22 (h) Day 20.61 (i) Day 180.00

SPIE Optics and Photonics 2022

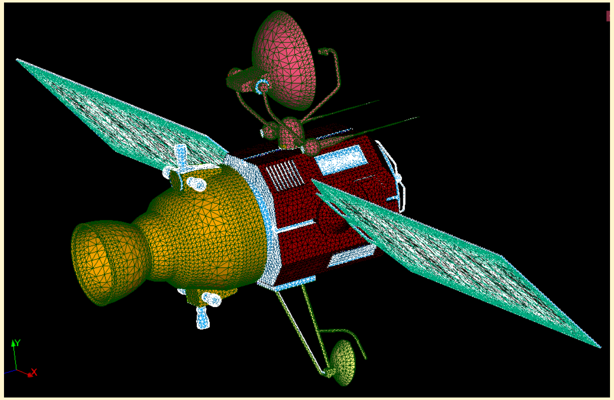
Modeling Approach



CAD model



create mesh



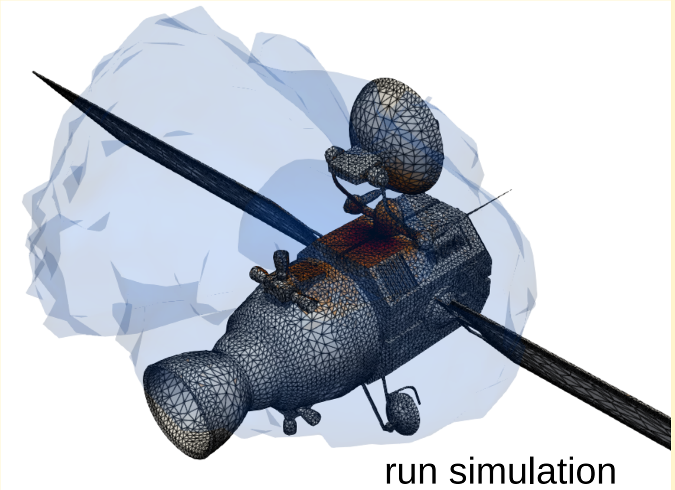
assign surface groups

45.56278	16.06691	15.04493	11.79354	80.18772	11.4268	9.787078	9.686701
45.56731	16.07102	15.04916	11.79765	80.19163	11.43084	9.790316	9.689591
45.57183	16.07509	15.05326	11.80175	80.19558	11.43487	9.793547	9.692451
45.57633	16.07913	15.05724	11.80584	80.19957	11.43891	9.796767	9.69528
45.58083	16.08314	15.0611	11.80991	80.20362	11.44293	9.799977	9.698078
45.58532	16.08713	15.06486	11.81396	80.20771	11.44695	9.803174	9.700848
45.58981	16.0911	15.06852	11.81799	80.21186	11.45097	9.80636	9.703592
45.5943	16.09505	15.07211	11.82201	80.21606	11.45497	9.809535	9.706314
45.59878	16.09898	15.07563	11.826	80.22031	11.45898	9.812702	9.709015
45.60326	16.1029	15.07909	11.82998	80.22461	11.46297	9.815861	9.711699
45.60774	16.10682	15.0825	11.83395	80.22894	11.46696	9.819014	9.71437
45.61221	16.11073	15.08589	11.8379	80.23332	11.47094	9.822163	9.717029
45.61669	16.11463	15.08925	11.84183	80.23773	11.47492	9.825308	9.71968
45.62117	16.11854	15.09259	11.84574	80.24218	11.47888	9.828452	9.722325
45.62564	16.12245	15.09592	11.84965	80.24665	11.48284	9.831596	9.724966
45.63011	16.12636	15.09925	11.85353	80.25115	11.4868	9.834741	9.727605
45.63459	16.13027	15.10258	11.85741	80.25567	11.49074	9.837887	9.730243
45.63906	16.13419	15.10592	11.86127	80.26021	11.49468	9.841036	9.732882
45.64353	16.13811	15.10927	11.86512	80.26477	11.49861	9.844187	9.735522
45.648	16.14205	15.11264	11.86895	80.26934	11.50253	9.847342	9.738165
45.65247	16.14599	15.11602	11.87278	80.27293	11.50644	9.8505	9.740811

load environments / temps

```
molecular_mat{name:water, weight: 18,
              mp_density:200, mpw_min:1e10, desorption_model:MURPHY_KOOP, r:1.9252e-10}

molecular_mat{name:vcm, weight: 54, mp_density:300, mpw_min:1e9,r:1.9252e-10,Ea:9,
             c_stick:-
[1.000@218.10,0.998@227.83,0.969@237.56,0.879@246.33,0.747@252.44,0.615@256.73,0.489@261.02,
                      0.361@265.41,0.227@270.08,0.097@277.43,
                      0.05@283.15,0.04@284.15,0.035@285.15,0.030@286.15,
                      0.0250@287.15,0.020@288.15, 0.0180@289.15, 0.016@290.15, 0.014@291.15,
                      0.012@292.15,0.010@293.15, 0@303.15],
                      desorption_model:c_stick, time_constant:0.2}

#specify surface properties
surface_props{comps:/.*/, mats:blanketing,temp:280}

surface_props{comps:df_foam,temp:233}
surface_props{comps:df_boxes,temp:280}
surface_props{comps:df_fins,temp:233}
surface_props{comps:df_rotors,temp:233}
surface_props{comps:df_legs,temp:233}
surface_props{comps:df_un,temp:273}


surface_props{comps:shell_hsa,temp:175}
surface_props{comps:shell_hsb,temp:188}
surface_props{comps:shell_seal,temp:153}
surface_props{comps:shell_bsa,temp:153}
surface_props{comps:shell_bsb,temp:175}
surface_props{comps:shell_bsc,temp:193}
surface_props{comps:shell_bsd,temp:248}
surface_props{comps:shell_bse,temp:270}
surface_props{comps:shell_parts,temp:196}
surface_props{comps:shell_outside,temp:270}


#Re-run sim with 1e-13 g/cm^2/sec VCM outgassing everywhere except for foam, foam is 3e-13
#Use 2x VCM rate for water
#Assume 1/sqrt(t) dependence

#add constant mass flux vent
source_cosine{comps:df_foam, mats: vcm, mass_flux:3e-12, v_drift:20}
source_cosine{comps:df_foam, mats: water, mass_flux:6e-12, v_drift:20}
source_cosine{comps:df_boxes, mats: vcm, mass_flux:1e-12, v_drift:20}
source_cosine{comps:df_boxes, mats: vcm, mass_flux:2e-12, v_drift:20}
```

