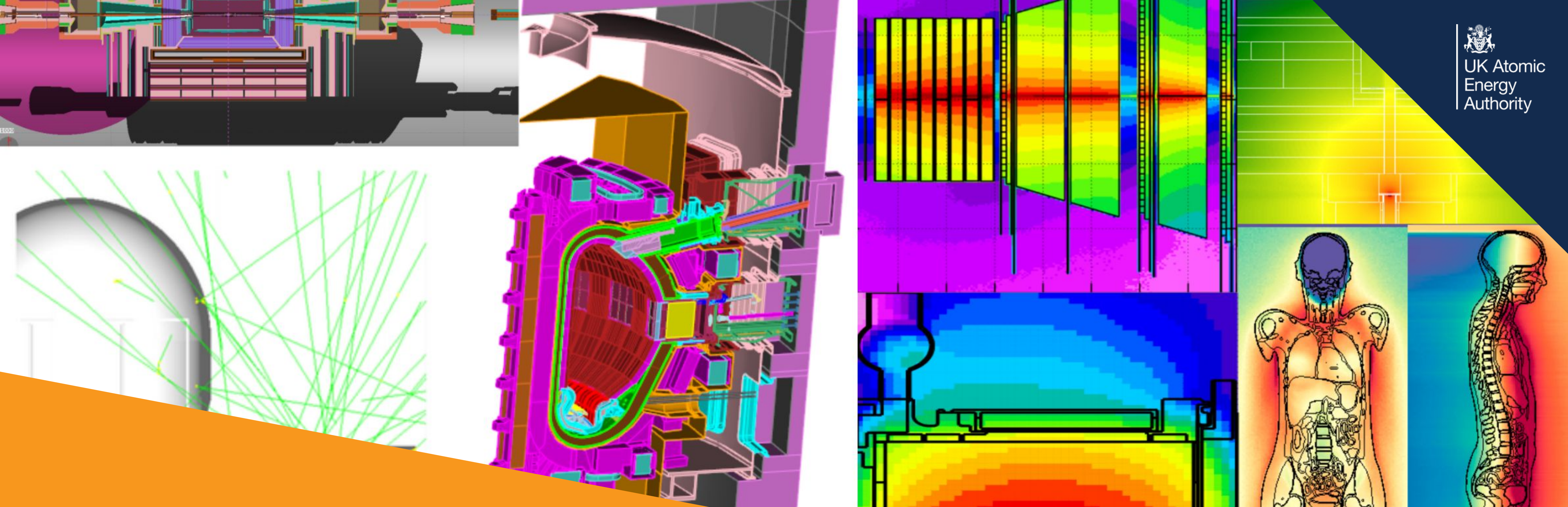

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Andrew Davis

CAD Based Radiation Transport: DAGMC Toolkit

Culham Centre for Fusion Energy

European Commission

Energy

Contract for the Operation of the JET Facilities Co-Funded by Euratom
This work was funded by the RCUK Energy Programme [Grant number EP/P012450/1]

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Contents

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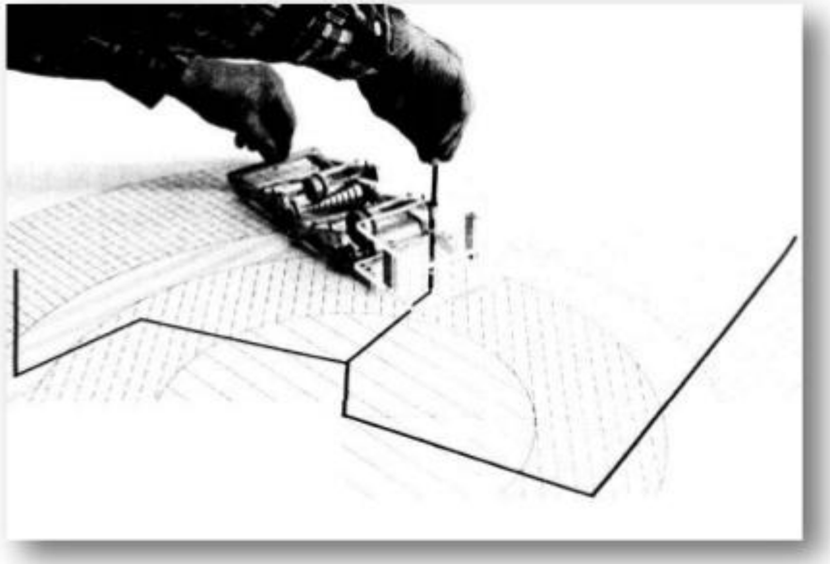
Monte Carlo Analysis

- Monte Carlo analysis was born in the Manhattan Project
- Von Neumann, Metropolis, and Fermi
- We define materials in regions of model, these regions have interaction probabilities, random numbers used to sample
- Traditionally we define regions using combinations of quadratic surfaces united with boolean operations

Let's Apply a Monte Carlo Simulation Tool



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The Monte Carlo trolley, or FERMIAC, was invented by Enrico Fermi and constructed by Percy King. The drums on the trolley were set according to the material being traversed and a random choice between fast and slow neutrons.

Another random digit was used to determine the direction of motion, and a third was selected to give the distance to the next collision. The trolley was then operated by moving it across a two dimensional scale drawing of the nuclear device or reactor assembly being studied.

The trolley drew a path as it rolled, stopping for changes in drum settings whenever a material boundary was crossed. This infant computer was used for about two years to determine, among other things, the change in neutron population with time in numerous types of nuclear systems.

CAD Based Workflows

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- CAD is desirable as a source of geometry for Monte Carlo calculations for several reasons
  - Allows very complex models to be represented (fidelity,accuracy)
  - Produced for manufacturing purposes (provenance)
  - The model usually already exists (you don’t need to make it)
  - User friendly, easier to fix and modify than CSG (effort)
  - Faster analysis turnaround (efficiency)
- CAD model integrity - “cleanliness”
- Several routes for use:
  - Translation - MCAM, McCAD, FastRAD, CATIA-GDML
  - Directly - DAGMC
  - Hybrid - OiNK

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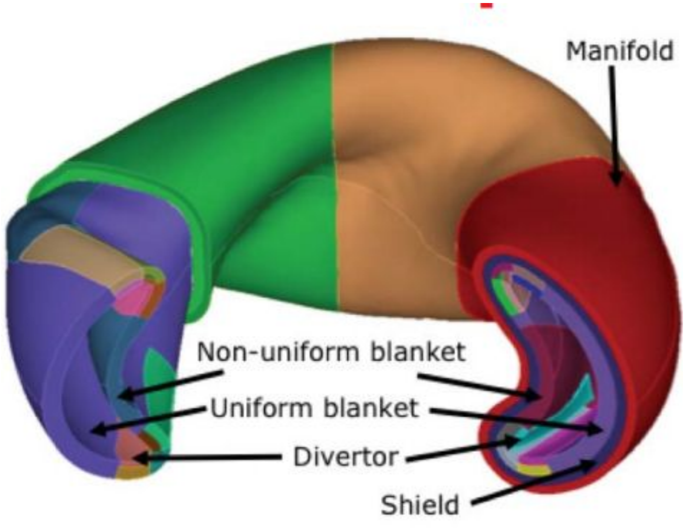
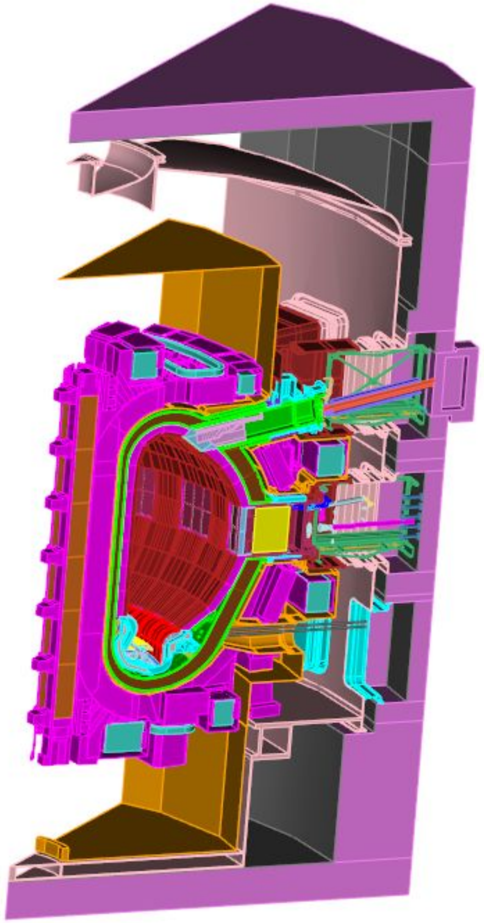
CAD Based Workflows

- Automation (including translation) provides:
  - Reduced human effort
  - Increased quality assurance
  - Direct geometry use provides **richer surface** representation
  - Facilitates coupling to other analysis types through common geon





What is DAGMC?

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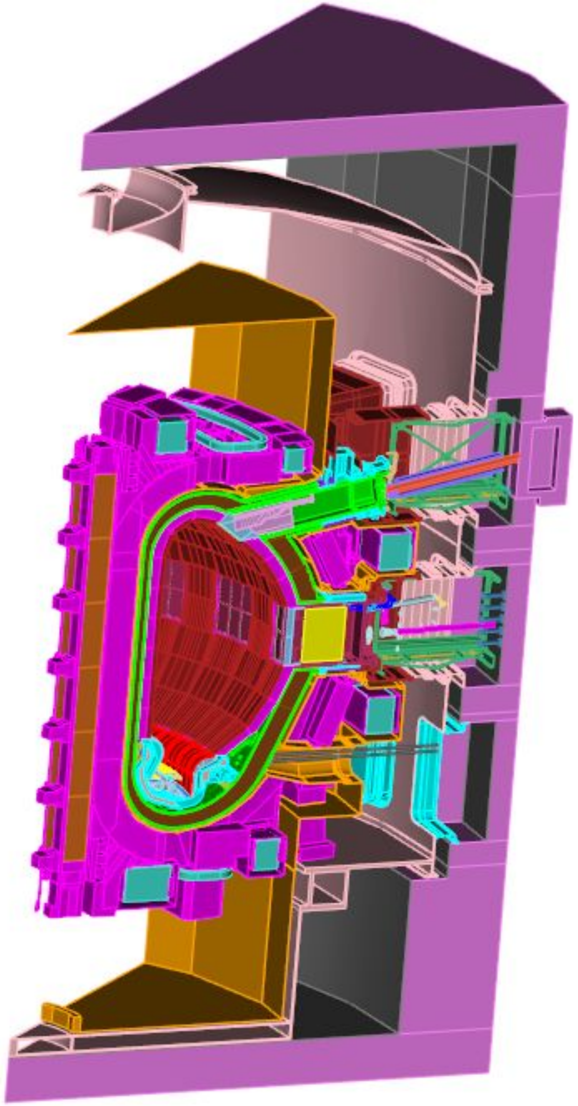
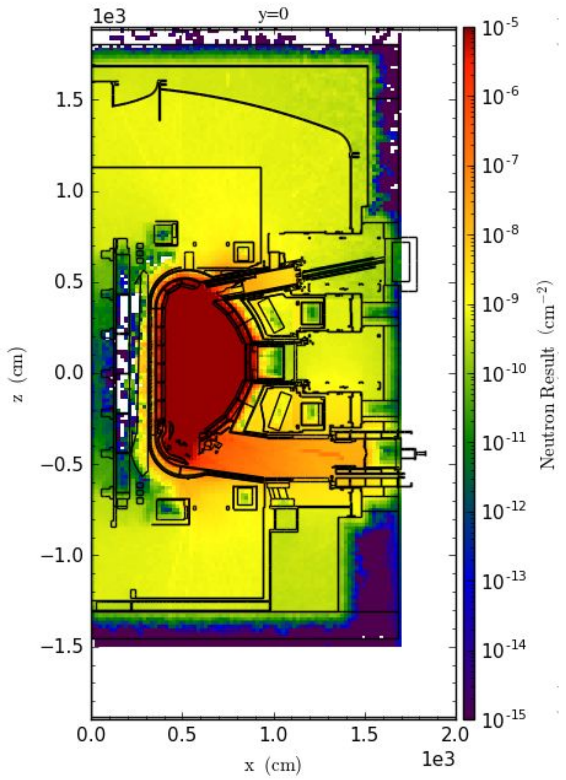
- DAGMC (http://svalinn.github.io/DAGMC) is an open source toolkit that allows a user to transport particles on CAD based geometries
- Developed by the Computational Nuclear Energy Research Group (CNERG - http://cnerg.github.io/) at the University of Wisconsin-Madison (and since I’m at UKAEA now) and UKAEA
- Its purpose is to enable particle transport on very detailed and complex geometries, by having a core geometry library which can be plugged into any Monte Carlo code





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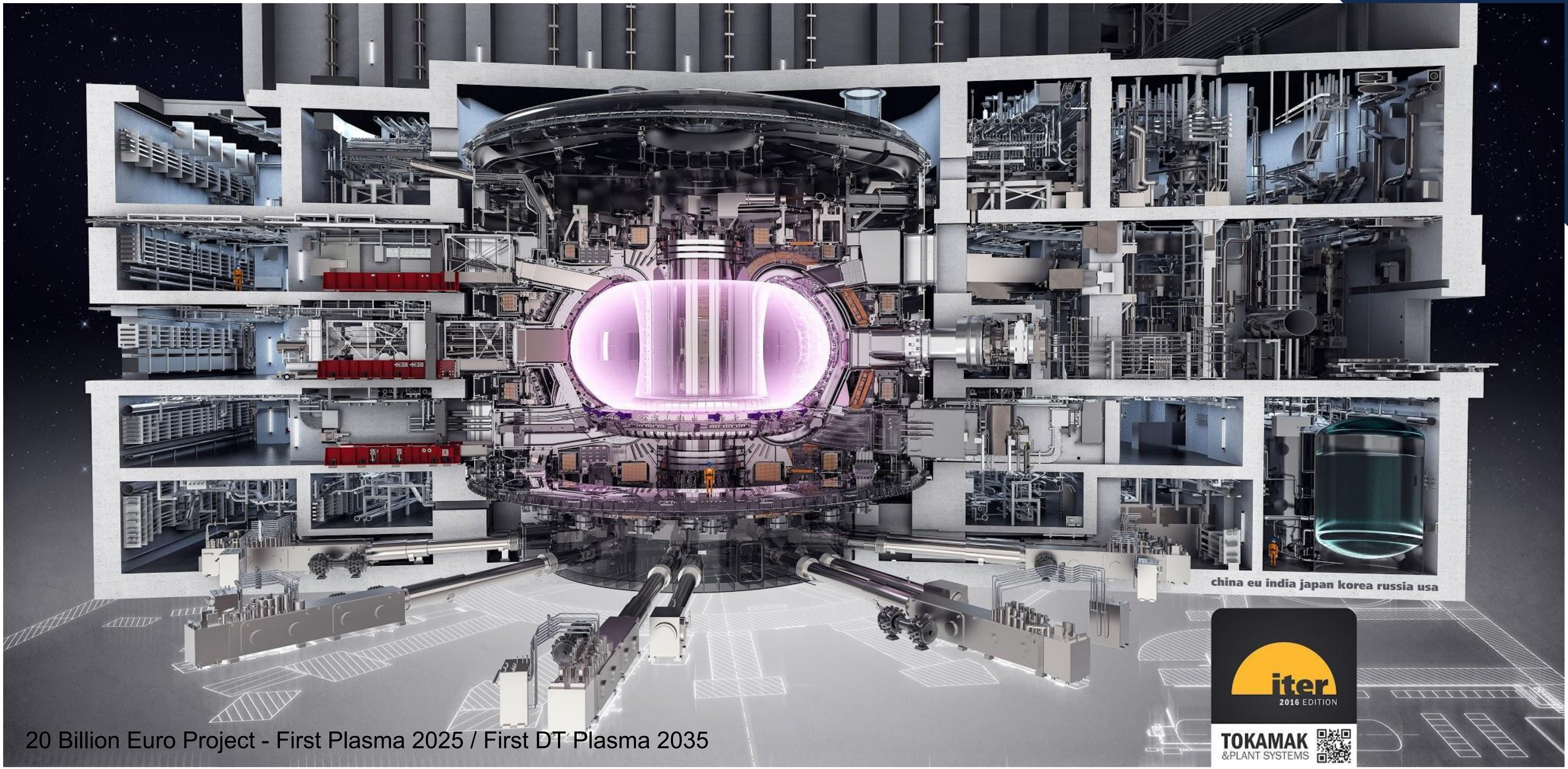
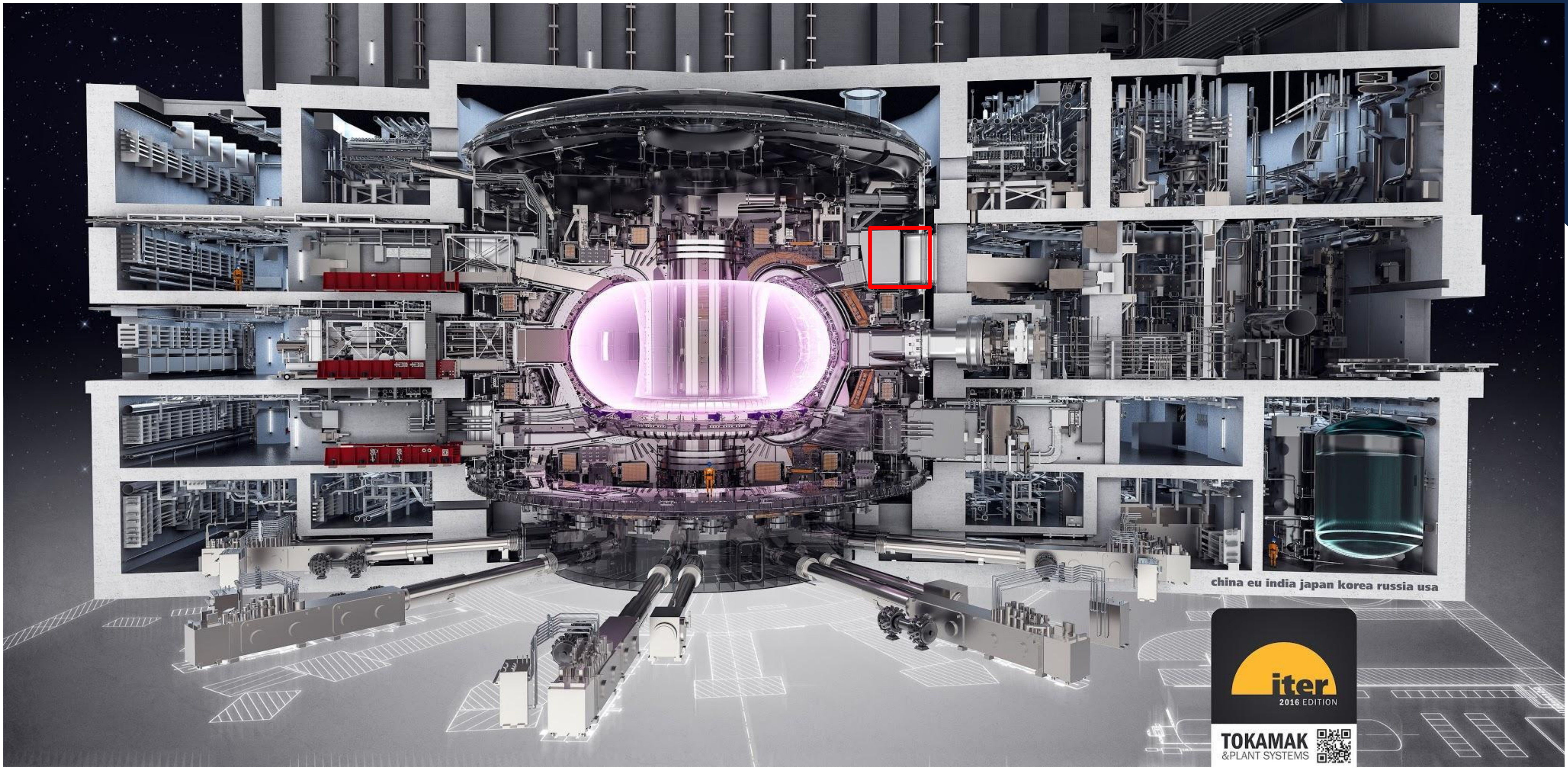


20 Billion Euro Project - First Plasma 2025 / First DT Plasma 2035


china eu india japan korea russia usa
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2016 EDITION
TOKAMAK
&PLANT SYSTEMS

What is DAGMC?

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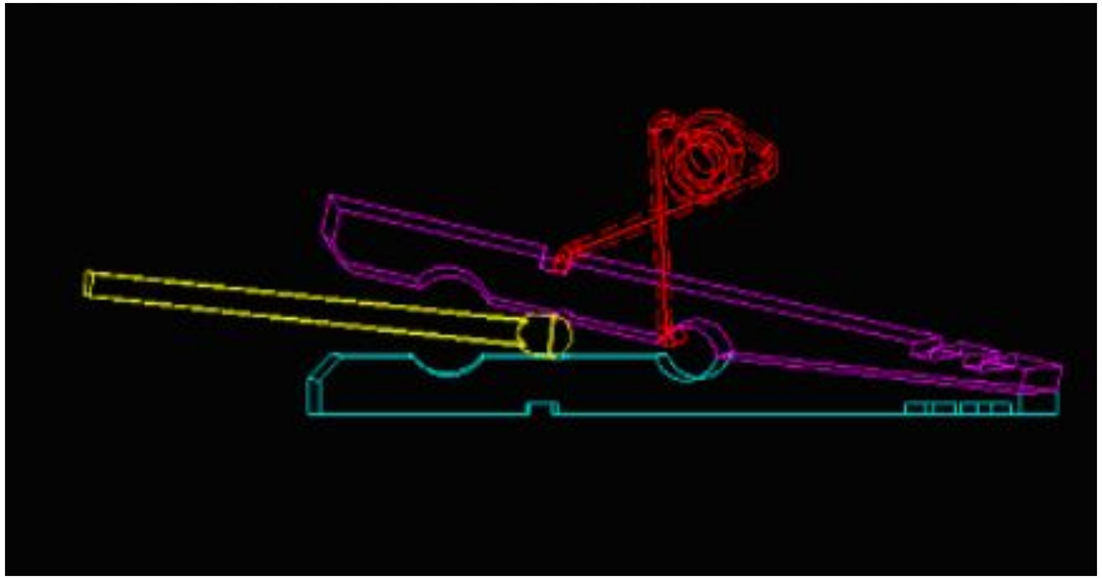
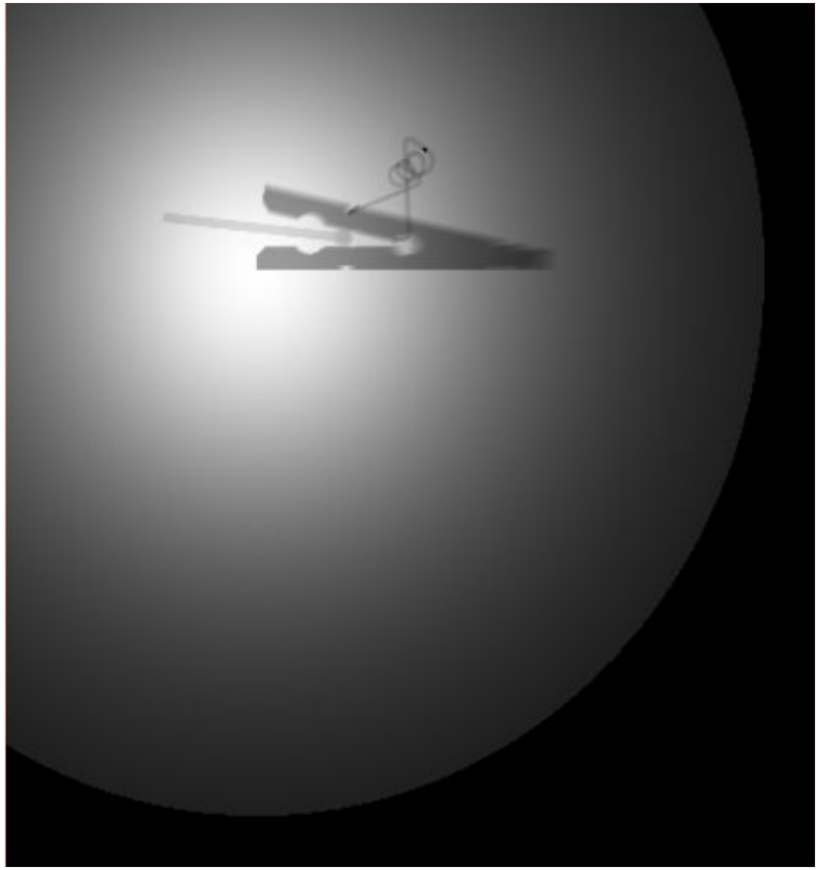
- Direct Accelerated Geometry Monte Carlo (DAGMC) started in 2001 (proof of principle by 2004) integrated directly into MCNP/X and tied directly into a CAD engine





Example use, Clothes peg defined in CAD with spiral winding in clasp, Right MCNP/X radiograph

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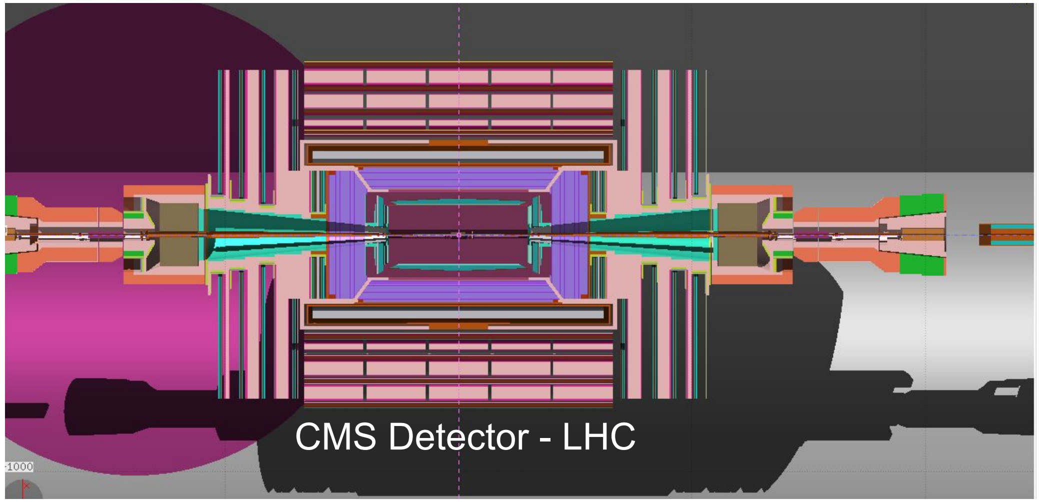
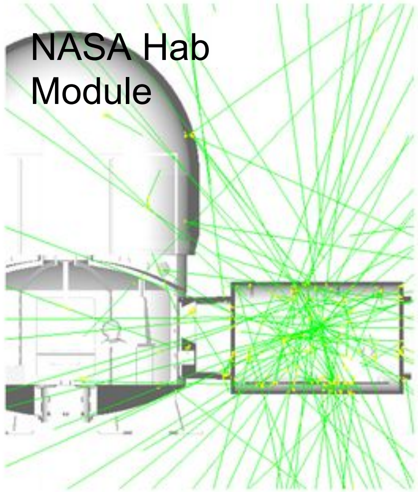
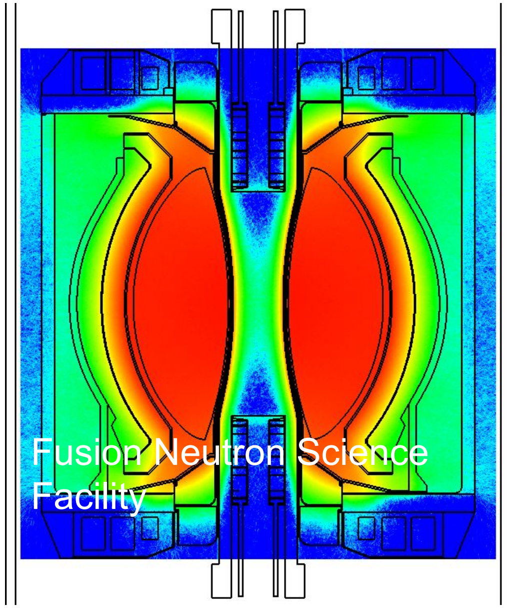
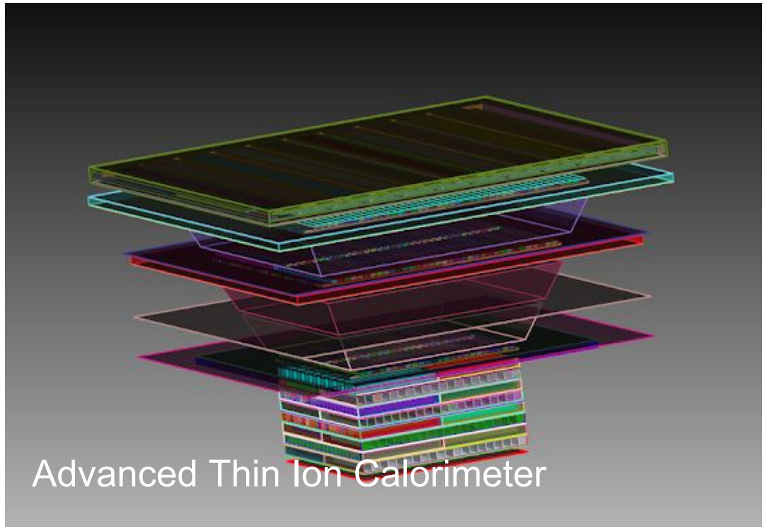
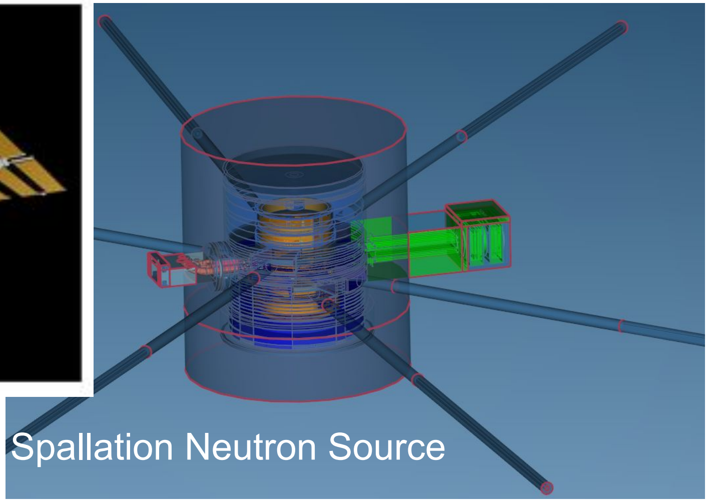
Examples of DAGMC Use











