Investigation of Unstructured Mesh Utilization in MCNP at LANSCE

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

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LANSCE, Spallation Physics

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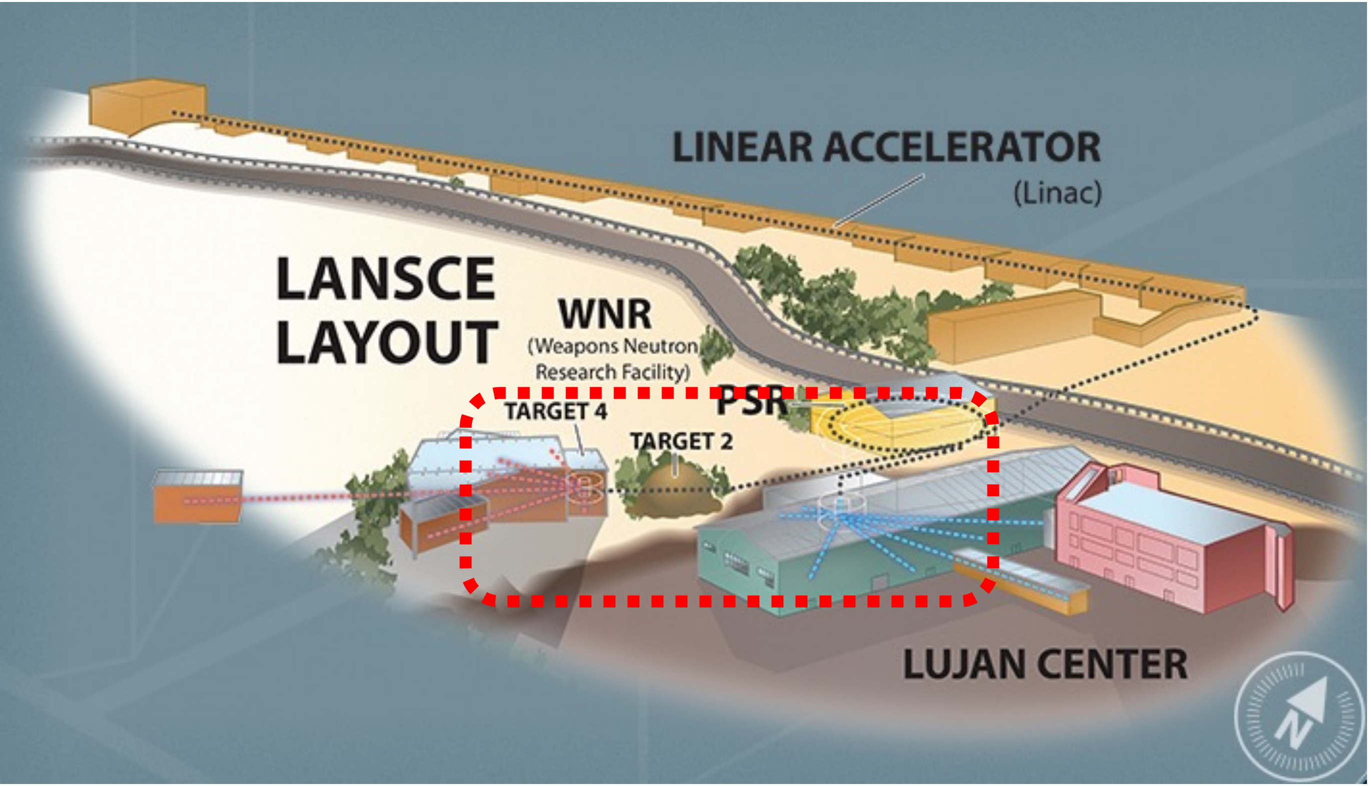
Content:

- LANSCE spallation targets intro. [LANSCE layout]
- How can we increase fidelity of complex simulations? [3D scans]
- Can we switch fully from CSG to UM? [Unstructured Mesh]
- Pros/cons - from MCNPX to MCNP63. ["results"]

Low histories calculation shown only, shown case study is opening potential novel approach to complex high fidelity calculations , benchmarking is in process currently

This project was accomplished thanks to a huge effort of my colleague Dusan Kral [LANL] who unfortunately, could not join this workshop.

LANSCE – Los Alamos Neutron Science Center @ Los Alamos National Laboratory (LANL)



<u>800 MeV Linac serves to:</u>

- IPF - Isotope Production Facility
  - ➢ Uses extracted 100 MeV
- pRAD – Proton Radiography
  - ➢ Diagnose dynamic experiments
- UCN – Utracold Neutron
  - ➢ spallation neutrons are cooled by solid deuterium
- Lujan Center
  - Target 1 (Mark-IV)
- Weapons Neutron Research Facility
  - Target 4

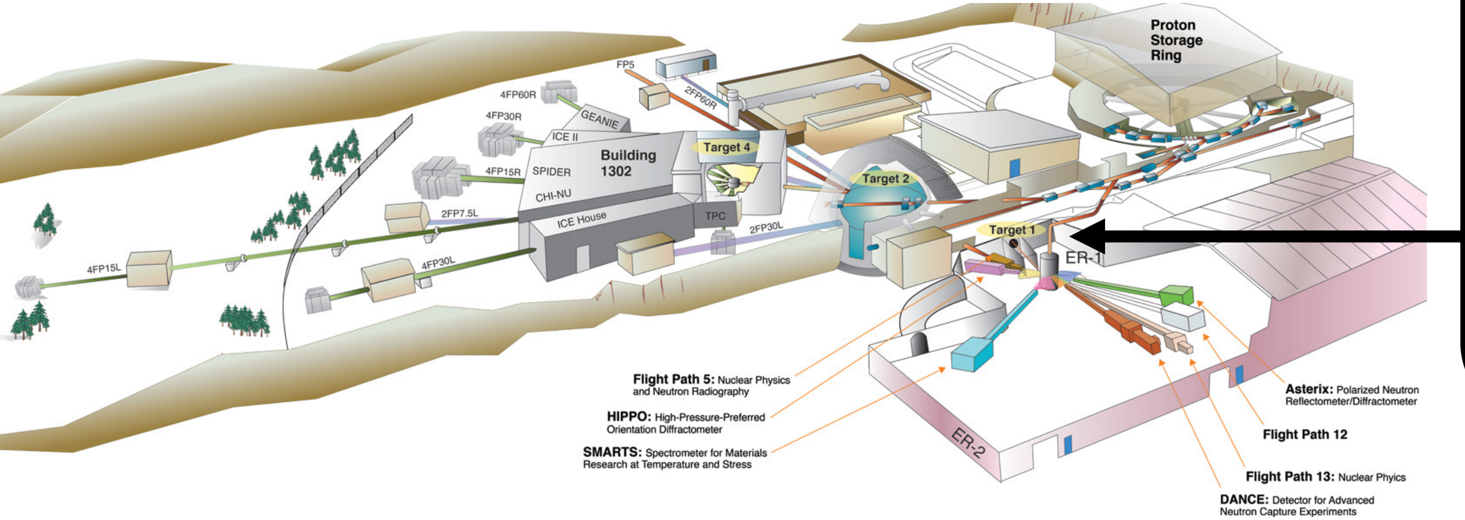
LANSCE layout visualization: https://lansce.lanl.gov/

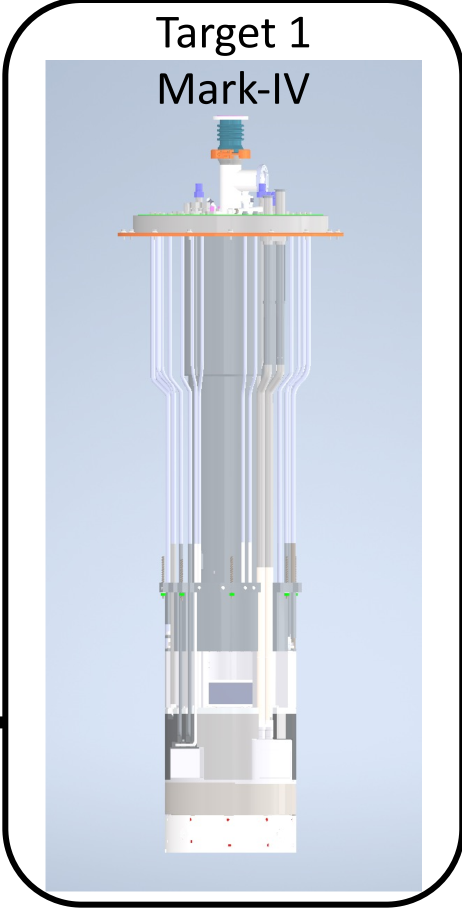
LANSCE Spallation Targets

Target 1 (Lujan Target)

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

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

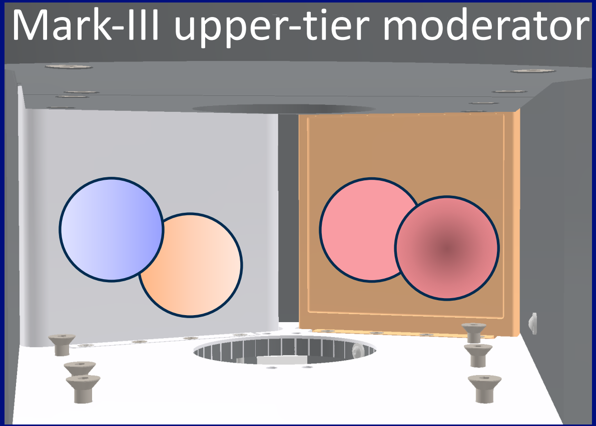




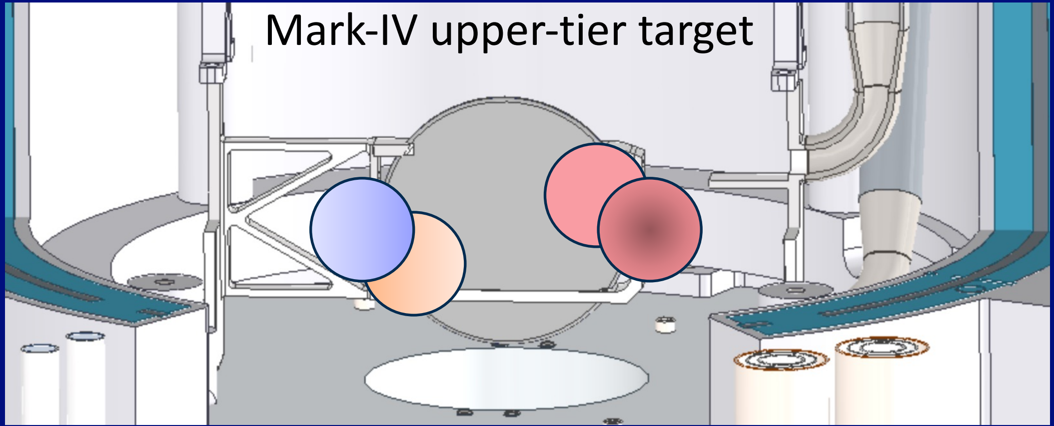
Target visualization: AOT, LANL; LANSCE visualization: https://lansce.lanl.gov/

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

- Mark-IV installed 2022
- New upper-tier target, upper-tier Flight Paths have direct FOV to part of the target
- Angle and absolute position now matters (previously large moderators)