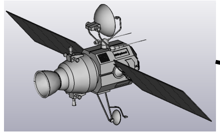
set outgassing rates / inputs



run simulation

CC responsibility

The ACTUAL Modeling Workload



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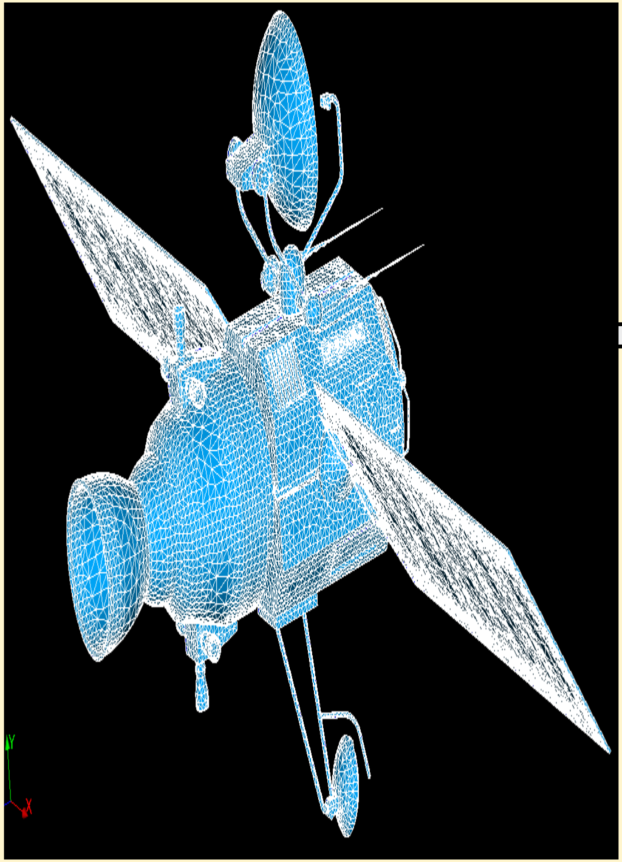
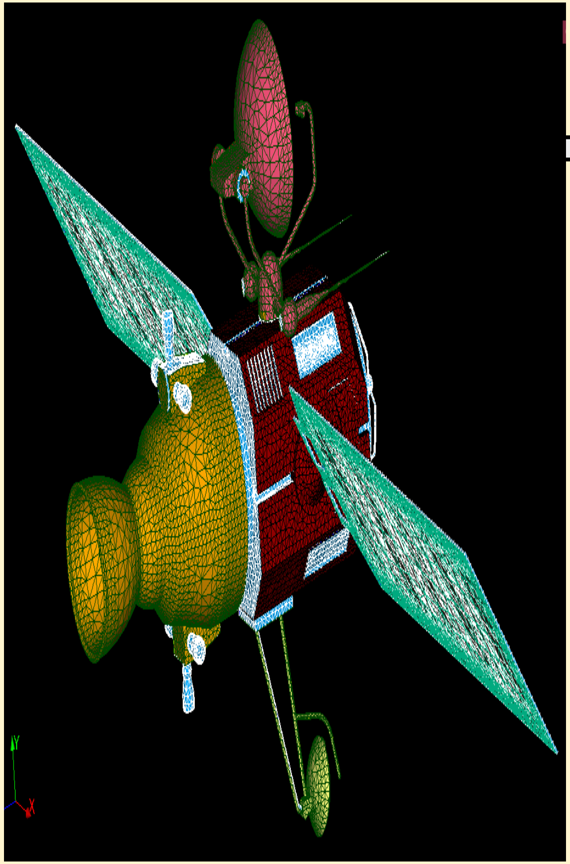
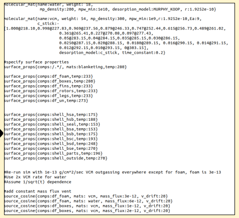
load environments / temps