DAGMC Theory

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- Ray-tracing: fundamental operation of Monte Carlo transport
  - Ray-tracing on 2nd order analytic surfaces is efficient
  - Ray-tracing on arbitrary high-order surfaces requires high-order root finding
  - Also need to detect curves where surfaces meet
    - More complexity with high-order surfaces

- **DAGMC has 3 main Accelerations**
  1. *Imprinting & merging*
  2. *Faceting*
  3. *Bounding Volume Tree*

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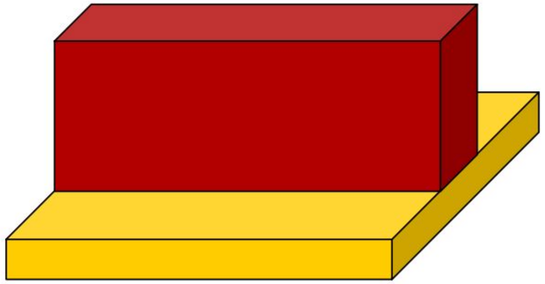
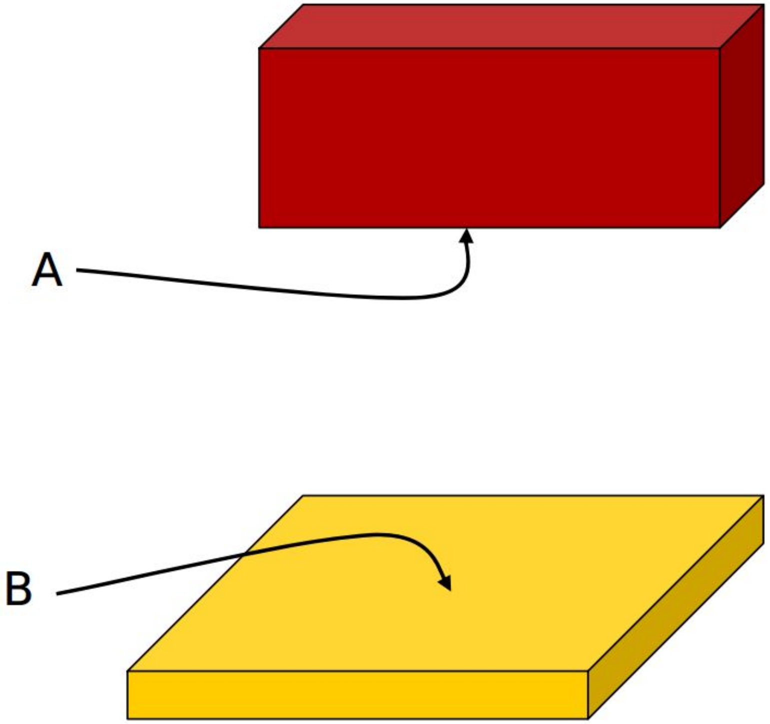
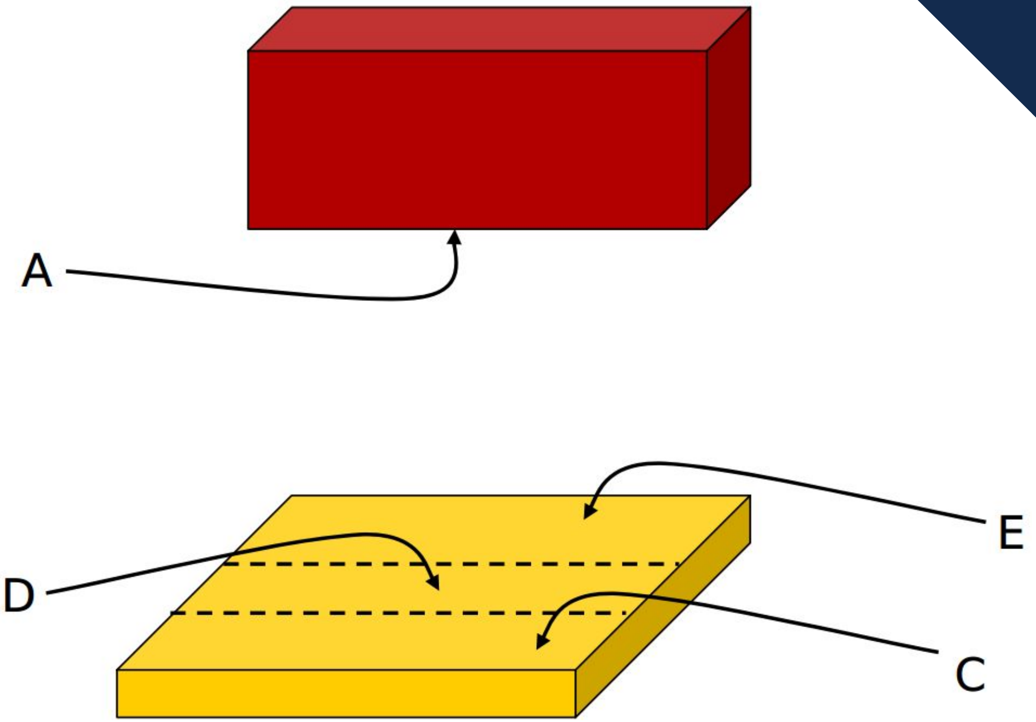
DAGMC Accelerations - Imprinting



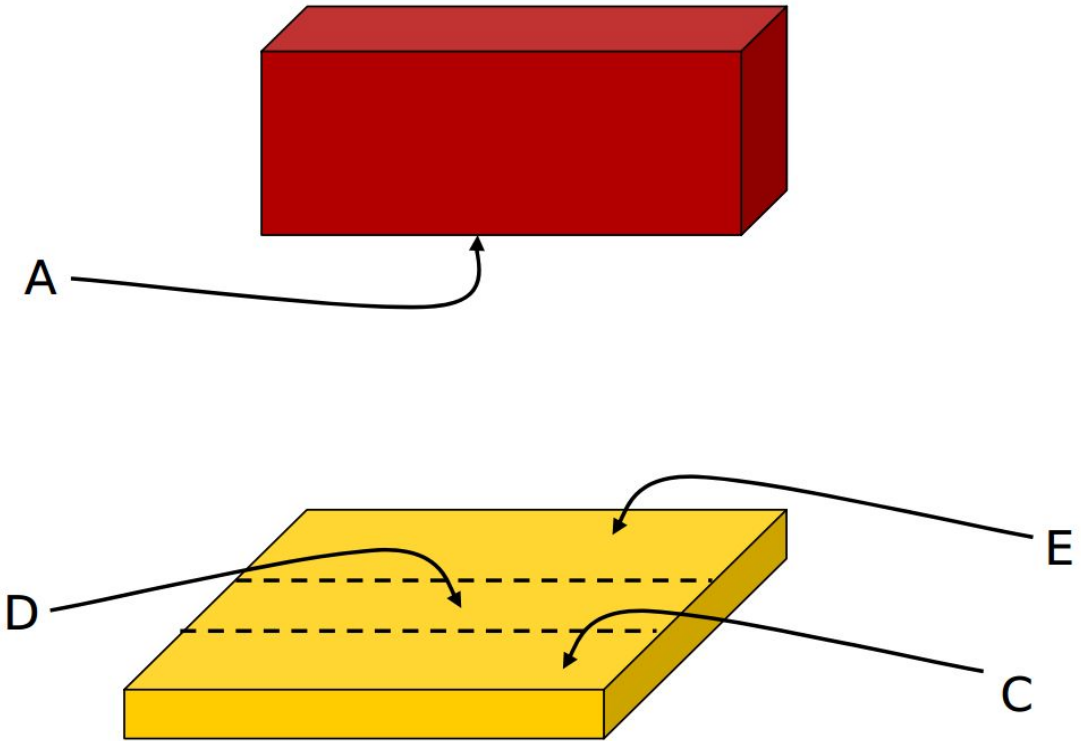




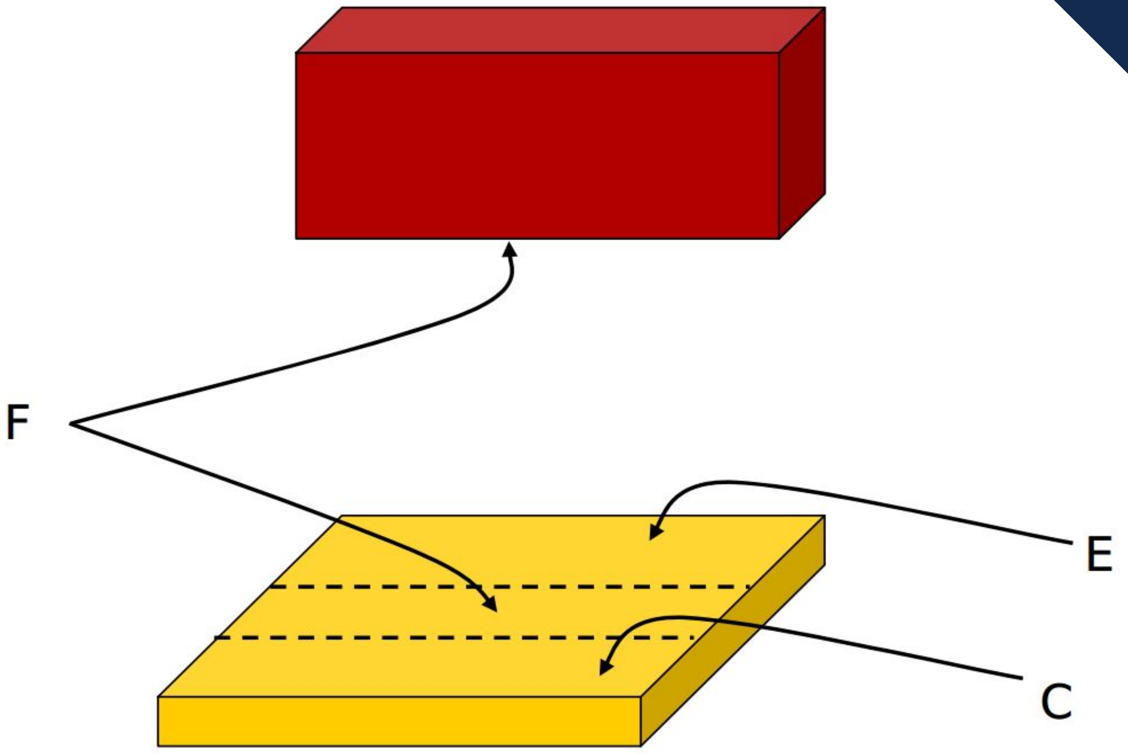
Reduces the complexity in determining neighboring regions of space

Surfaces A & B shared between the volumes

DAGMC Accelerations - Merging



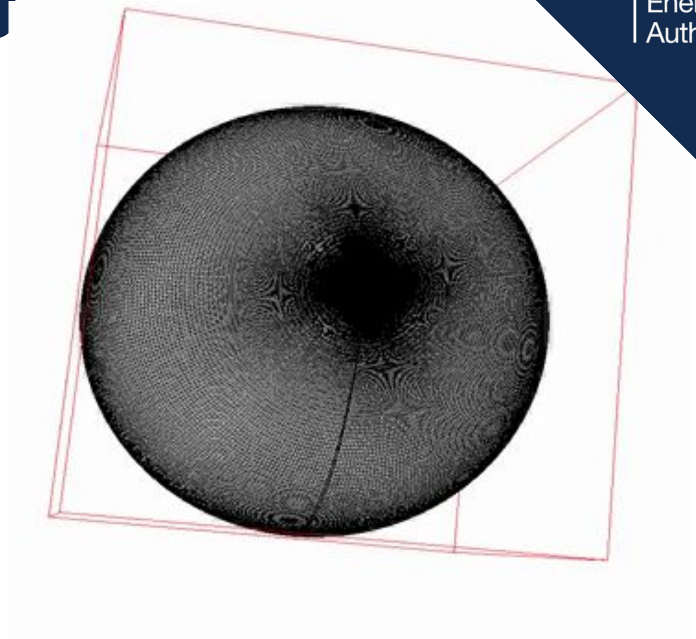
4 surfaces (3 new ones created during imprint), surface A imprinted upon surface B to create C,D,E

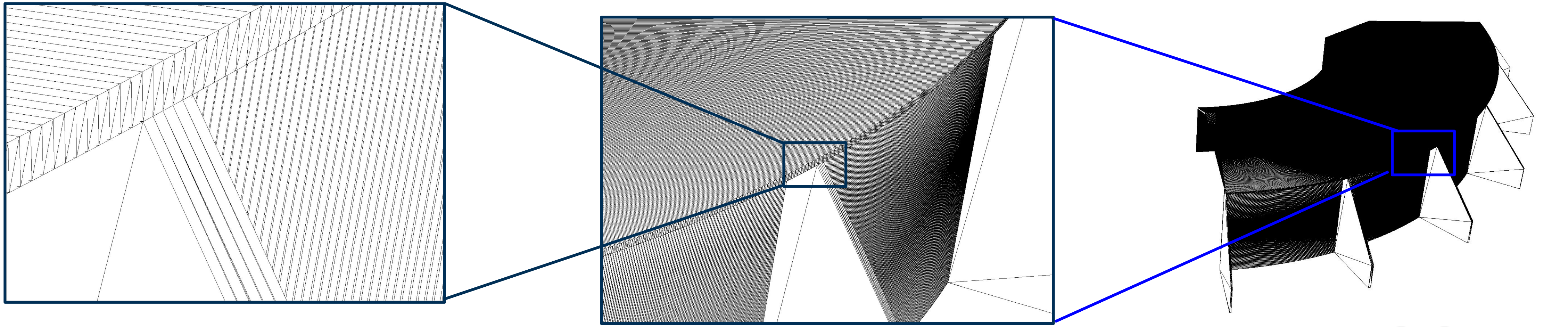


Merging surfaces F & A, now any surface can only be shared by no more than two volumes

DAGMC Accelerations - Faceting

- Reduces ray tracing to always be on planar facets
  - introduces approximation
  - millions of facets
- Axis aligned bounding box often larger than needed
  - Oriented boxes make for smaller boxes
  - OBB on facets allow for finer granularity boxes





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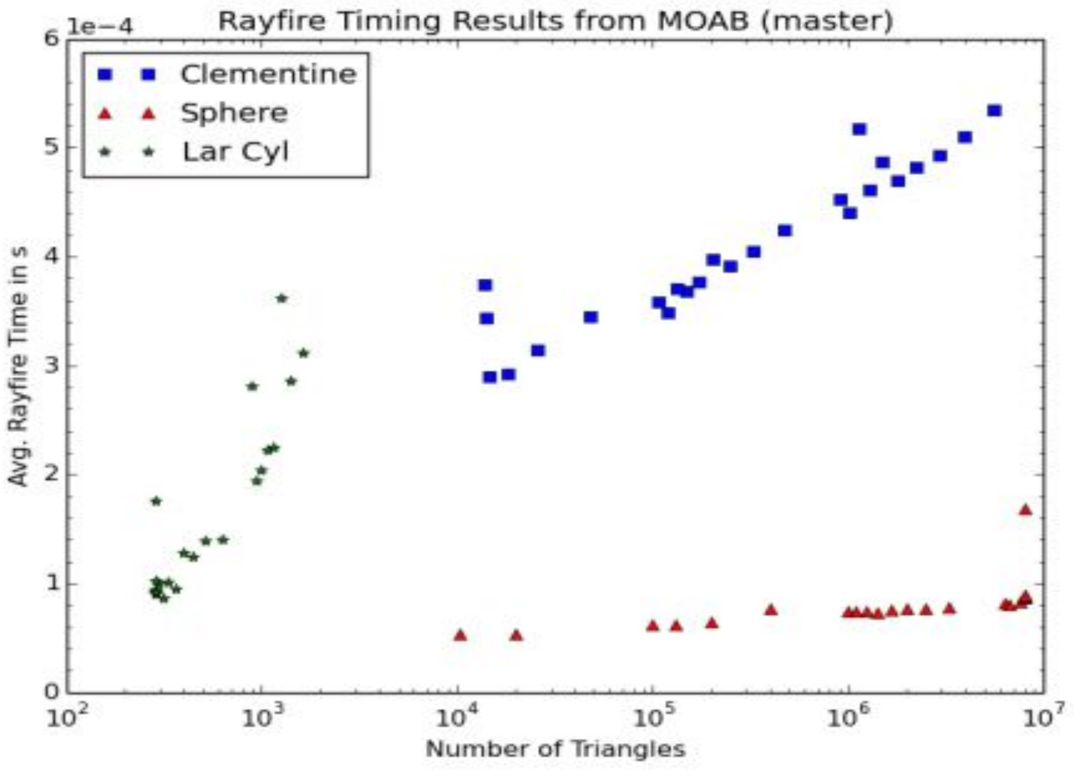
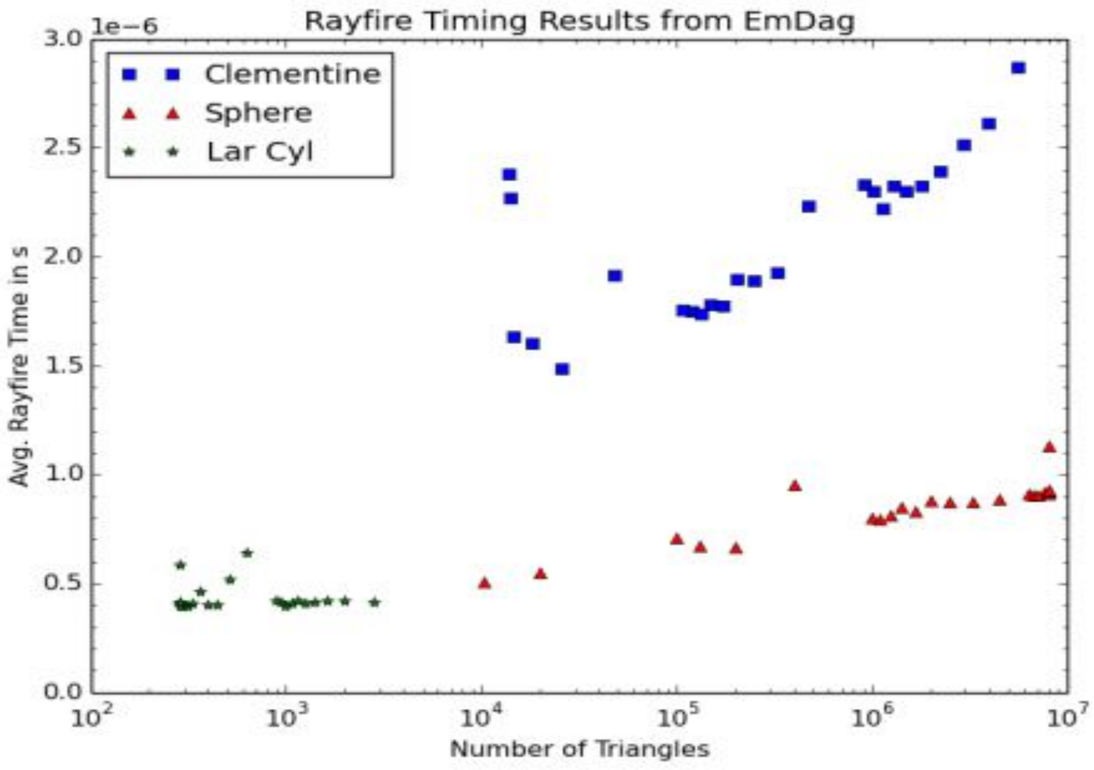
DAGMC Accelerations - BVH Trees



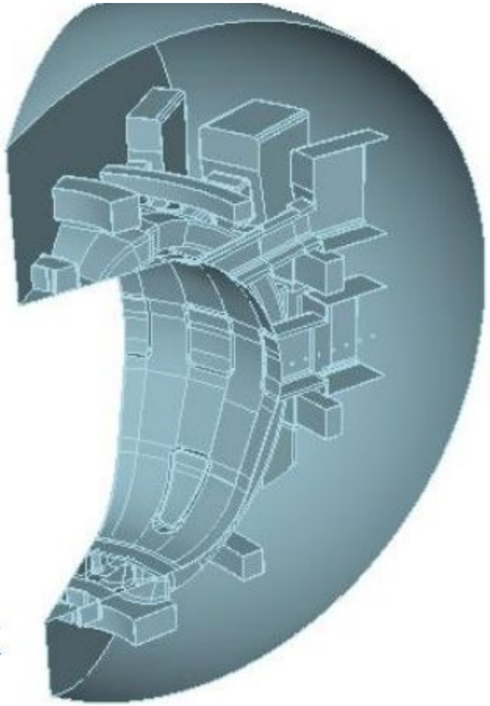
MOAB OBBs

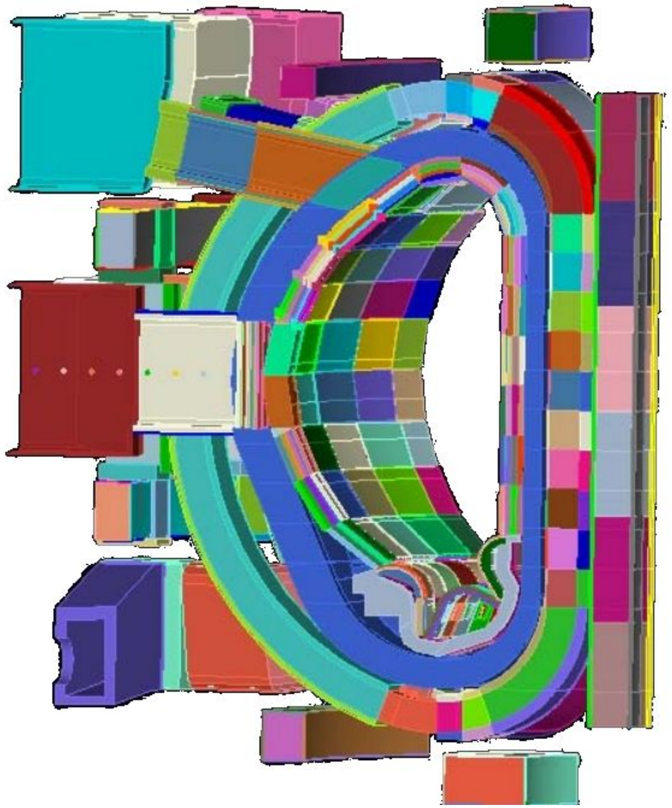


Embree AABB

DAGMC Convenience - Implicit Compliment

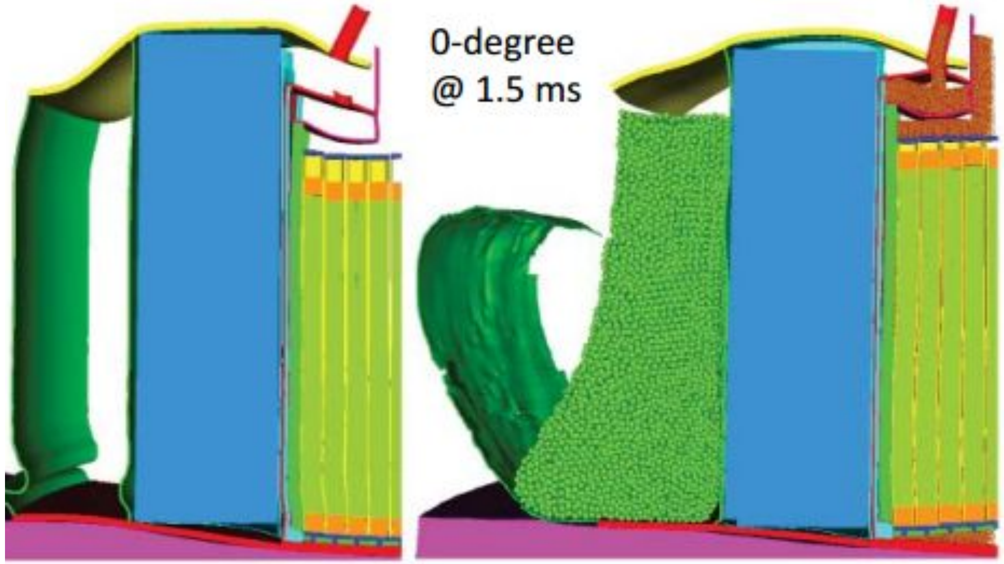
- CAD models generally do not define “void space”, including:
  - Coolants
  - Vacuum
  - Air
- DAGMC
  - Any surface that does not associate with 2 volumes must bound this compliment space (due to imprinting a surface can only be associated with 1 or 2 volumes)
- Is **automatically** generated
- On going work to have multiple logically derived implcit complements

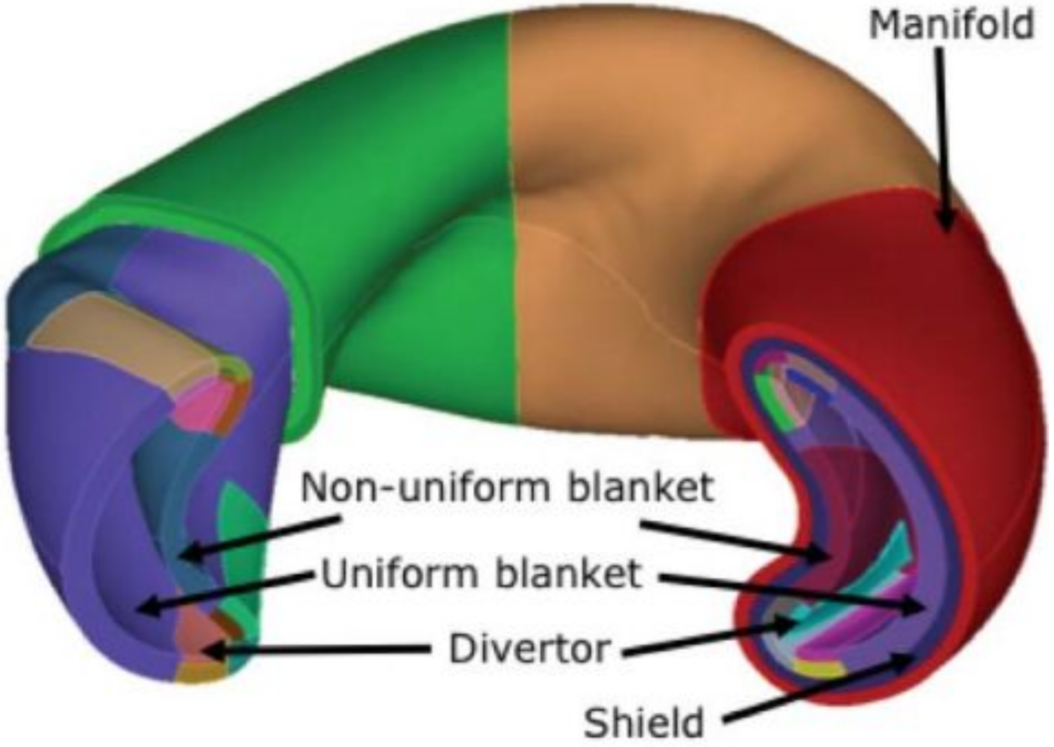




DAGMC Advantages

- Richer surface description
  - Stellarator only possible to model in DAGMC - Andre Haussler (KIT)
- Implicit Complement
  - Complex negative space geometry not needed to be defined
- All volumes implicitly derived from triangle surface representation





- Tighter coupling to other physics
  - Facet based model can be deformed due to external input

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Access to DAGMC

- Fundamentally open source
  - http://svalinn.github.com/DAGMC
- Software stack:
  - Free & Open: MOAB, HDF5, (optional PyNE), DAGMC
  - Licensed: Cubit/Trelis
    - Maybe use Attila mesher?
  - Working on OS solution for geometry
- Community forum:
  - dagmc-users@groups.google.com
- Please try it!

