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Title: Study of Unstructured Mesh Utilization for Large and Complex Models at Los Alamos Neutron Science Center (LANSCE) Case study: Neutron dose rate at FP14 (DANCE instrument)

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Study of Unstructured Mesh Utilization for Large and Complex Models at Los Alamos Neutron Science Center (LANSCE)

Case study: Neutron dose rate at FP14 (DANCE instrument)

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Motivation after last symposium:

- Can we easily mesh large & complex CAD model to UM and simply run it with MCNP63?
- Does it going to make our work more efficient in the future?
- What are the difficulties and potential complications?

Content:

- LANSCE spallation targets intro. [LANSCE layout]
  - More info: Thanos's talk on Tuesday 11:10 am, + other LANSCE talks
- How can we increase fidelity of complex geometries? [3D scans]
- Can we switch fully from MCNPX&CSG to MCNP63&UM?
  - Pros – one "as-built" model, fully updated, easier to tracking changes
  - Cons – initial time consumption, computation time + RAM [old clusters]
- Challenges with proton source

Acknowledgement:

L. Zavorka (ORNL) – consultations

Hoonify – HPC

SilverFir – Attila4MC support

Credit:

D. Kral – CAD model, UM trouble shooting

J. Svoboda – UM troubleshooting

M. Mocko – funding, consulting

V. Kuhns – computation power, benchmarking

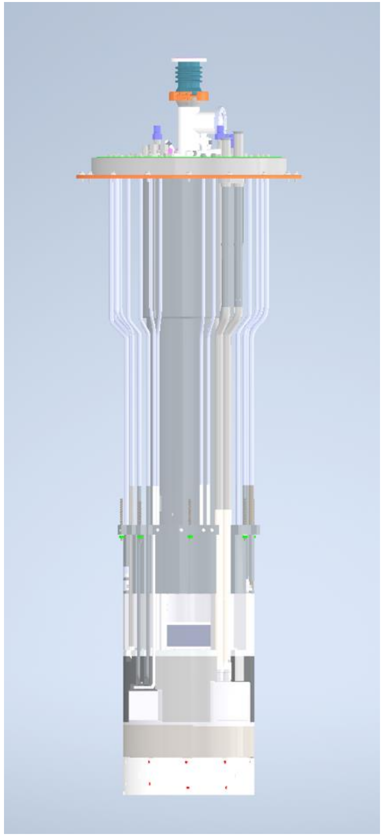
Spallation Target 1 (Mark-IV)

Combination of target-moderator-reflector-shield (TMRS)

TMRS is a shape of cylinder with about 60cm in diameter and height of 3m

- consists of ~2,500 parts - many pipes, screws, holes, thin layers and curvatures

Target 1
Mark-IV



Credit: CAD model - AOT, LANL; Lujan Center photo: https://lansce.lanl.gov/

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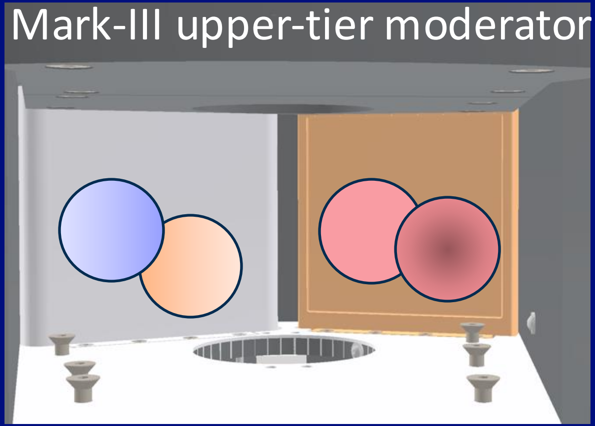
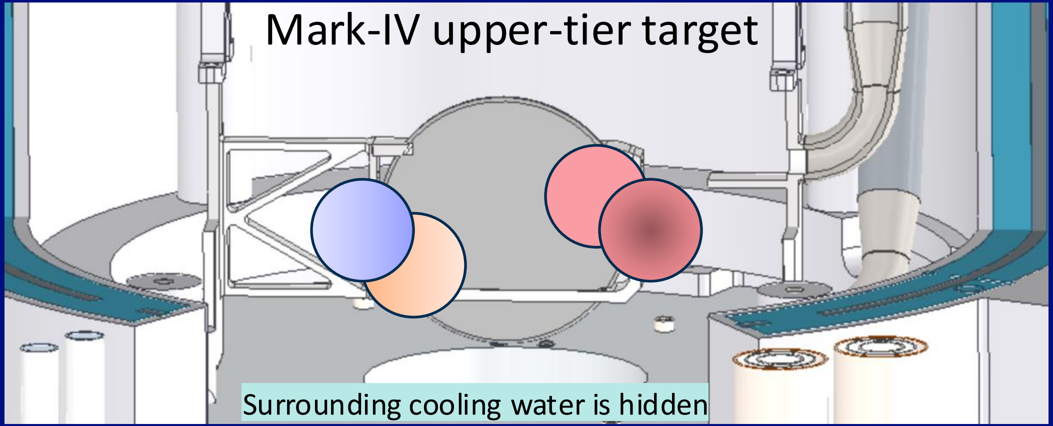
Where is Mark-IV located and why do we need to know?

- Mark-IV installed 2022
- New upper target design
- Absolute position needed due to direct flight paths FOV (previously larger moderators)



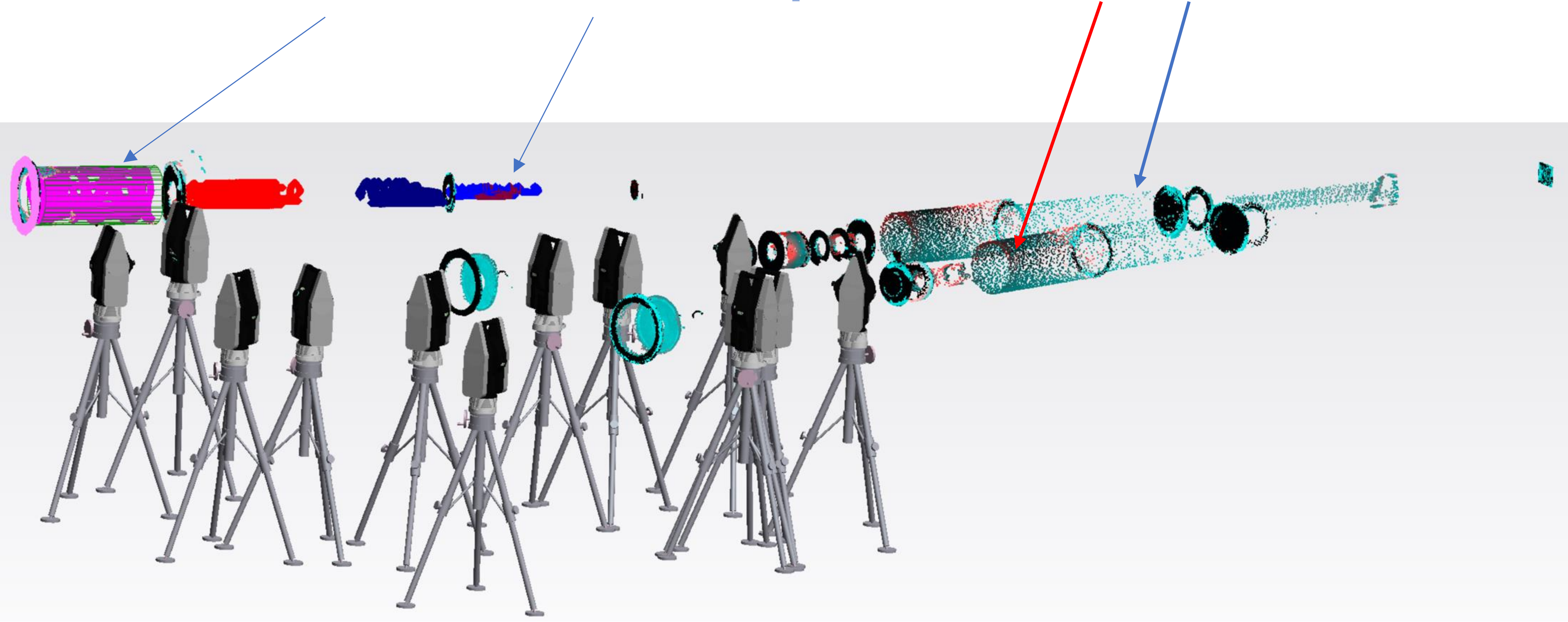
accurate position of FOV did not matter so much for large MARK-III moderators with uniform n-distribution



In the case of MARK-IV, due to its design, the accurate position of FOV matters due to part of FOV on water, another part on W target having harder nFlux

From ”as-designed” to “as-built” - Laser Tracker Survey (LTS)

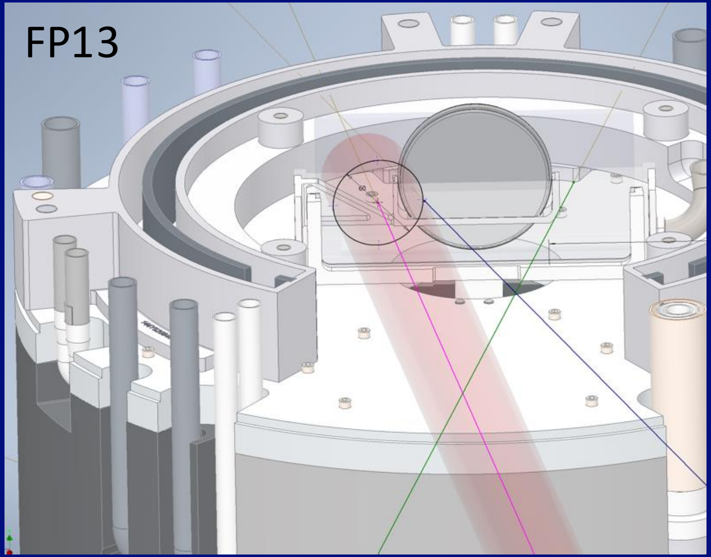
FP14 bore, collimator1 and ports of FP12&13 LTS scan