create mesh



assign surface groups



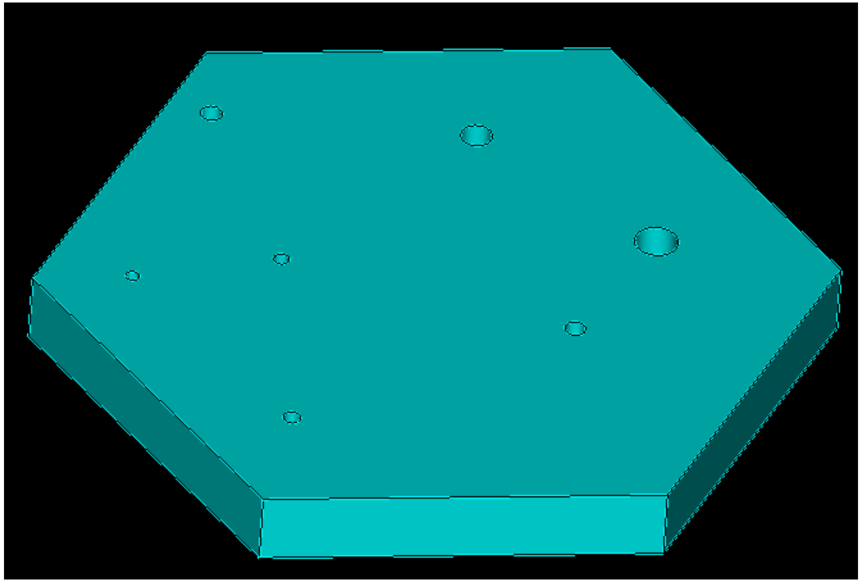
set outgassing rates

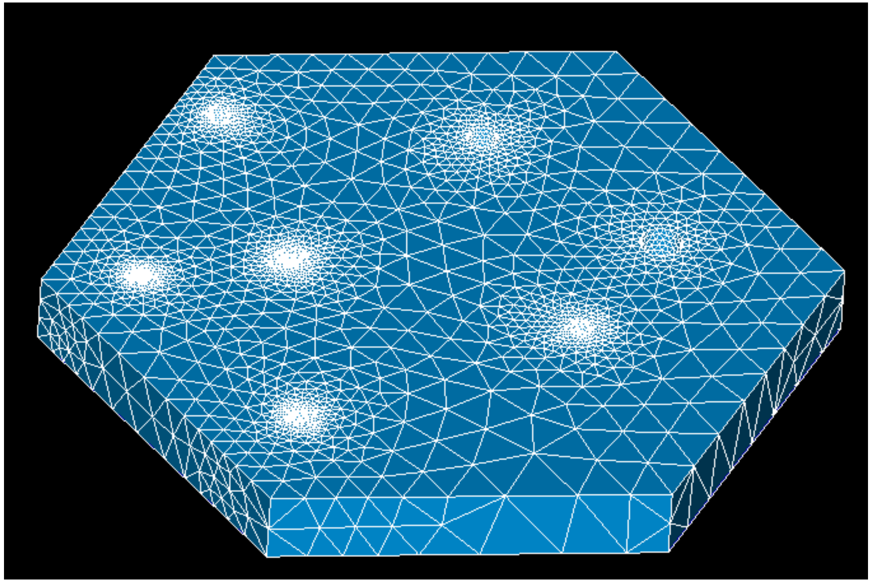
run simulation

CC responsibility

Meshing Challenges

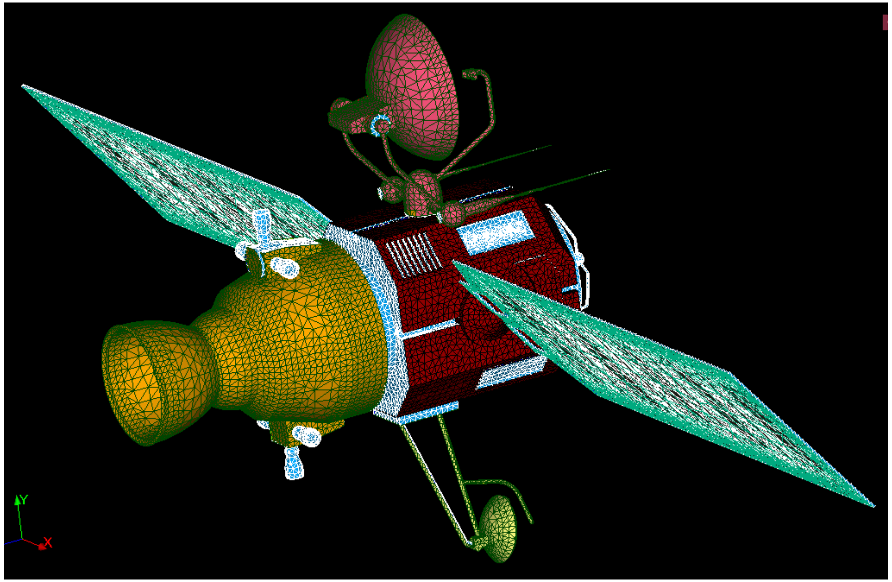
- Legacy modeling tools utilize surface mesh to store model geometry
  - Triangular/quadrilateral mesh, or assembly of analytical shapes in TD/TSS
  - Inefficient: remeshing required when mechanical design changes
  - Analysis often lags behind latest mechanical design
- Mechanical models tend to contain small features such as drill holes or screws
  - Lead to meshing challenges or an excessive number of surface elements
  - **Often requires substantial work to redraw / simplify CAD model!**





Grouping

- Surface elements also need to be organized into groups to assign material properties, surface models, etc.
- Challenge: mechanical and thermal grouping typically NOT compatible with CC needs
- Example: JWST thermal components grouped by external material. Majority of material was kapton to capture MLI outer layer. CC cares about what is *underneath* the MLI!
- Extremely tedious manual work involving selecting groups of coplanar elements.
- Must be redone whenever the mesh changes.
  - Interns come in handy…



Mesh-Free Alternative

- The surface mesh has dual role:
  1) Used for particle-geometry boundary checks (did the particle hit something?)
  2) Used to store surface data including results (deposition thickness, PAC, etc.) and surface-adsorption model inputs (surface temperature, roughness, material, etc.)
- Mesh not needed in the volume! Can use point clouds to load airflows or electric fields.

CAD models are internally composed of analytically defined shapes (faces). Can we do **line-CAD** intersection test instead of the legacy **line-triangle** to check for surface impact?