DAGMC - Integration

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FLUKA

MCNP6

MCNP5

GEANT4

Tripoli4

Shift

Complete and Available

OpenMC

In Progress

EGSnrc

PHITS
Particle and Heavy Ion Transport code System

Serpent2

Proposed

19

Penelope

Mercury

MARS

Not Currently Planned

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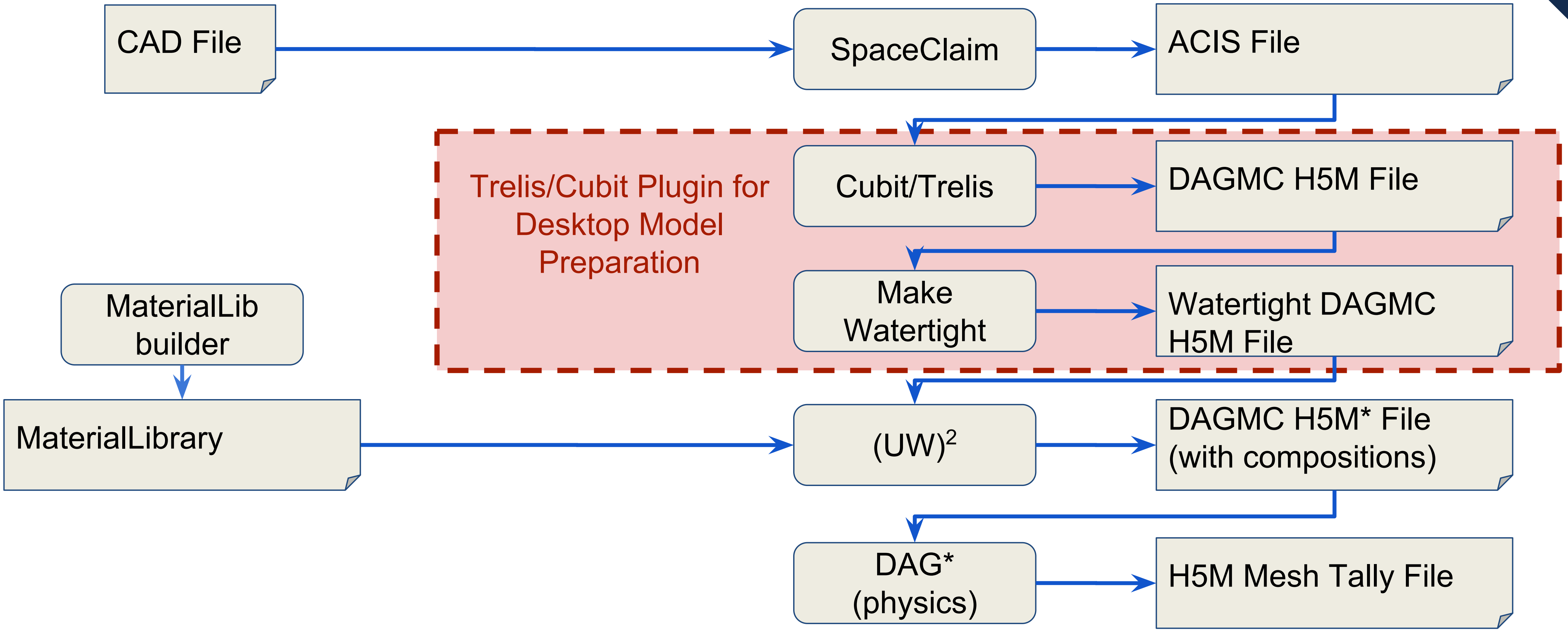
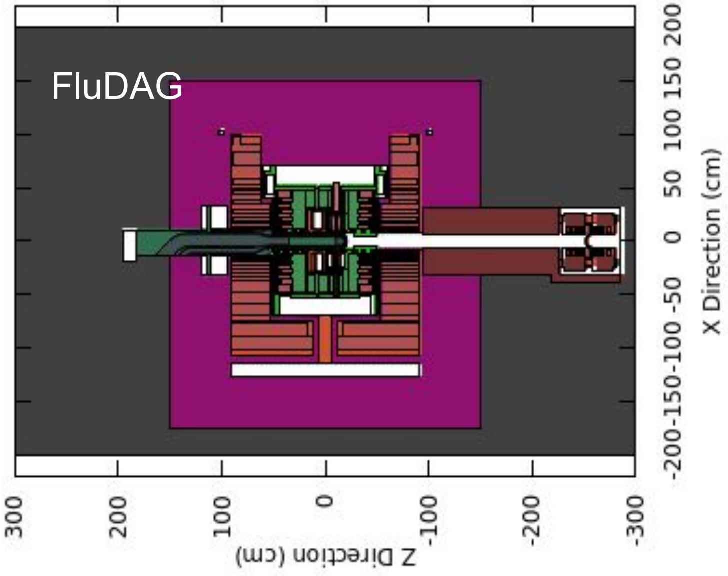
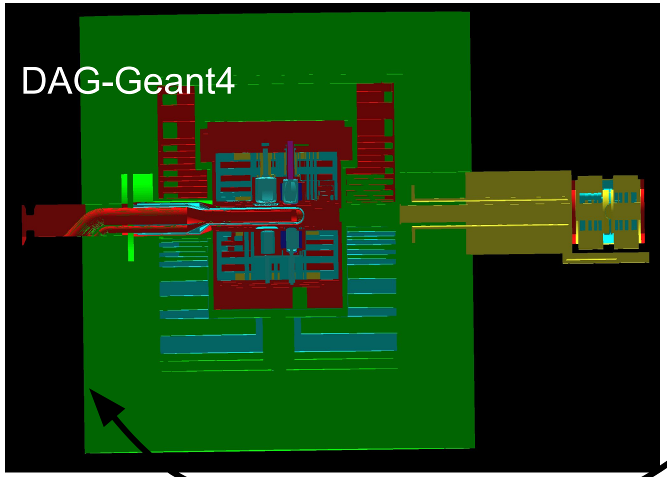
DAGMC Workflow

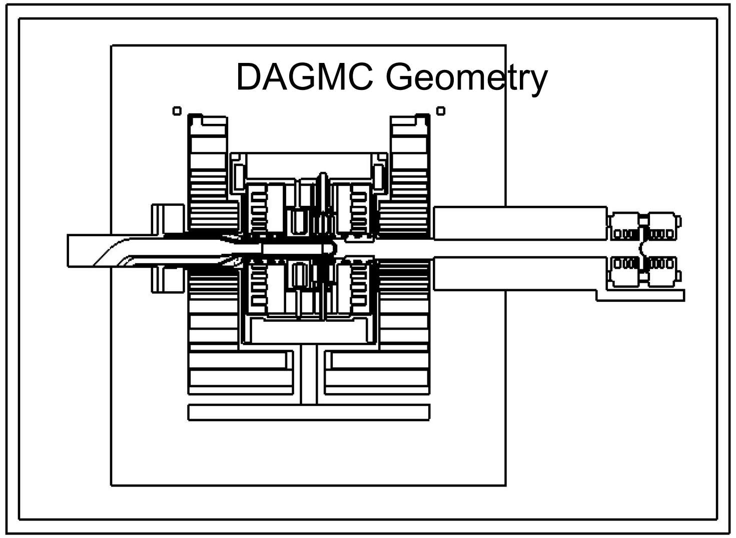


Geometry as a Service

- We have MC code agnostic workflow where materials are encoded in generic form







mat:Mercury
mat:StainlessSteel
mat:ParaHydrogen
mat:Cadmium
….

- Deploy the literal same geometry in supported codes - no changes needed

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DAGMC Software Testing

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- Fundamental library tests within MOAB
  - Run nightly
  - Run on demand with pull requests
- Fundamental DAGMC Code Interface tests
  - Run nightly on the baseline branch
  - Run on demand with Github pull requests
- DAG-MCNP5/MCNP6 Verification and Validation
  - Sinbad, Several code comparisons, MCNP5 test suite
- FluDAG
  - Sinbad, Several code comparisons, bespoke test suite

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DAGMC Examples - ITER NBI Sector

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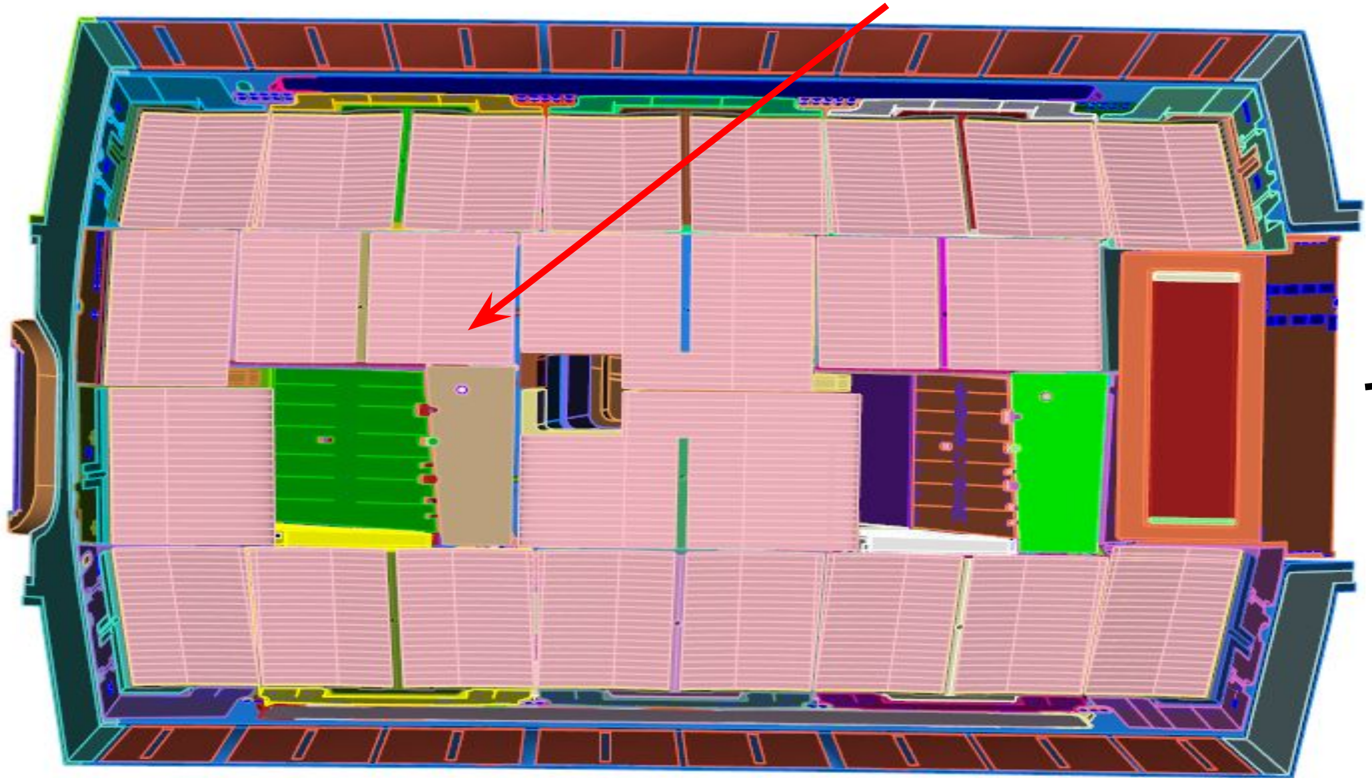
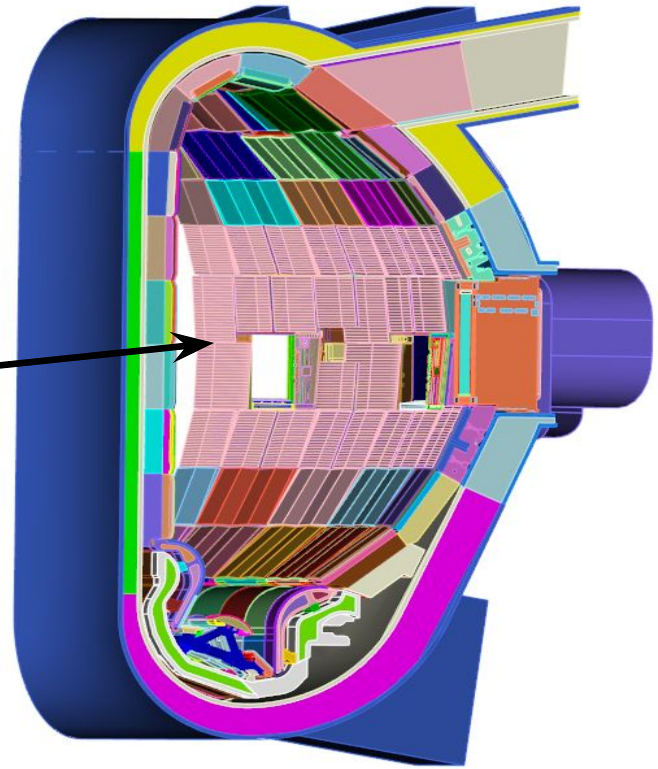
- A detailed, updated model of the NB port region was integrated into the BL-Lite model (40° model) - 2646 volumes, 72019 surfaces, 171361 curves





Calculations run using DAG-MCNP5 and FENDL-2.1 cross section library

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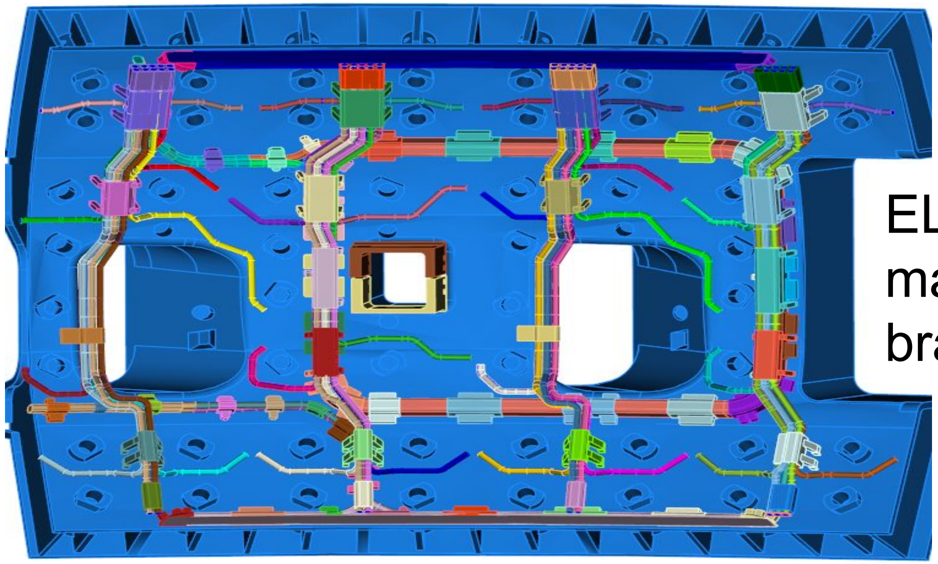
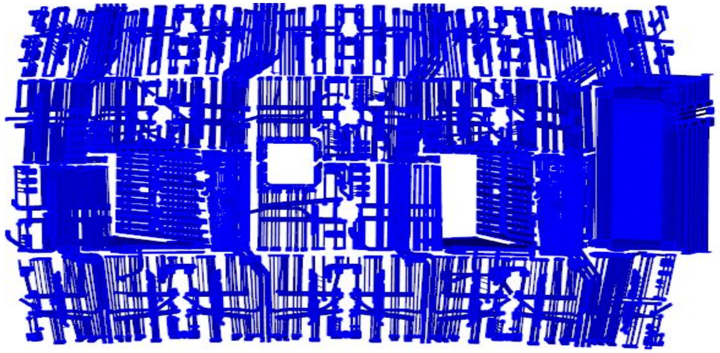
DAGMC Examples - ITER NBI Sector

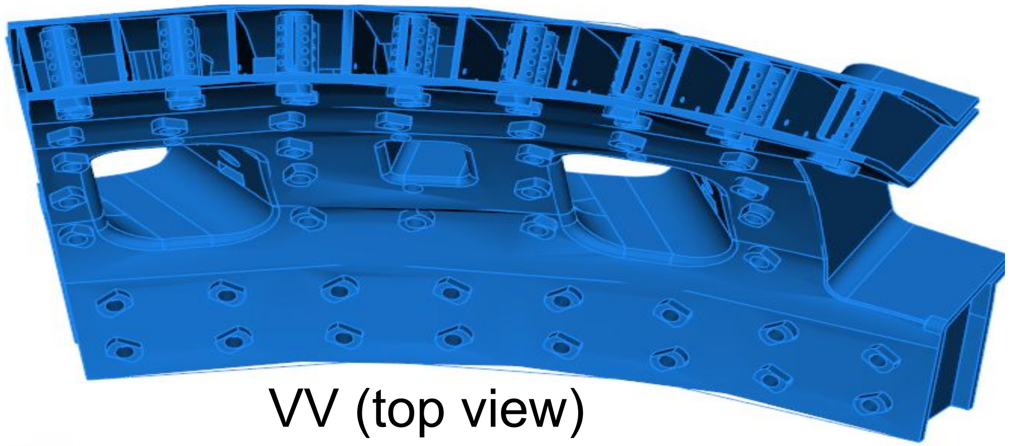
- A lot of detail in the BM13-16 region:



ELM coils, manifolds, brackets



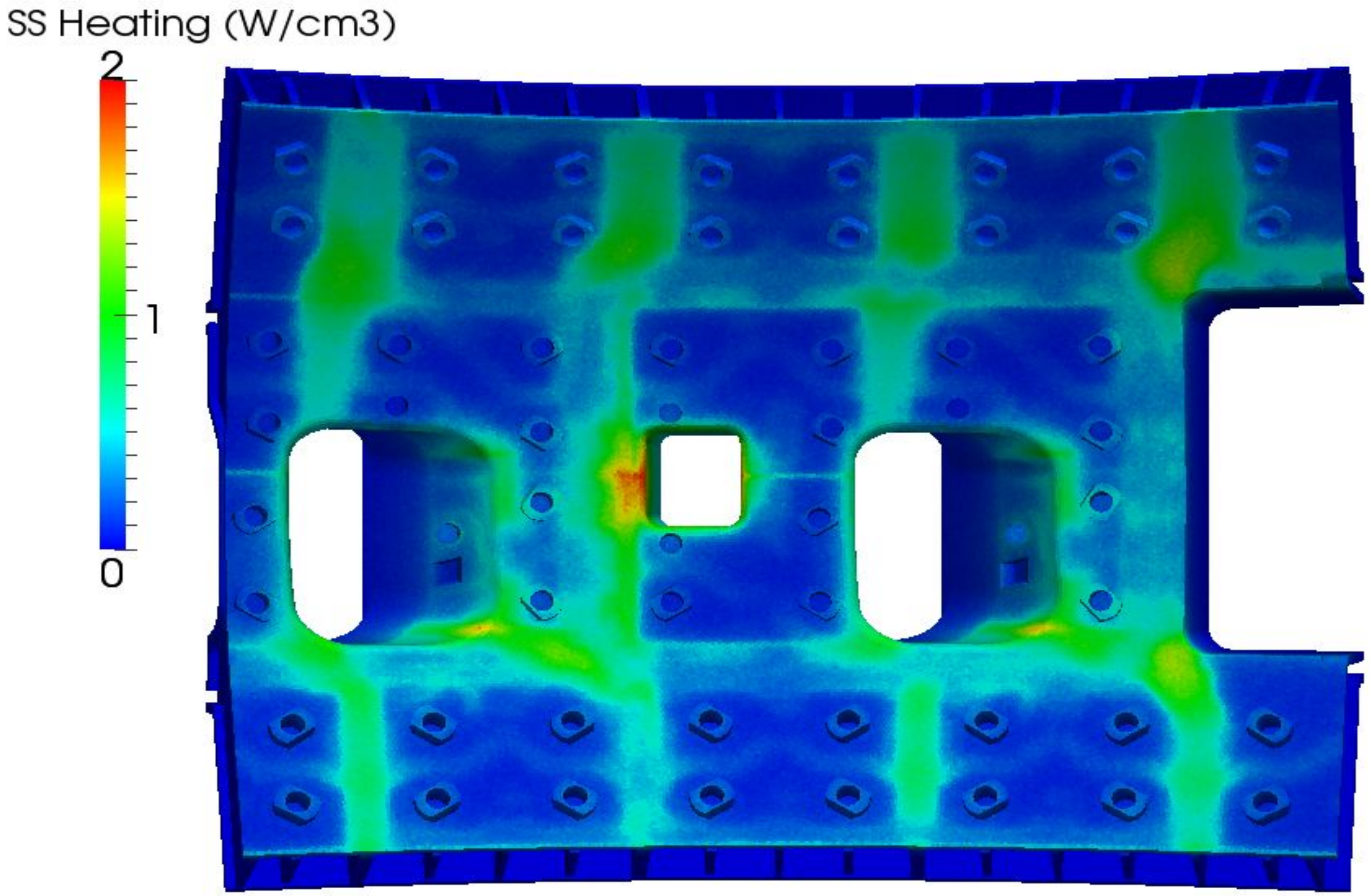
Water coolant channels

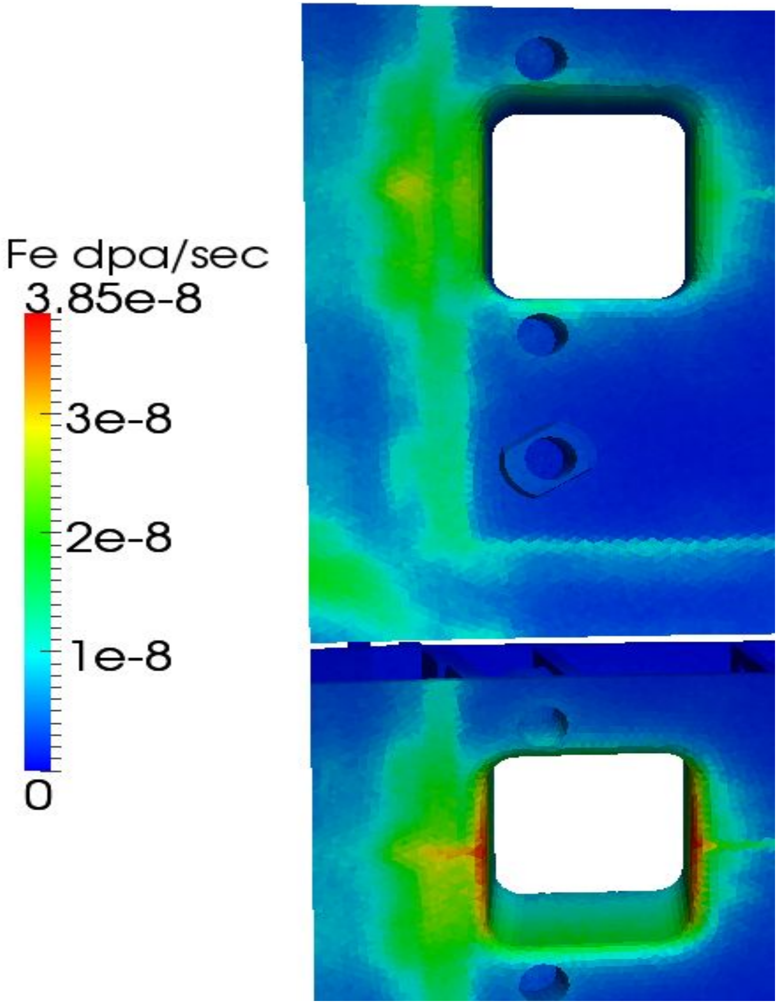


VV (top view)

SB (rear view)