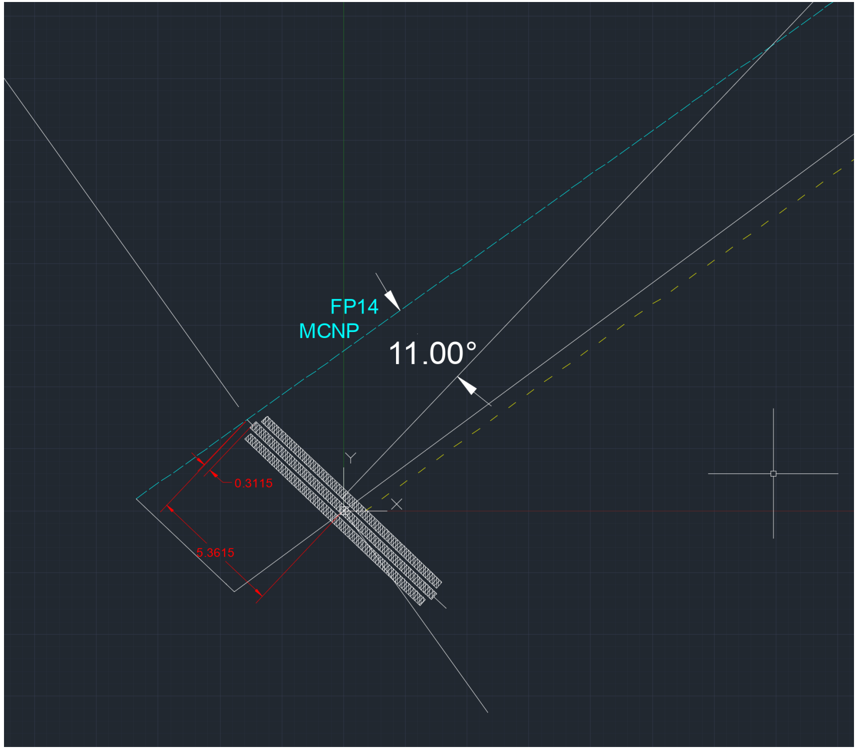
accurate position of FOV did not matter so much for MARK-III large moderators with uniform n-distribution



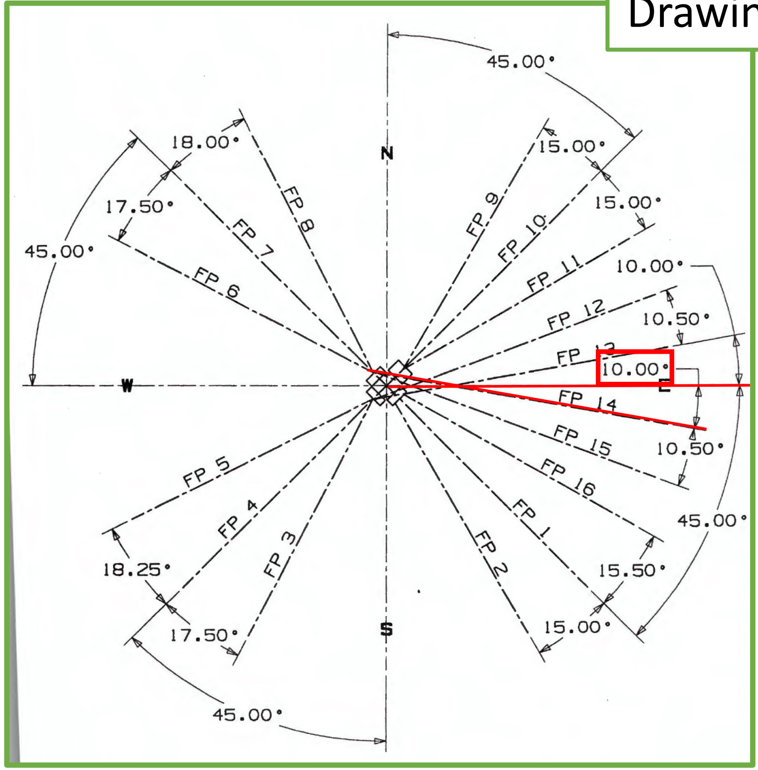
In the case of MARK-IV, due to its design, the accurate position of FOV matters due to part of FOV on water, another part on W target having harder nFlux

MCNP “as-designed” geometry model

Estimates intersection of FP14 axis with upper-tier target ~53.5mm off the

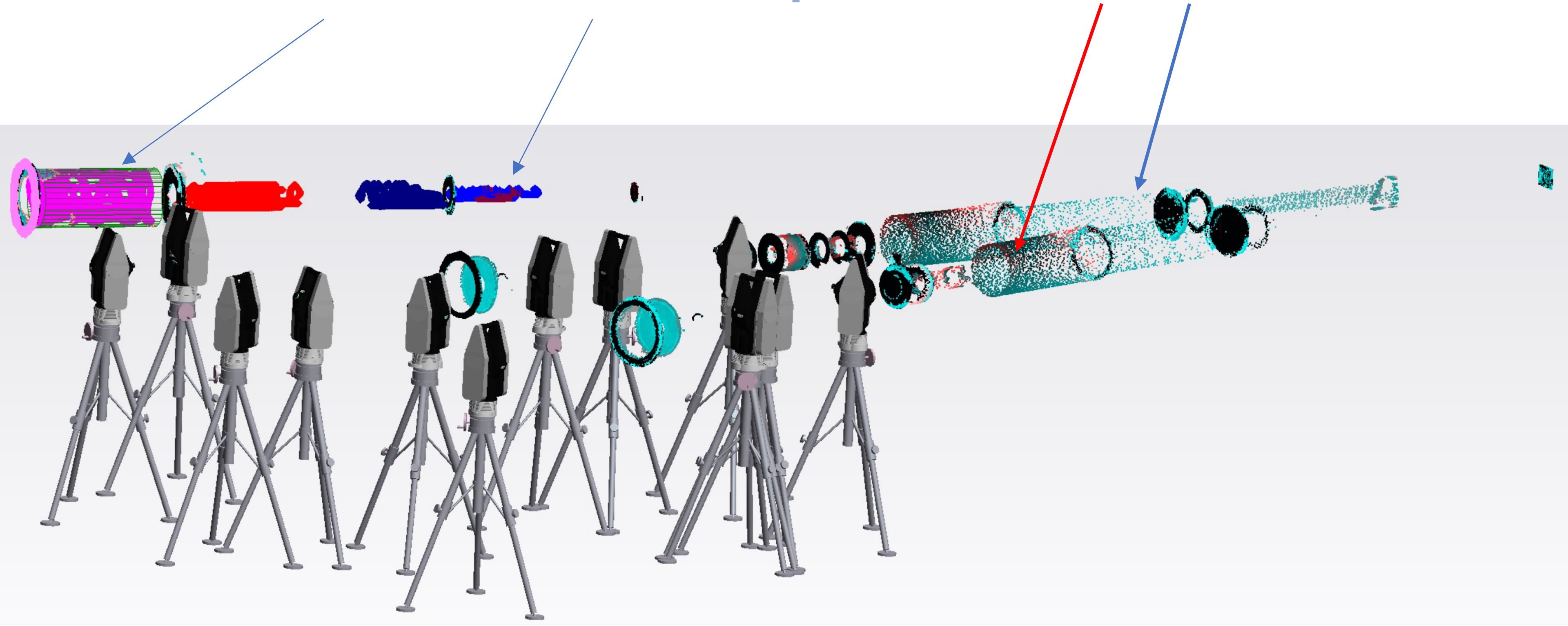


Drawing 1996



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

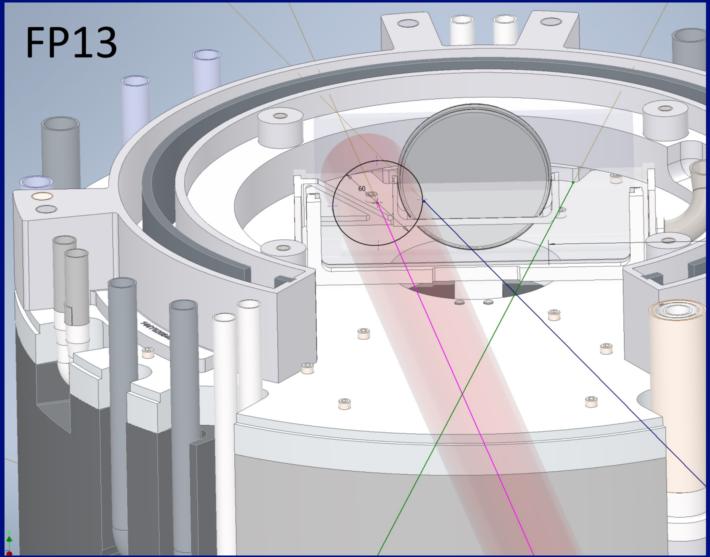
FP14 bore, collimator1 and ports of FP12&13 LTS scan

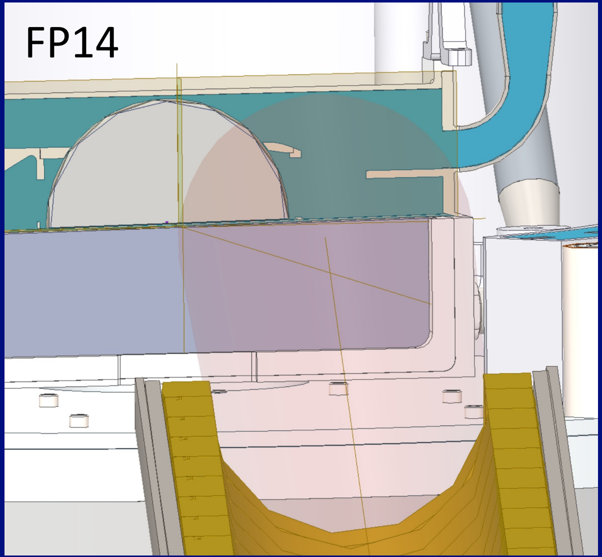


FOV for FP13 (DICER) & FP14 (DANCE) based on LTS

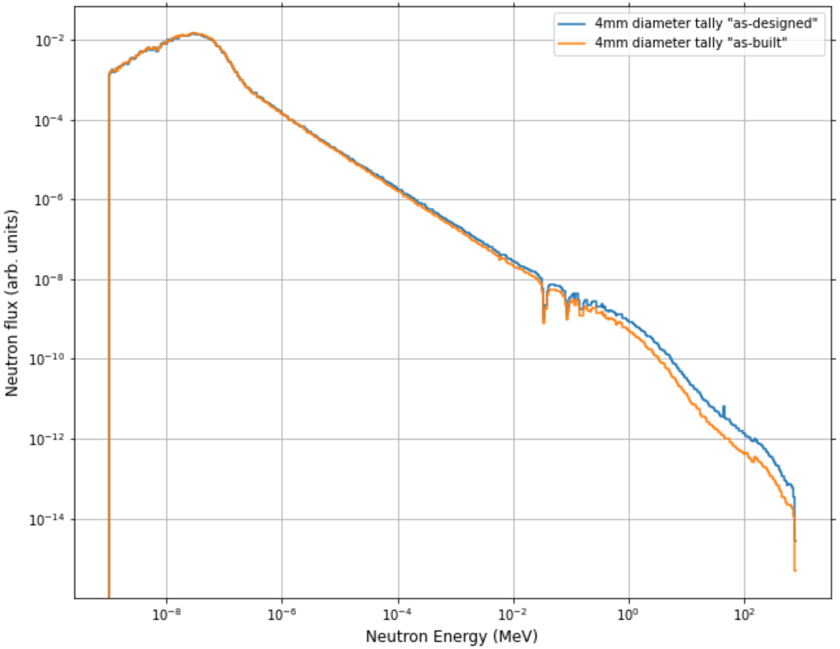
FOV=Field-Of-View for Flight Paths (FP); LTS=Laser Tracker Survey