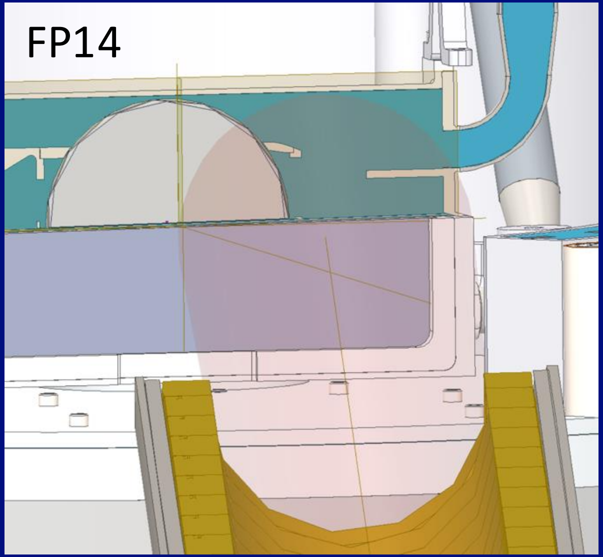


FOV for FP13 (DICER) & FP14 (DANCE) based on LTS

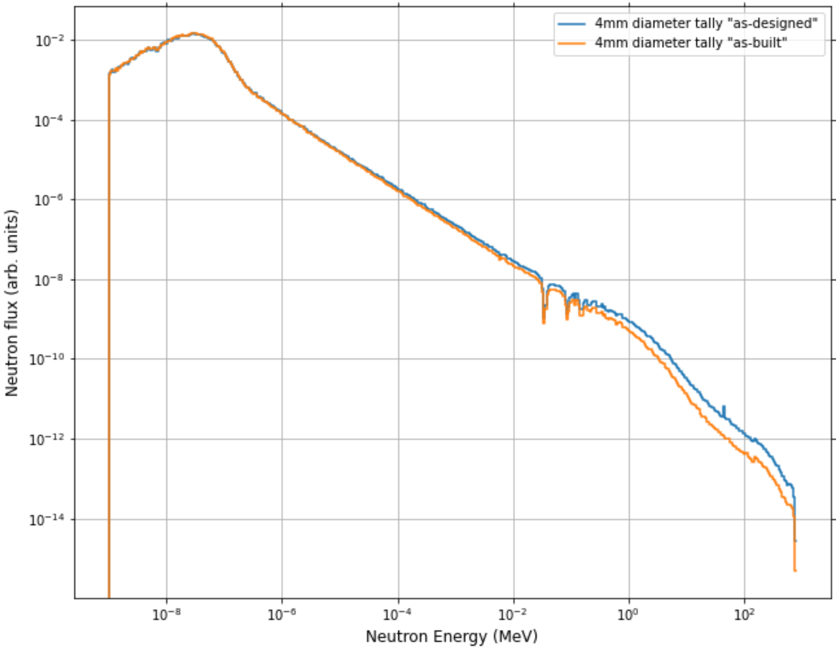
FOV=Field-Of-View for Flight Paths (FP); LTS=Laser Tracker Survey

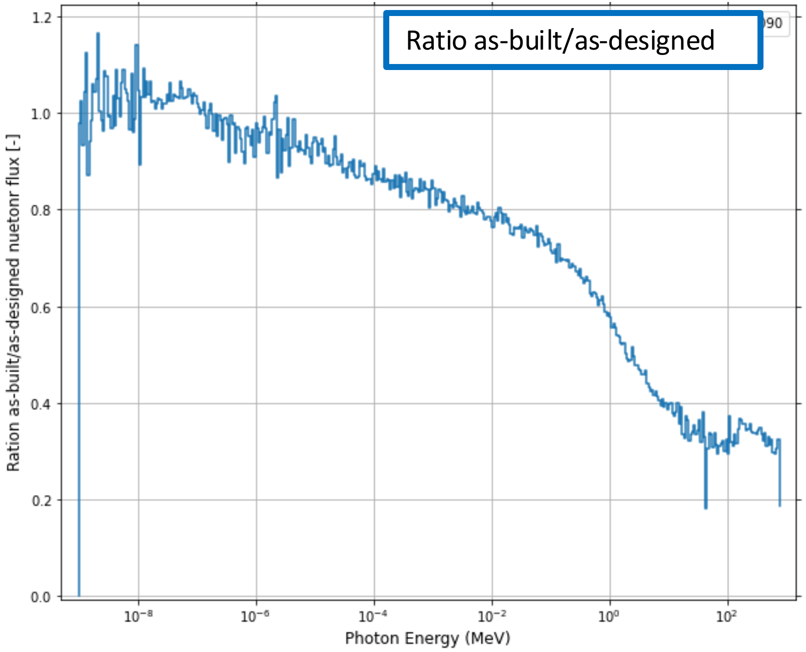
- DICER is not sensitive to non-uniform beam spot, so its absolute FOV position does not affect results of sample irradiation greatly (problem seems to be in greater background)
- DANCE instrument requires neutron beam spot uniformity in full energy range for experimental studies of samples having disc shape of ~4mm in diameter





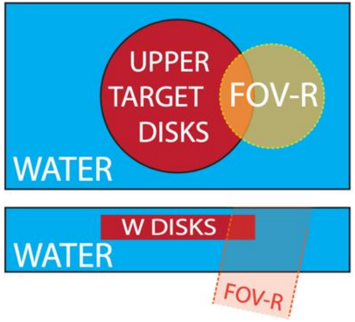
Is a high-fidelity geometry important for our MCNP





intersection point determination before and after LTS

As-designed:	As-built:
X=53 mm	X=65.17mm
Y=0 mm	Y=-5.84mm



J.Svoboda, NIMA, 2024

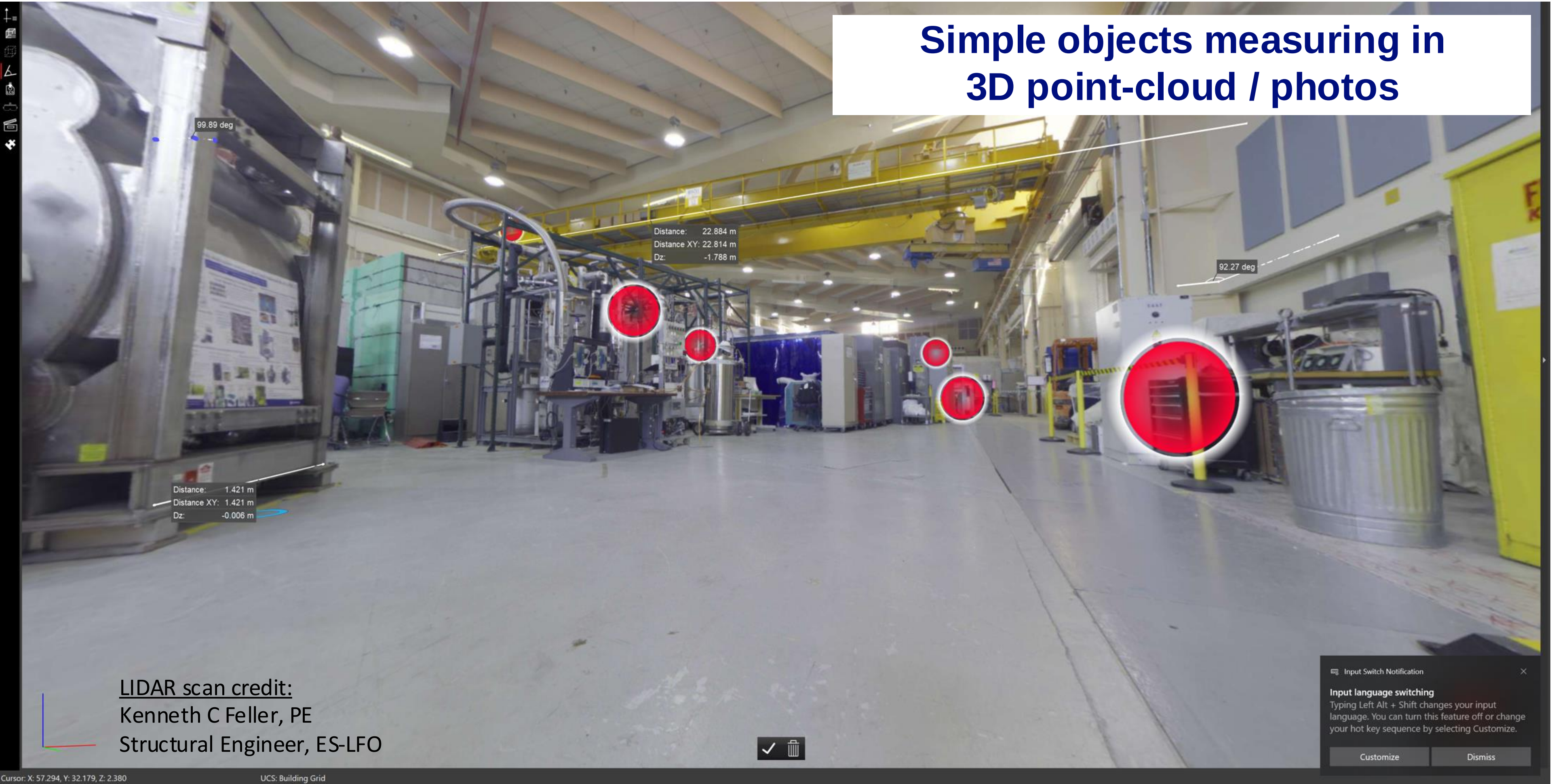
Enhancing MCNP Geometry Fidelity:
Current Progress at LANSE, Lujan Center

- 3D LIDAR scan with high quality panorama photos
  - (allows measure geometry of experimental hall from the office)
- LTS connected with LIDAR for detailed CAD modeling
- Conversion of 3D scan into CAD
- CAD-MCNP geometry conversion by using Unstructured Mesh (UM)
- MCNP63 simulation {TurbOS benchmarking}

MCNP UM simulation:
High level of confidence
Low time-cost for geometry updates
Ready of optimization process