DAGMC Examples - ITER NBI Sector





ITER lifetime is 0.54 FPY (1.7e7 sec) so 2.94e-8 dpa/sec corresponds to 0.5 dp

Detailed Blanket Module Heating

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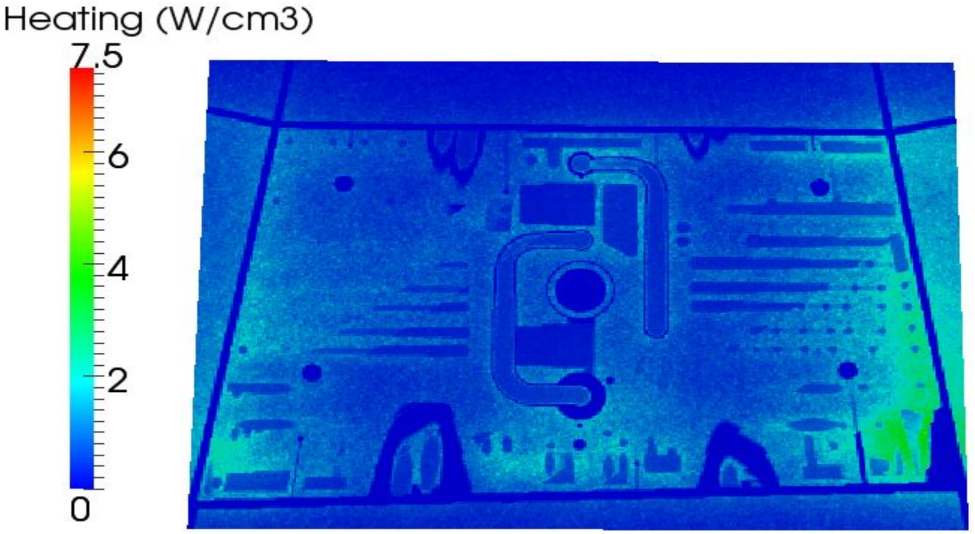
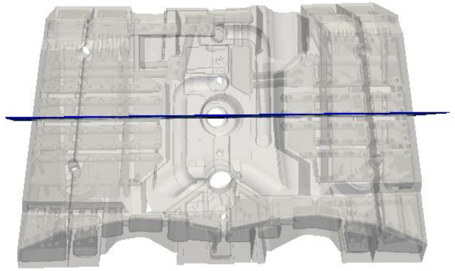
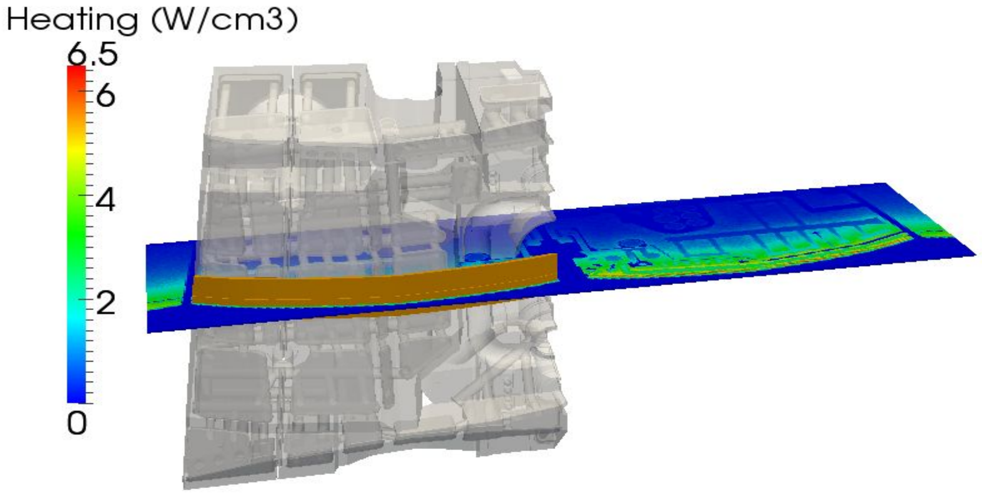
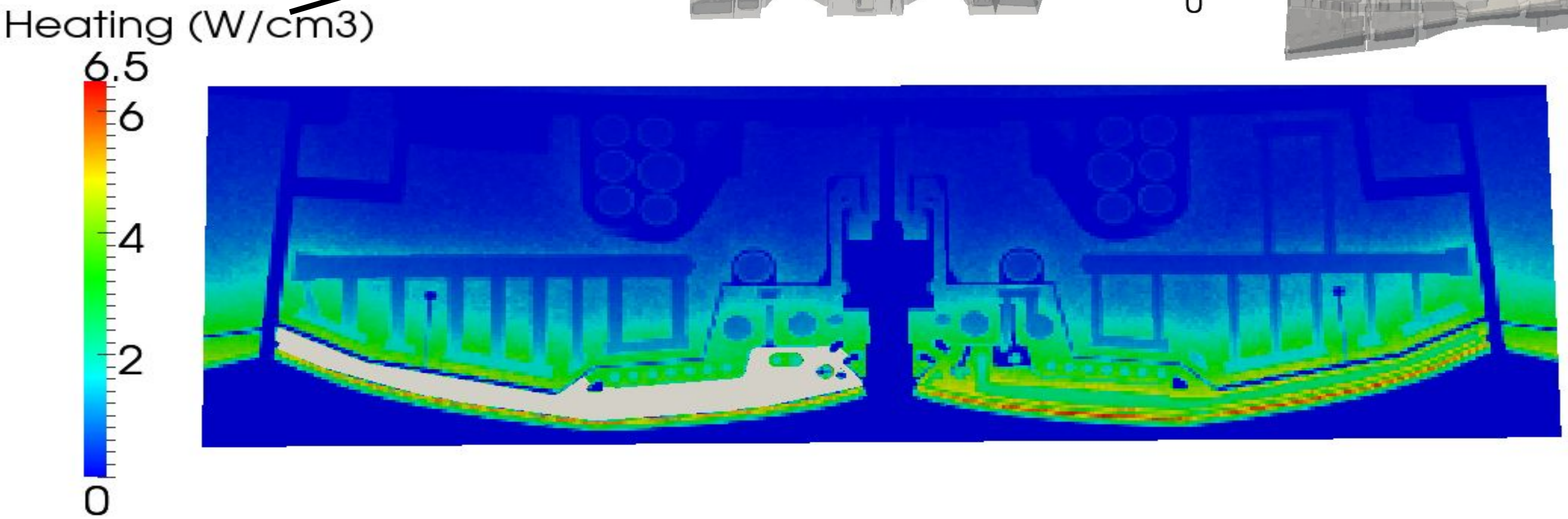


Slice through mid-plane

- Entire BM08 model covered with a rectangular (non-conformal) mesh tally







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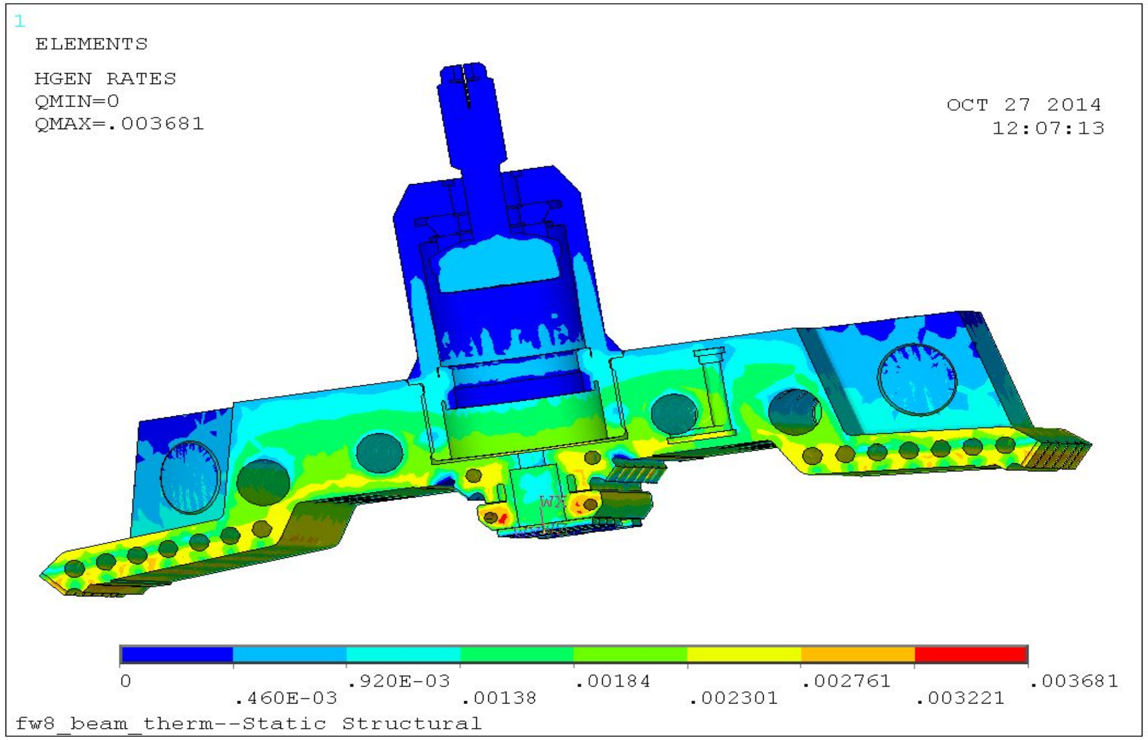
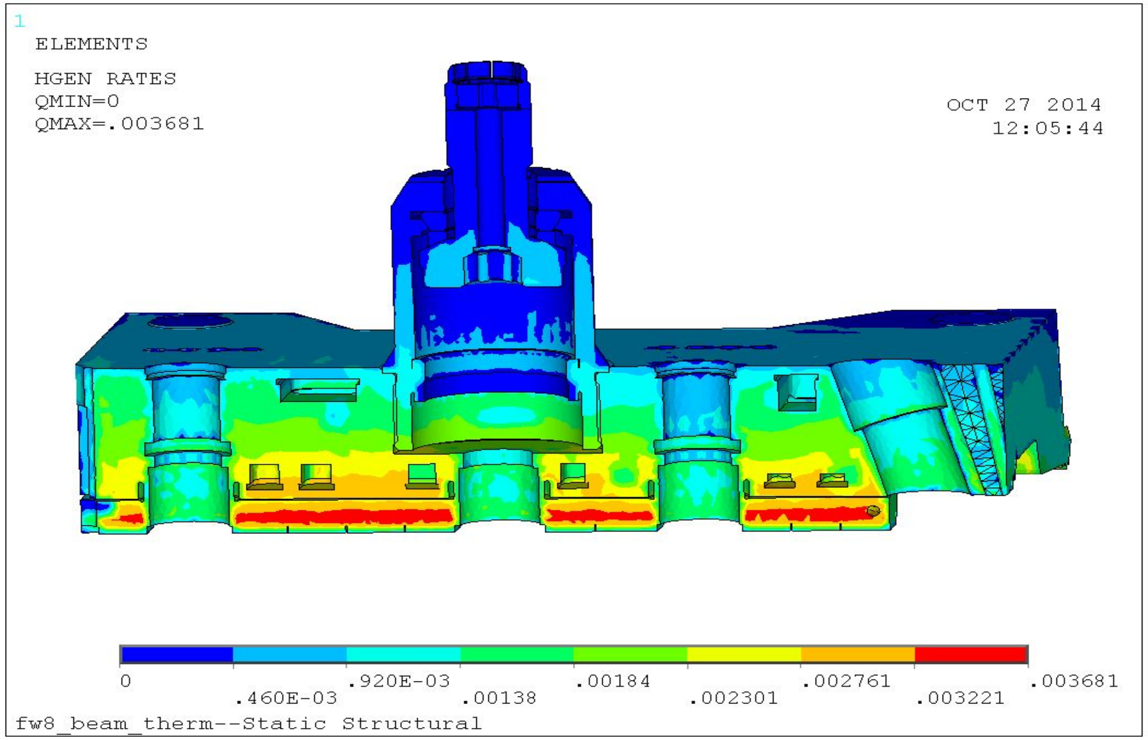
Detailed Blanket Module Heating

- The IO requested nuclear heating mapped onto an ANSYS mesh of the BM08 beam with units of W/mm^3
- The nuclear heating generated with the Cartesian mesh was used for this mapping:





SNL Space Reactor

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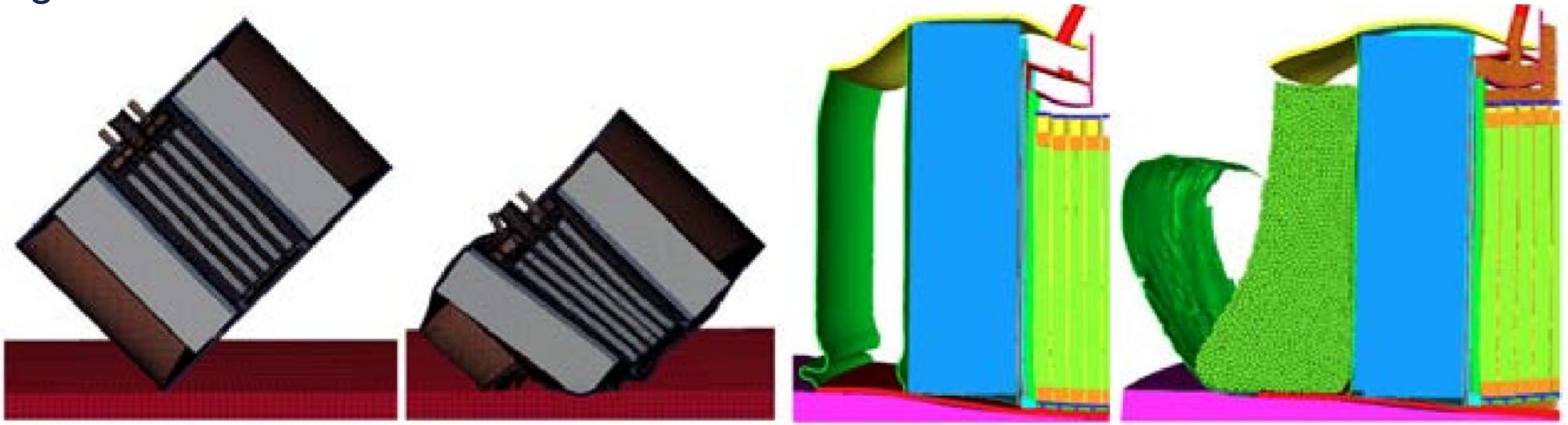
- CAD geometry of the SNL Space reactor was was meshed, structural mechanics of the FE mesh used to determine deformation of the geometry when the reactor was dropped ‘during launch conditions’
- Need to determine the k_{eff} of the system under various failure modes, drop angles



45-degree 0 ms | 45-degree 2.1 ms | 0-degree 1.5 ms | 0-degree SPH 1.5 ms

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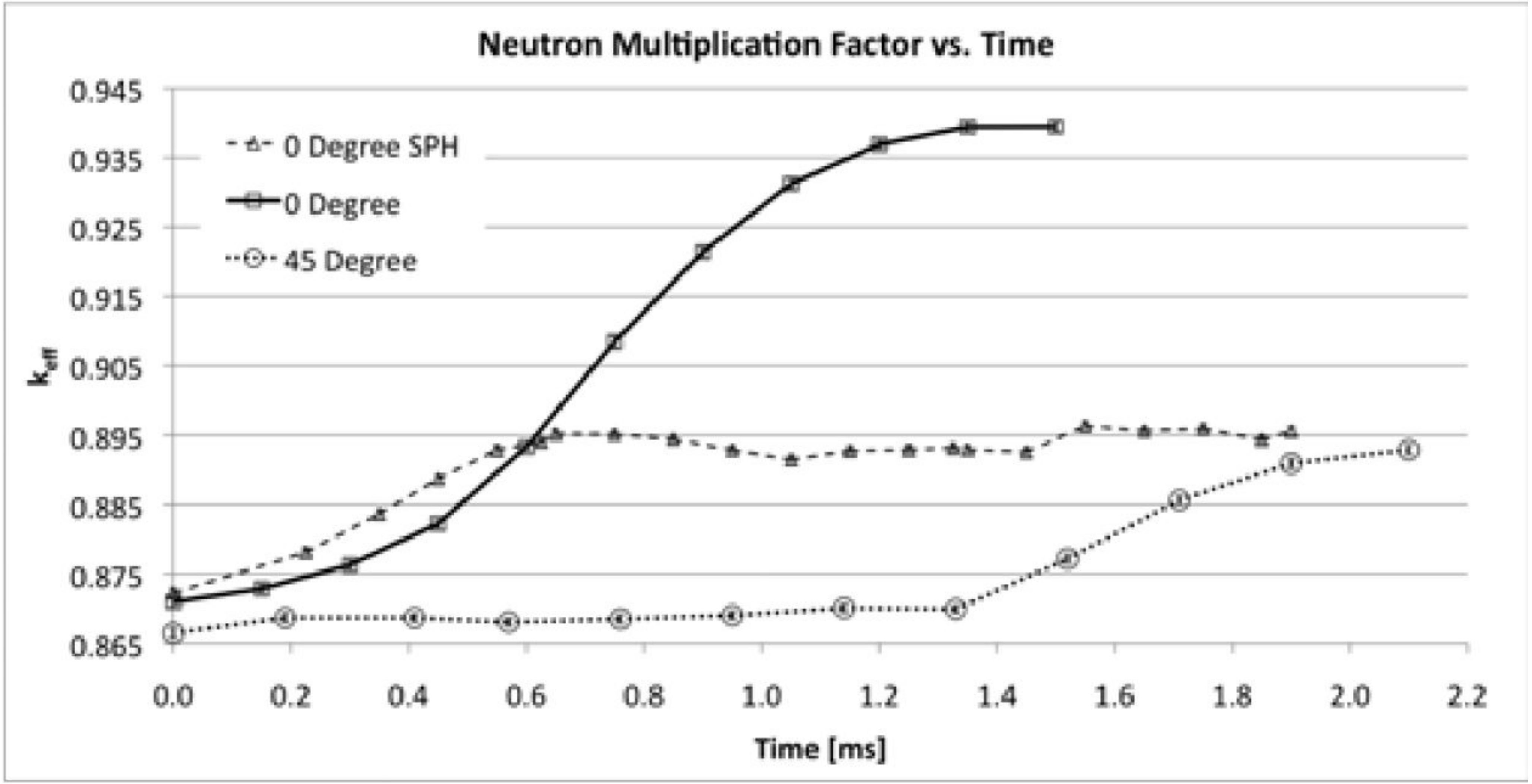
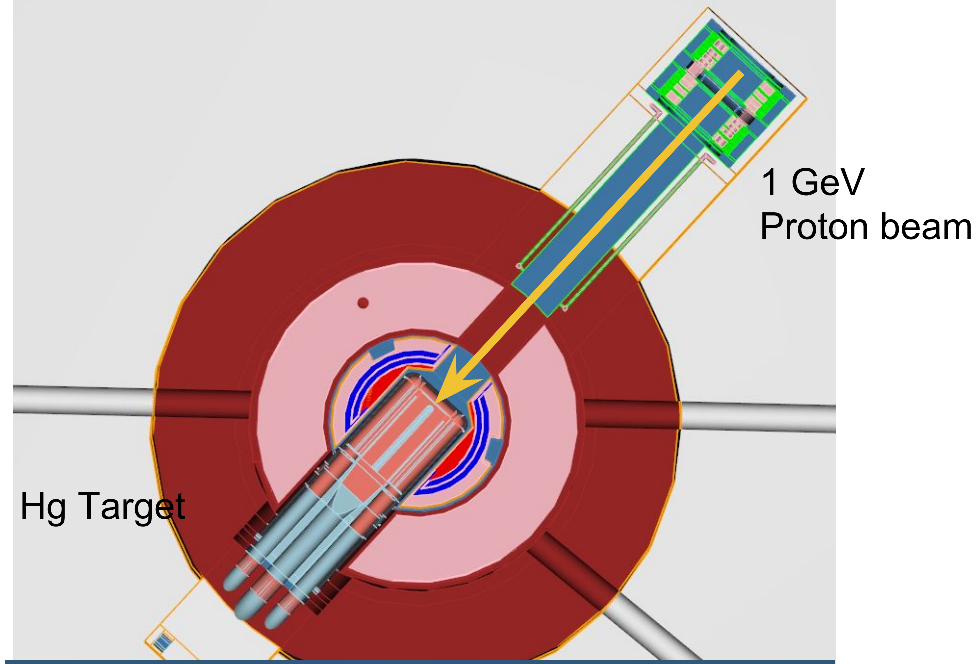
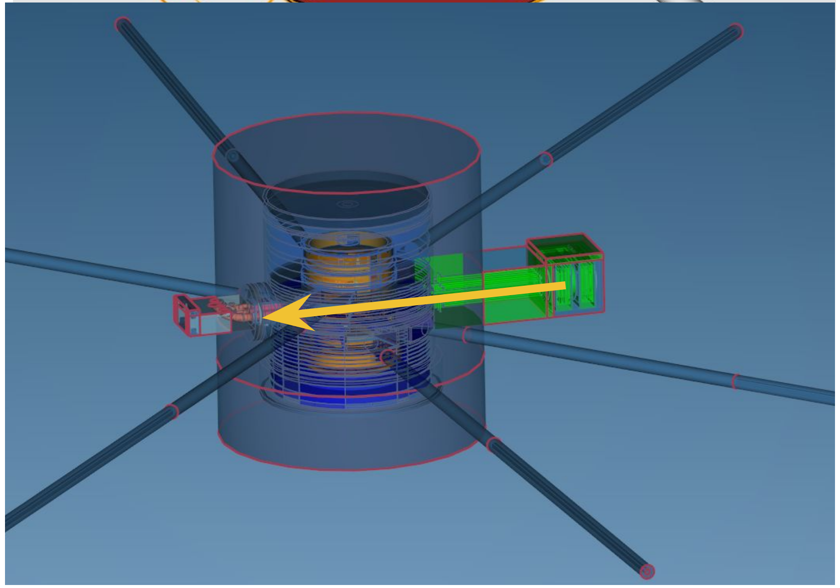
SNL Space Reactor



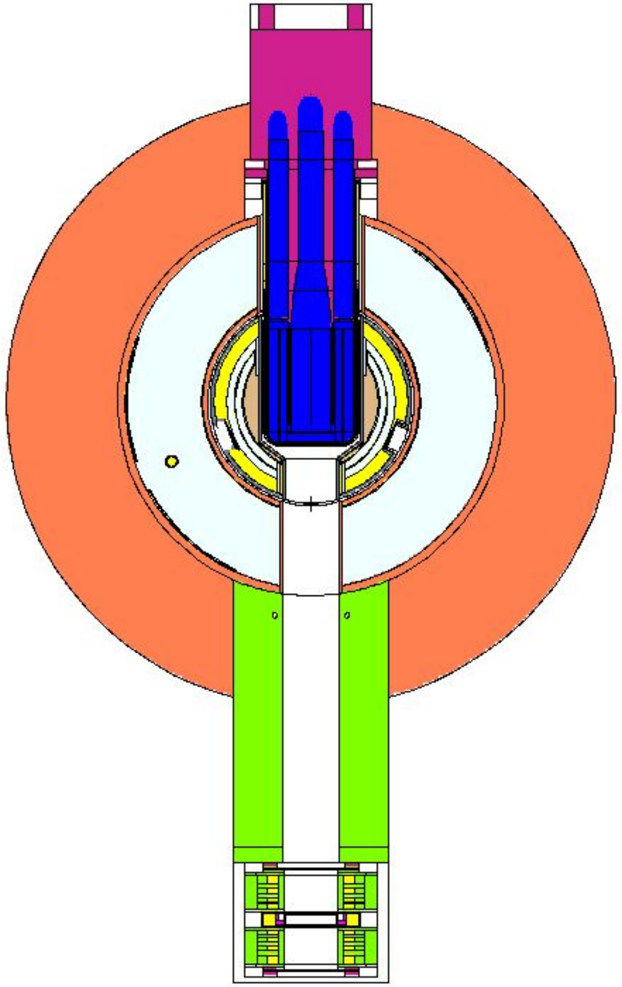
DAG-MCNP6 SNS

- Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS) are interested in shifting to a complete CAD based workflow
  - They have extensive CAD models of the facility and a planned upgrade
- SNS 1 GeV proton beam impinges on liquid mercury target delivering 1 MW of heat into the target, producing around 20 spallation neutrons for each source neutron
  - The neutrons are then ‘encouraged’ along beamlines to target stations

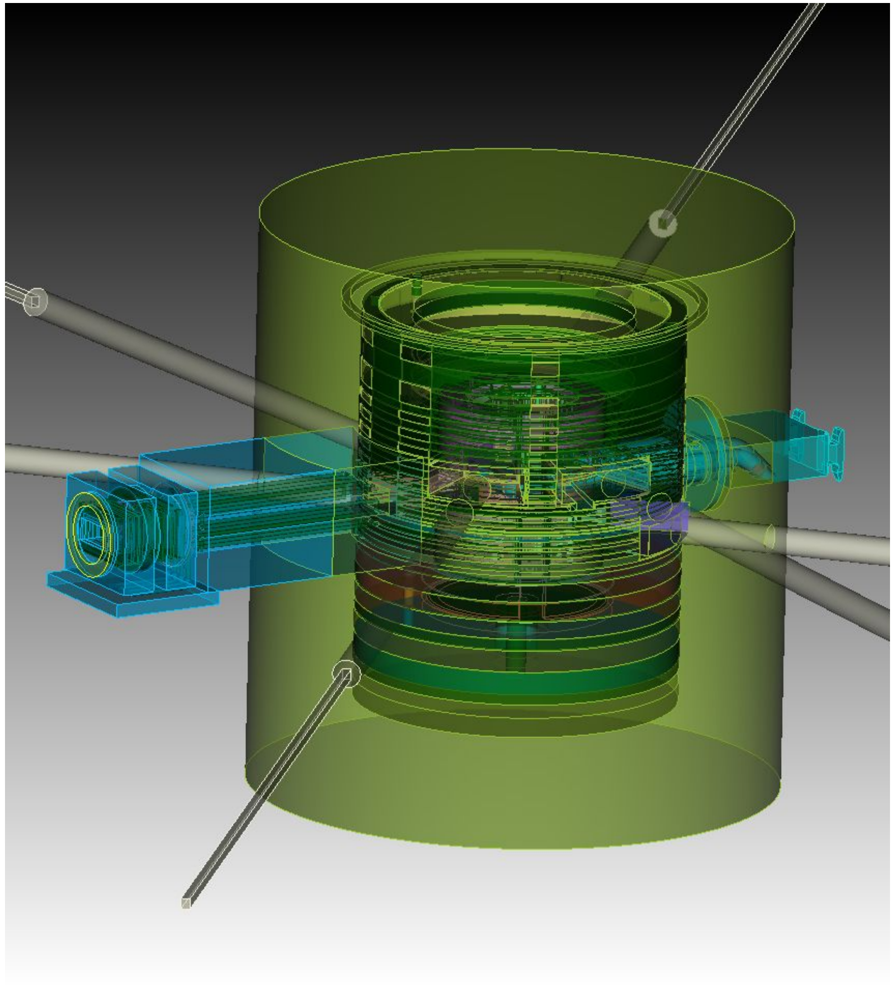




DAG-MCNP6 SNS



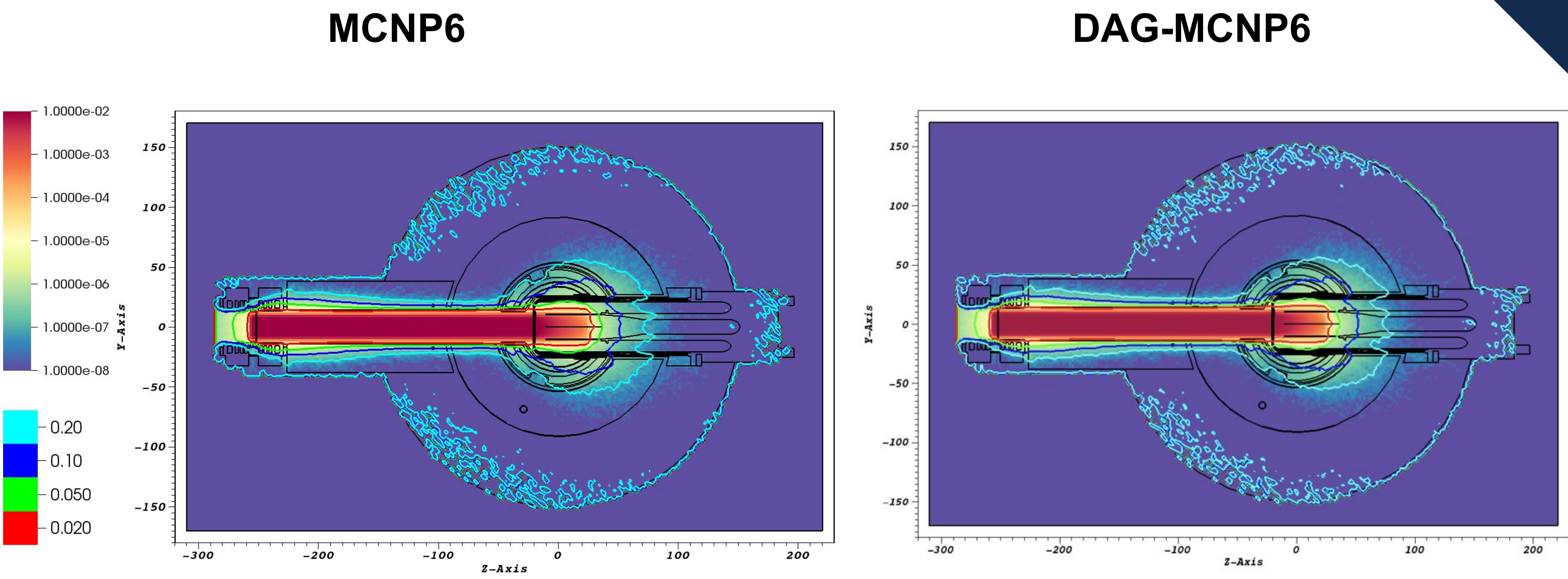
MCNP geometry



CAD model

- Oak Ridge National Laboratory (ORNL) provided native MCNPX model
- Converted to CAD geometry using the mcnp2cad tool (automatic)
- The native MCNP model was created by hand at great expense of time and effort (6 months)