And perhaps there is some way to store data on CAD geometries?

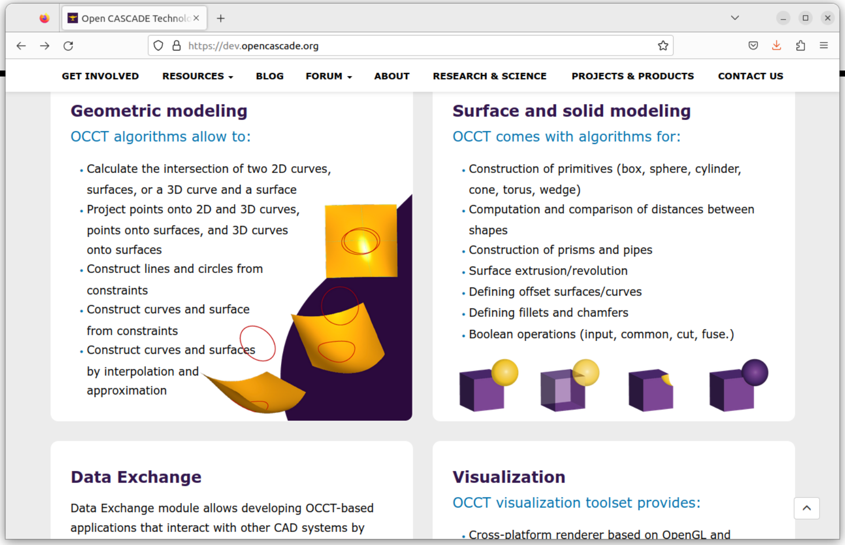
OpenCascade

- Elimination of meshing expected to lead to **significant reduction in labor cost** and **ability to automatically re-run analysis** when mechanical model is changed

- But how to work with CAD files?

- Open Cascade Technology (OCCT) to the rescue!
  - Open source C++ software for performing 3D CAD analysis
  - Developed by Open Cascade SAS company
  - LGPL 2.1 license, allows use in proprietory applications

- **The Bad: documentation very limited, much of our effort involved trial and error**




```
const TopoDS_Shape &aComp2 = ((AIS_Shape*)myObject3d.First().get())->Shape();

//  Handle(Geom_Line) l = new Geom_Line(gp_Pnt(100, 0, 0), gp_Dir(-1, 0, 0));
Handle(Geom_Line) l = new Geom_Line(gp_Pnt(300, 0, 1000), gp_Dir(0, 0, -1));
NCollection_Vector<Handle(AIS_InteractiveObject)> myPts;

TopTools_IndexedMapOfShape faces;
TopExp::MapShapes (aComp2, TopAbs_FACE, faces);
int i, j=0;
for (i = 1; i <= faces.Extent (); i++) {
  TopoDS_Face face = TopoDS::Face(faces(i));
  Handle(Geom_Surface) S = BRep_Tool::Surface(face);
  GeomAPI_IntCS in(l, S);
  if (in.NbPoints() > 0) {
    const gp_Pnt &pp = in.Point(1);
    Handle(Geom_Point) ppp = new Geom_CartesianPoint(pp);

    myResult << " " << pp.X() << " " << pp.Y() << " " << pp.Z() << std::endl;
    myObject3d.Append(new AIS_Point(ppp));

    j++;
  }
}
myResult << "done " << j << std::endl;
```

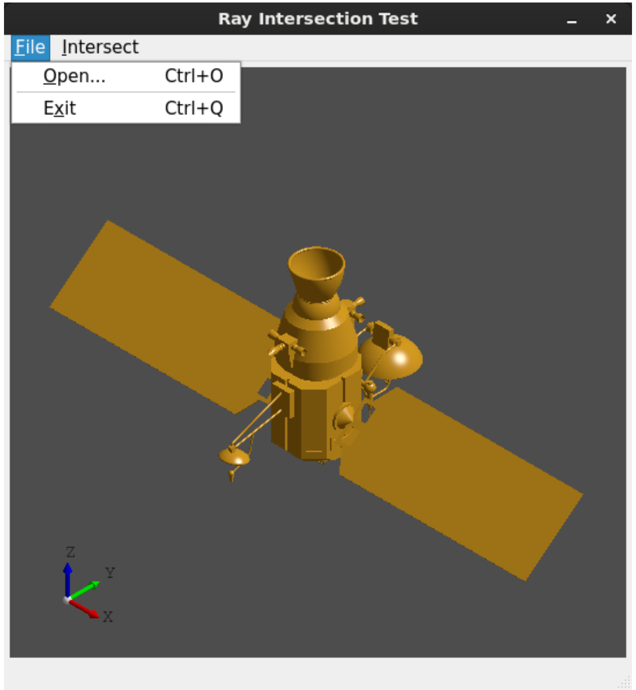
◆ SetDisplayMode() [2/2]