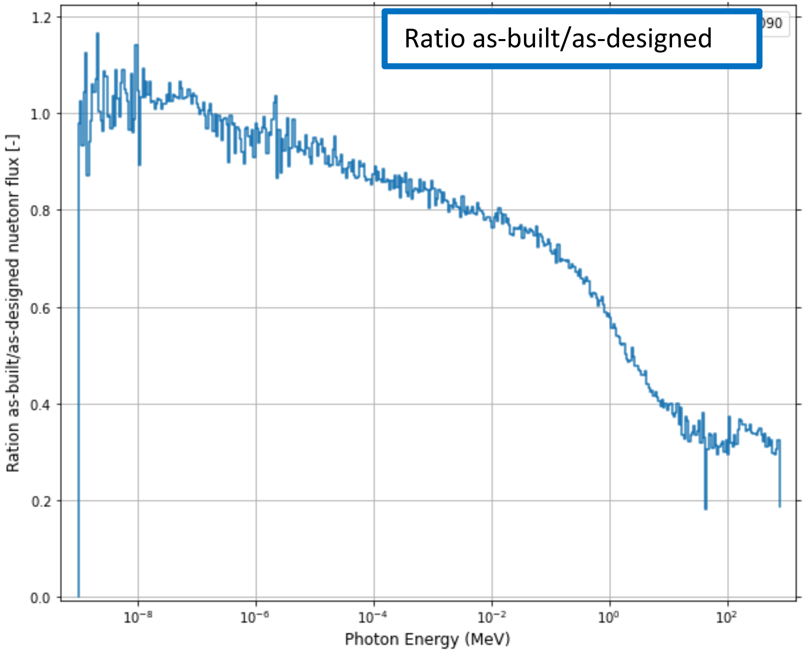
- DICER is not sensitive to non-uniform beam spot, so its absolute FOV position does not affect results of sample irradiation greatly (problem seems to be in greater background)
- DANCE instrument requires neutron beam spot uniformity in full energy range for experimental studies of samples having disc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





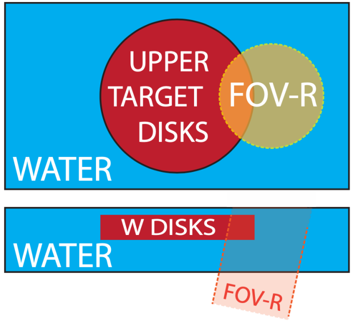
Is a high fidelity geometry important for our MCNP





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

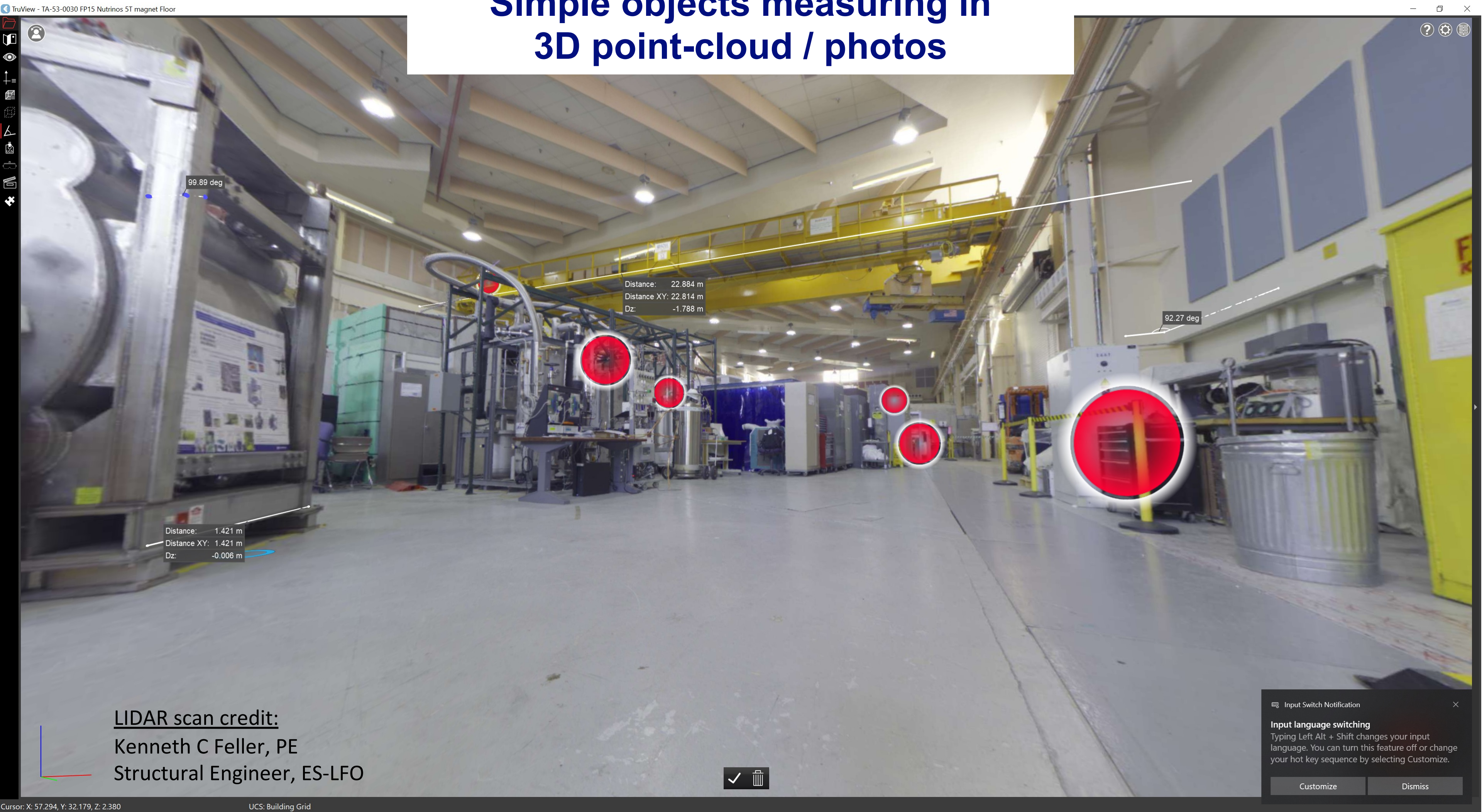
Enhancing MCNP Geometry Fidelity:
Current Progress at LANSE

MCNP simulation:
High level of confidence
Low time-cost of geometry updates

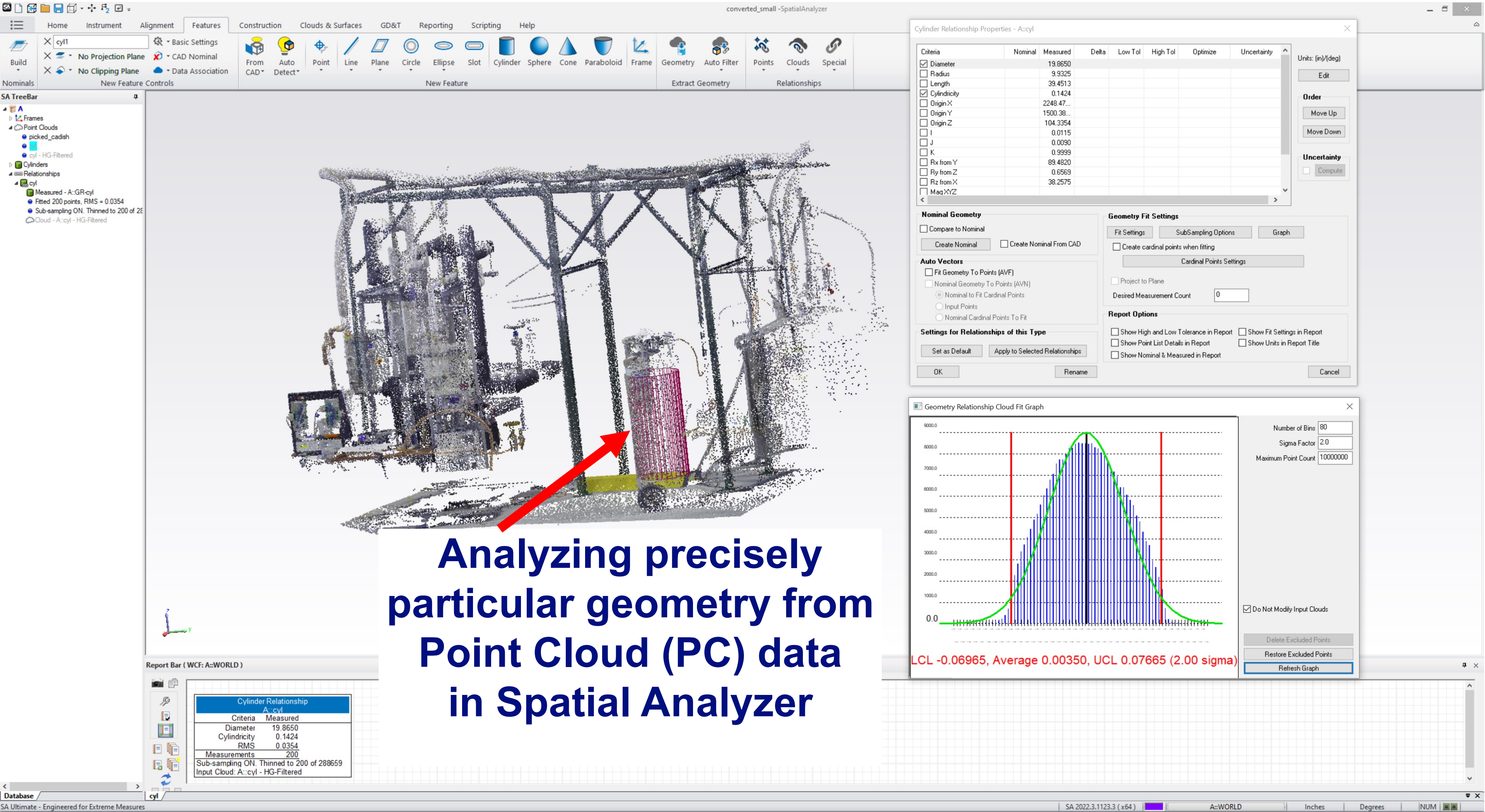
- 3D LIDAR scan with high quality panorama photos
  - (allows measure geometry of experimental hall from the office)
- LTS connected with LIDAR for detailed CAD modeling
- Conversion of 3D scan into CAD
- CAD-MCNP geometry conversion by using Unstructured Mesh (UM)
- MCNP63 simulation {TurbOS benchmarking}
- Design changes involved? -> mesh redesigned part and run MCNP again

❖ If optimization (future plan):
  - Currently studying 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

Simple objects measuring in 3D point-cloud / photos



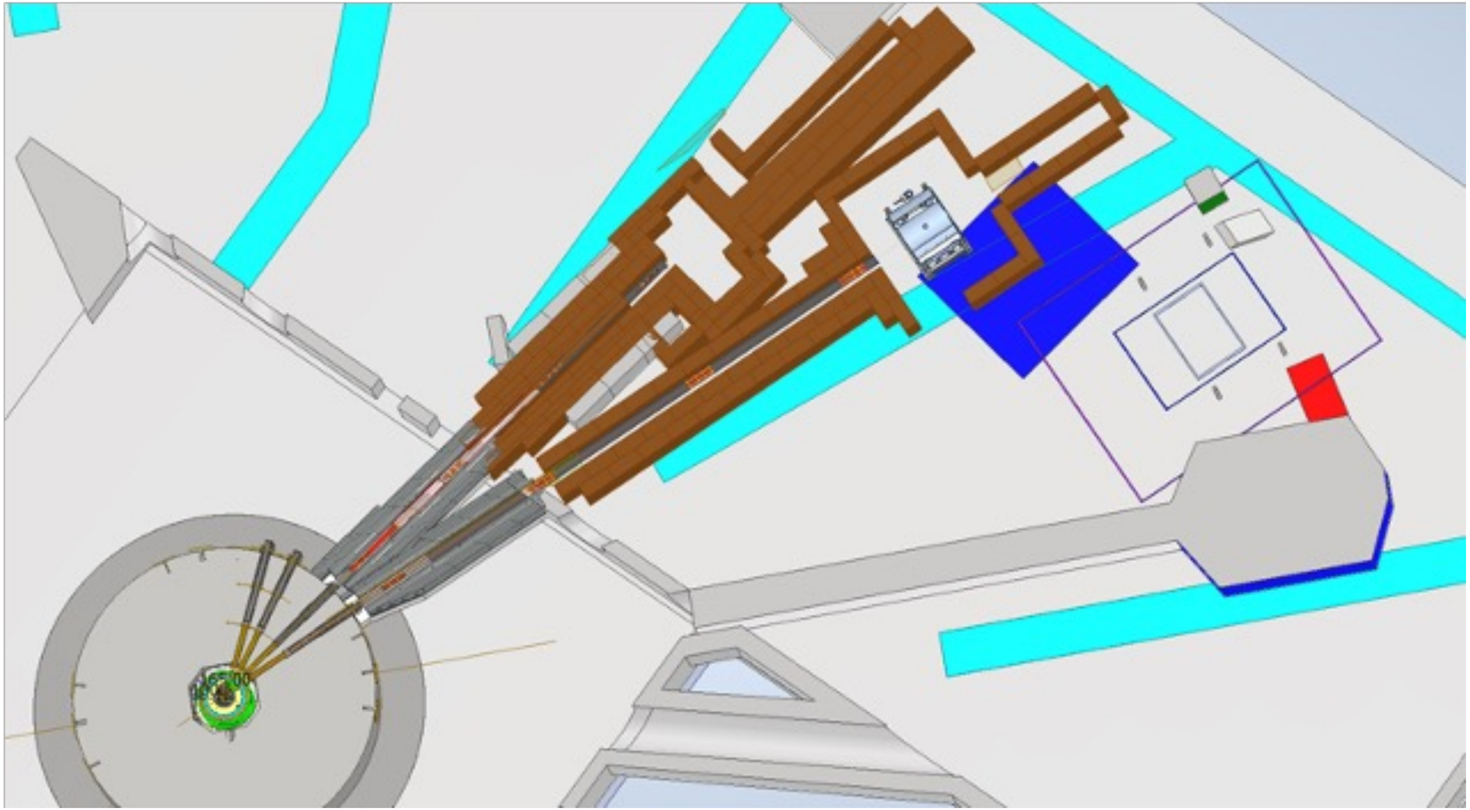
LIDAR scan credit:
Kenneth C Feller, PE
Structural Engineer, ES-LFO