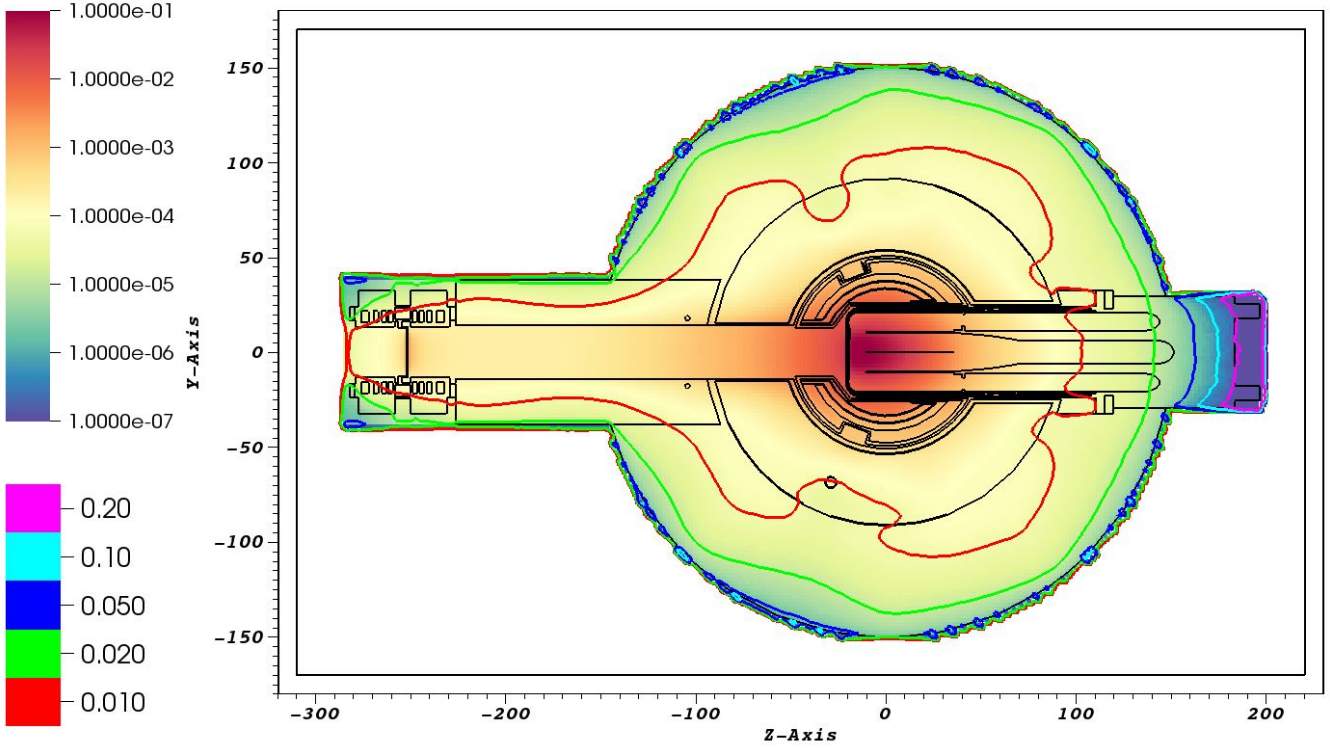
DAG-MCNP6 SNS



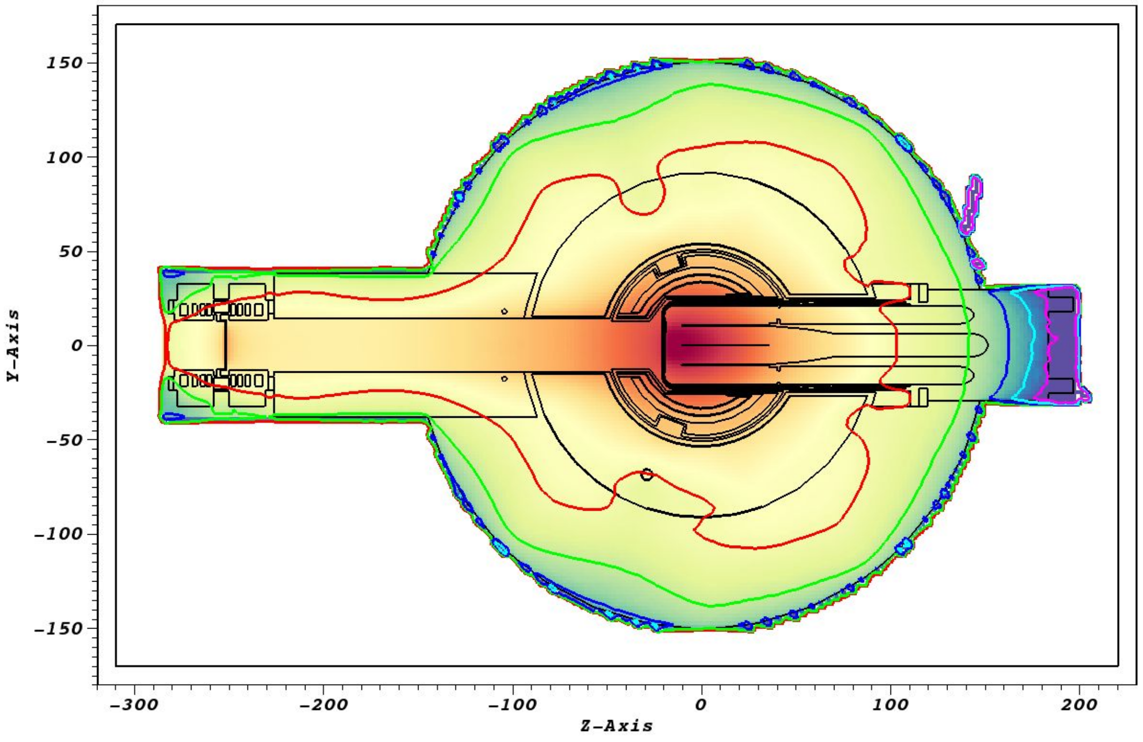
Proton Flux

DAG-MCNP6 SNS

MCNP6



DAG-MCNP6



Neutron Flux

UK Atomic Energy Authority

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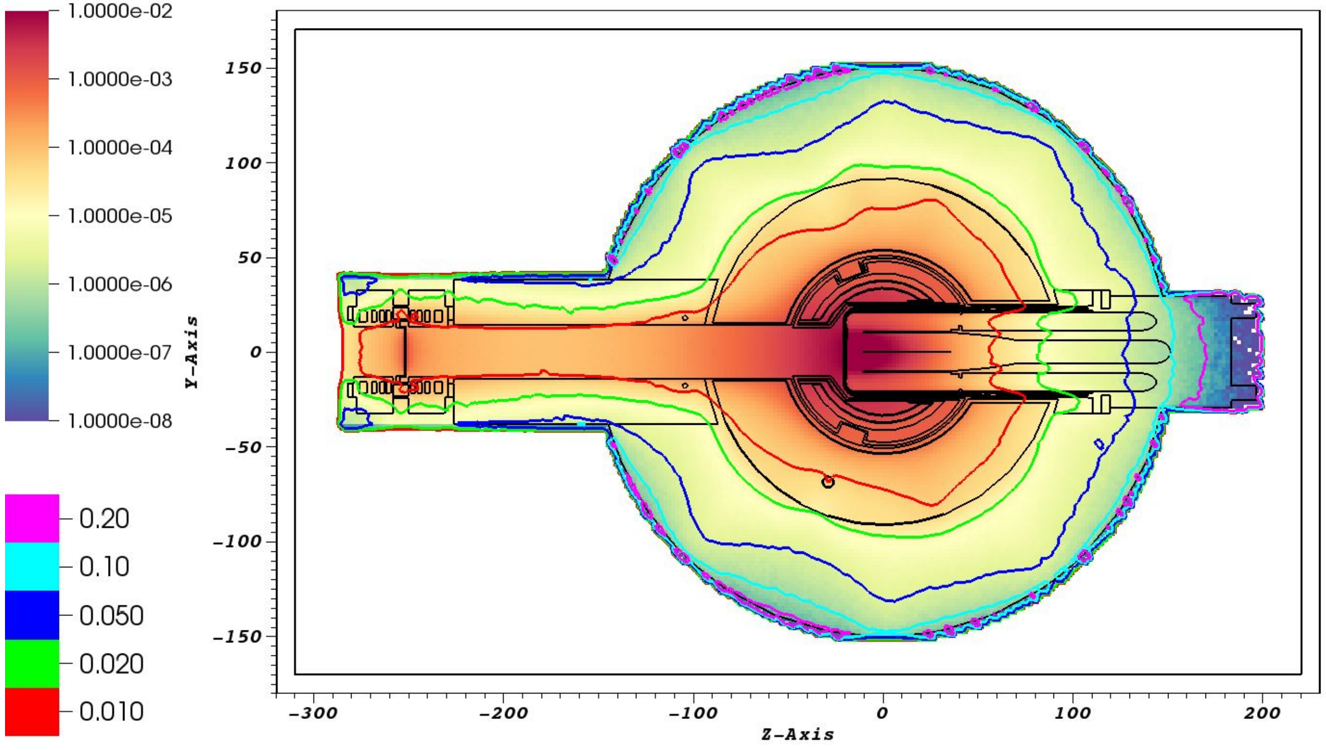
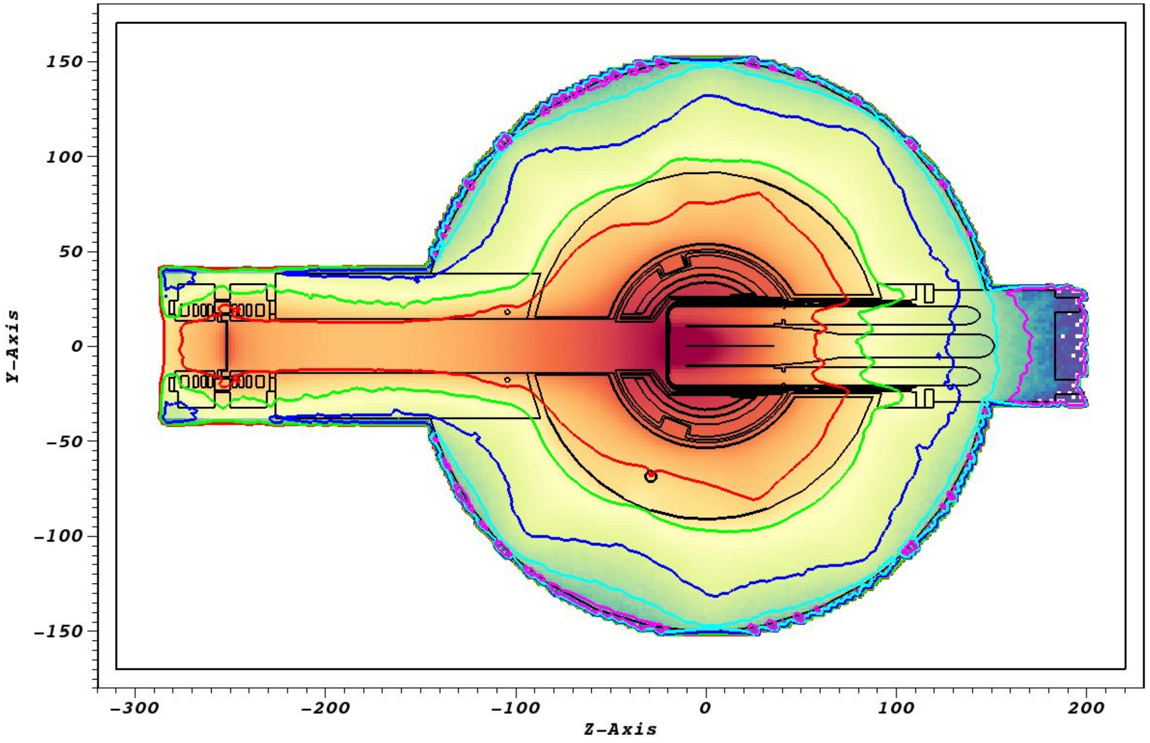
DAG-MCNP6 SNS

UK Atomic Energy Authority

MCNP6



DAG-MCNP6



Photon Flux

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Specific Tally Comparison in SNS

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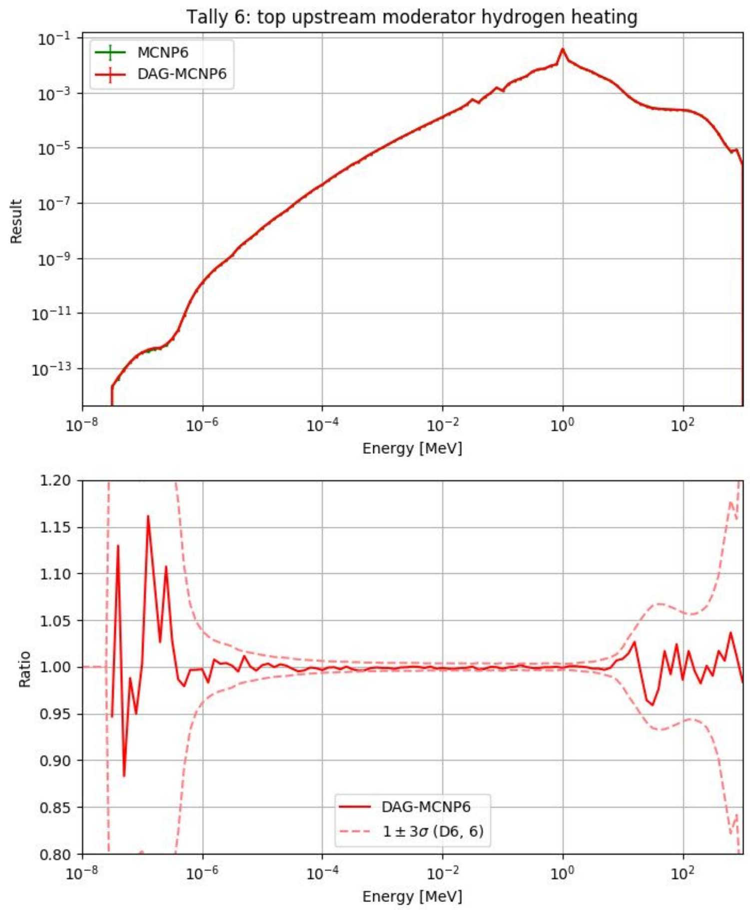

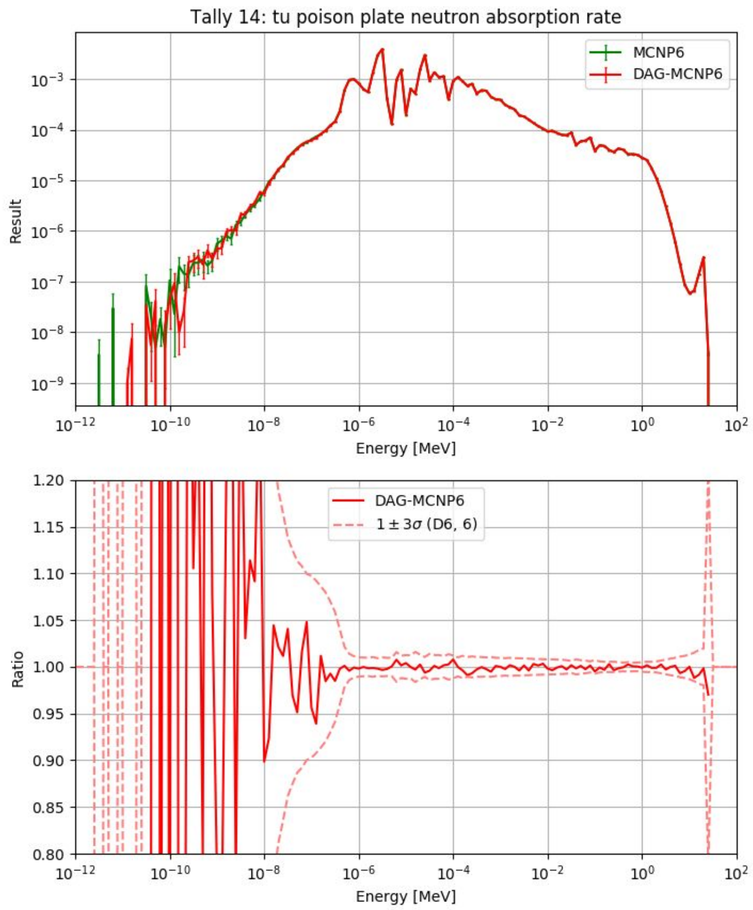

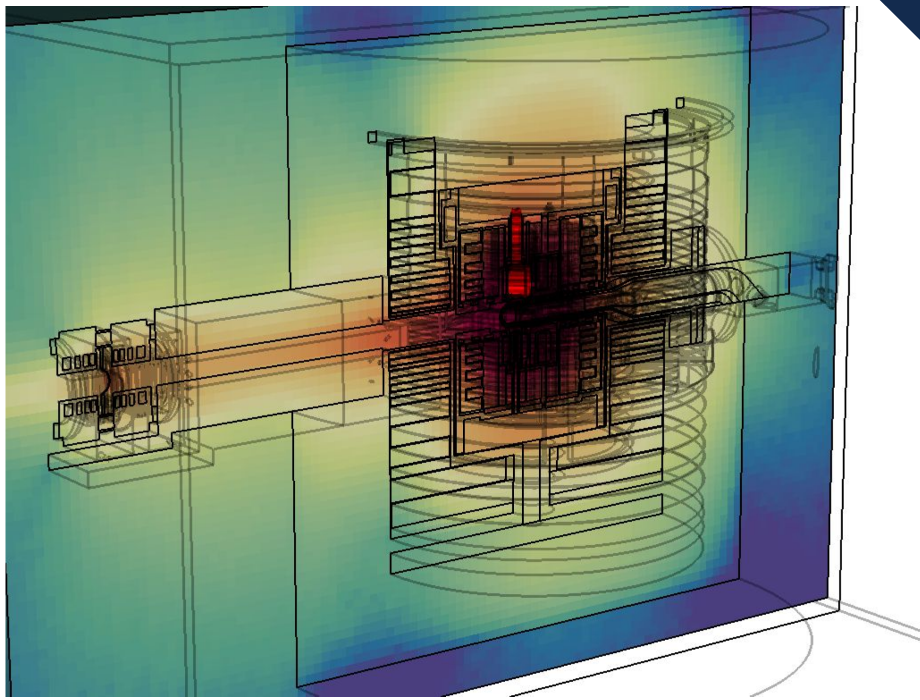

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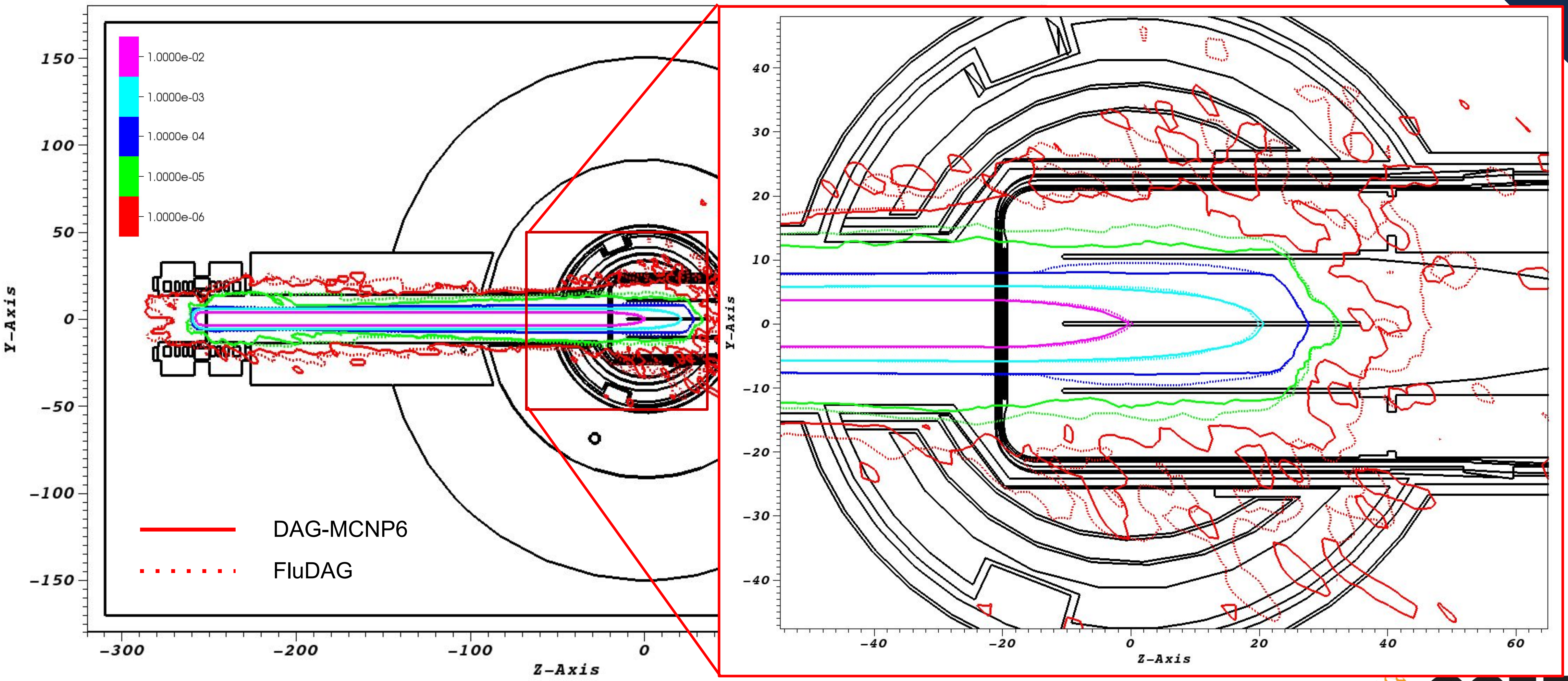
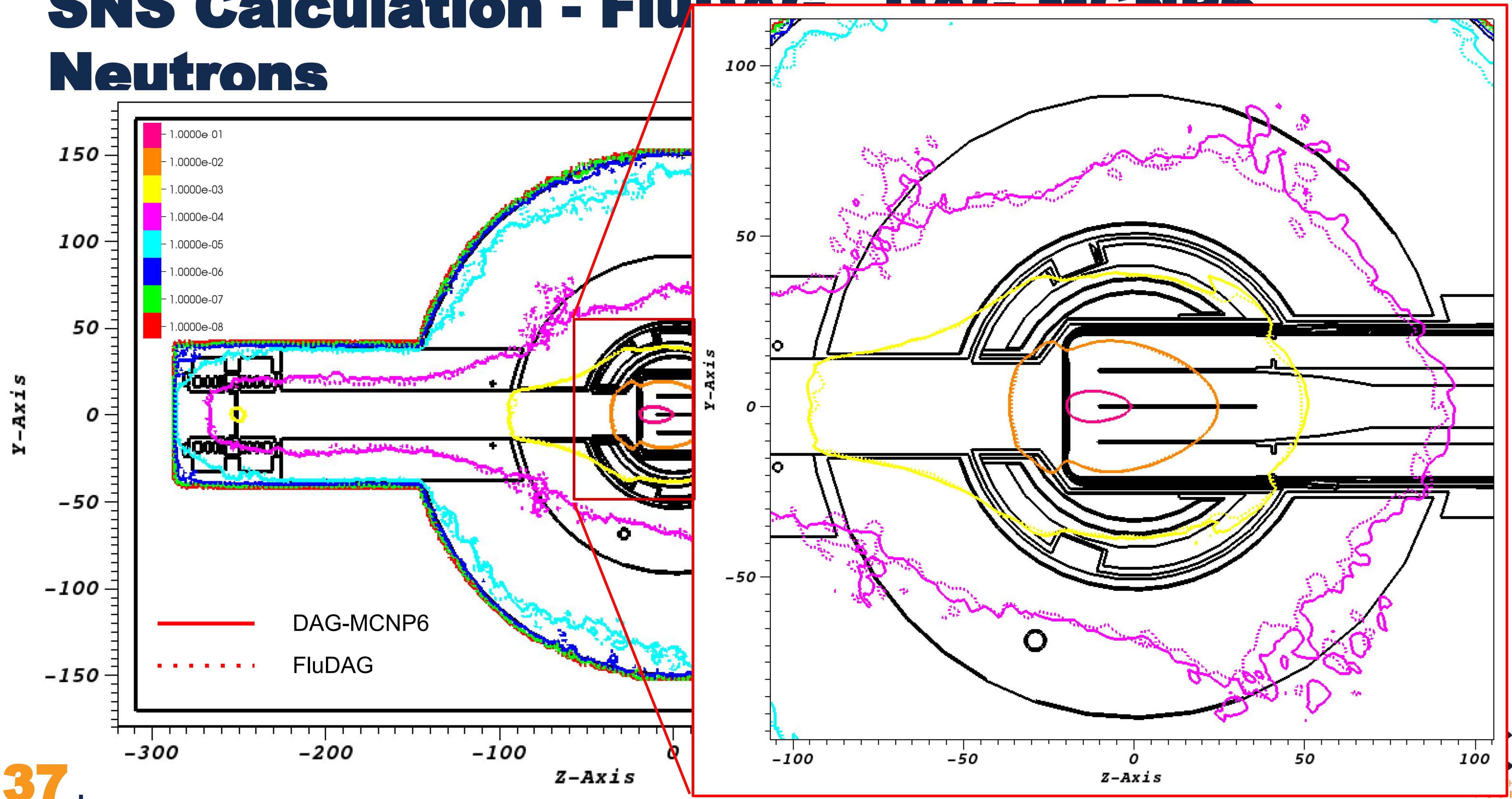
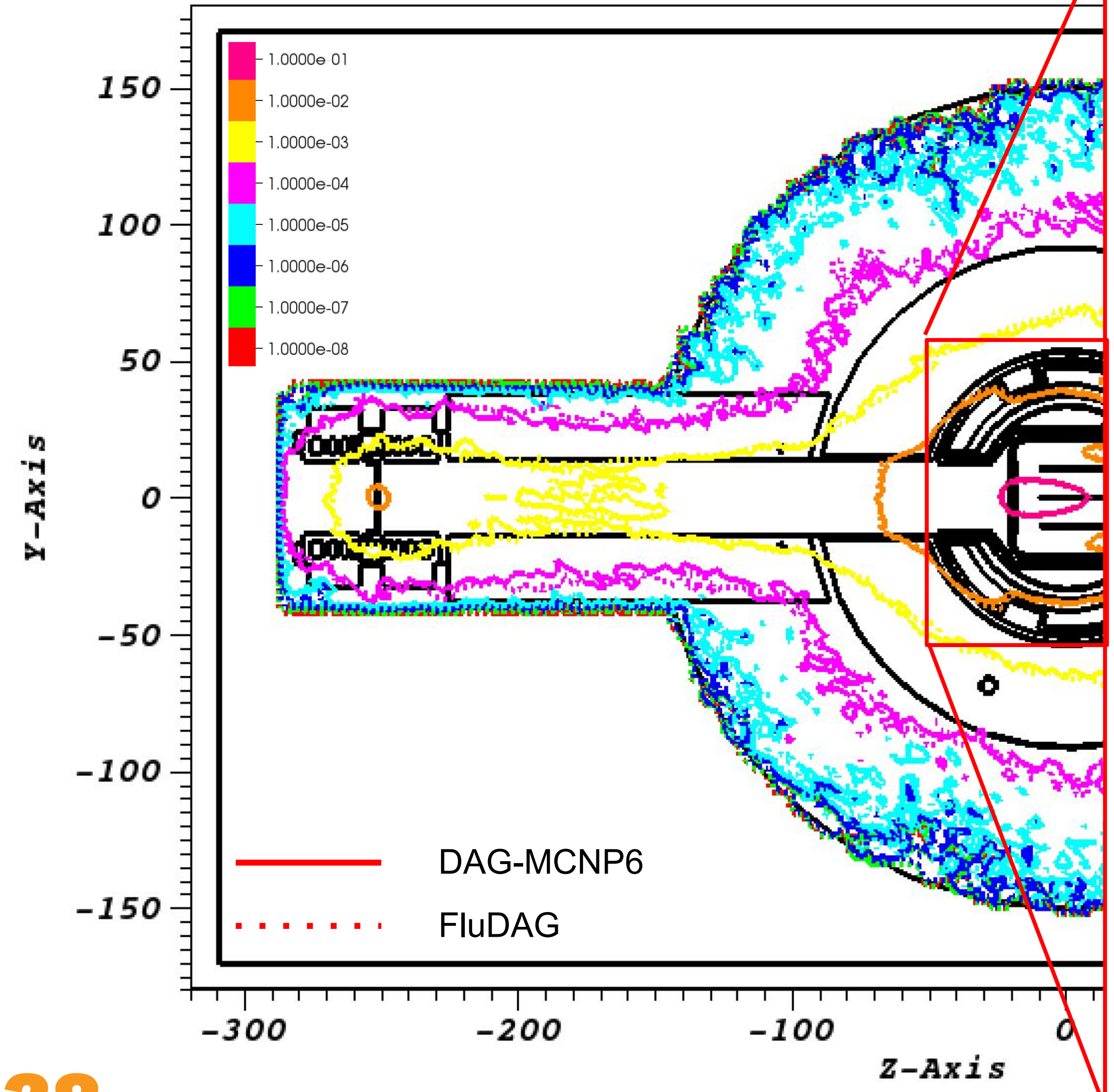
SNS Calculation - FluDAG/DAG-MCNP6 - Protons