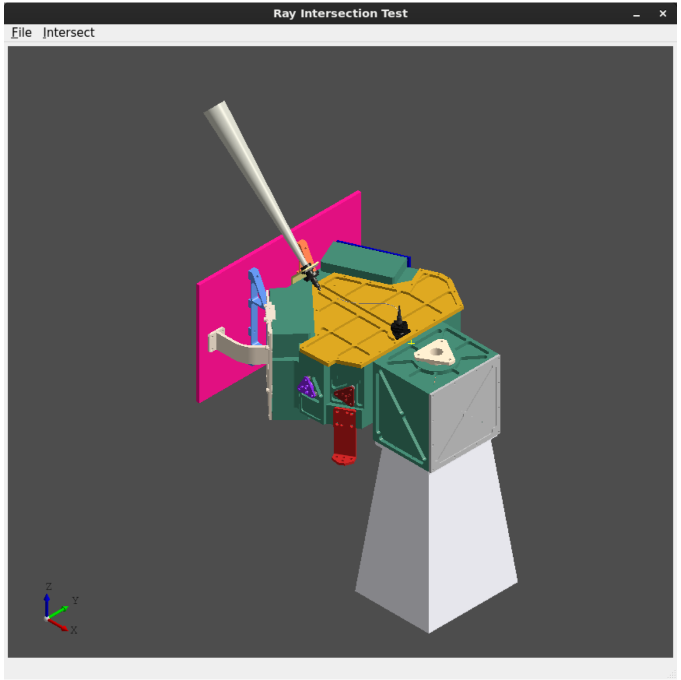
void AIS_InteractiveContext::SetDisplayMode (const **Standard_Integer** theMode,
const **Standard_Boolean** theToUpdateViewer
)

Sets the display mode of seen Interactive Objects (which have no overridden Display Mode).

File Loading

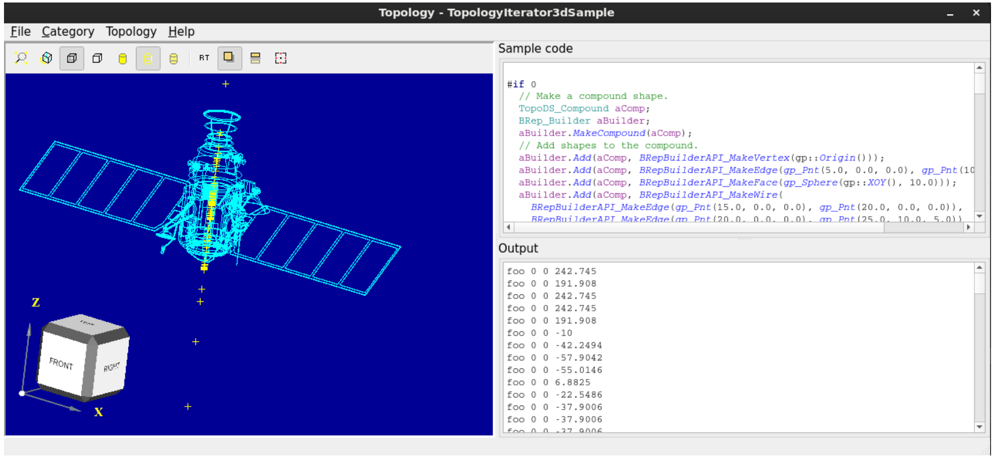
- Developed standalone application to study the feasibility of this CAD-based modeling approach
  - OCPT: OpenCascade Particle Tracer
- First step involved learning how to load and visualize STEP files, and to identify different element groups

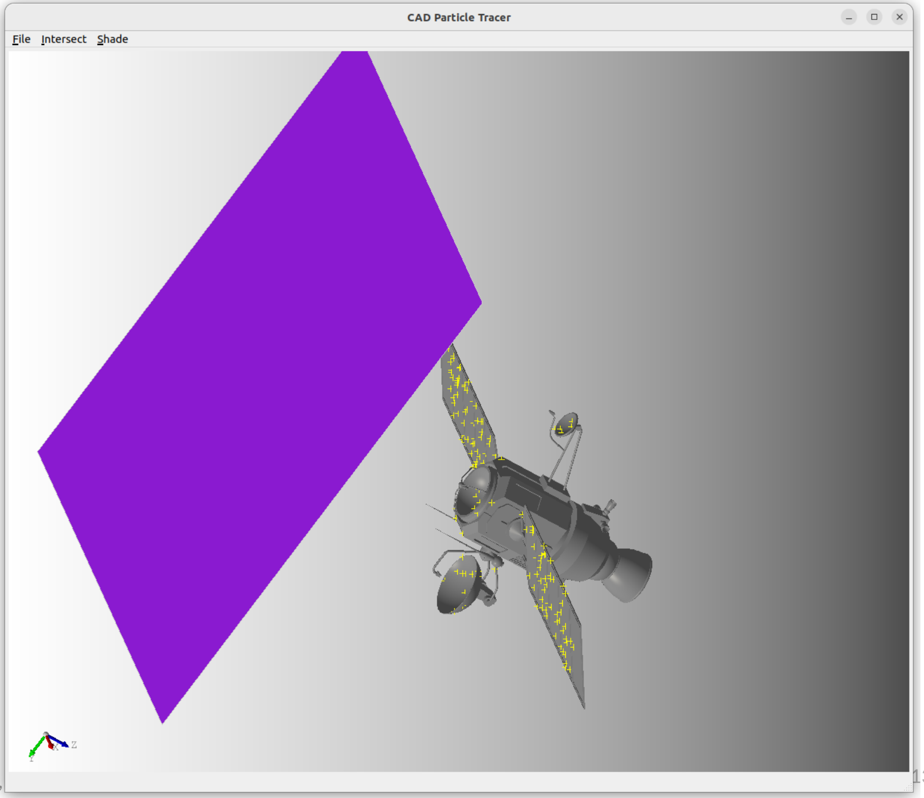




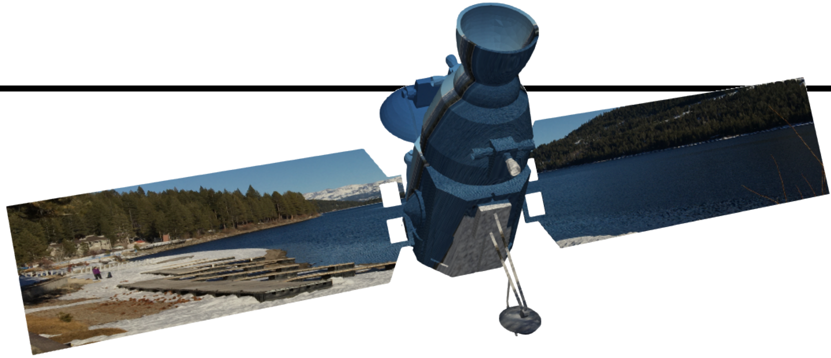
Surface Intersections

- Next had to figure out how to use OpenCascade to find intersections between an arbitrary line and the loaded surface
- Effort greatly complicated by documentation consisting mainly of API documents with very limited information and multiple classes seemingly doing the same thing