Analyzing precisely particular geometry from Point Cloud (PC) data in Spatial Analyzer
converted_small - SpatialAnalyzer
Cylinder Relationship Properties - A::cyl
Geometry Relationship Cloud Fit Graph
LCL -0.06965, Average 0.00350, UCL 0.07665 (2.00 sigma)
Cylinder Relationship
A::cyl
Criteria Measured
Diameter 19.8650
Cylindricity 0.1424
RMS 0.0354
Measurements 200
Sub-sampling ON. Thinned to 200 of 288659
Input Cloud: A::cyl - HG-Filtered
SA Ultimate - Engineered for Extreme Measures

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

+ simple editing, new part may be quickly designed or the old one remodeled/removed



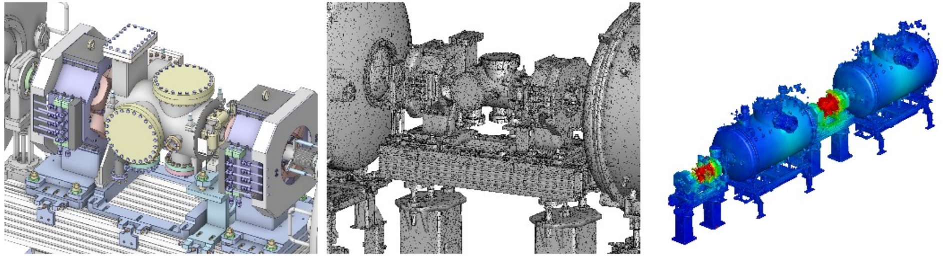
LIDAR+LTS -> CAD -> MCNP UM geometry -> Optimization?

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

Silver Fir SOFTWARE

& Hoonify – HPC (benchmarking)

https://www.silverfirsoftware.com



European Spallation Source: Courtesy of Elena Donegani

hoonify

ALWAYS ACCESSIBLE

ON-PREMISES

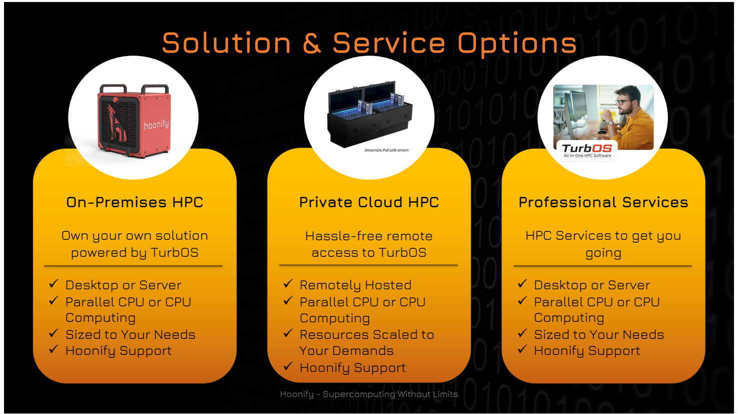
PRIVATE CLOUD

MCNP6 FLUKA

Ask us about more software...

www.hoonify.com

info@hoonify.com



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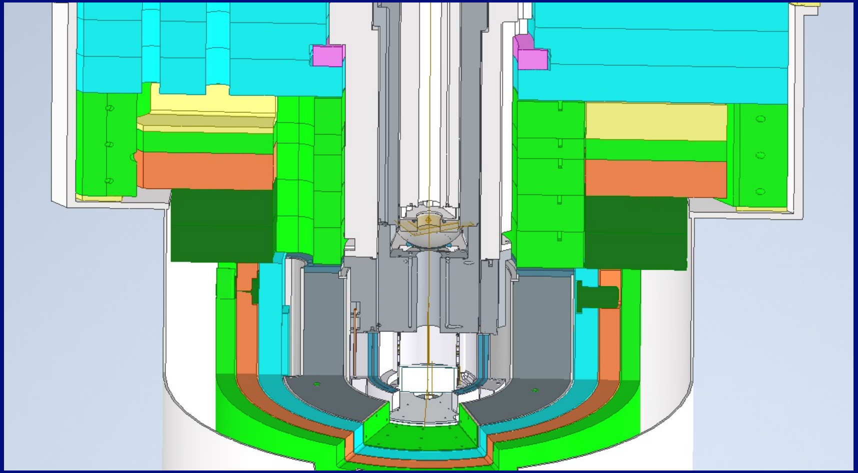
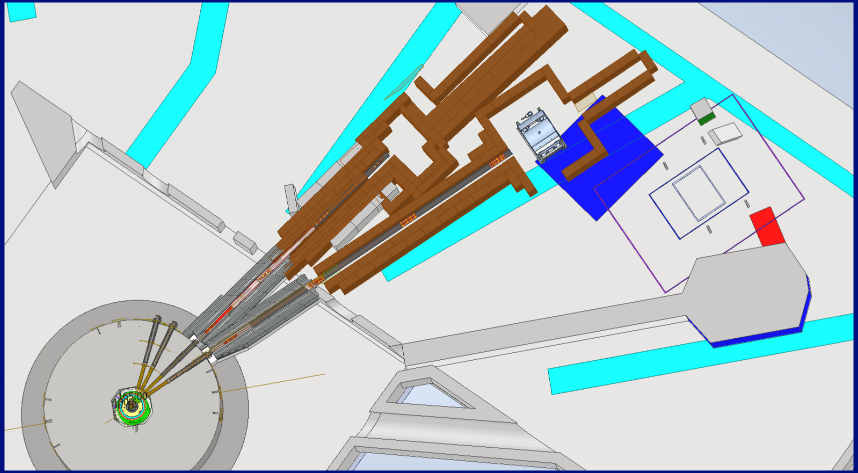
Large and complex CAD model

~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

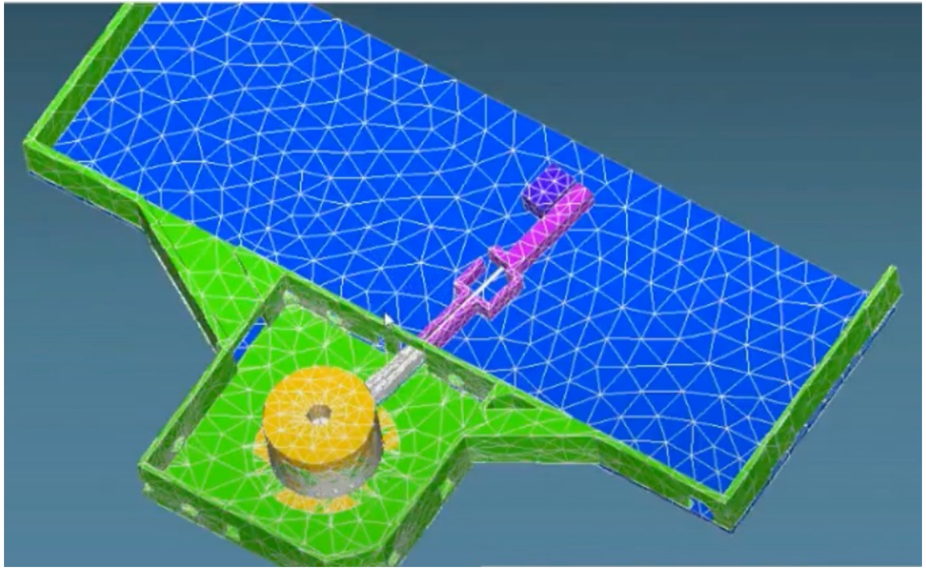
- CSG is mostly based on original drawings with some updates from 3D CAD models
- UM Increasing fidelity by using ”as-designed” CAD and “as-built” data from LTS

Attila4MC - creating UM for large and complex model

How good mesh we have? What is a GOOD?

- From CAD model (SpaceClaim)

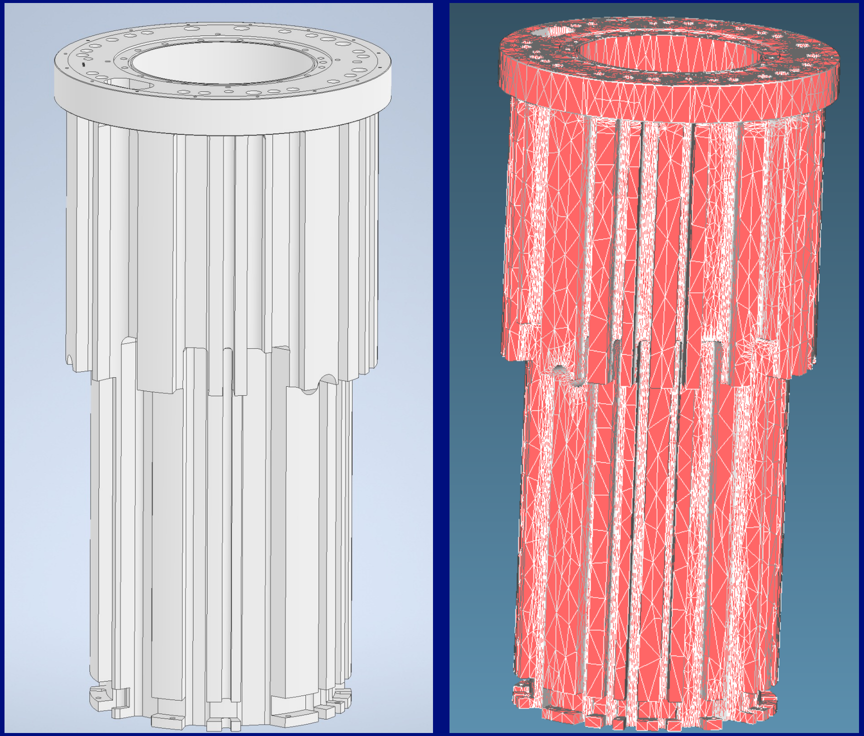
- To UM in Attila4MC



Credit: Attila4MC, Dusan Kral (P-3), Chris Fairbank (P-2) [LANSCE]

Part-by-part Mesher (PBP)