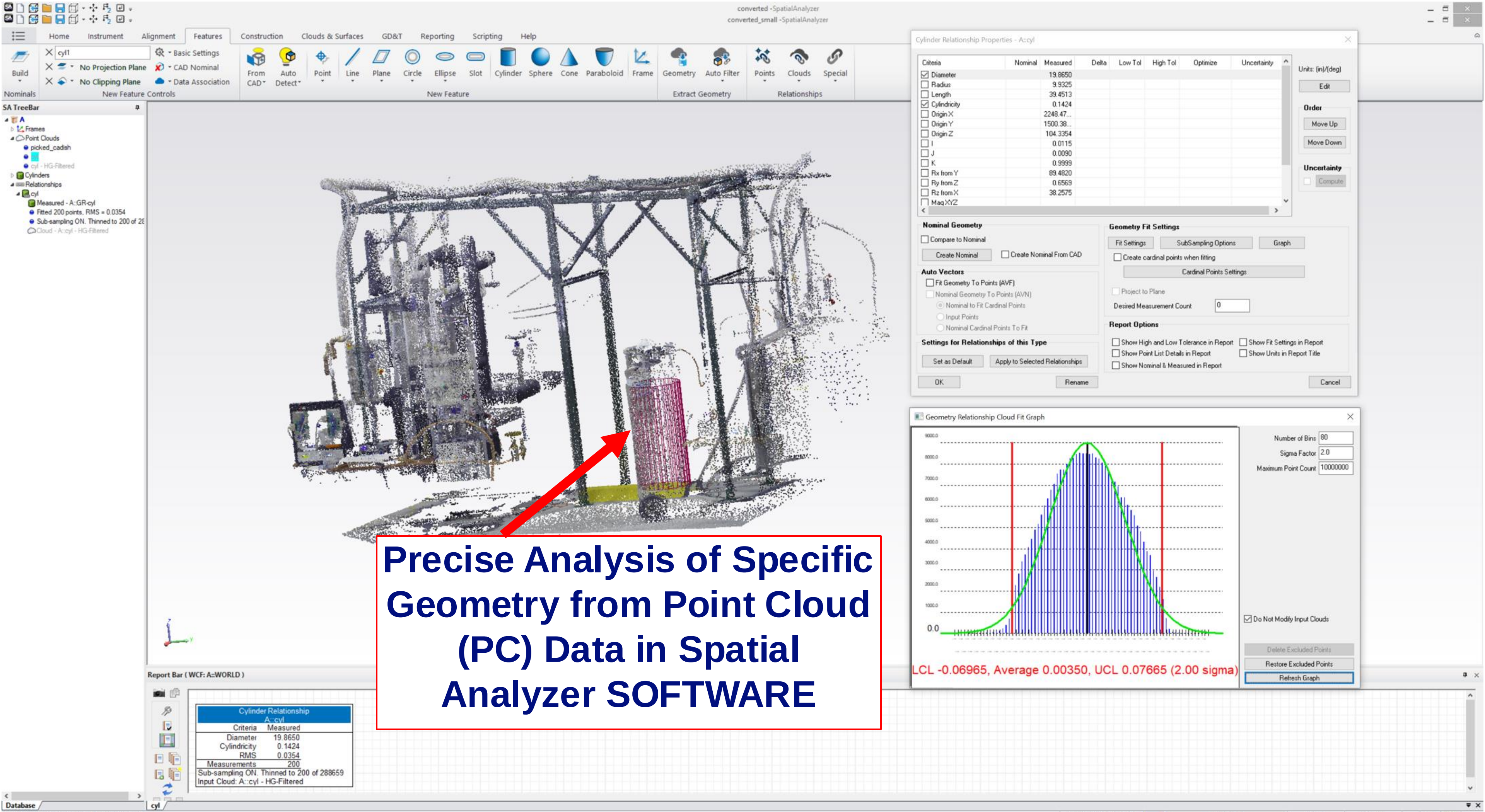
❖ If optimization (future plan):
  - Currently exploring Machine Learning (ML) options for simple geometries (UMICH, Omer Erdem)
  - DAKOTA?
    - Parametrization of geometry for optimization (shielding // target design)
    - MCNP run, extract results, automatic CAD changes, run again

LIDAR+LTS -> CAD -> MCNP UM geometry -> Simulation



LIDAR scan credit:
Kenneth C Feller, PE
Structural Engineer, ES-LFO

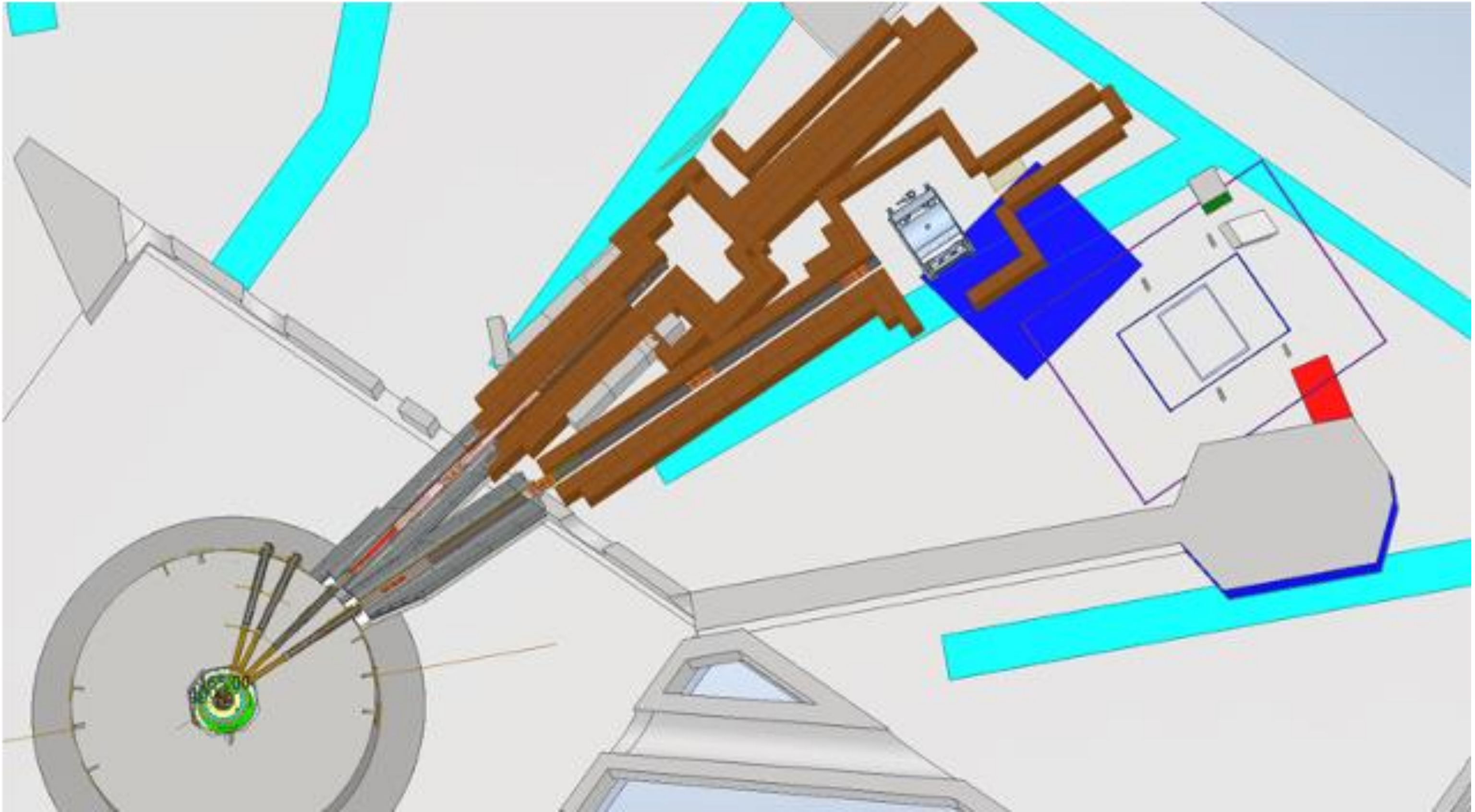
Precise Analysis of Specific Geometry from Point Cloud (PC) Data in Spatial Analyzer SOFTWARE



LIDAR+LTS -> CAD -> MCNP UM geometry -> Simulation

3D scan allows to build high-fidelity “as-built” CAD model

+ simplifies editing, new part may be quickly designed / old one redesigned



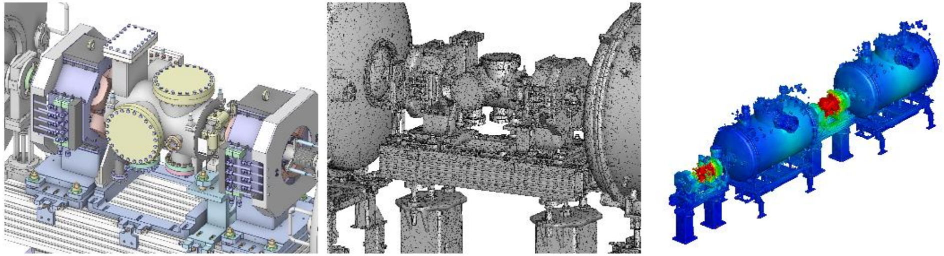
LIDAR+LTS -> CAD -> MCNP UM geometry -> Simulation

- Cooperation with Silver Fir (Attila4MC): UM, Variance Reduction (VR)

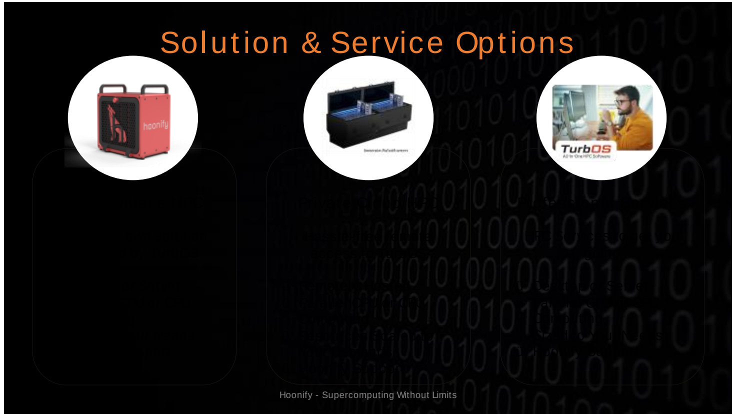
  & Hoonify – HPC (benchmarking)