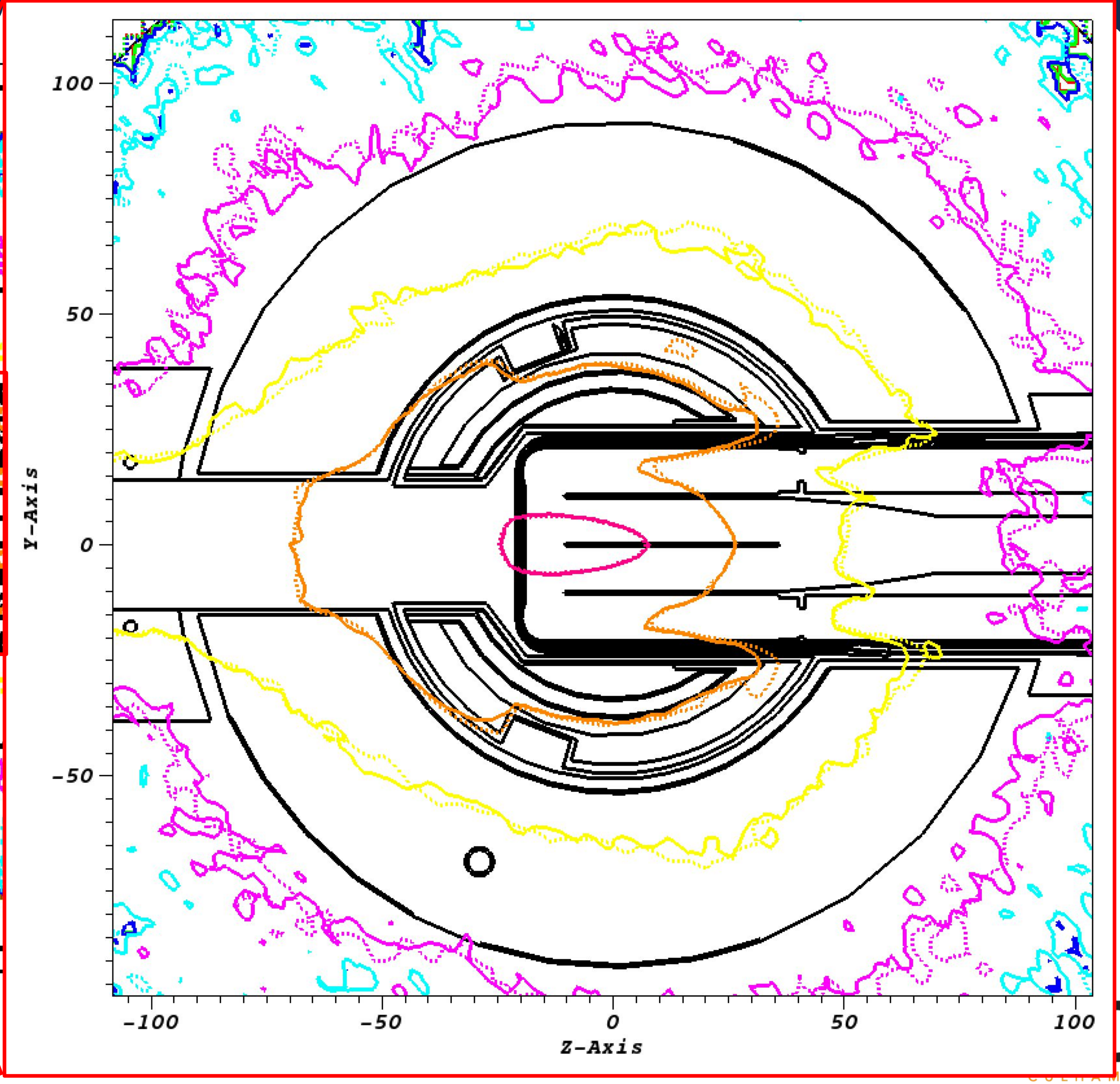


SNS Calculation - FluDAG - DAG-MCNP6 Neutrons



SNS Calculation - FluDAG – DAG-MCNP6 – Photon

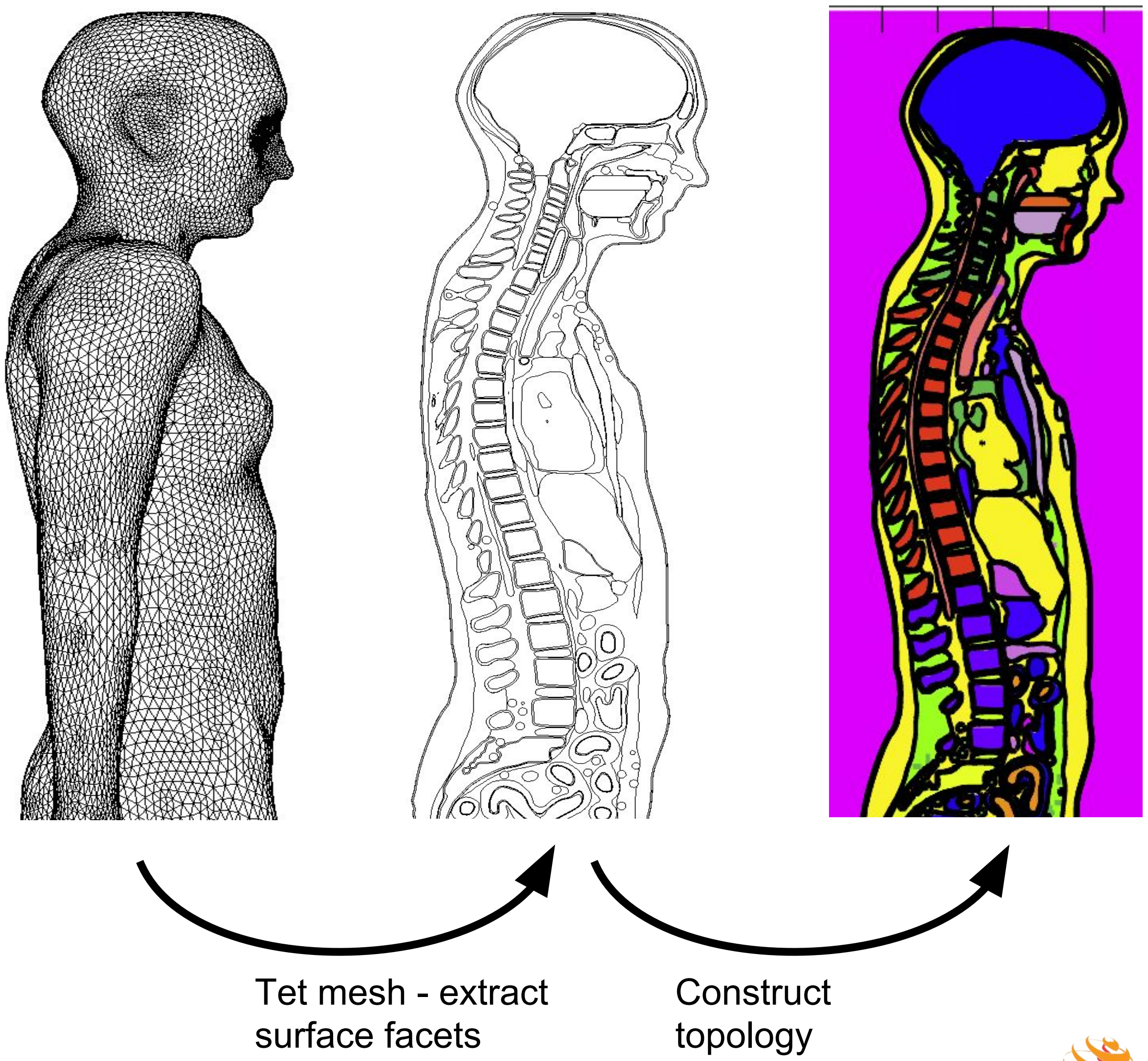




Human Mesh Phantom

UK Atomic Energy Authority

- Adult female **M**esh-type ICRP **R**eference **C**omputational **P**hantom
- Created by HUREL @ Hanyang University
- 2.6 million triangular facets
- Tet mesh originally - extract surface triangles



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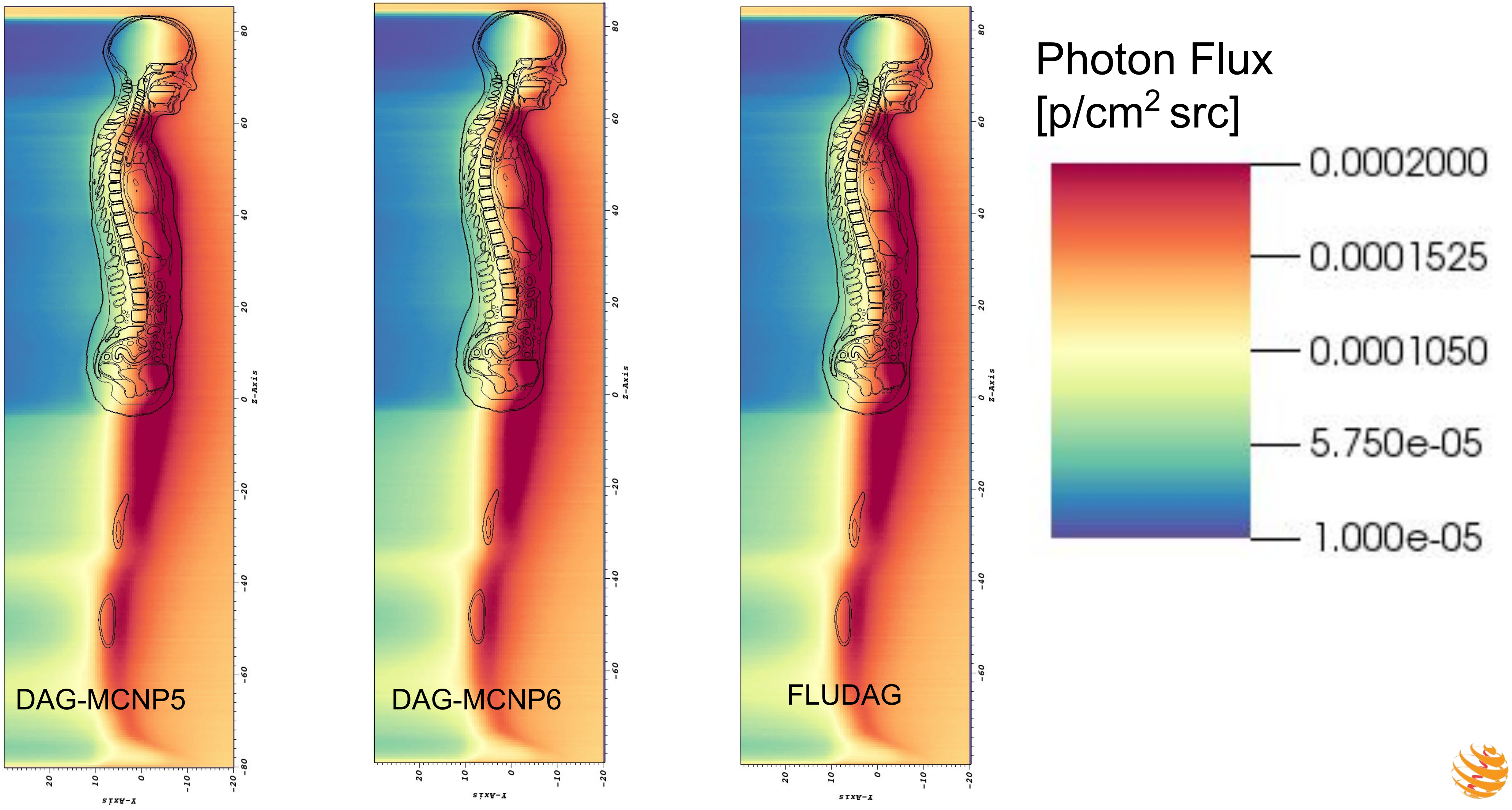
Human Mesh Phantom

Results: 0.1 MeV Photon Source



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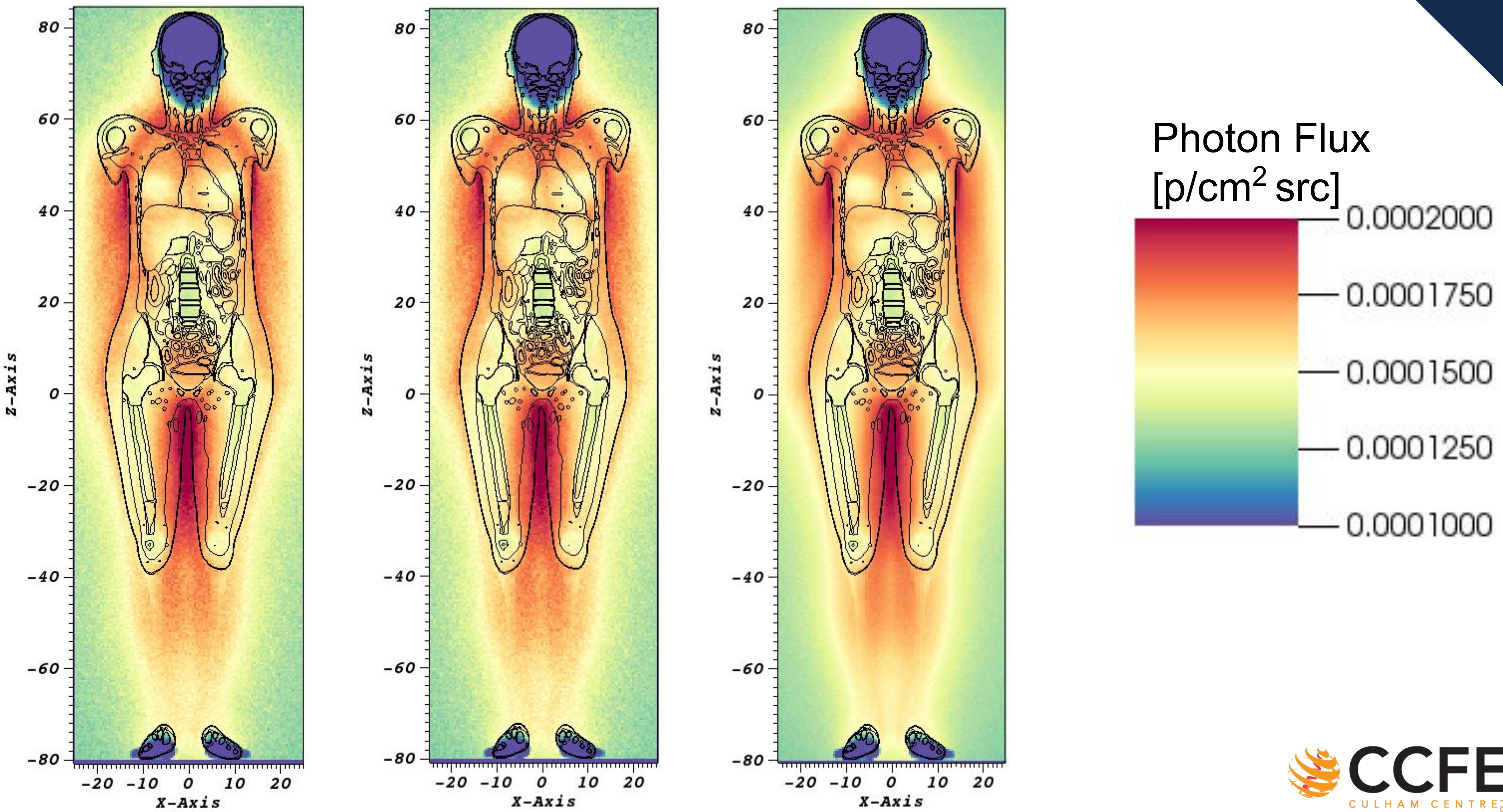
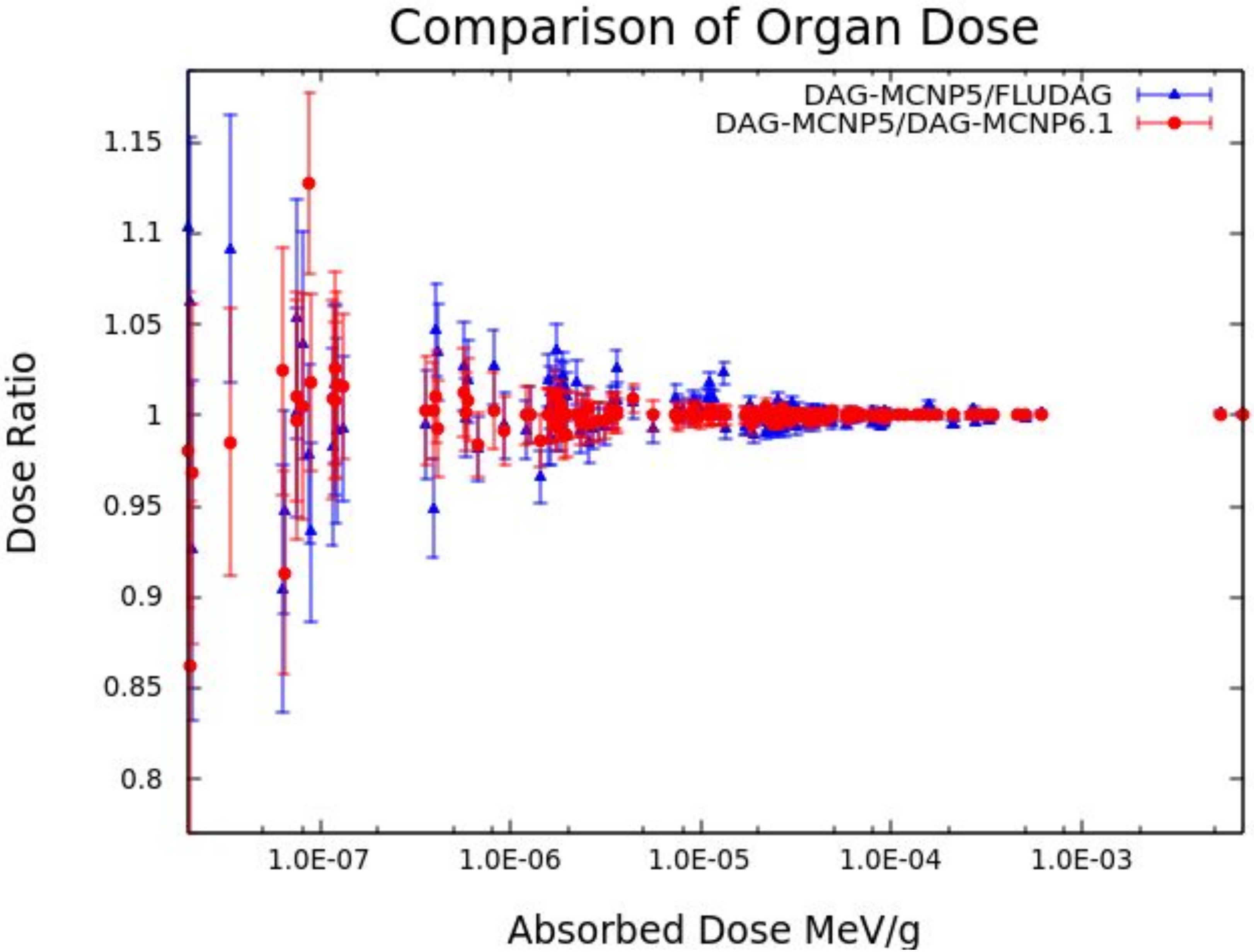
Human Mesh Phantom



Human Mesh Phantom



ATIC Benchmark

NASA Radiation Detector flown on high altitude balloon Advanced Thin Ionization Calorimeter (ATIC), used to measure cosmic ray spectra

Relatively complex & intricate geometry

- ~ 6200 volumes

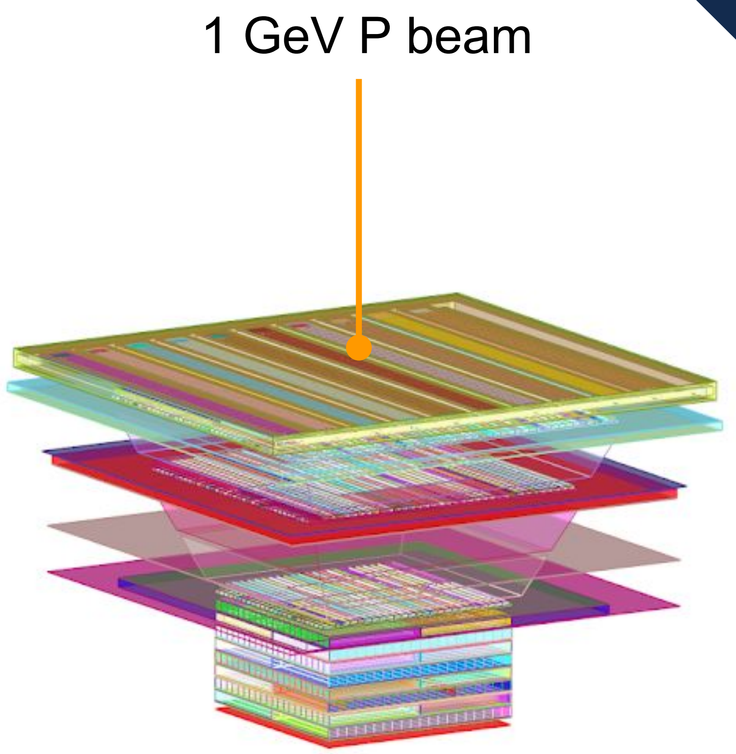
Used as acceptance case to validate FluDAG

- Results expected to match exactly with Fluka results.

Layers of Silicon, Mylar, Aluminium, BiGeO

1 GeV protons incident from above the geometry

Interested in Proton Flux, Neutron Flux, Photon Flux, Energy Deposition and a few others