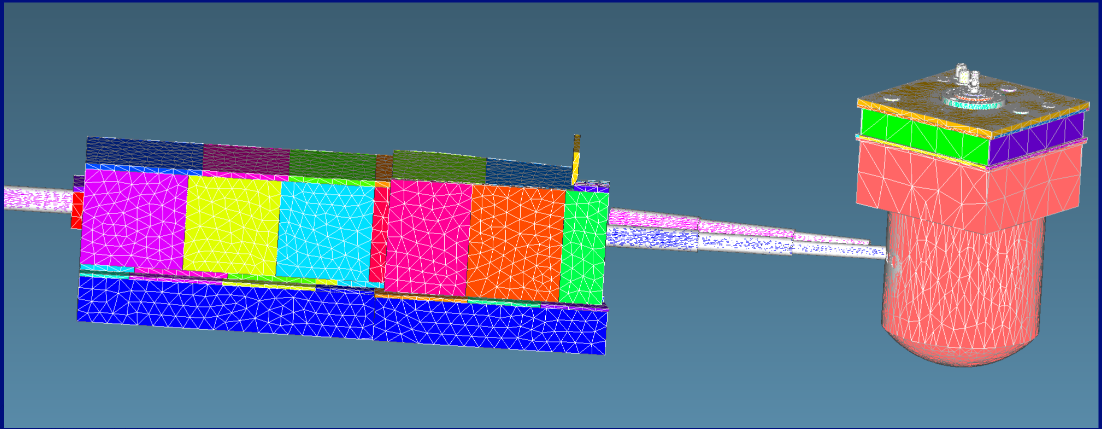
- Silver Fir's stand-alone package for discontiguous mesh preparation
- Tested beta version running in Linux
- Just released Attila 10.3 coming with PBP implemented in GUI
- Supports parallel processing (SMP) => assembly with more parts
- Parasolid input from CAD software (we used Autodesk Inventor)
- Variety of settings – cell volume, curvature, global/specific part settings, volume cutoff,…
- Output goes to Attila4MC (now implemented)

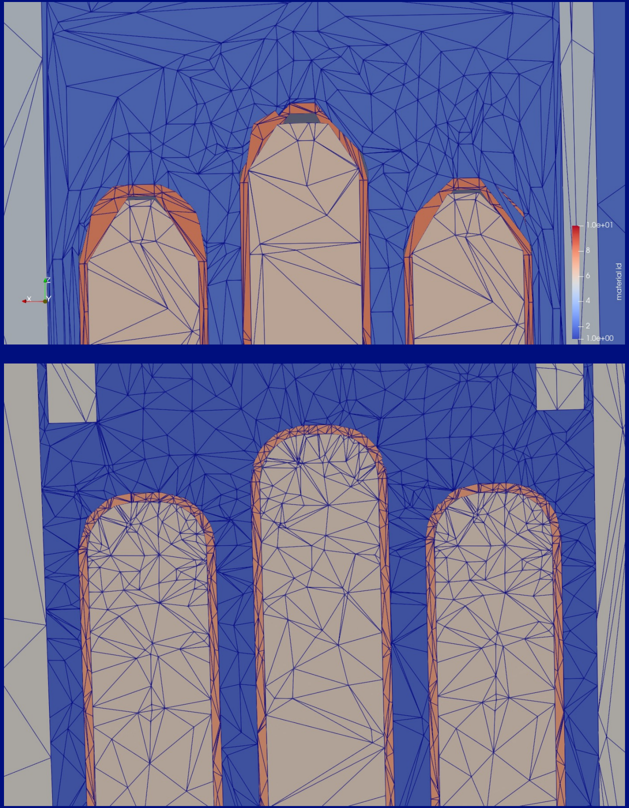


(a) CAD model, (b) PBP mesh

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 million cells
(allows rotations and translation)

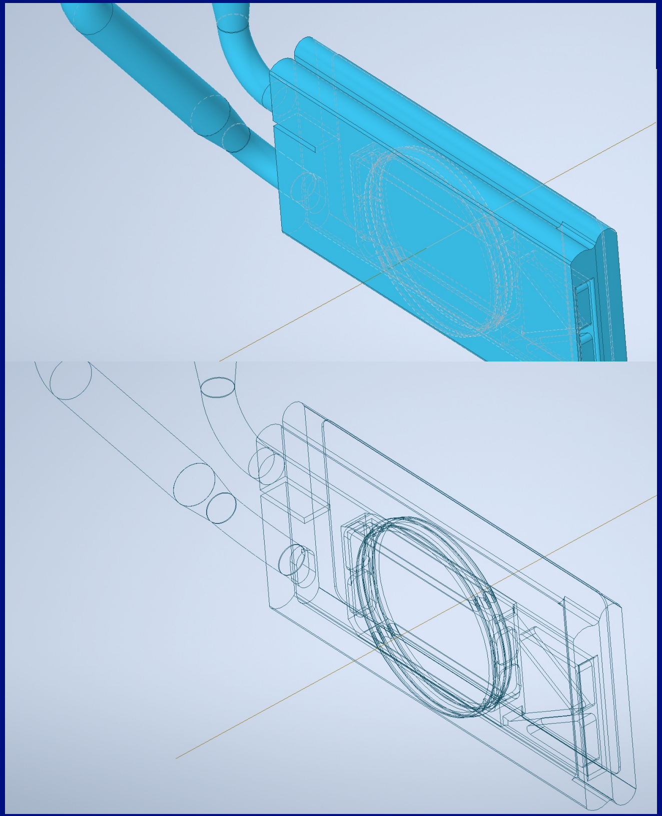




A comparison of a curvature quality for Mark 4 Upper Target mesh – different settings

Preparation for Unstructured Mesh (UM) I.

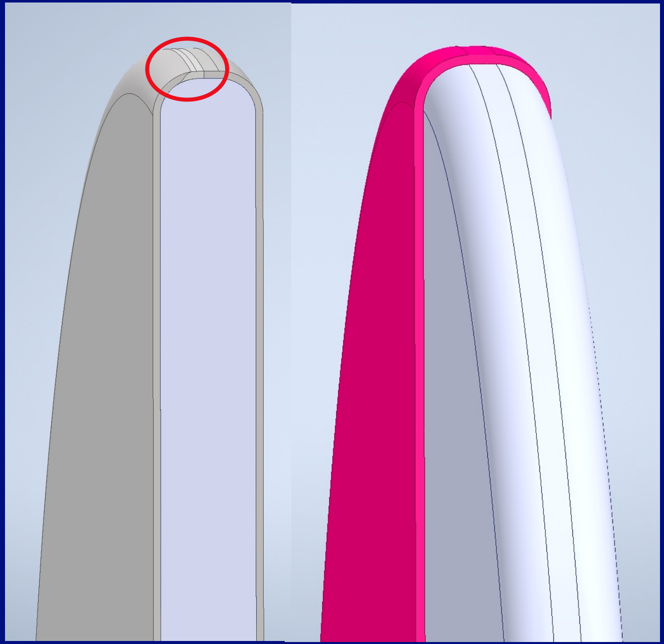
- We have set a limit for mesh size to ~5mil cells
- Real facility contents liquids, gases, thin layers from neutronics specific materials → model adjustments:
  - Create parts which represent liquids (water with different temperatures, liquid hydrogen, etc) (filling cavities)
  - Find the larger geometry 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



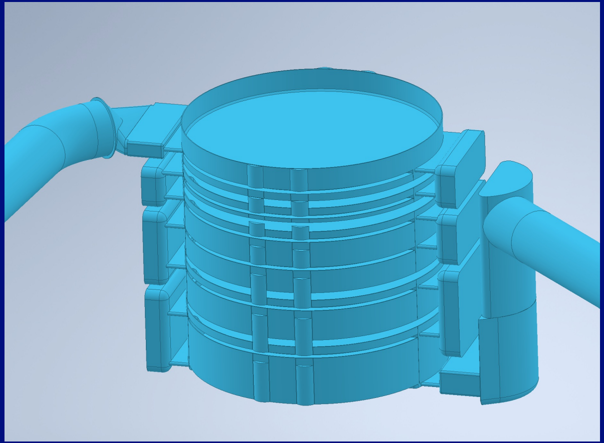
Example of Upper Target cooling water and moderator with detailed view in an inner structure

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)

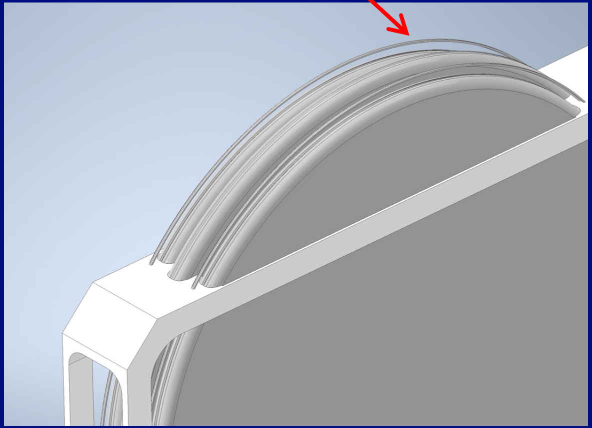


Water filler with thin volumes

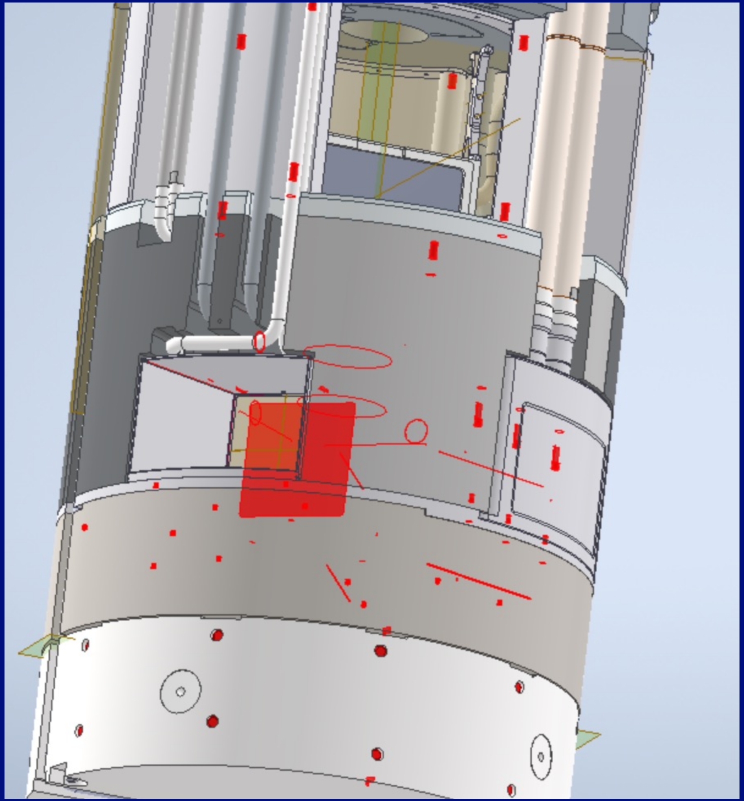
Fillers =
filled cavities

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.