Silver Fir SOFTWARE

https://www.silverfirsoftware.com



European Spallation Source: Courtesy of Elena Donegani



hoonify

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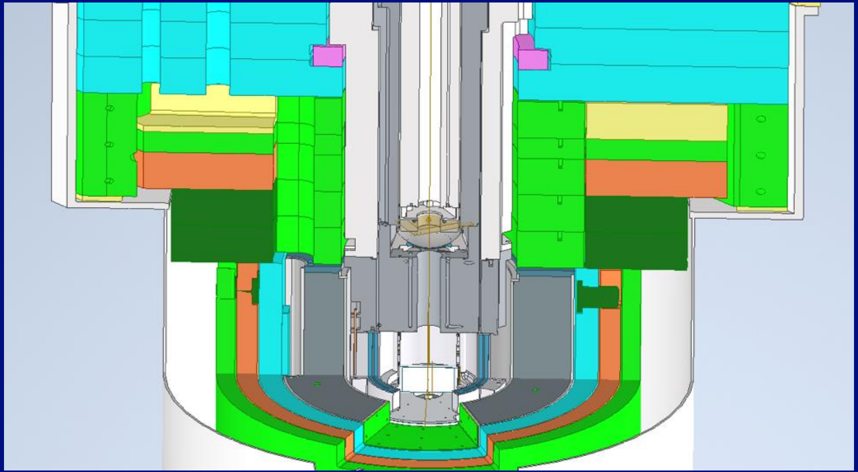
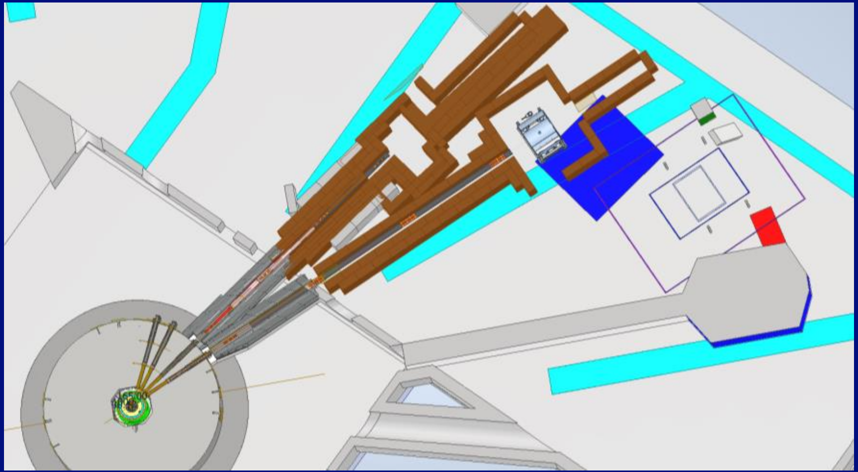
Context of Large and Complex CAD model

~2,500 parts, parts dimension from *xx* um to *xx* m
complex curvatures D{mm-m}



Target-Moderator-Reflector-Shielding + Crypt components



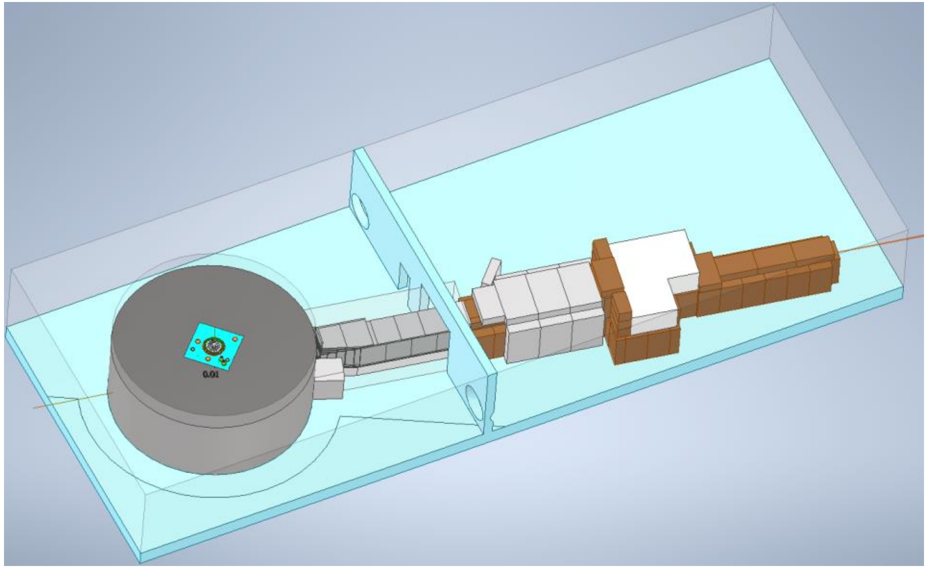
Lujan Center – buildings ER-1 and ER-2 with FP14 and design of FP15

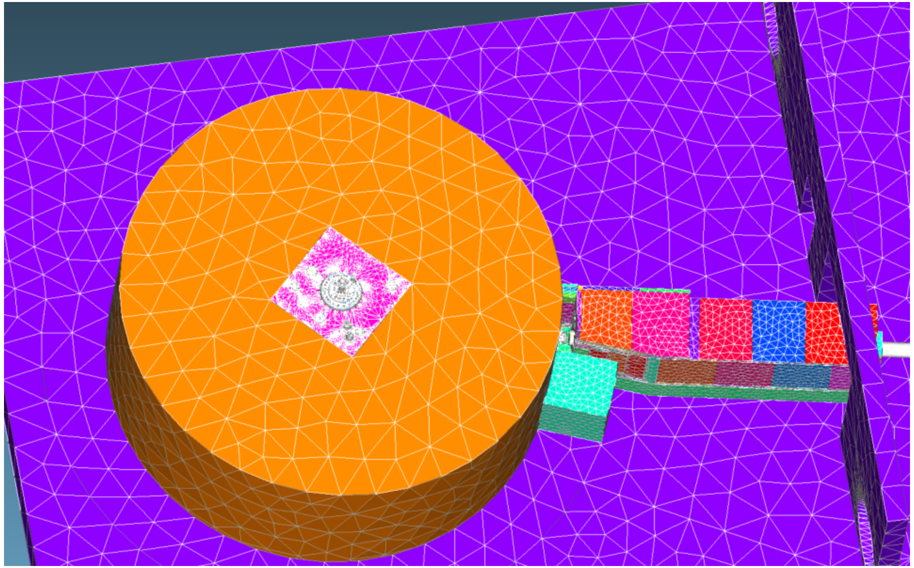
- CSG is mostly based on original drawings with some updates from 3D CAD models
- UM Increasing fidelity by using ”as-designed” CAD and “as-built” data from LTS

Attila4MC - creating UM for large and complex model

How good mesh do we have? What is a GOOD MESH?

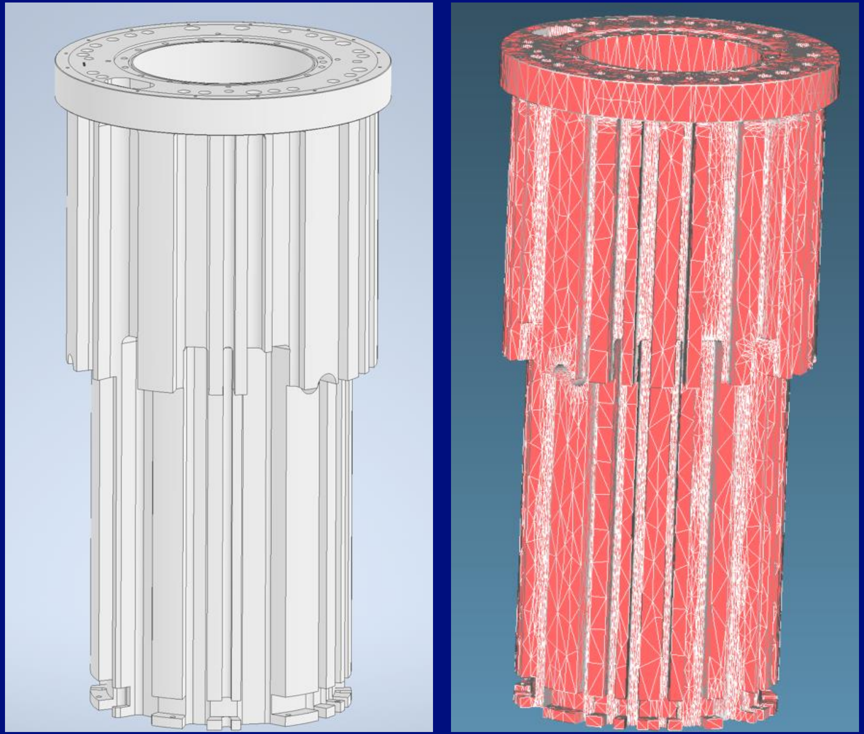
- From CAD model (Autodesk Inventor)
- To UM in Attila4MC





Part-by-part Mesher (PBP)

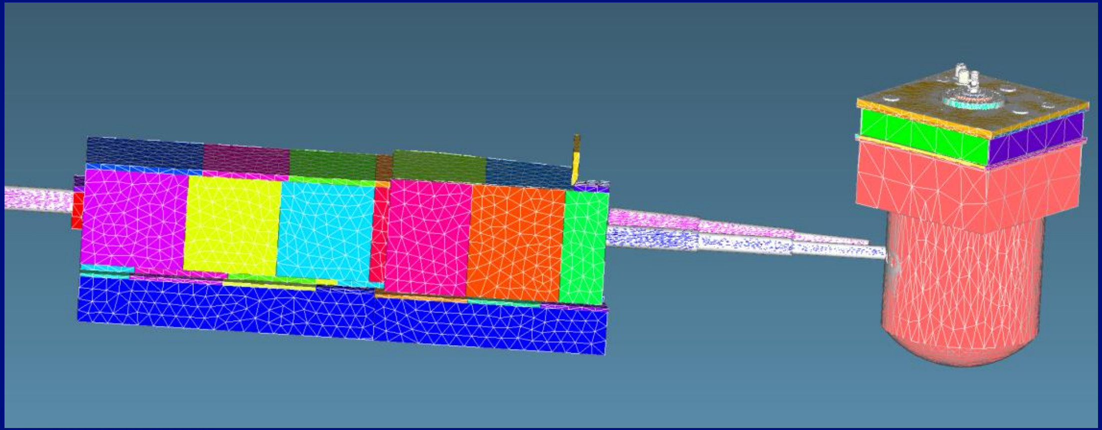
- Silver Fir’s stand-alone package for discontiguous mesh preparation
- Tested beta version running in Linux
- Lately released Attila 10.3 came with PBP implemented in GUI
- Supports parallel processing (SMP) => assembly with more parts
- Parasolid input from CAD software (we used Autodesk Inventor)
- Variety of settings – cell volume, curvature, global/specific part settings, volume cutoff,…
- Output goes to Attila4MC (now implemented)
- UPDATE: all was later tested in Attila10.3, works well