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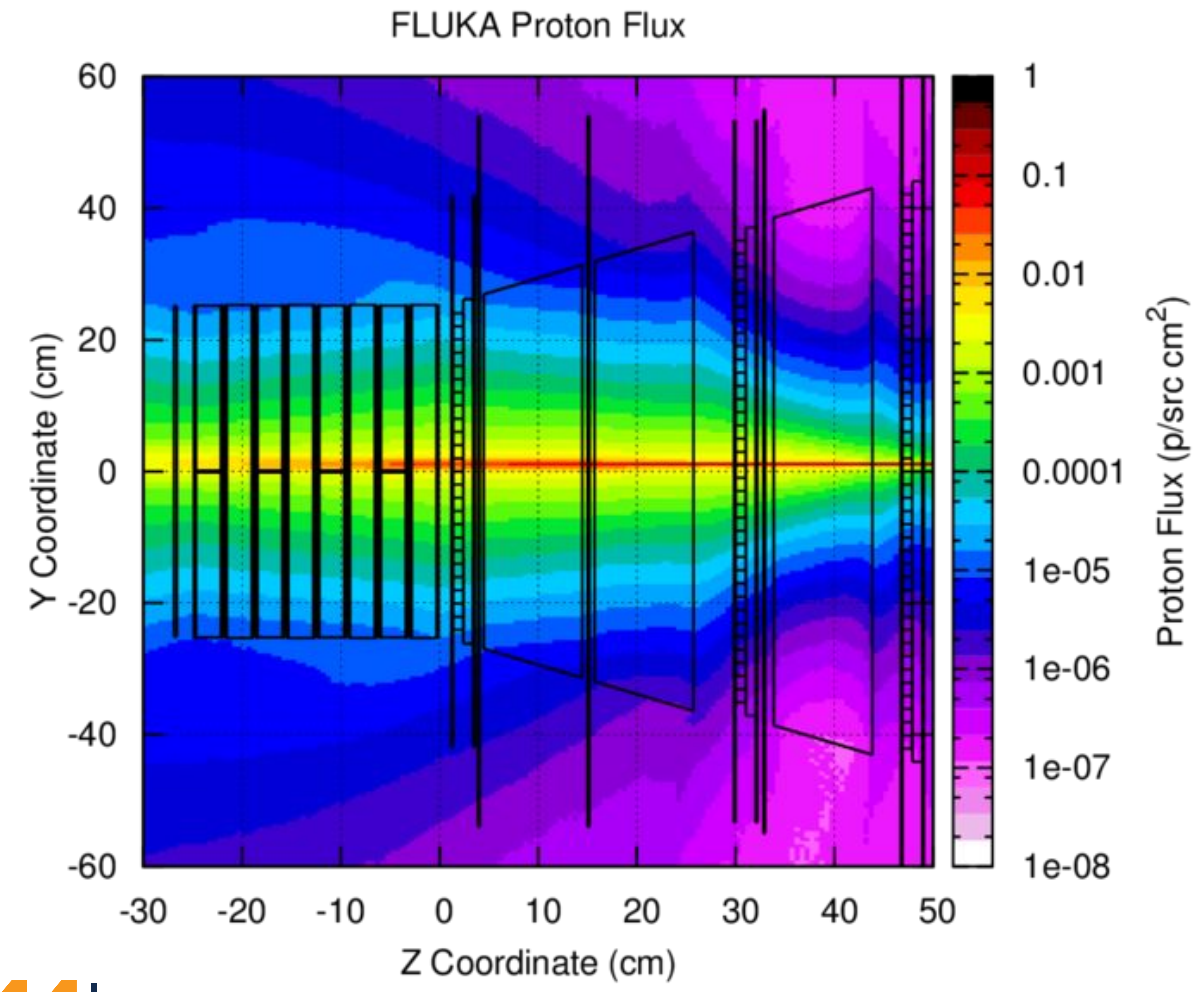
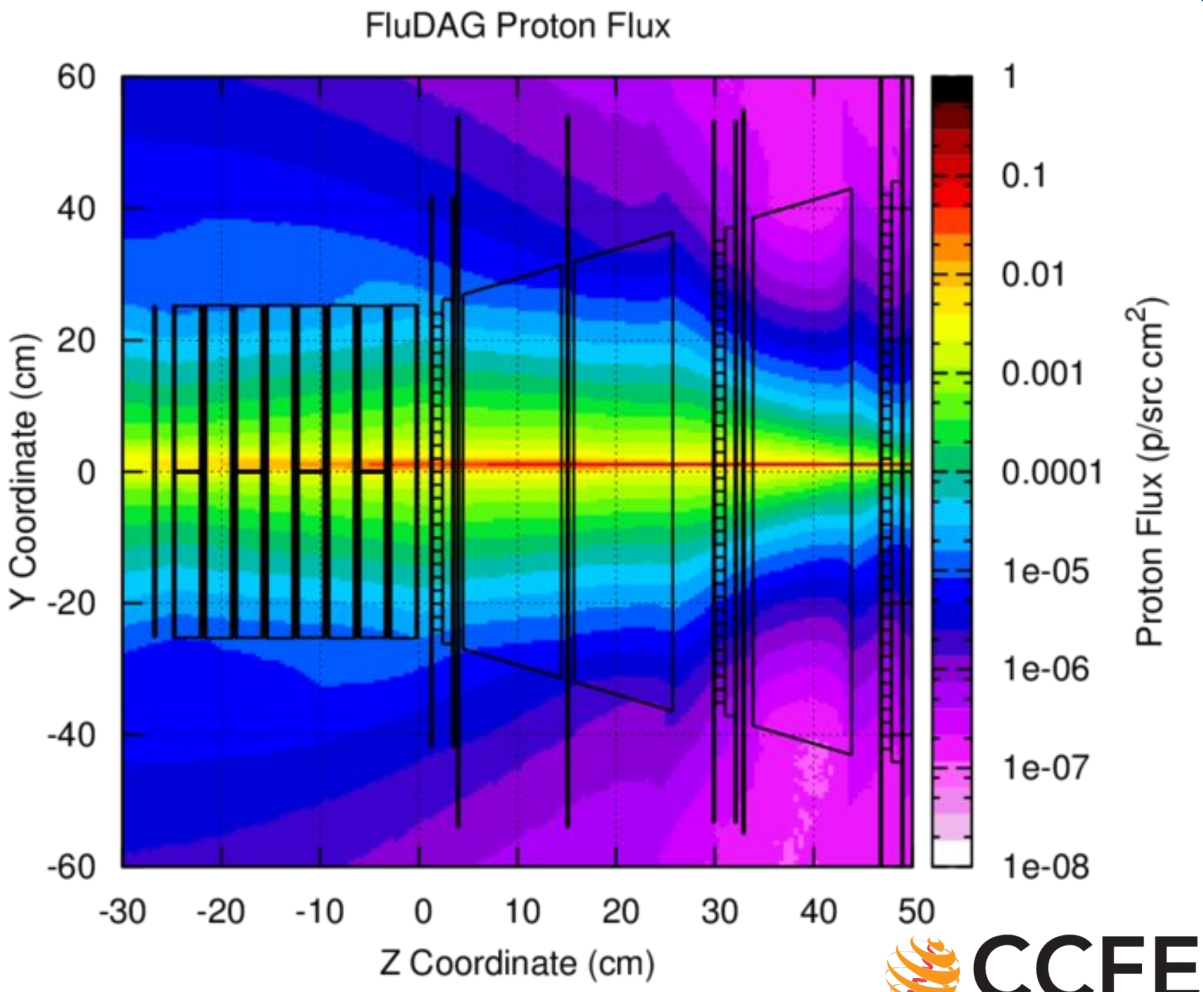
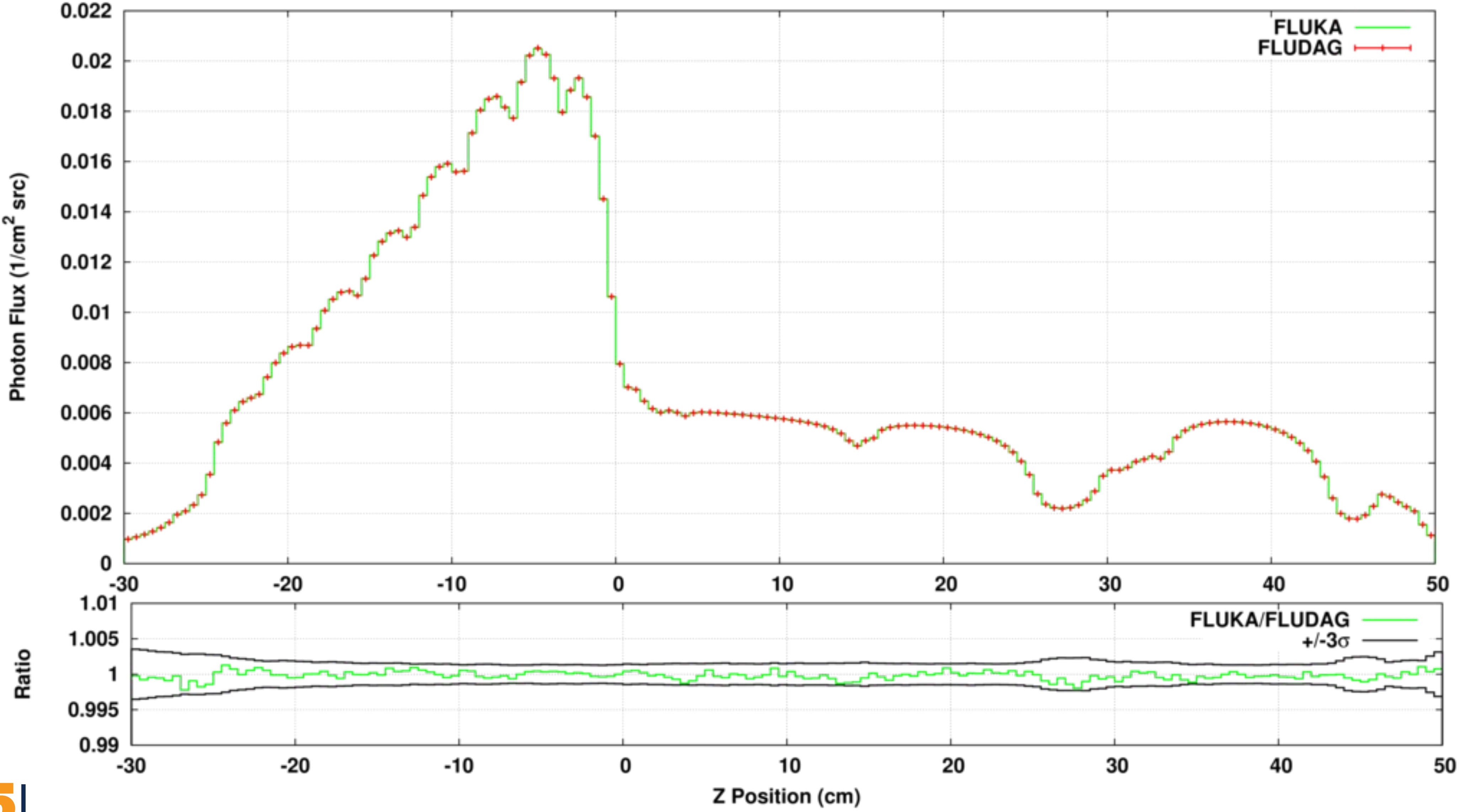
Proton Flux

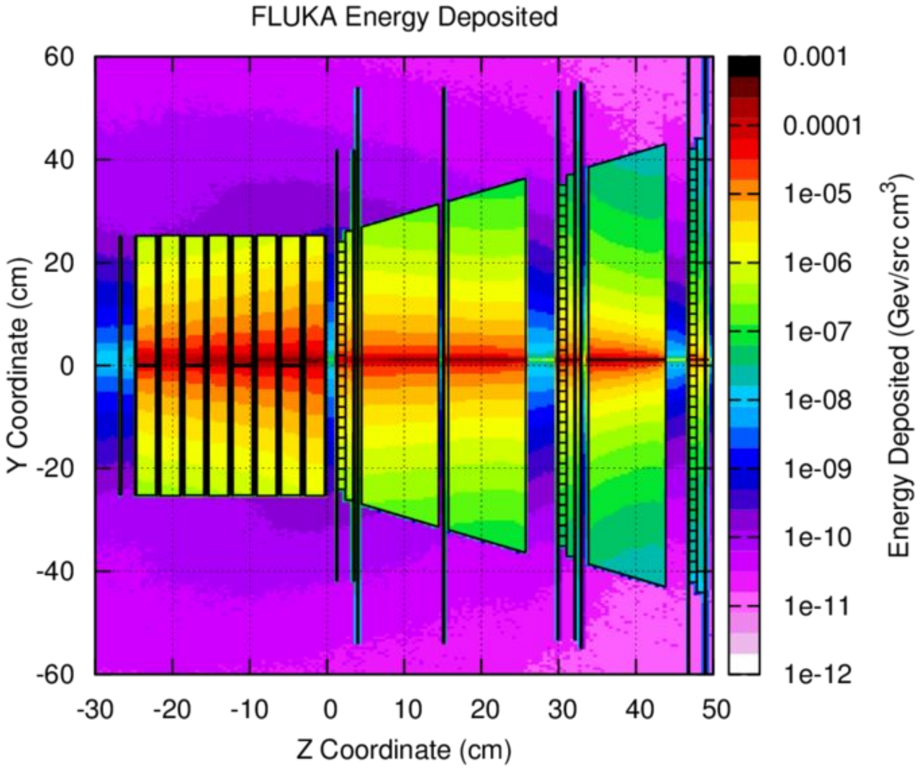

FLUKA Proton Flux
60
40
20
0
-20
-40
-60
Y Coordinate (cm)
-30 -20 -10 0 10 20 30 40 50
Z Coordinate (cm)
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
Proton Flux (p/src cm^2)

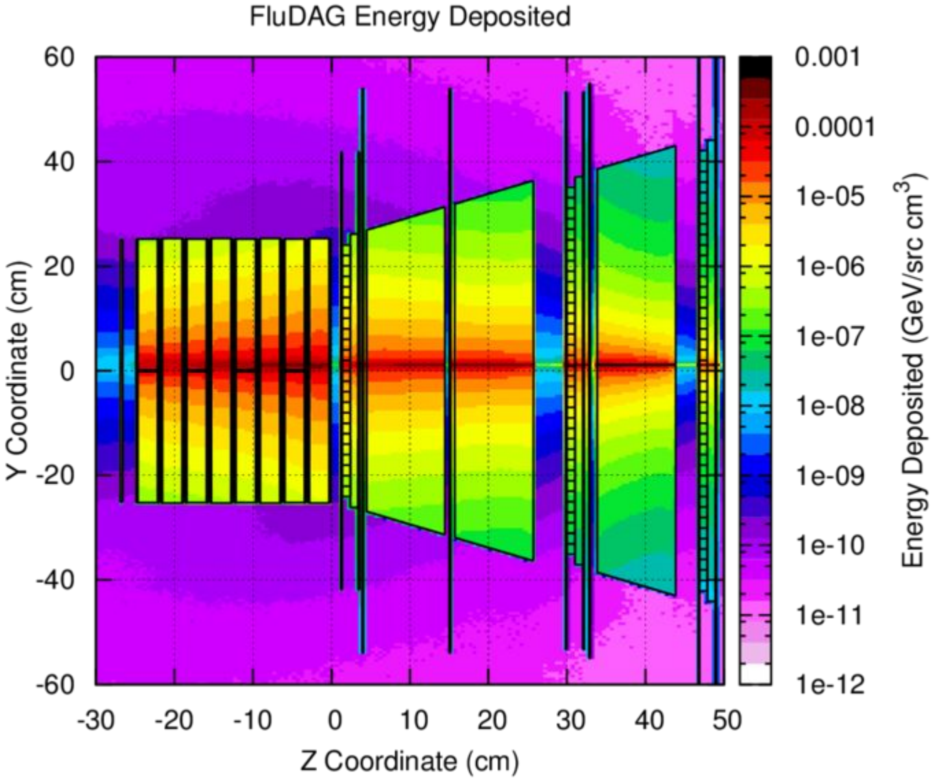

FluDAG Proton Flux
60
40
20
0
-20
-40
-60
Y Coordinate (cm)
-30 -20 -10 0 10 20 30 40 50
Z Coordinate (cm)
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
Proton Flux (p/src cm^2)

Proton flux lineout



Energy Deposition Profile





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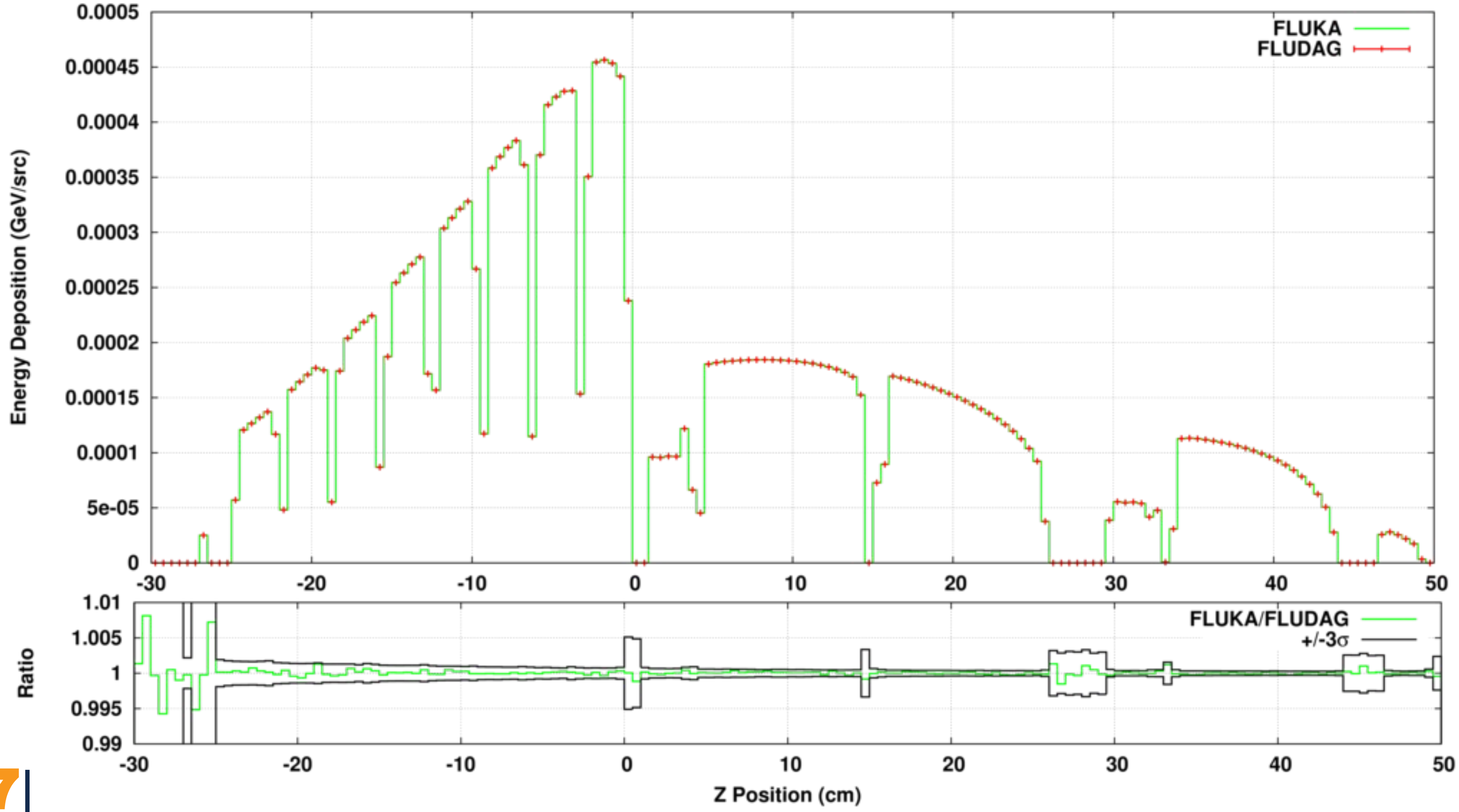
Energy Deposition lineout



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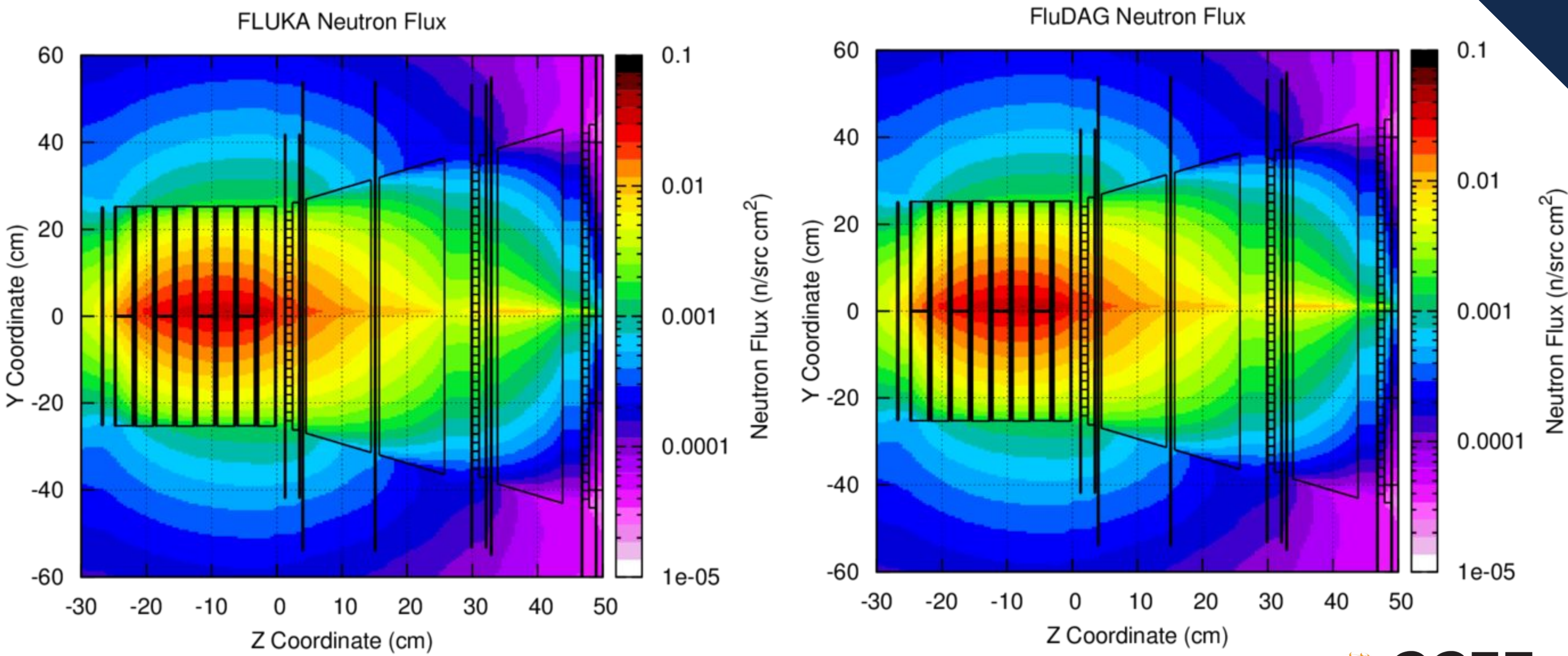
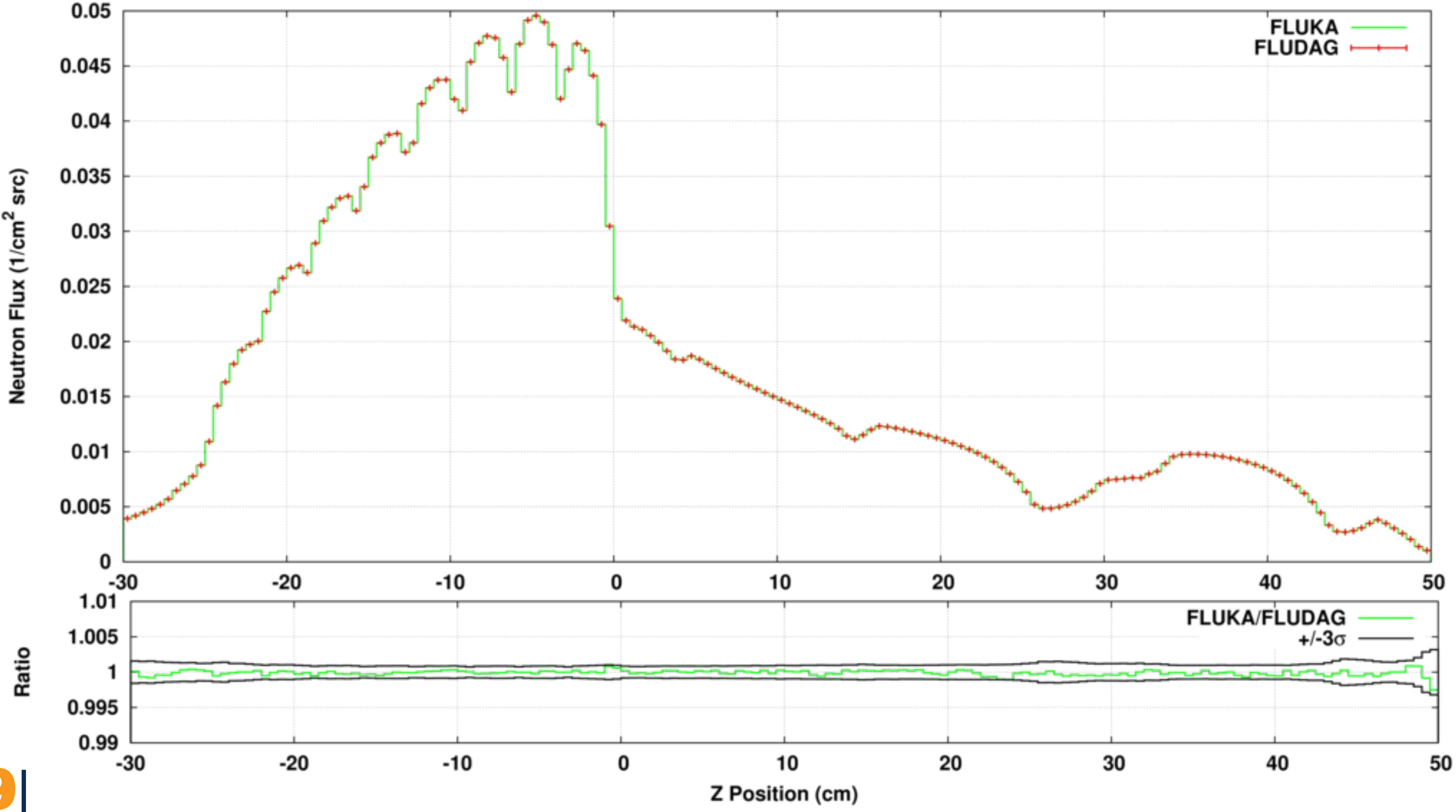
Neutron Flux Profile



Neutron flux lineout



High Energy Physics Example

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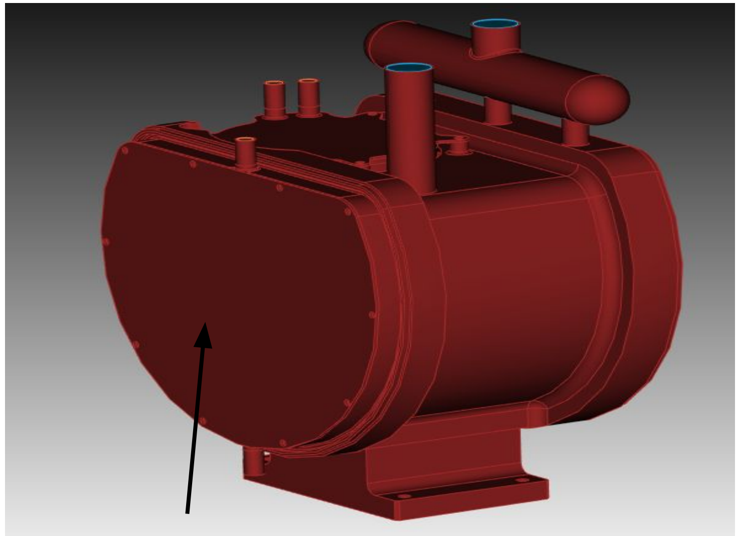
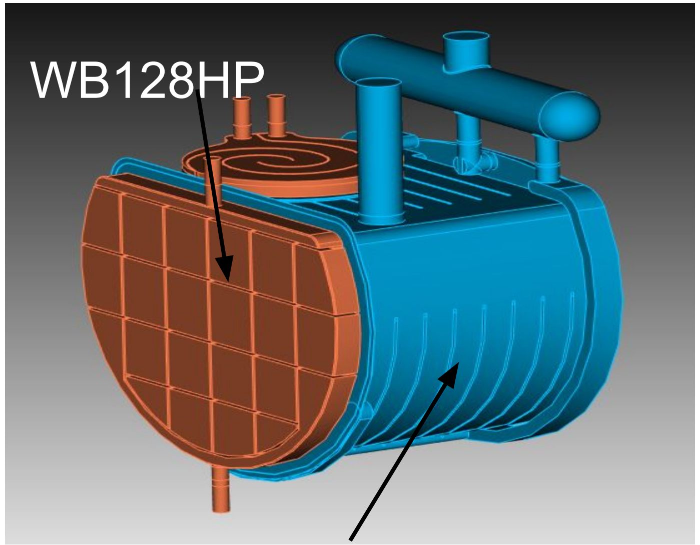
- 20 (ish) GeV proton beam onto a largely lead target
  - For a STEP file CAD was very clean :)
  - Needed some repairs in the spiral section
  - Model was rotated to the appropriate coordinate system and shifted



SS316LN



Water

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nTOF Geometry

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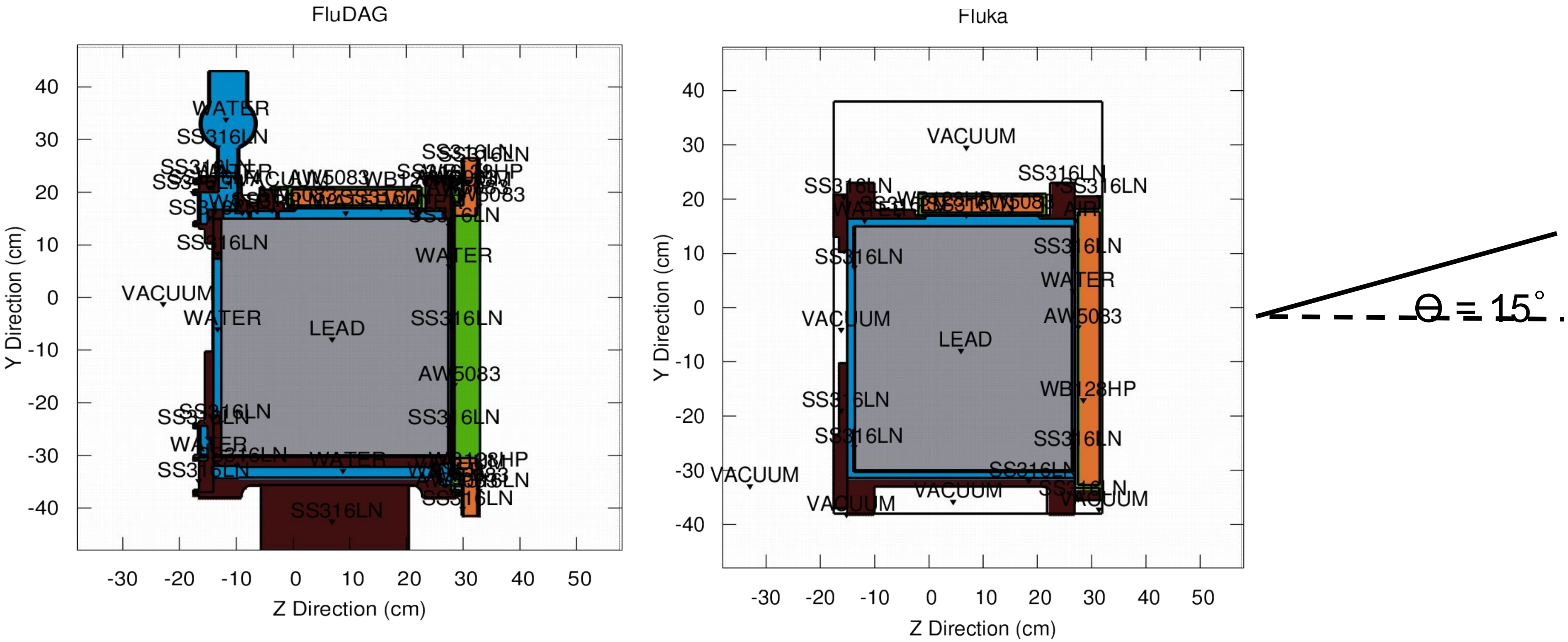