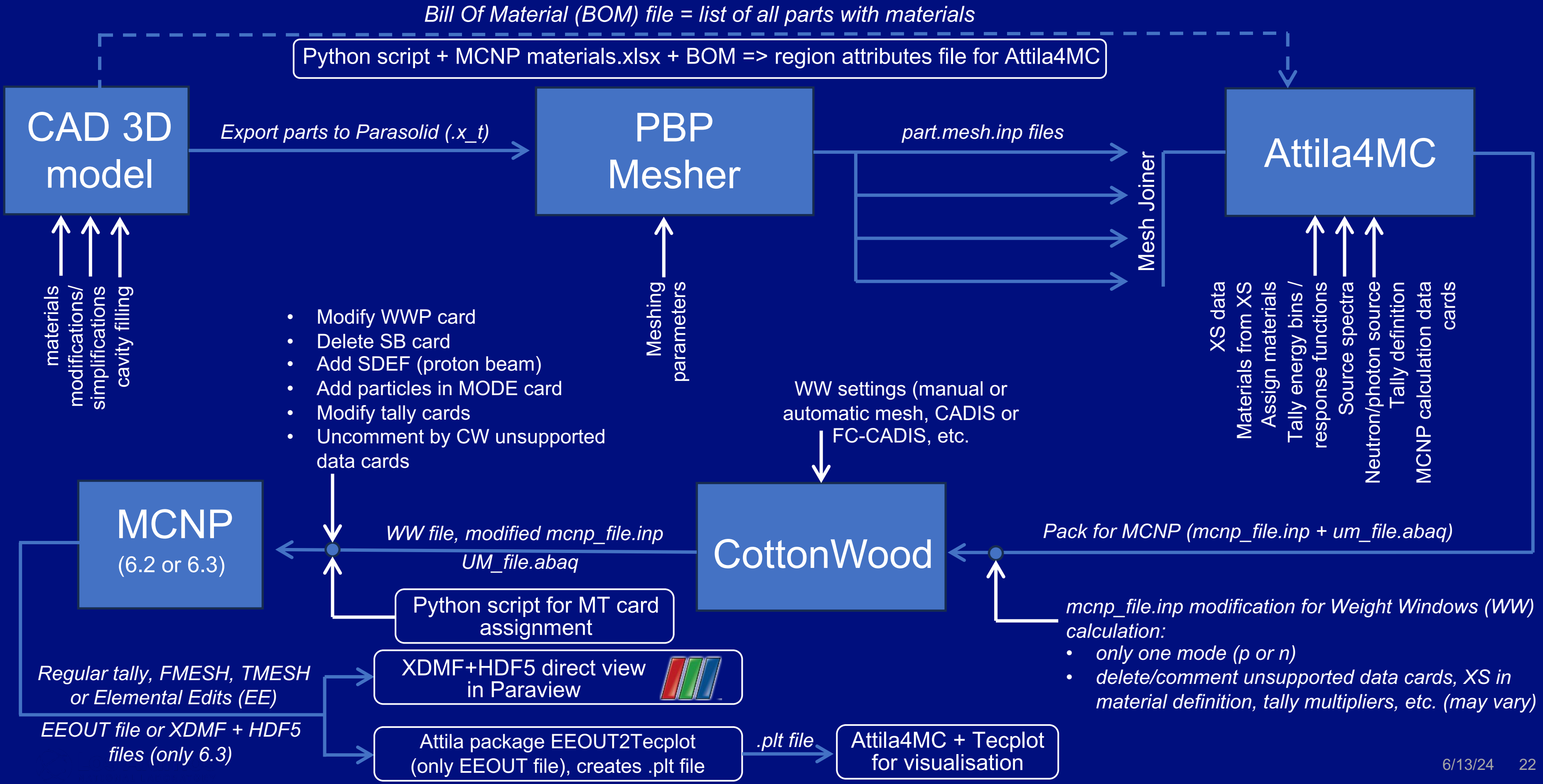


Incorrect design of previous Tantalum cladding



Findings of an inspection tool in Autodesk Inventor

UM calculation workflow



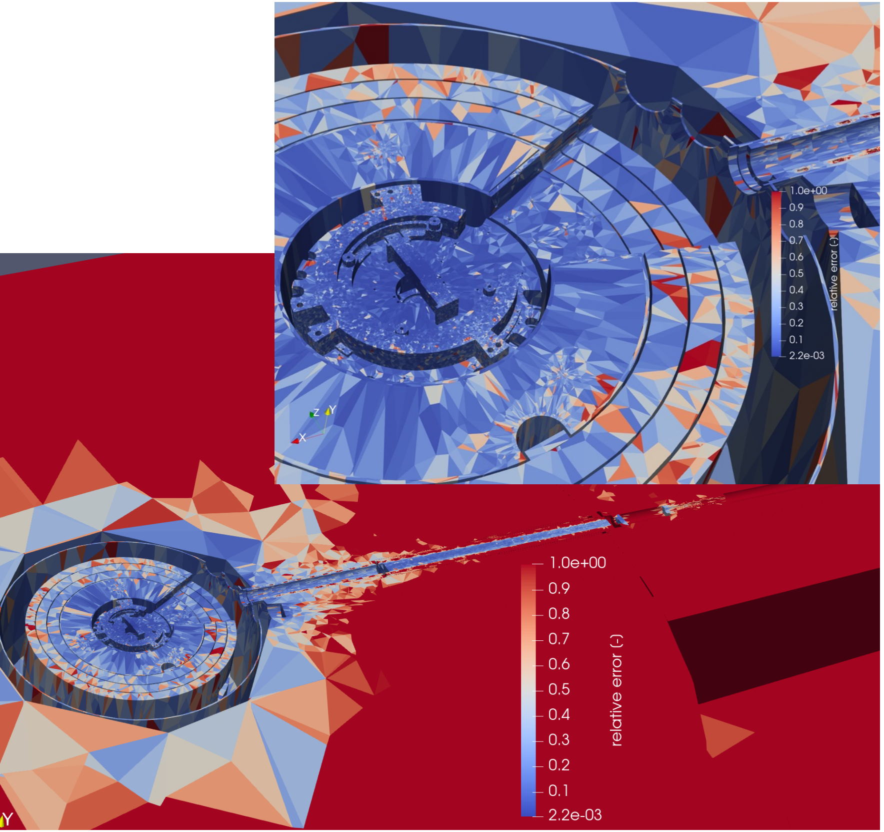
MCNP simulation with UM geometry

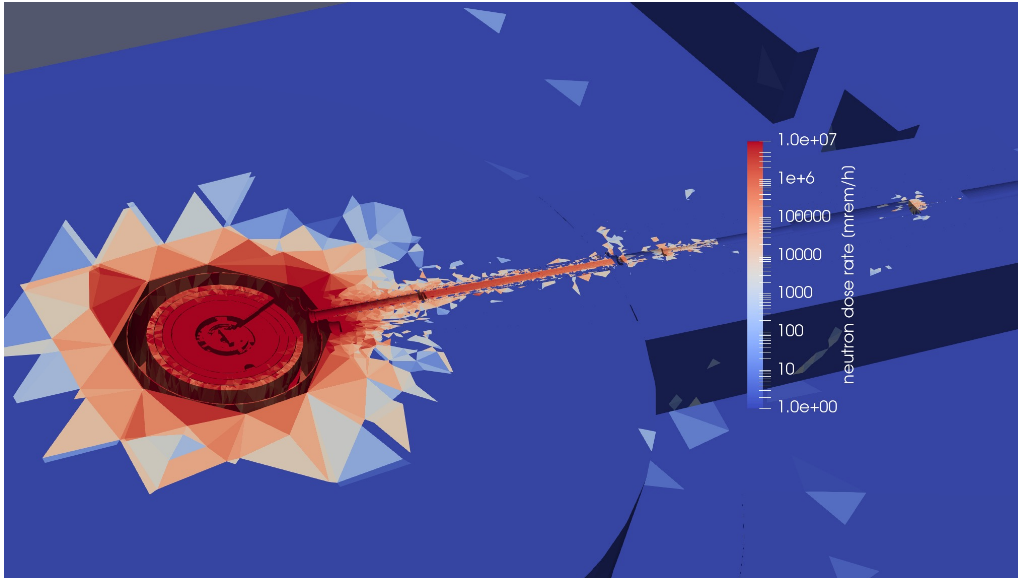
- Only MCNP6.2 and MCNP6.3 supports UM mesh
- Optional step: rtt_mesh_editor is Attila's independent module for Abaqus mesh modifications – used to increase distances between nodes to reduce overlap problems
- Many hours spent with troubleshooting (calculation stalled without raising error while cores are still loaded, crashing with charged particles, etc.)
- Currently we have "so so" stable type of simulation in some cases we have to use a Bash script with CONTINUE run to control good behavior or run
- A huge difference between 6.2 and 6.3 found (comparing the same model on 6-cores laptop 6.2/6.3)
  - Abaqus mesh processing time before particle transport start is significant longer in 6.2 (40min/0.3min)
  - Memory consumption: 6.2 needs almost 5× more memory per one core than 6.3 (10BG/2GB)
  - 6.3 offers HDF5 format which decrease time needed for dump write significantly (10min/~s)
- Very positive improvement with last MCNP version (thank you developers!)

Proton - Spallation based UM MCNP63 simulation

HPC Hoonify 256 cores; ~5M cells; 1e8 ~4days; ~110 stall; WW applied to delivered neutrons to

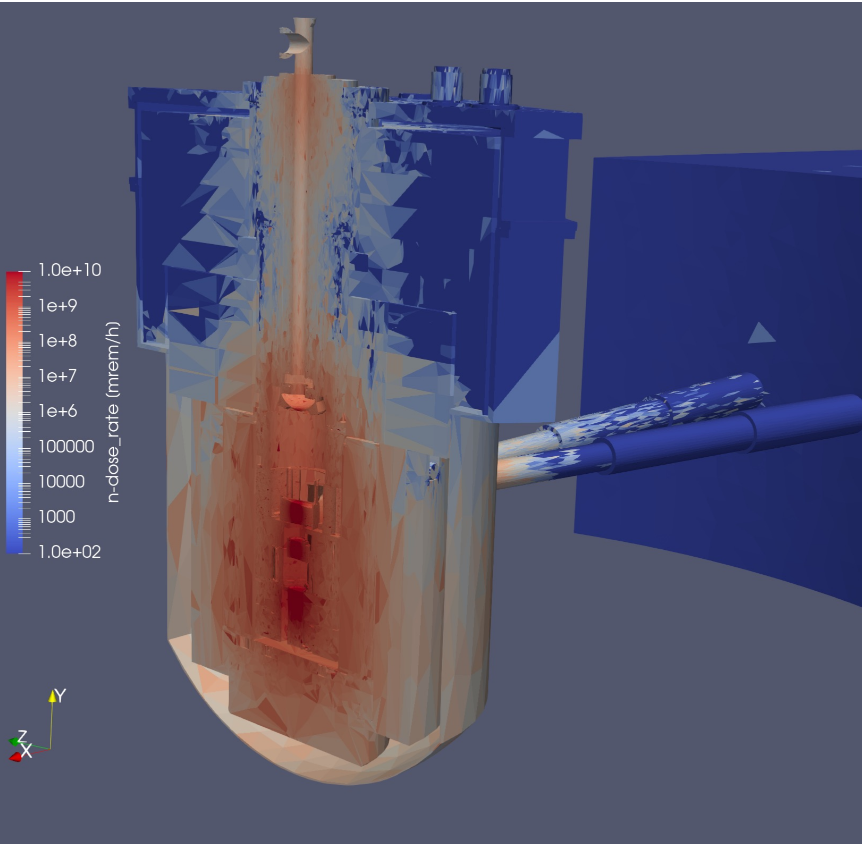
800 MeV proton –> tungsten, spallation, WW, Elemental Edit

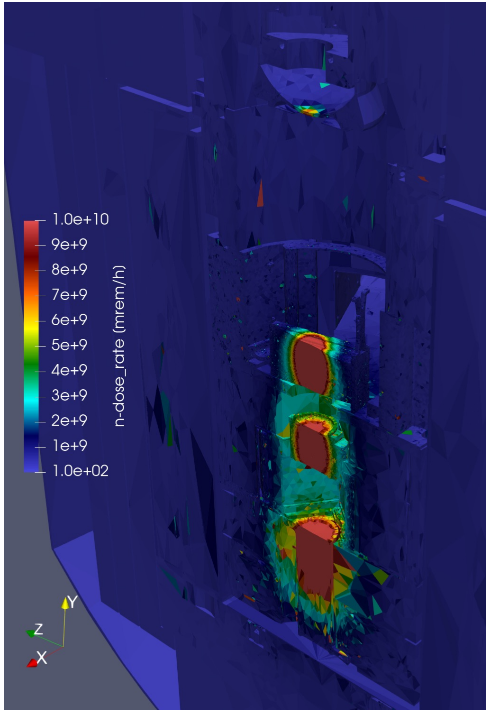


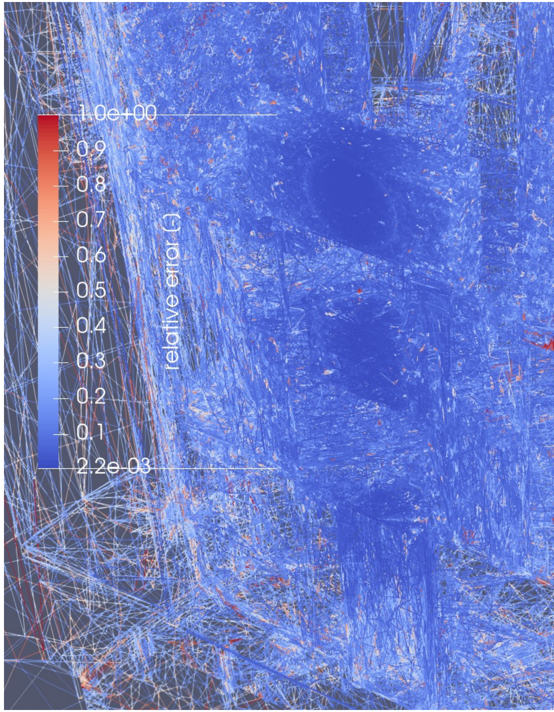


Proton - Spallation based UM simulation (MCNP63)