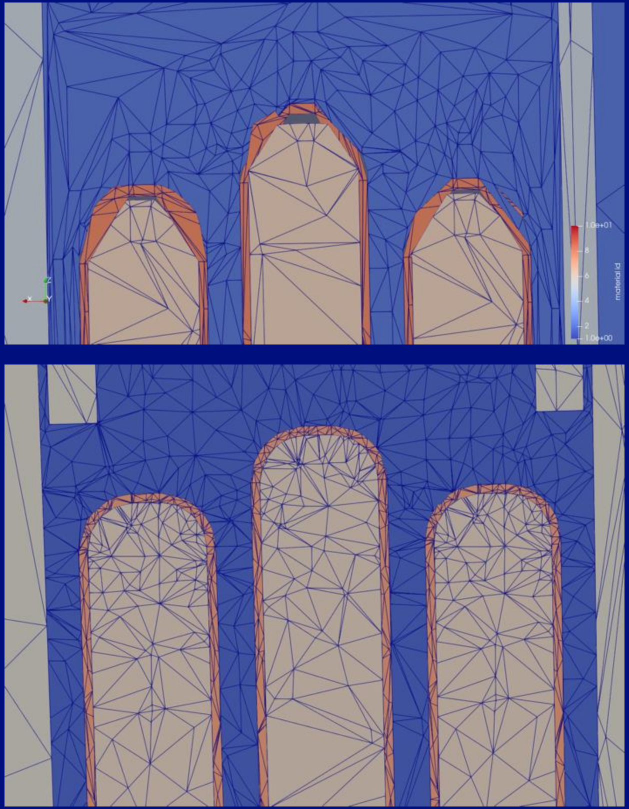


(a) CAD model, (b) PBP mesh

Part-by-part Mesher (PBP)

- MCNP sensitivity to some overlaps has been seen (more pronounced if changed particle occurs)
- Mesh quality controlling needed some steps (Cottonwood => .GSV => Paraview)
- Full mesh created in Attila4MC by Mesh Joiner, approx. 5-7 million cells
(Mesh Joiner is great for rotations and translation)

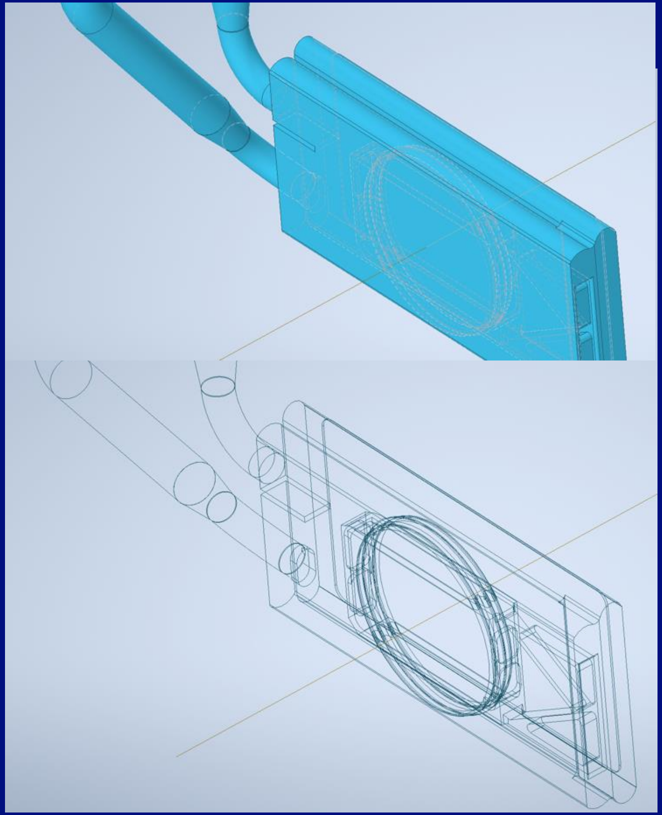




A comparison of a curvature quality for Mark 4 Upper Target mesh – different settings

Preparation for Unstructured Mesh (UM) I.

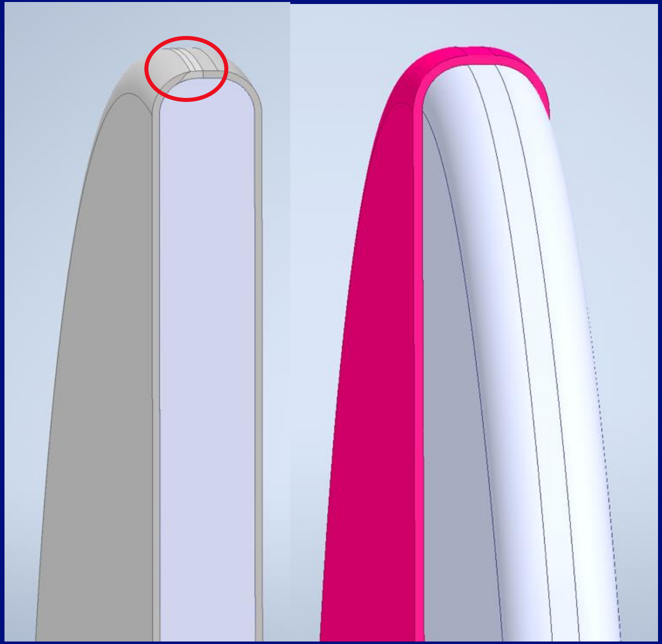
- Constrains - We have set a limit to ~5-7mil cells
- Real facility contents liquids, gases, thin layers from neutronics specific materials → model adjustments:
    - Create parts which represent liquids (water with different temperatures, liquid hydrogen, etc) (filling cavities)
    - Find the larger geometry overlaps
    - Simplified complicated designs with low impact
    - Focus on important parts with higher number of collisions (thin layers of Cadmium or Gadolinium)
    - Add correct materials (several different options how to add material in Attila4MC)
    - Some big or complicated (a lot of curvature) parts had to be divided into sub parts due to MCNP does not like pseudo cells being assembly with too many cells



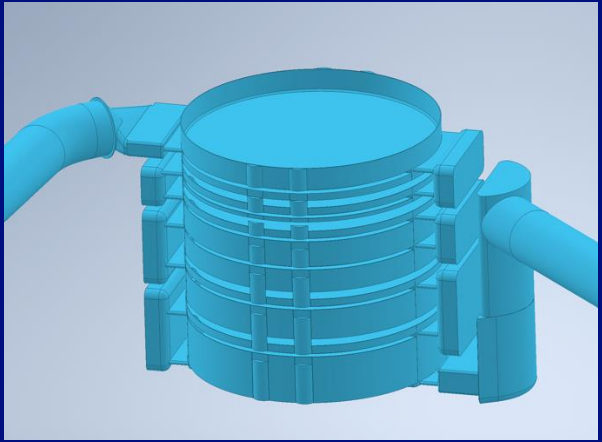
Example of Upper Target cooling water and moderator with detailed view in an inner structure

Preparation for Unstructured Mesh II. – fillers

- Fillers usually had to be modified due to big amount of very thin layers <= original model has spaces between components (weld placement)
- Curvatures are potential problem (overlaps)
- Some parts or assemblies were simplified – Tantalum cladding from tungsten targets were replaced by one part



Three parts (a) replaced by one (b)

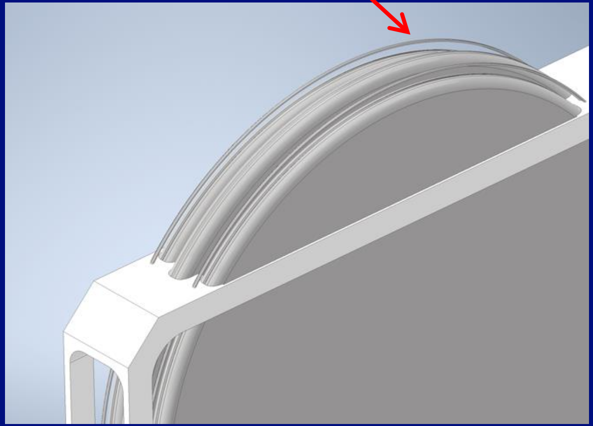


Water filler with thin volumes

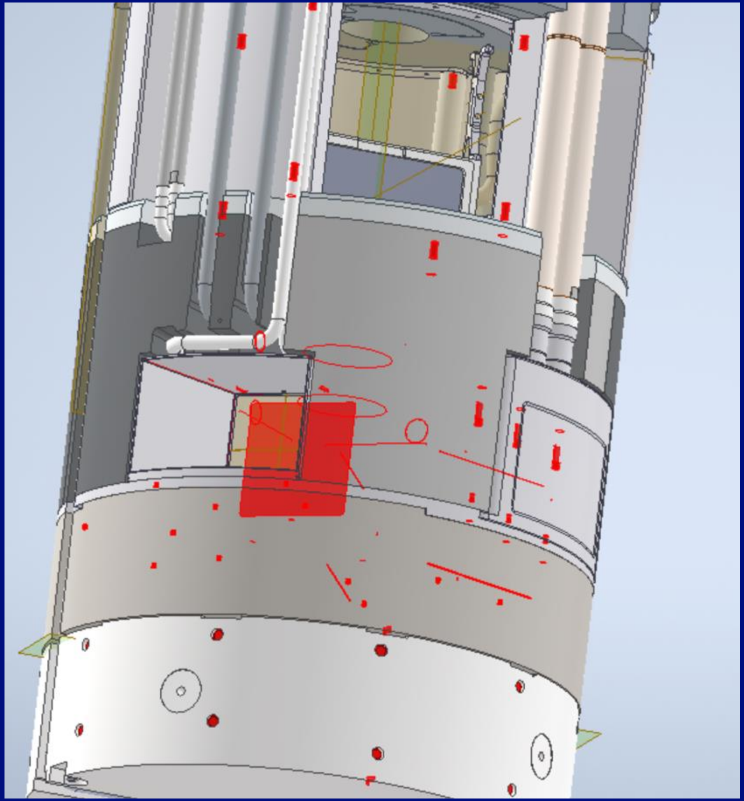
Fillers =
filled cavities

Preparation for Unstructured Mesh III. – model cleaning

- PBP Mesher officially doesn't need overlaps cleaning BUT we had a bad experience and wanted accurate model
- This step very depends on quality of the source model.