Slice through x=0

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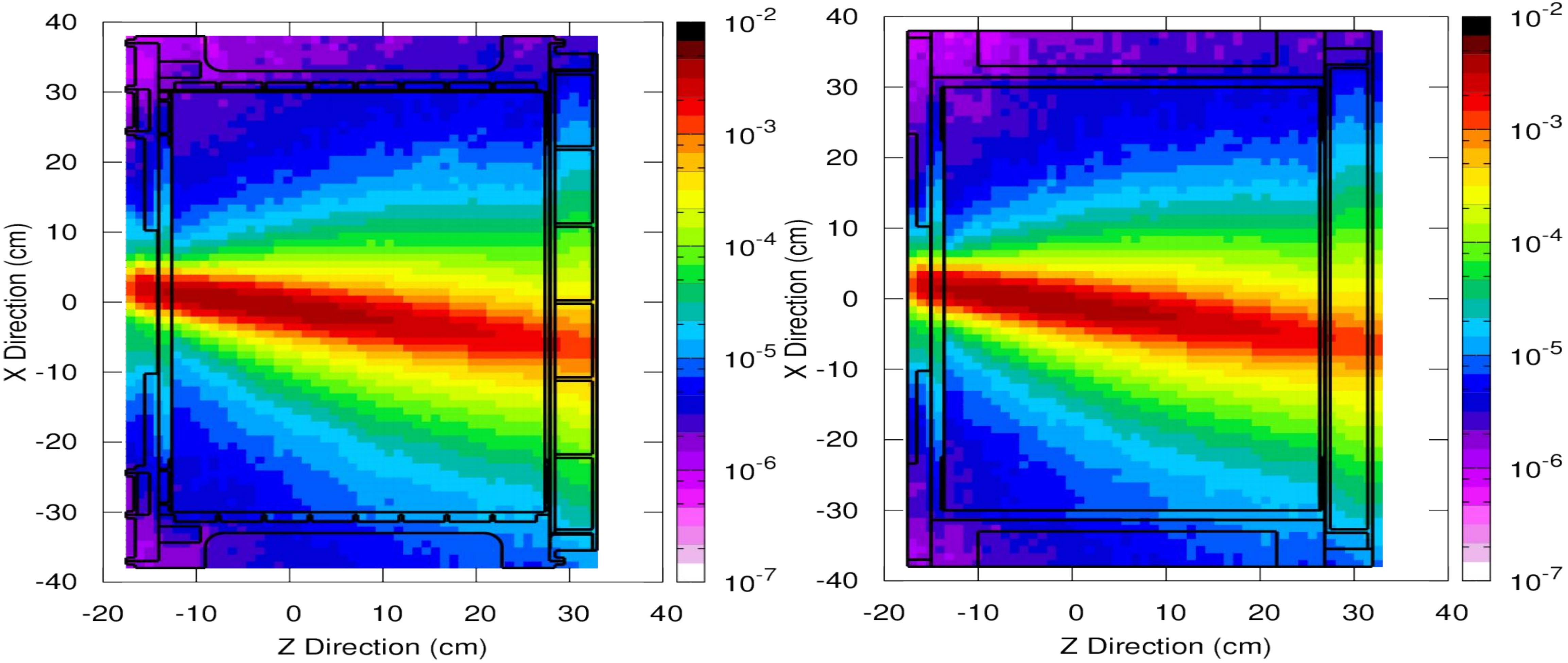
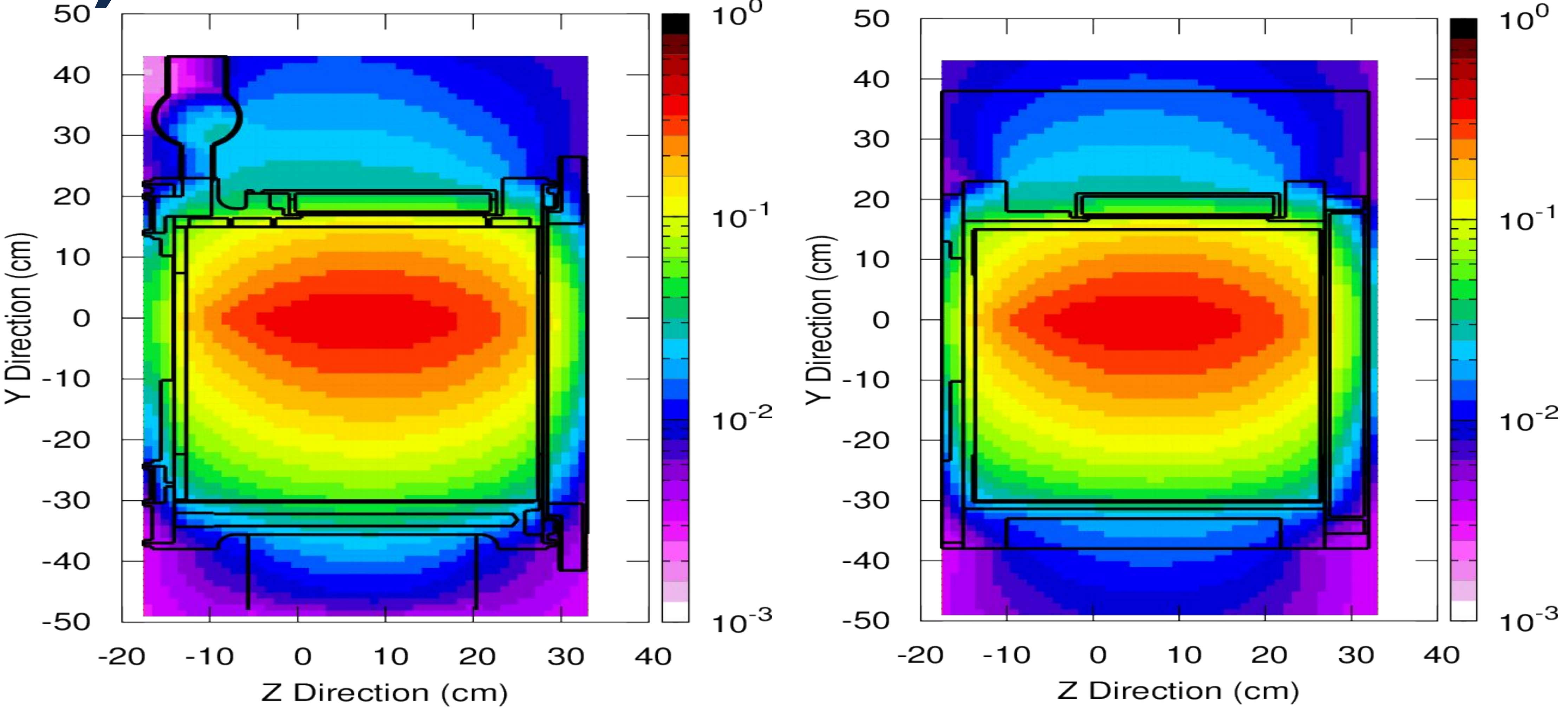
nTOF Comparisons - Proton Flux



nTOF Comparisons - Neutron Flux (per src)



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nTOF Comparisons - Neutron Spectrum

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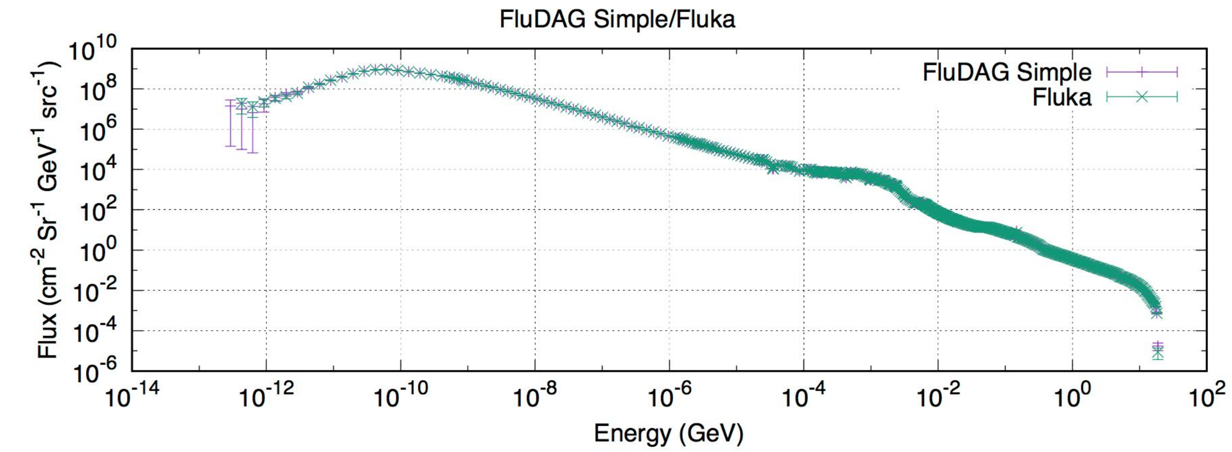

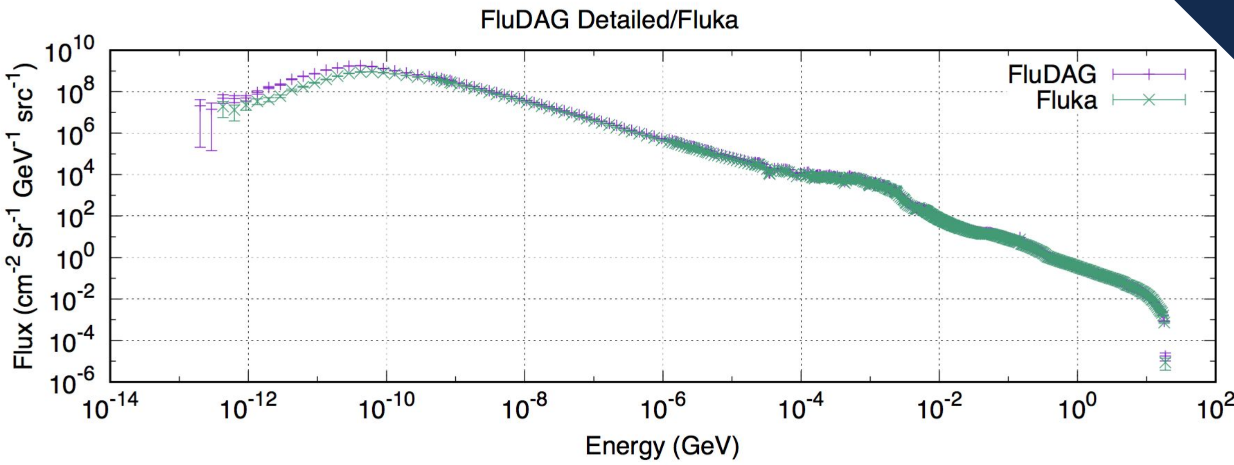

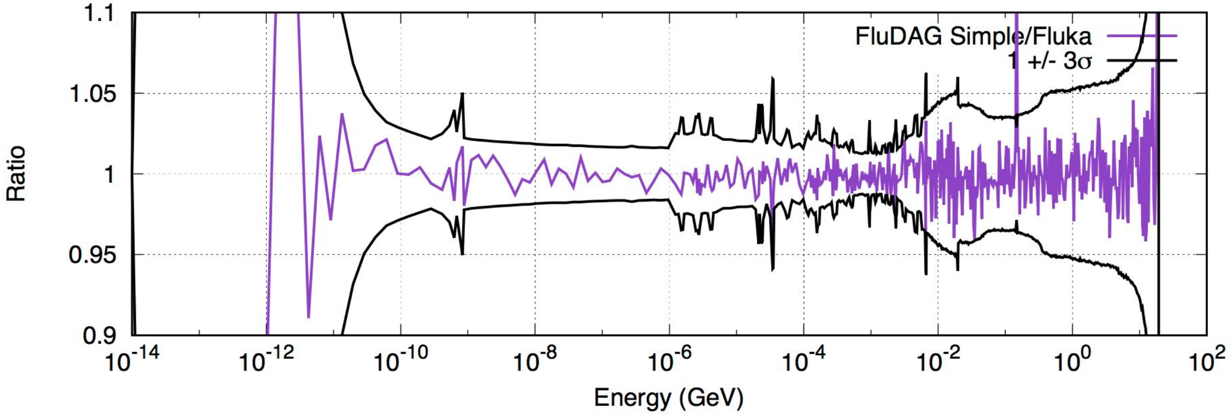

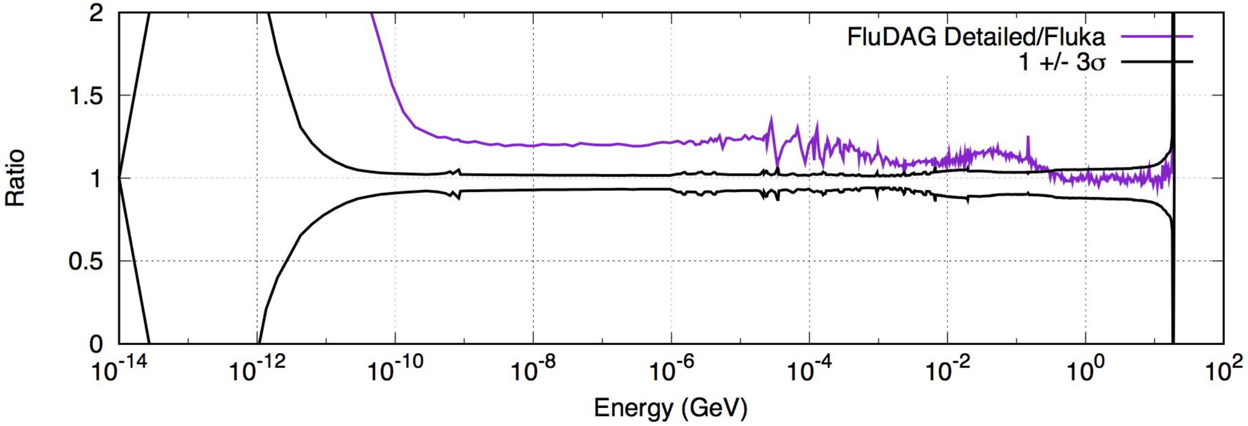

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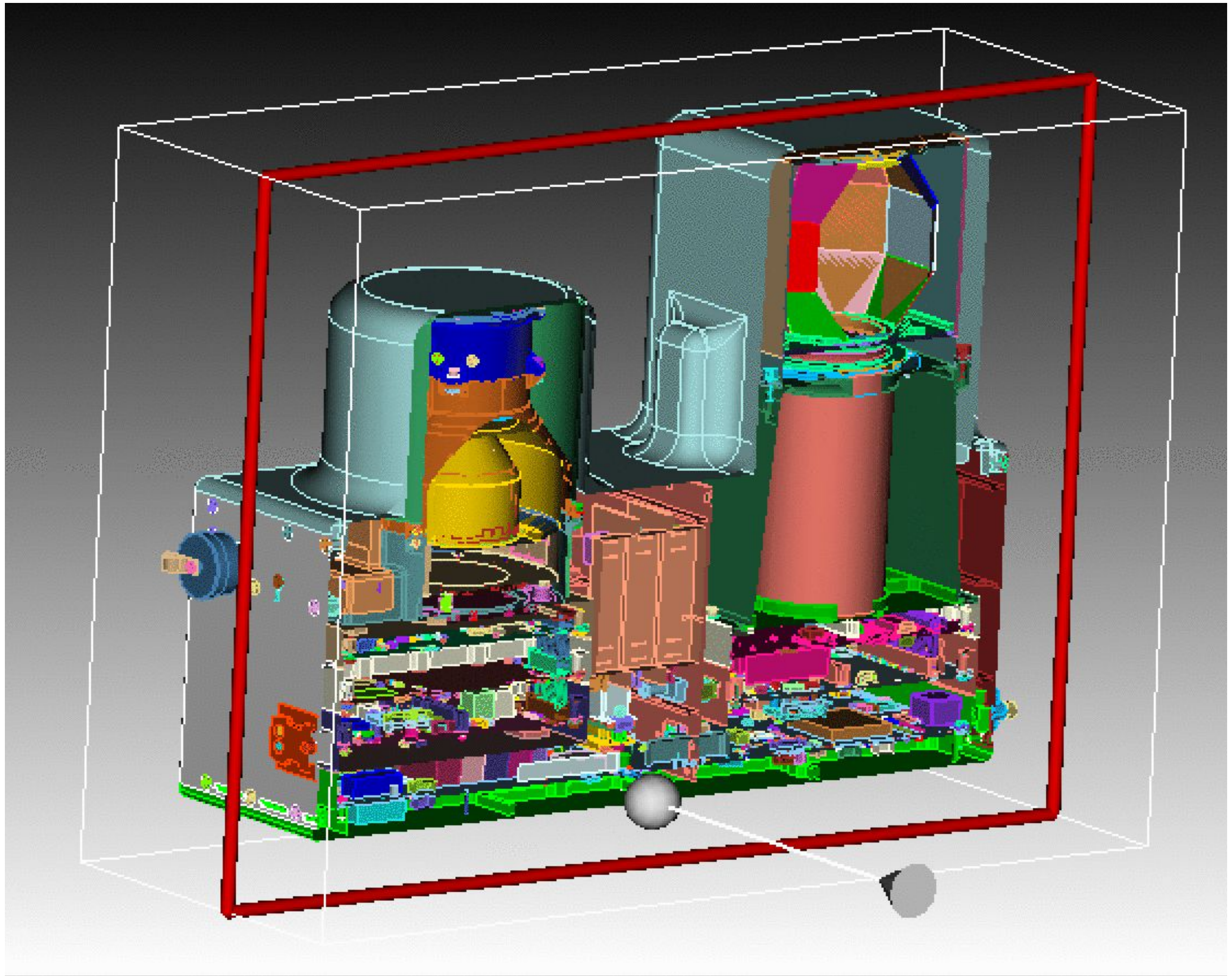
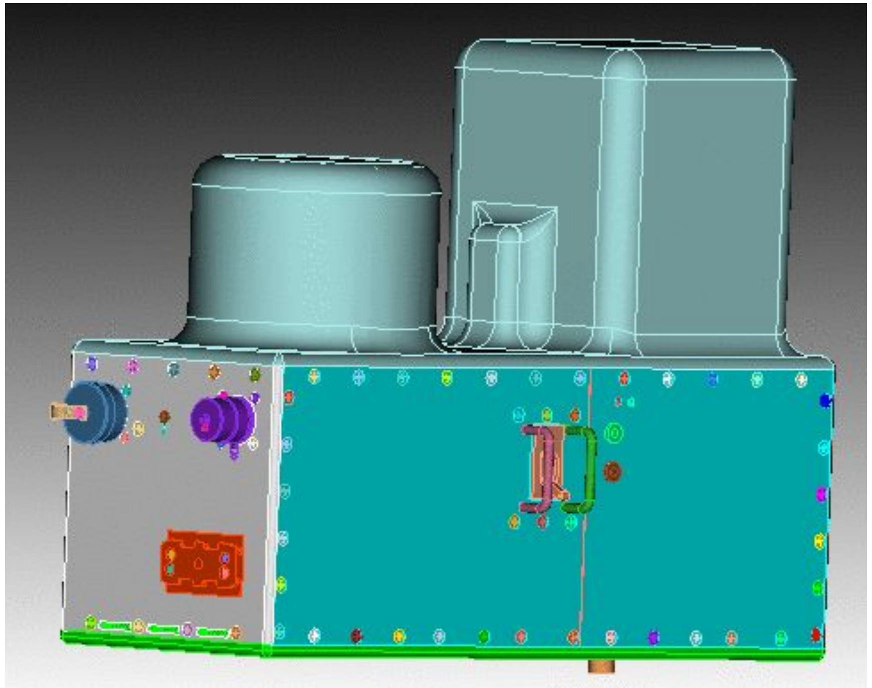
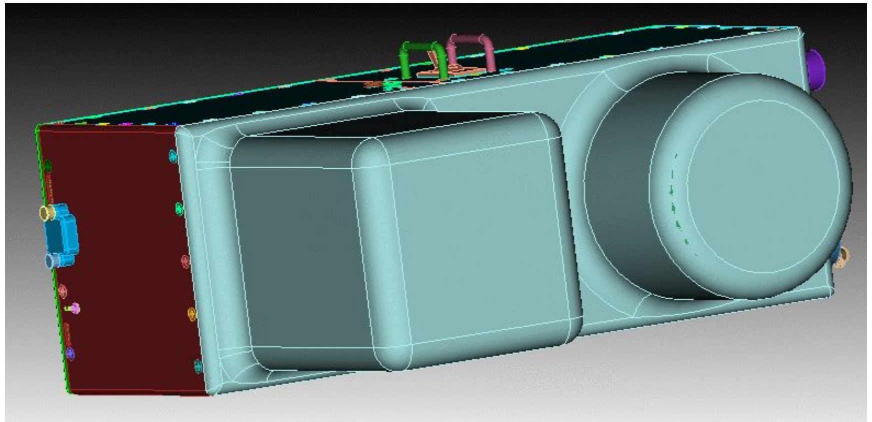
Space Radiation Example

- NASA wanted to simulat the RAD detector that flies on the ISS
- CAD model taken from drawing office
  - Simplified in SpaceClaim (2 weeks)
  - Running in FLUDAG & DagGeant4

Space Radiation Example

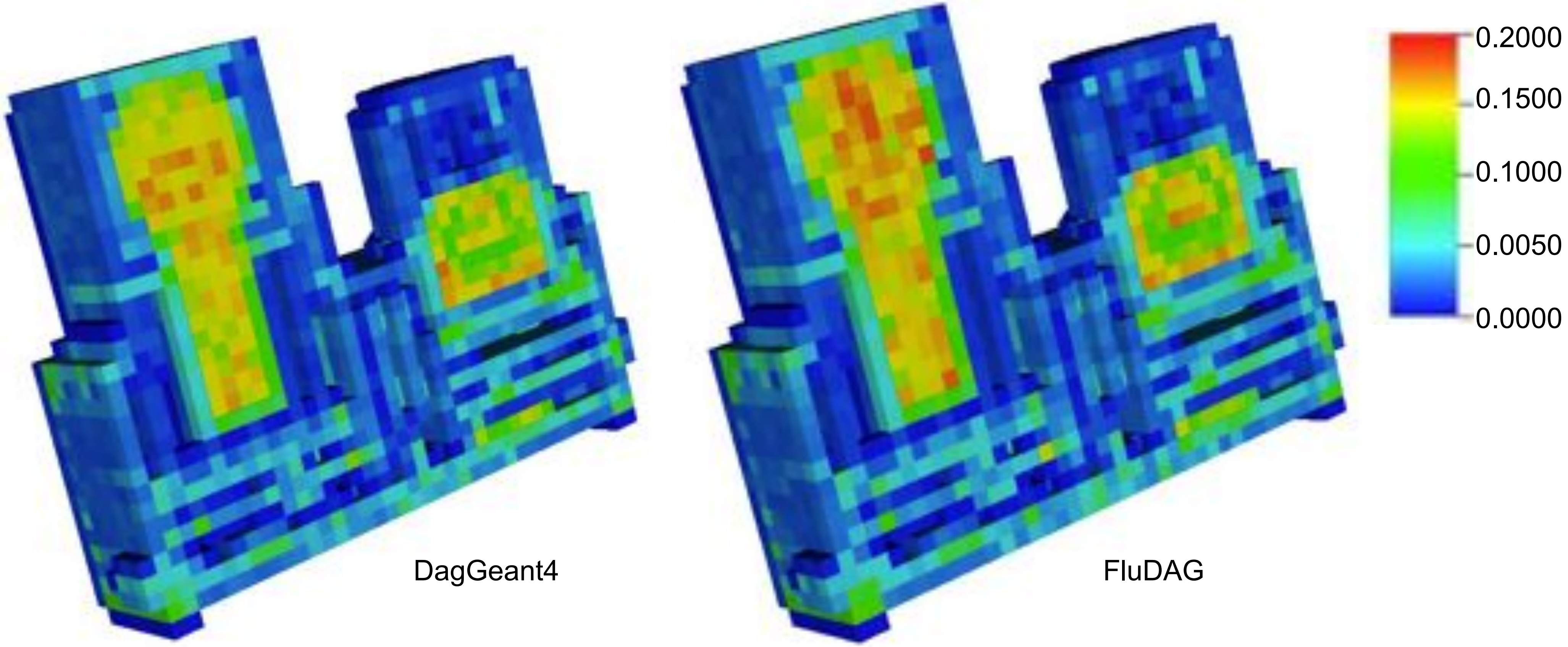






This work performed by SRAG - NASA

Space Radiation Example

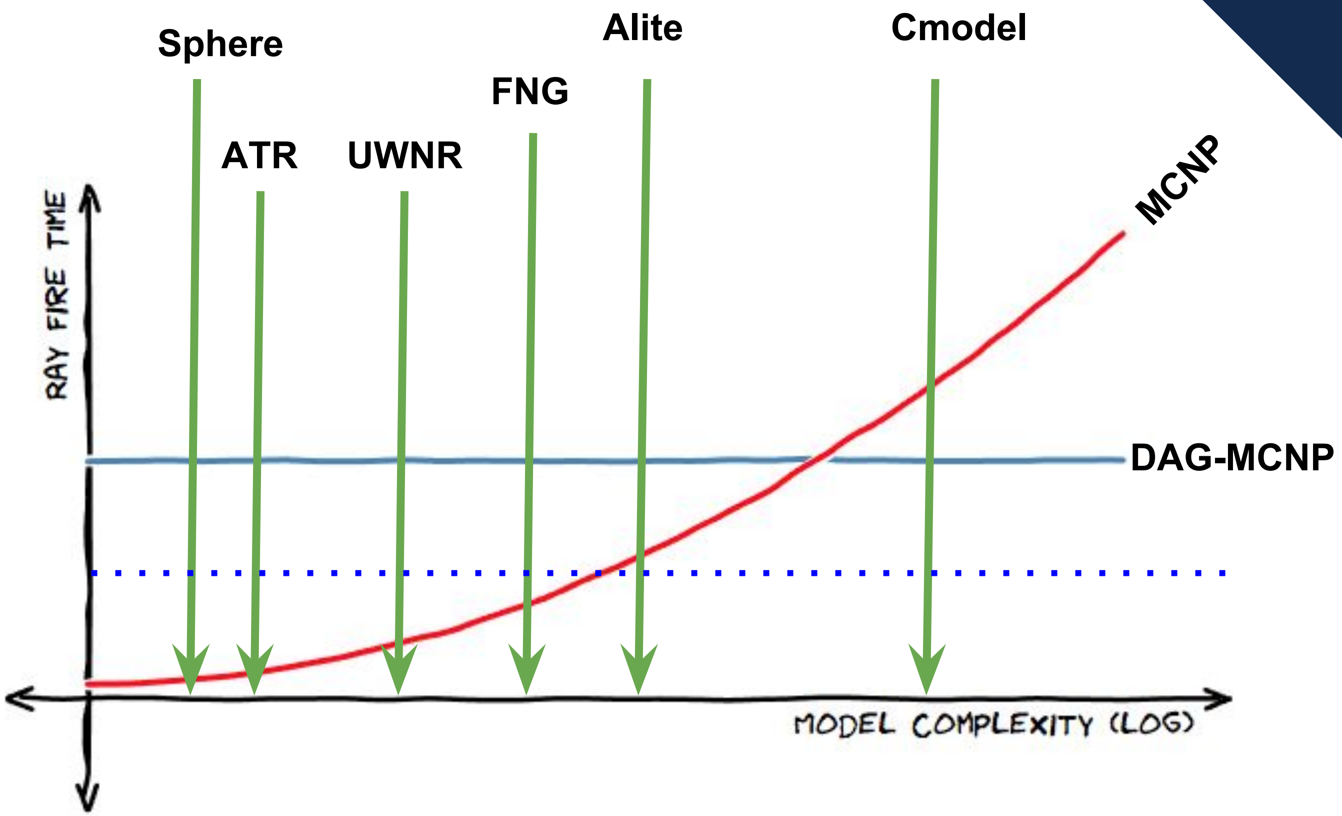


DagGeant4

FluDAG

The Future

- DAGMC is approaching being a finished project
- Work in progress
  - DAGMC ‘parallel’ universe
  - Cubitless workflow
  - MC code integration(s)
  - Integration of DAGMC like workflov using NVidia OPTIX as ray fire engine
- CERN are interested in integration DAGMC directly into Geant4 as a prime geometry member
- Argonne National Lab want the san for OpenMC



Advantages of DAGMC

- Faster model creation time
- Easier integration with existing CAD models
- MC Code independence
- Not native MCNP
- Stresses the right part of the workflow (CAD)
- Simple coupling with other multiphysics analysis
- Represents the boundary of the volume only
    - no expensive extraneous boundary crossings

Questions

Any questions, sorry for all the slides :)

andrew.davis@ukaea.uk

https://github.com/svalinn/dagmc