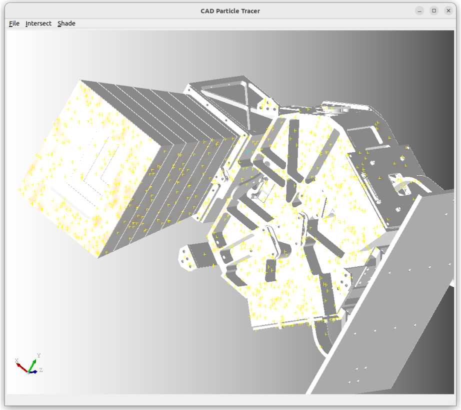


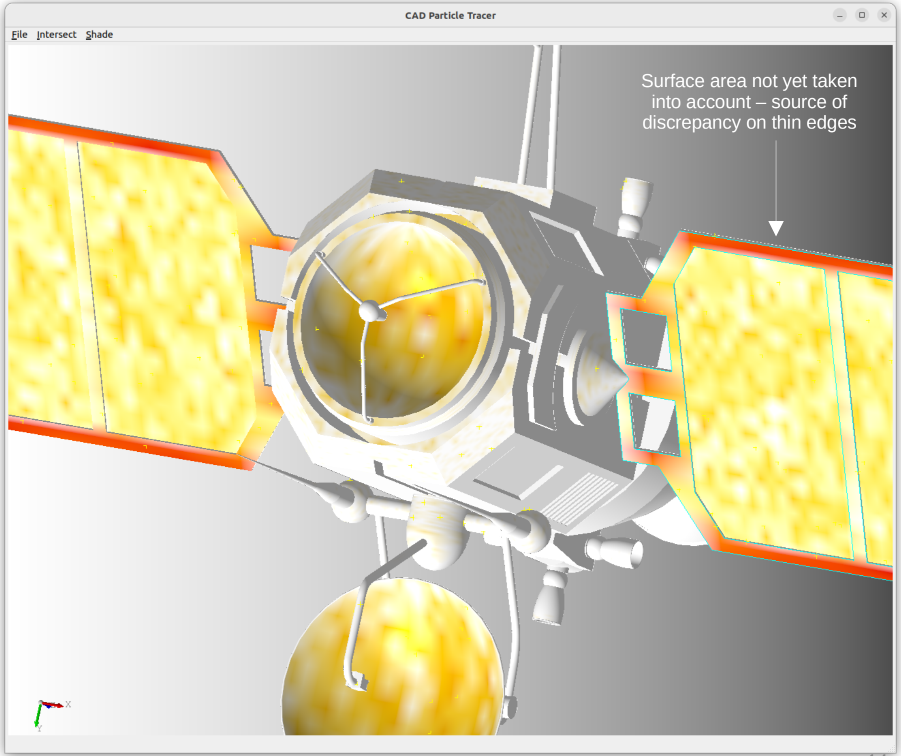


Surface Data



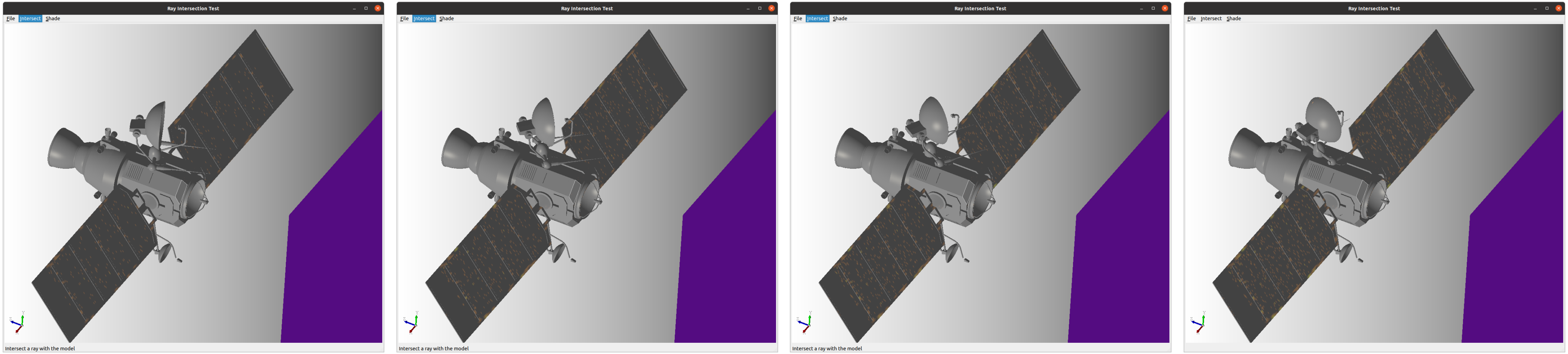
- Initial surface impacts visualized using markers – not practical for visualizing analysis results
  - Prefer to paint “contour map” on the surface
- Can be accomplished by mapping texture data to the CAD model
  - Intersection code determines texture coordinate and increments corresponding data
- Texture coordinates can also be used to sample surface data to control particle behavior