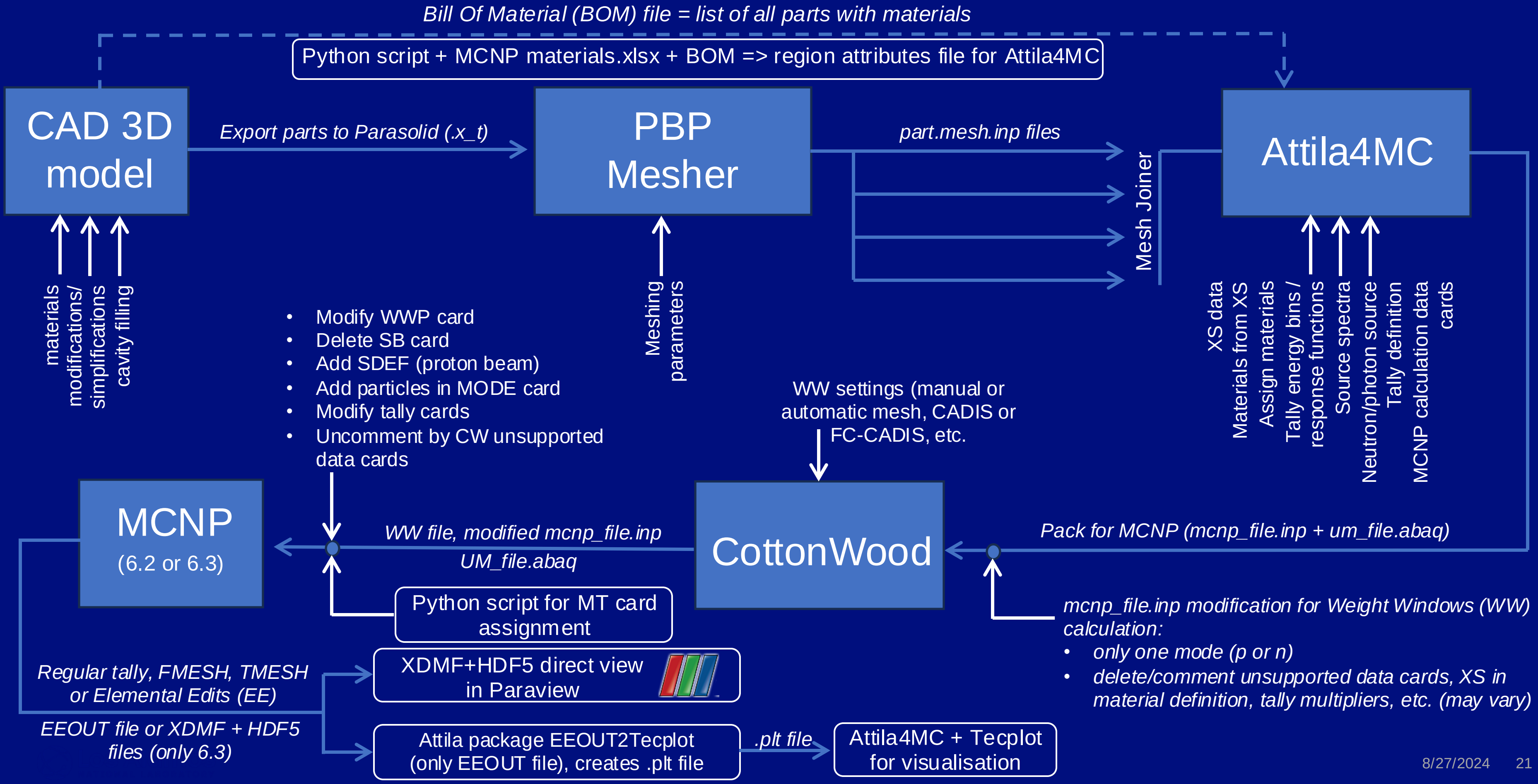


Incorrect design of previous Tantalum cladding



Findings of an inspection tool in Autodesk Inventor

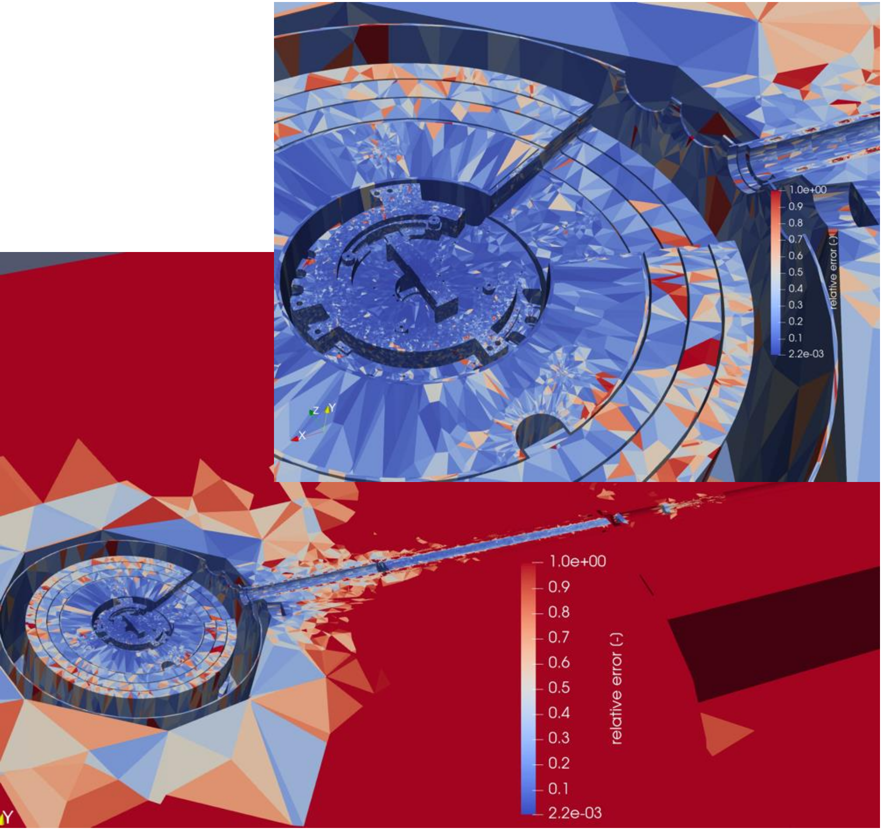
UM calculation workflow (back in Spring 2024)

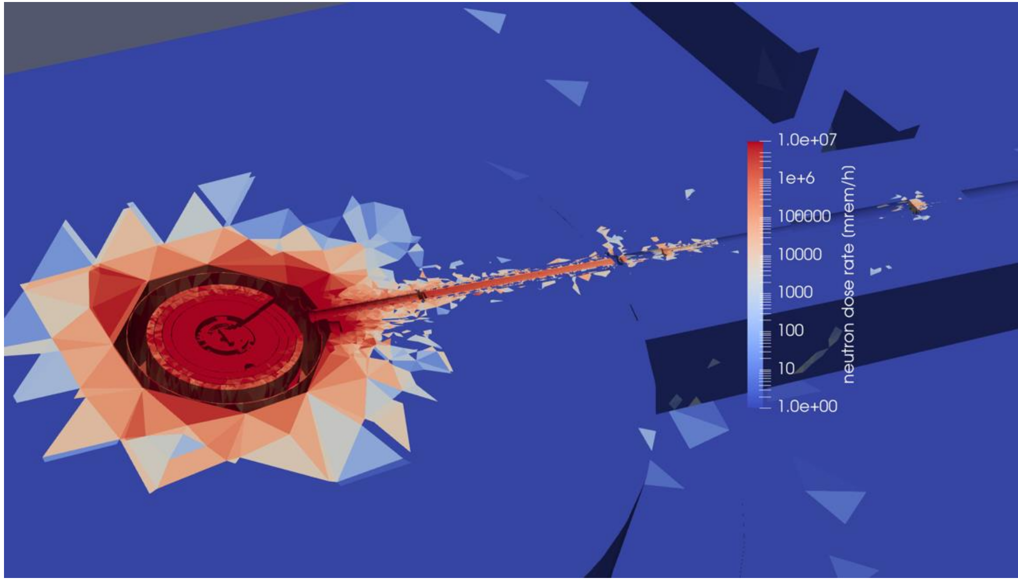


Proton - Spallation based UM MCNP63 simulation, Dose study (mrem/h)

HPC Hoonify 256 cores; ~5M cells; 1e8 ~4days; ~110 stalled, Without WEIGH WINDOWS