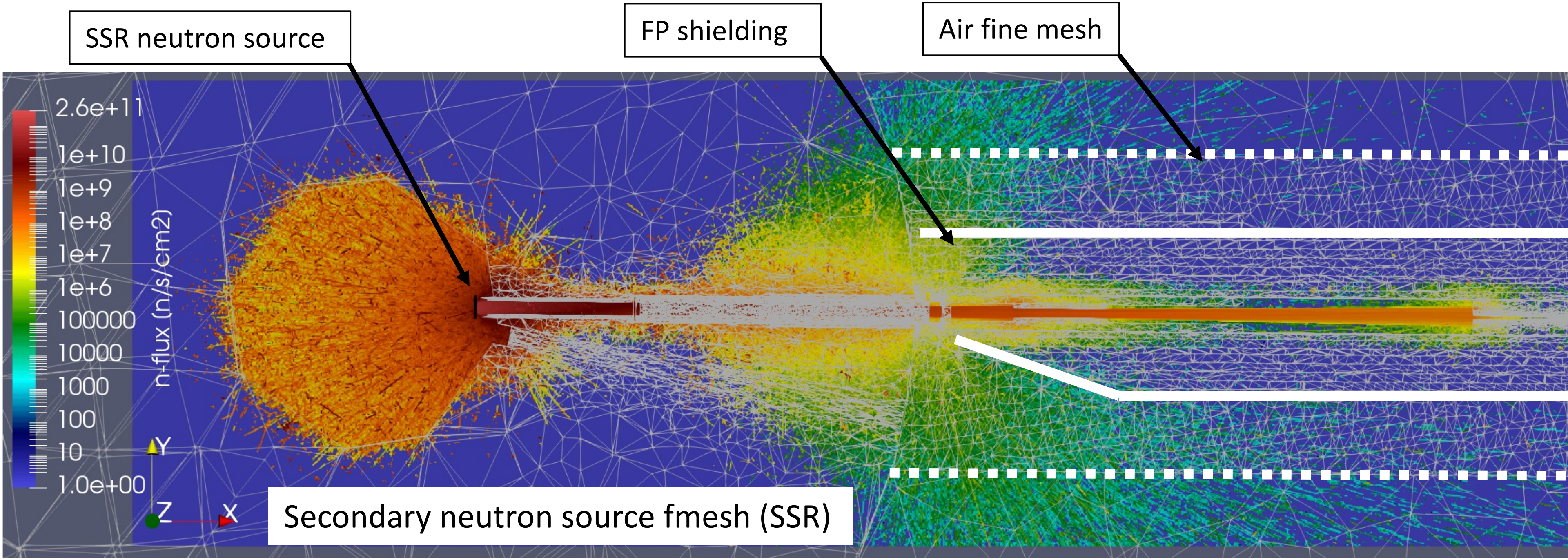
4 nodes Hoonify HPC 256 cores; ~5M cells; 1e8 ~4days; ~110 stall; WW usage; {neutron dose rate}



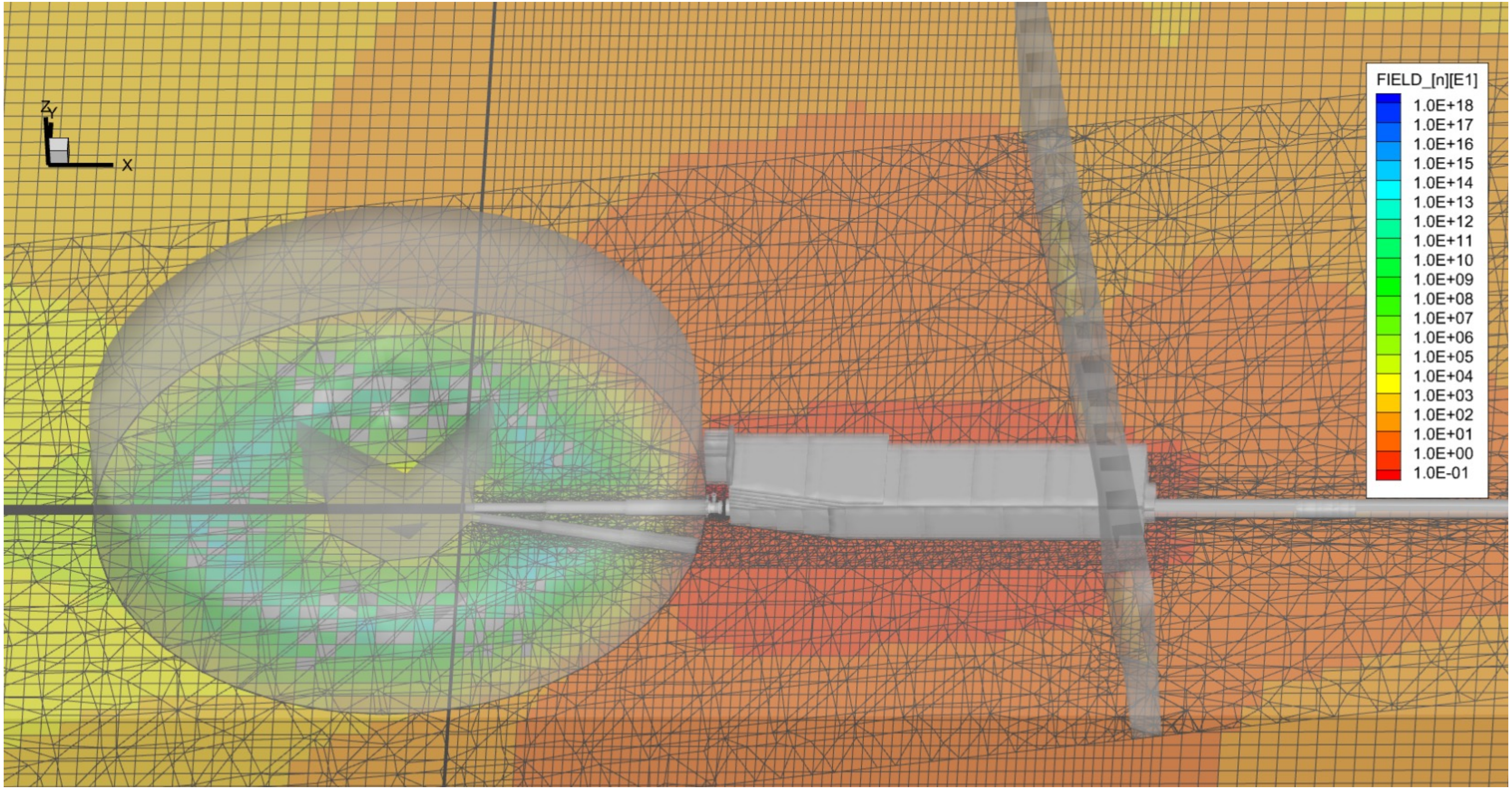




2. Step - Calculation of Surface Source File (SSW) and its reading SSR
- we have removed target for secondary n-source simulation: UM from 5mil to 1mil cells

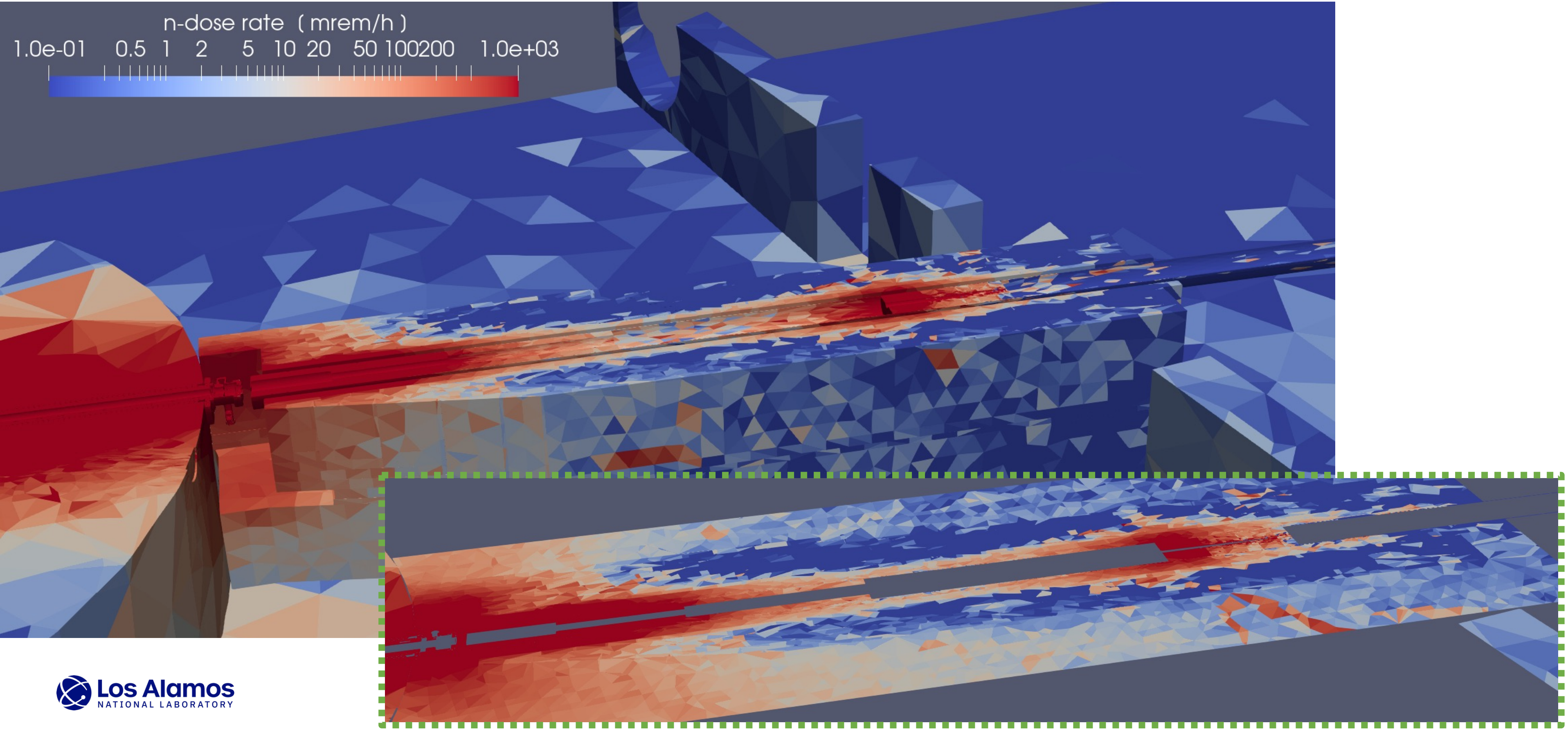


SSR source + Weight Windows applied from CW



Neutron dose rate with secondary neutron source (SSR)

3e7 histories, 7.5h @5cores; HPC experiences very slow run (in discussion with developers)