Transformations

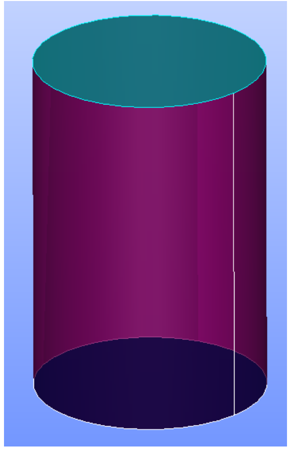
- STEP files describe geometry using analytical shapes
- Surface parts can be easily transformed
- Could be very useful for modeling deployments of stowed components, instrument slew, rotation of antennas, and planetary body surface operations

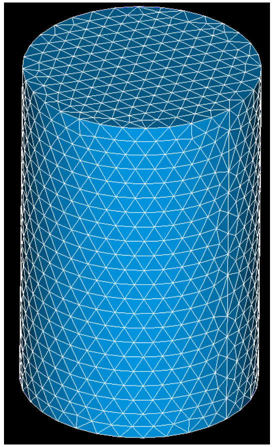


Frames from a simulation with a continuous translation and rotation of the antenna dish

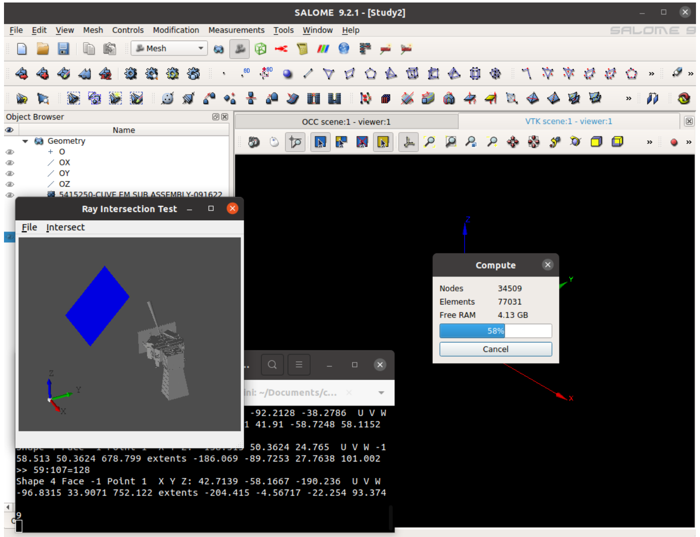
Timing Comparison

- CAD-based time per particle push currently about 100,000 slower than using triangulated surface
  - CAD model in general contains far fewer faces than FEM model (i.e. cylinder can be represented by only 3 shapes) but intersection check more computationally expensive
  - But OCPT not optimized – rays intersections tested against entire CAD model
  - CTSP uses octree to limit triangle search only to elements withing the ray's bounding box – similar ordering required in OCPT
- OCPT **faster** when considering entire workflow – can load STEP file and complete analysis while meshing algorithm still running



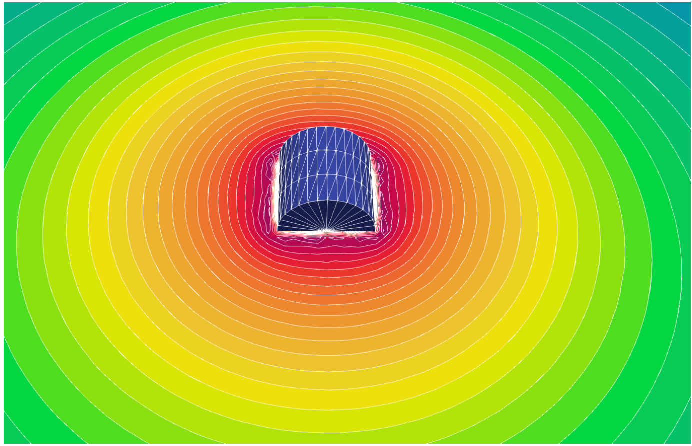


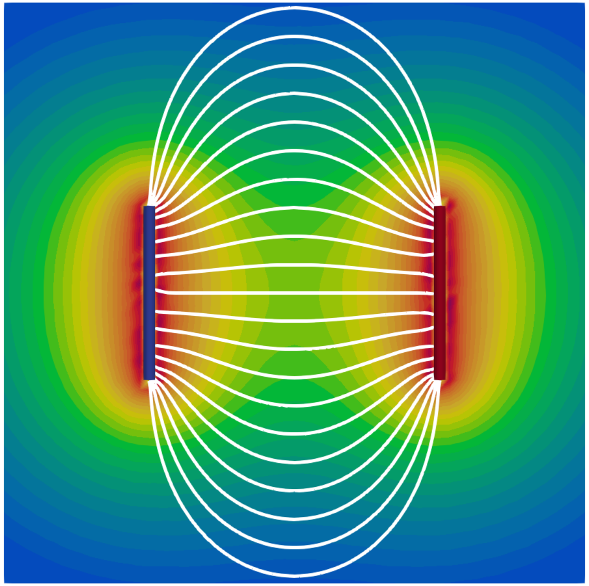
Case	meshing	geometry load	time per particle
OCPT, Satellite, 3.6 Mb STEP	N/A	0.9	0.012 s
CTSP, Satellite 7.5 Mb UNV UNV	30 min	2 s	5.05e-7 s
OCPT, Instrument, 18 Mb STEP	N/A	10.6 s	0.34 s
CTSP, Instrument	FAIL		
OCPT, Dragonfly, 48 Mb STEP	N/A	16.3 s	0.49 s