800 MeV protons –> tungsten, spallation, DOSE Elemental Edit

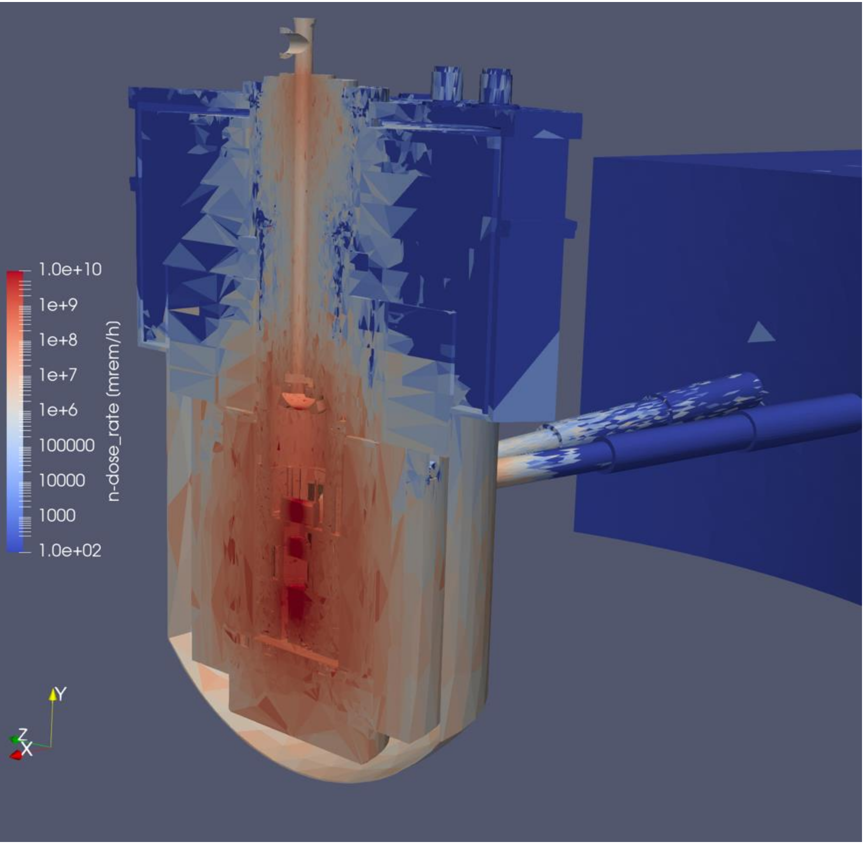


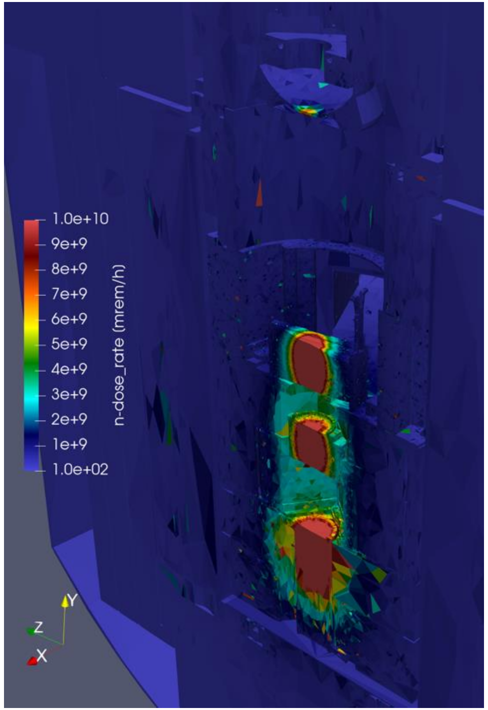


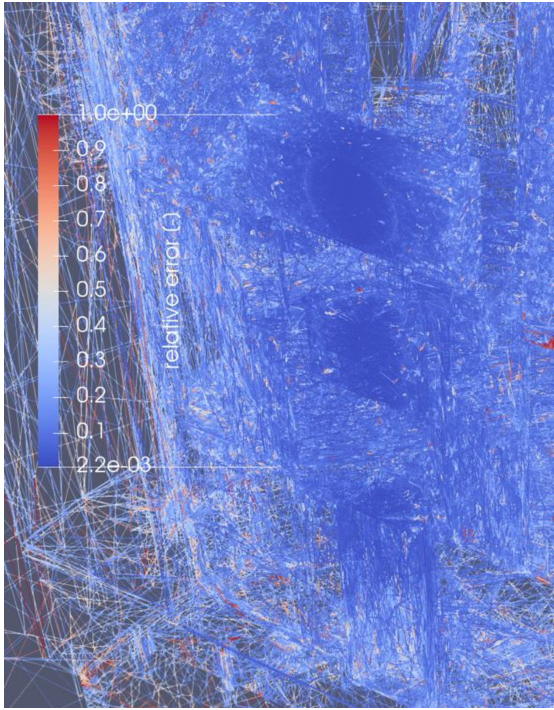
<- left-rel.error, right-dose ->

Proton - Spallation based UM MCNP63 simulation, Dose study (mrem/h)

HPC Hoonify 256 cores; ~5M cells; 1e8 ~4days; ~110 stalled, Without WEIGH WINDOWS



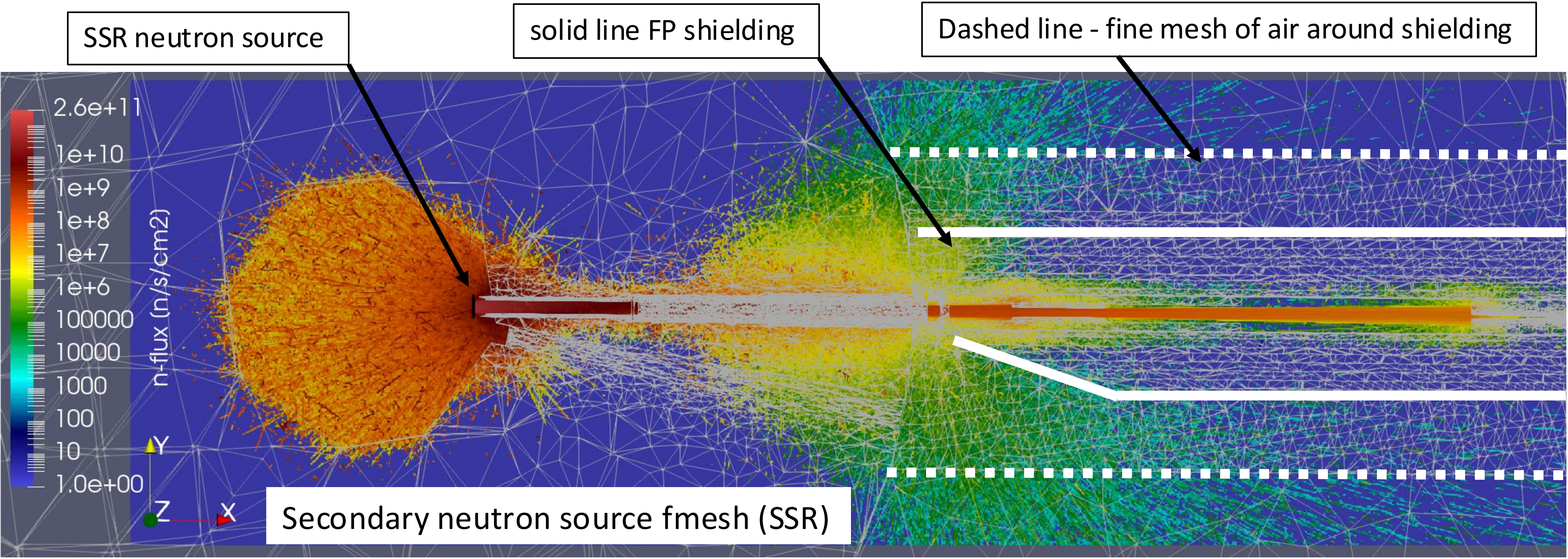




Visualization of Upper, middle and lower target dose of Mark-IV TMRS

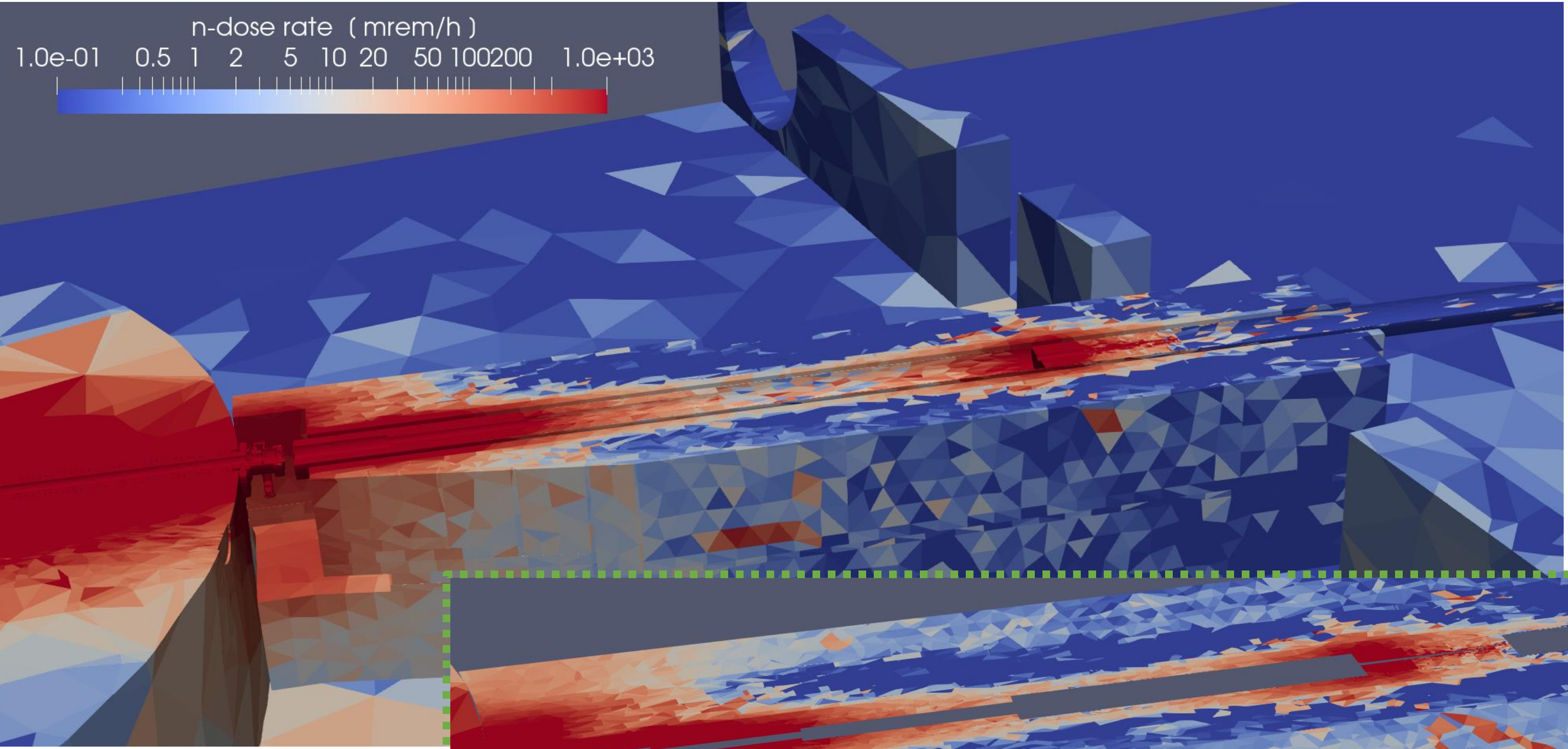
Calculation of Surface Source File (SSW) and its reading SSR

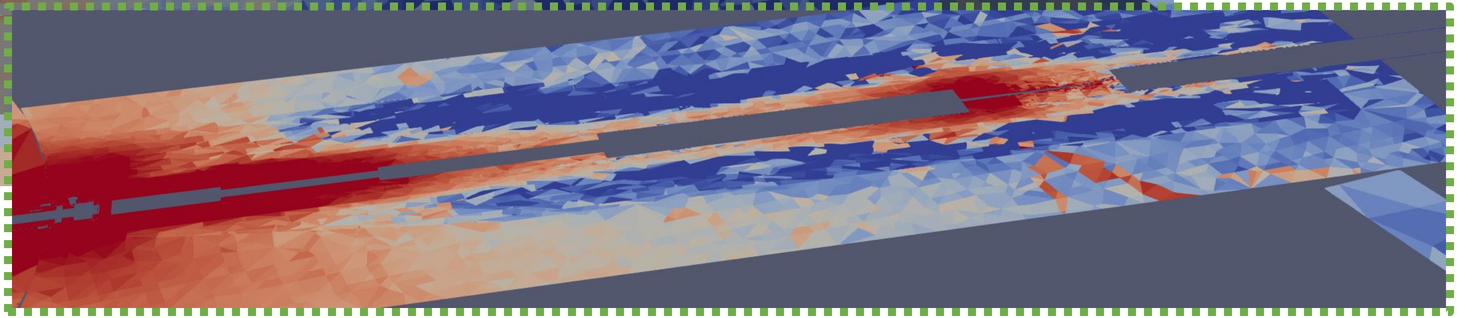
- Due to stalling issue on proton-based UM simulation, we have removed the TMRS (target) and used secondary n-source calculated with CSG through SSW card
- Neutrons only, UM from 5mil to 1mil cells, quick run, no problems at 6-core laptop
- We have been experiencing very slow run on HPC (256cores), writing/accessing rssa file?