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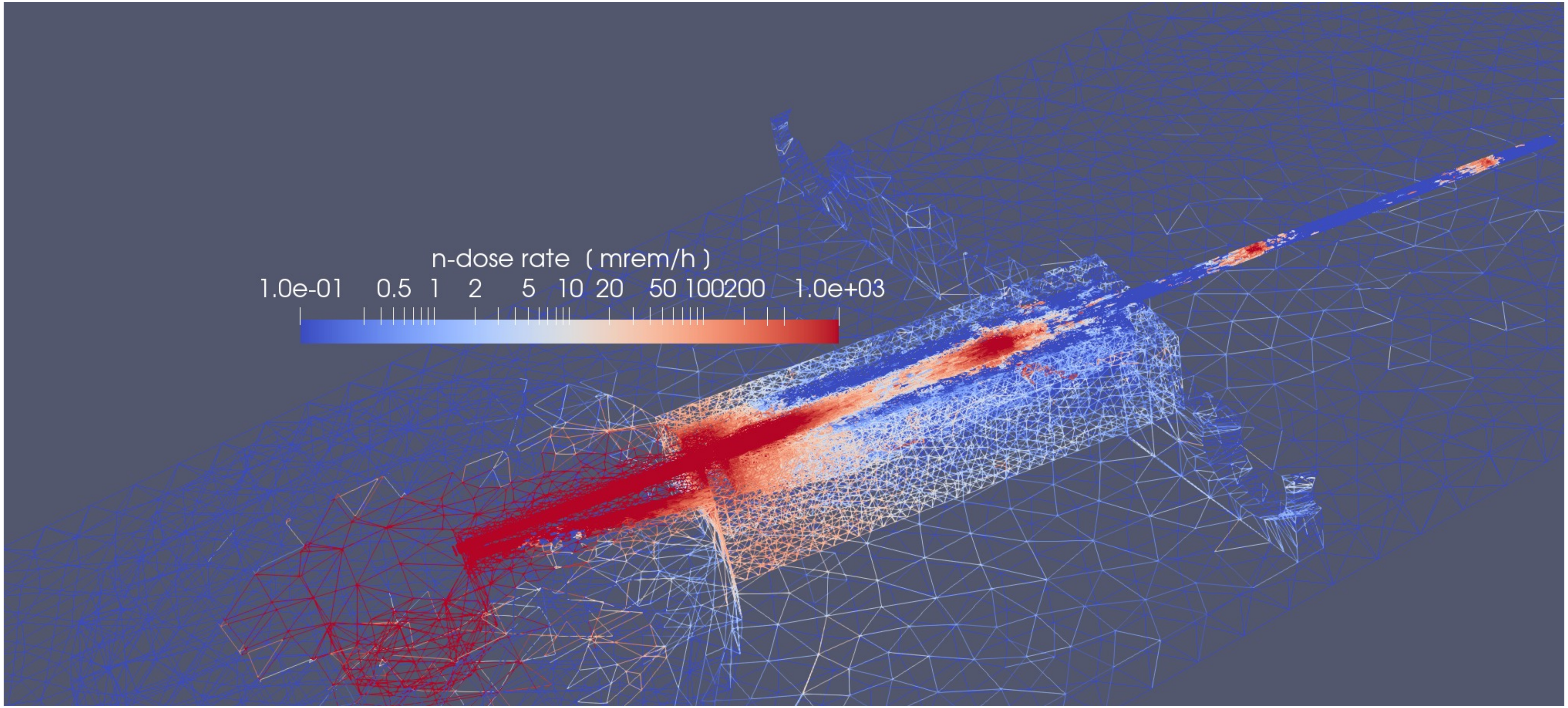
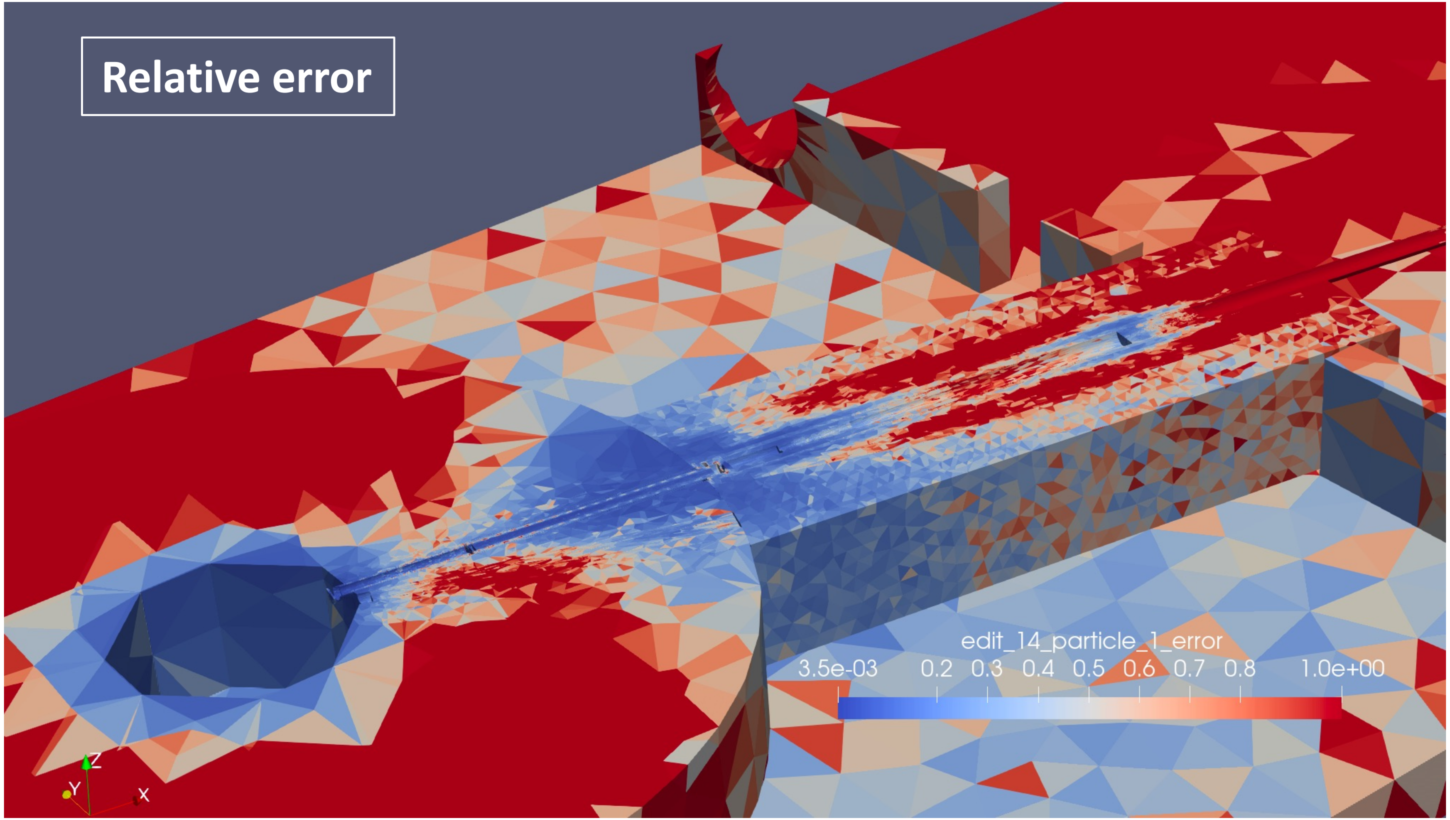
Various visualization options in Paraview

Option to turn on/off individual parts (without main air)



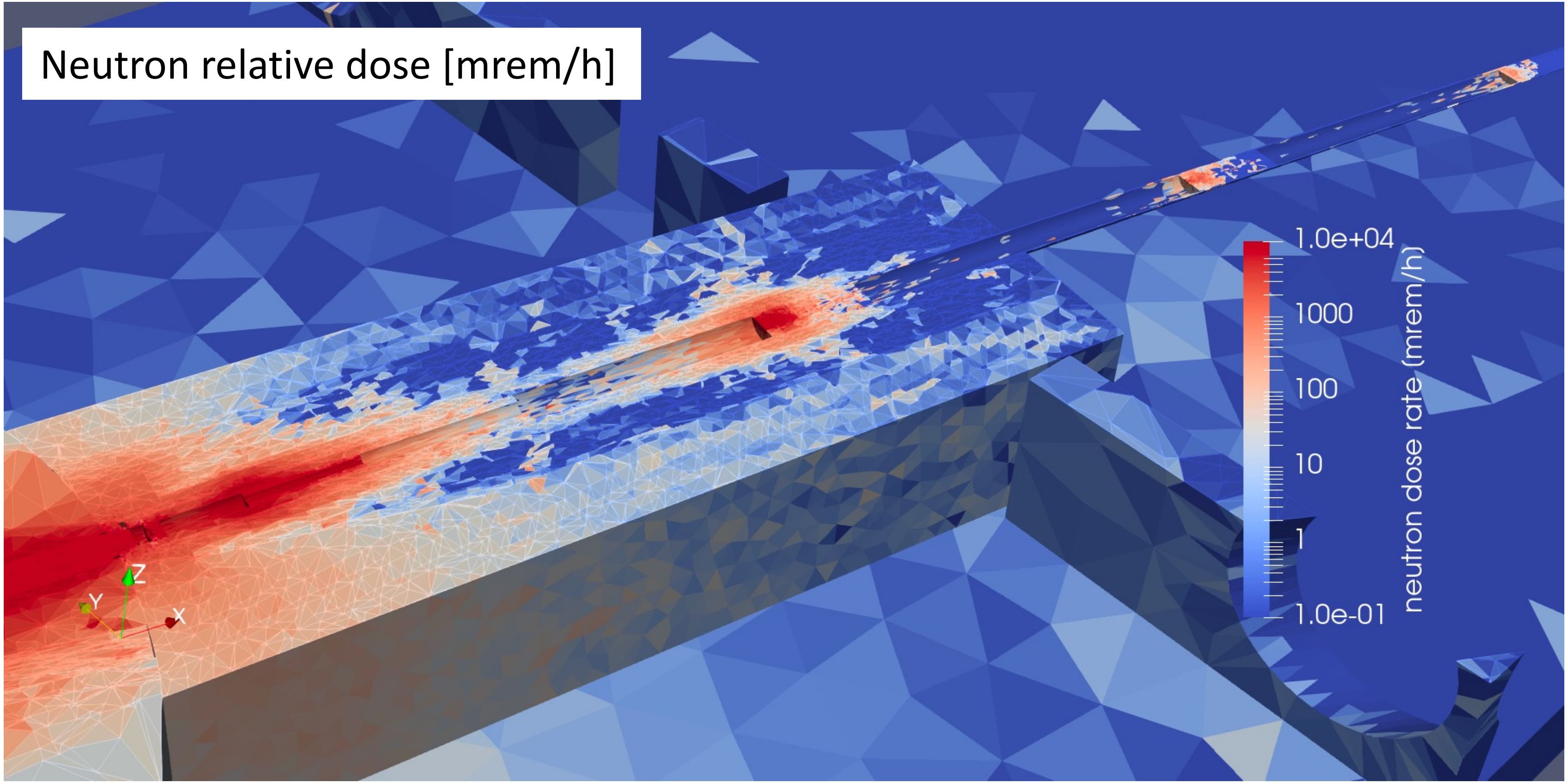
Neutron dose rate with secondary neutron source (SDEF)

Laptop ~2.5x faster than SSR



Neutron dose rate with secondary neutron source (sdef)

Laptop ~2.5x faster than SSR



Summary

- It is feasible to use of UM in big & complex; currently updating our ~4000 core cluster to Hoonify TurbOS+mcnp63
- Studying the reason of calculation stall for primary source particles (protons)
  - Tiny overlaps of PBP meshes were partly cured by RTT_mesh_editor to increase space between nodes, [Attila developers discussion]
  - Bash script used for killing MCNP if dump time>2x avg, SEED-2, continue run
- MCNP6.2 uses about 5x more RAM per core for 5M cells than MCNP6.3 (old clusters)
- Large EEOUT file storage ~10min vs ~s for HDF5file
- SSR usage for UM - seen weird behavior of accessing to file on clusters as CTM so its normalization (if NPS SSR<NPS UM calculation)
- Meshing of a complex geometry by PBP is fast, however, careful with meshing setup (backward control of skipped volumes)
- SSR vs SDEF (non-uniform source is averaged; 2.5x faster)

Thank you for your attention.

Josef Svoboda & Dusan Kral

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