Volumetric Electric Field

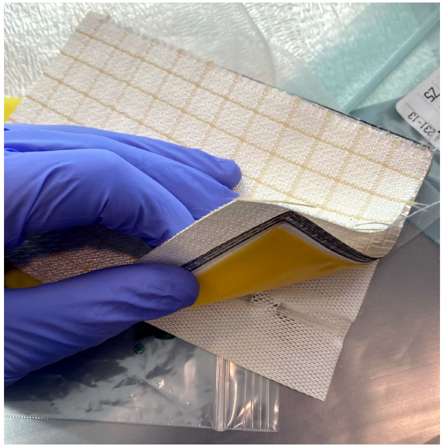
- CAD-based modeling approach also very attractive for modeling space weather instruments
  - Analysis involves simulating trajectories of charged particles in an electric field imposed by instrument electrodes
  - Discretized elements used in legacy codes cannot accurately capture the curvature of actual hardware
- Molecular contaminants can also become photo-ionized and subsequently return to the spacecraft
- Developed a standalone code to demonstrate feasibility of calculating volumetric electric field using solely surface data (surface charge density) coupled with Coulomb force.
- Future work involves investigation of the Boundary Element Method, as well as coupling with volumetric mesh to perform kinetic plasma simulations.

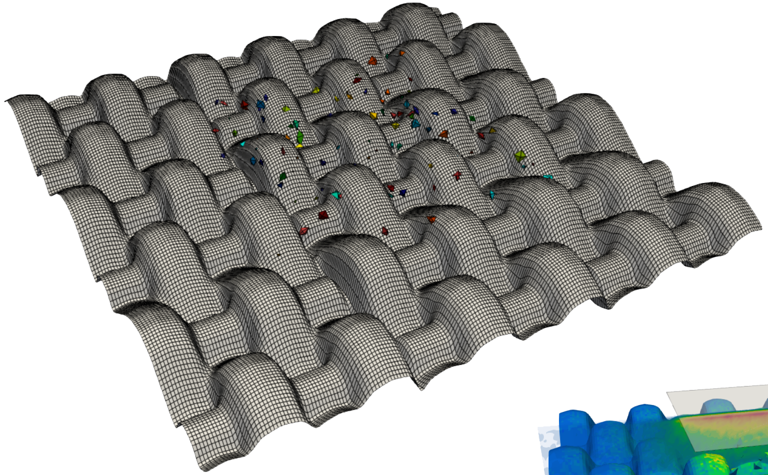


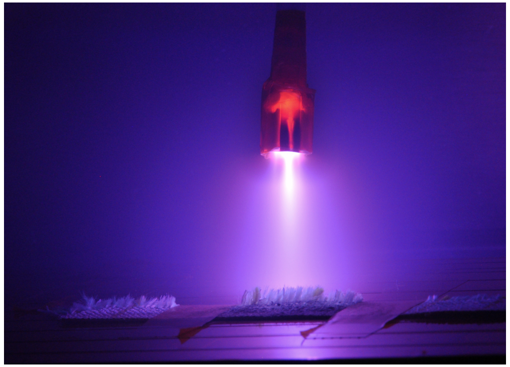


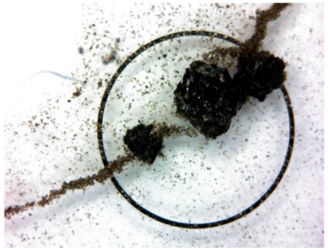
Other Work

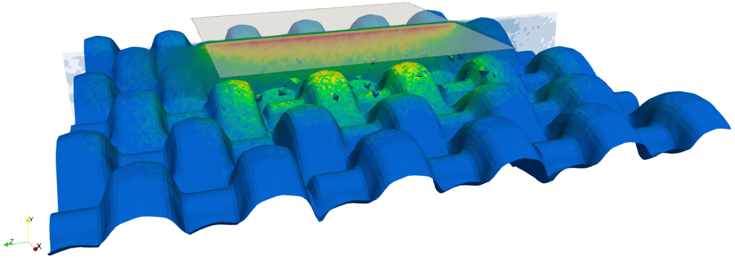
- Also interested in modeling dynamic objects – specifically dust grains individually represented by unique geometry shapes interacting with ambient plasma and other surfaces
- Being used to model lunar regolith adhesion to spacesuits, experimental work conducted at USC
- Preliminary results just published in IEEE TPS, update at ASEC

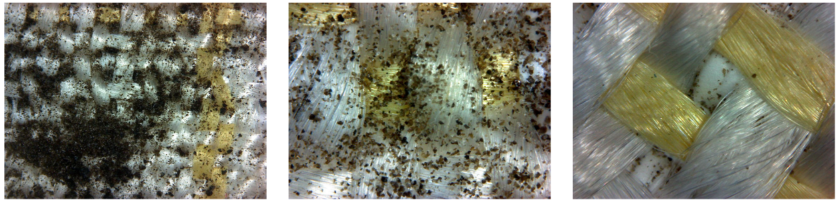












Summary and Future Work

- Developed a proof of concept simulation code to demonstrate the feasibility of performing contamination transport analysis directly using CAD geometries
- Proved out the required technology: ability to load STEP files, ability to perform line-CAD intersections, ability to access surface data
  - Also demonstrated ability to compute volumetric electric field using surface charge density
- Several steps remaining before the tool can be used by the CCE community:
  - Code optimization and speedup – shapes need to be sorted into an octree to limit search space
  - CC specific algorithms – ability to set outgassing rates, assign surface temperatures, specify particle-surface behavior – primarily port from our legacy mesh-based code
  - Graphical user interface as well as input files
  - Spring 2024 ECD for beta version
- Contact: *lubos.brieda@particleincell.com*

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