Neutron dose rate with secondary neutron source (SSR card)

3e7 histories, 7.5h @5cores; HPC very slow (probably communication with rssa file?)





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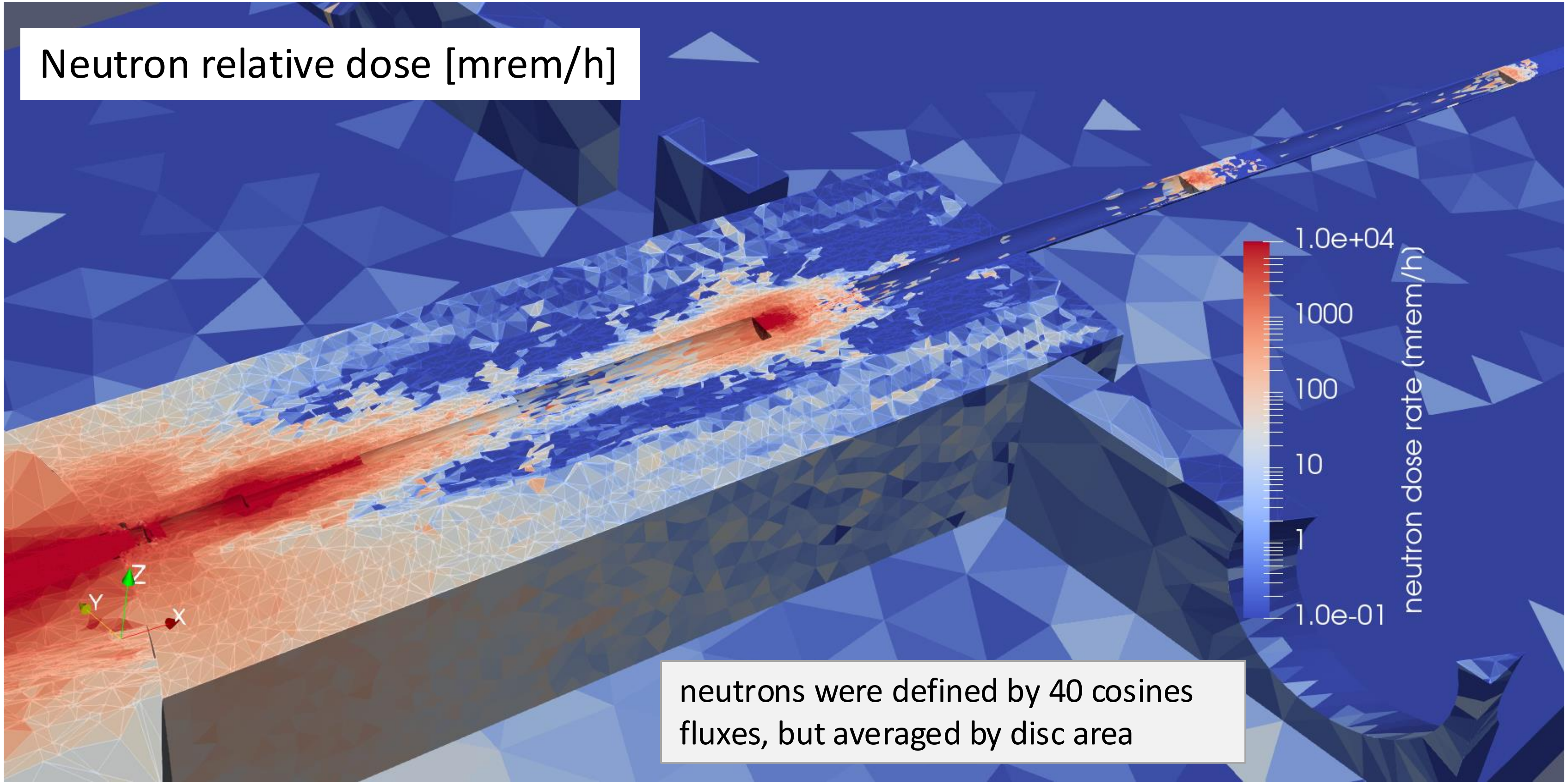
Neutron dose rate with secondary neutron source (sdef)

Laptop ~2.5x faster than SSR; loosing fidelity due to averaging non-uniform source

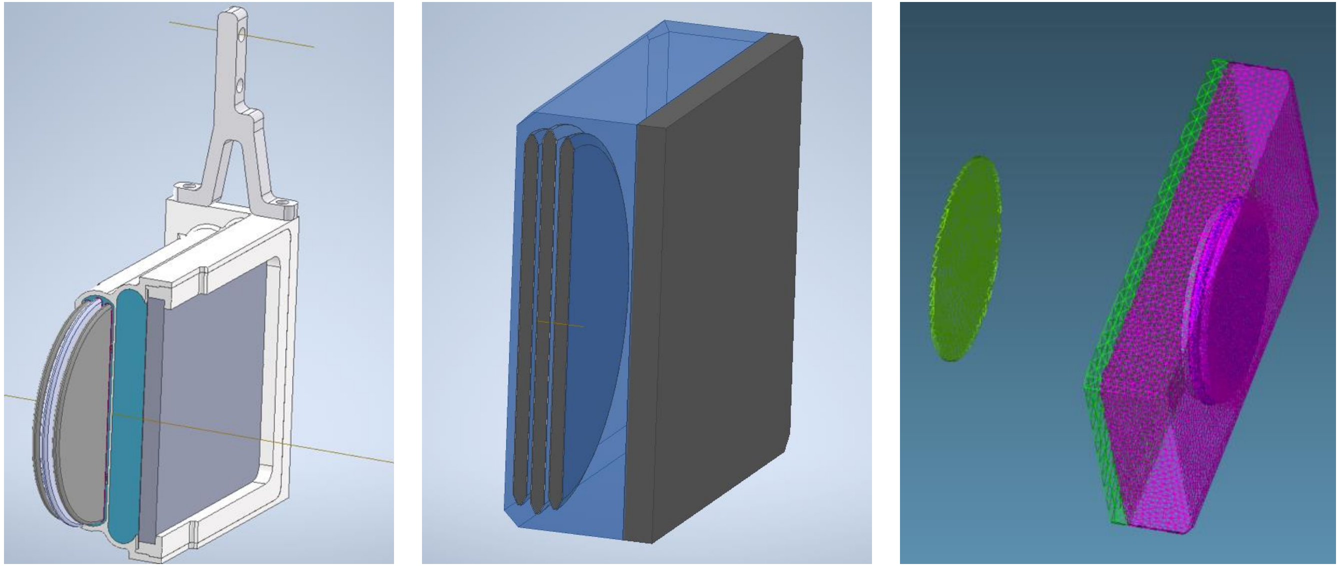


Focusing on MCNP Stalling - problem of protons with UM

- We have simplified UM upper target model for testing with charged particles (800 MeV p^+)
- Most of the parts from TMRS (Target 1) were removed

  1st step: Precise engineering model with high fidelity UM (+1million cells) – doesn't help

  2nd step: Simplified model – all structural parts deleted; target discs simplified (edge rounding removed); added 10 µm of void between Tungsten-Tantalum cladding and Cladding-Water – doesn't help



- Even we have simplified model into simple shapes, stalling problem did not disappear
- instead of stalling at 1e6 (it was common for fine mesh of upper target), simulation stalled at 16e6

(a) Engineering CAD model, (b) simplified CAD model, (c) Meshed simplified model with tally disc

Summary

We attempted to investigate the cause of calculation stalling for primary source particles (protons):

- Tiny overlaps of PBP meshes were partially addressed using RTT_mesh_editor to increase the space between nodes [Attila developers discussion]—this did not resolve the issue.
- Killing protons below the fine upper target mesh—this did not resolve the issue.
- Focusing only on the upper target with the proton-spallation reaction—this did not resolve the issue.
- Simplified target with no curvature and no complicated geometry—this did not resolve the issue.
- A Bash script was used to terminate MCNP if dump time exceeded 2x the average. The SEED was adjusted by -2, and the run was continued - this did not resolve the issue but allow us to reach 1e8 histories.

Observing improvement between MCNP6.2 and MCNP6.3:

- MCNP6.2 uses approximately 5x more RAM per core for 5M cells compared to MCNP6.3 [default settings].
- For large EEOUT files, saving time was around 10 minutes versus seconds for HDF5 files.
- When SSR was used for UM, unusual behavior was observed—likely due to accessing RSSA on HPC, plus crashing occurred if UM dose calculations involved more source particles than those calculated for SSW.
- Complex geometry meshing with PBP was fast but required some skill. Careful with volume skipping (screws/absorbing layer).
- SSR vs. SDEF disc source definition: Non-uniform sources are averaged by disc surface area, but it runs 2.5x faster.
- We are currently updating our ~4000 core clusters to Hoonify TurboOS and fully transitioning to MCNP6.3.
- We found no advantage in using older versions. Thank you, developers!

Thank you for your attention.

Josef Svoboda & Dusan Kral

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