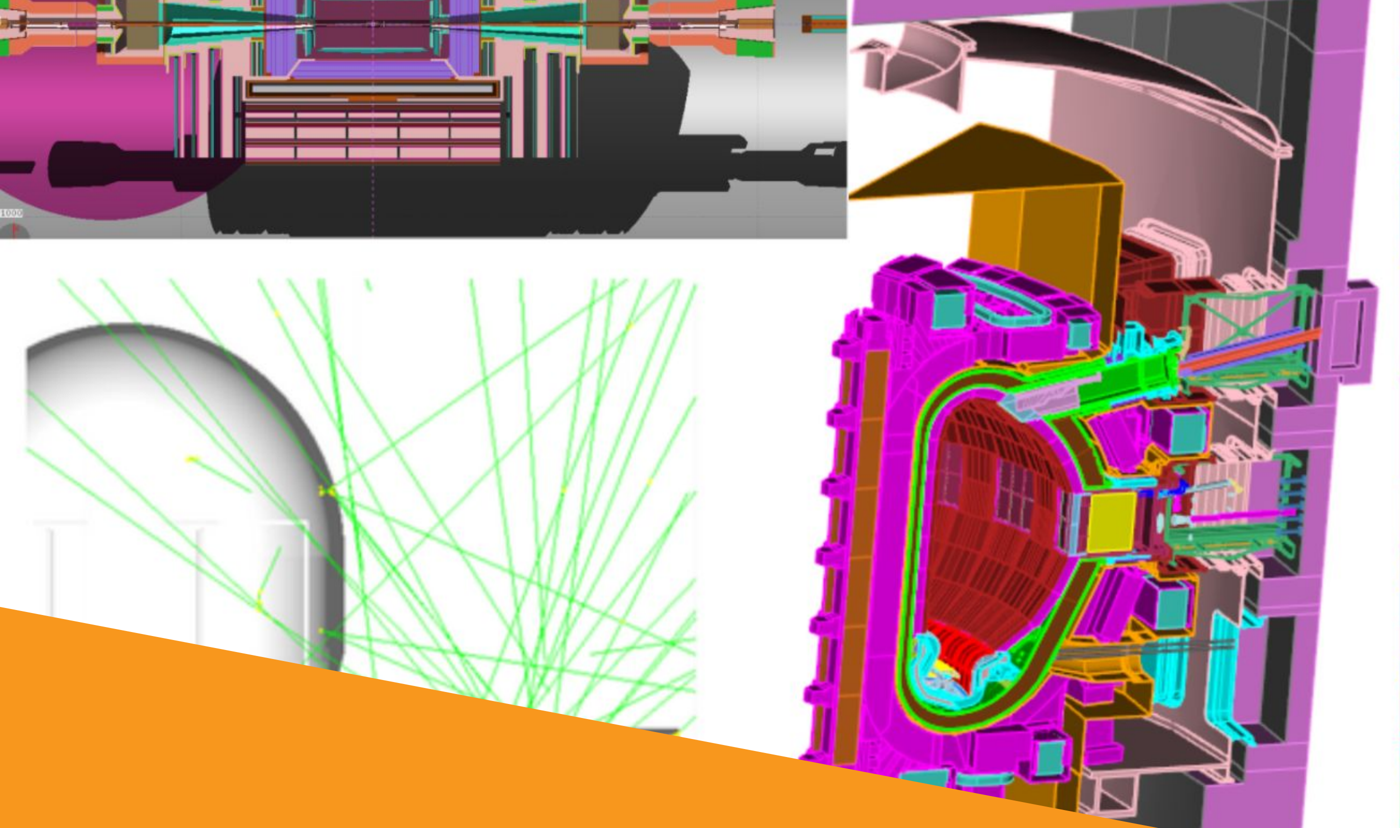

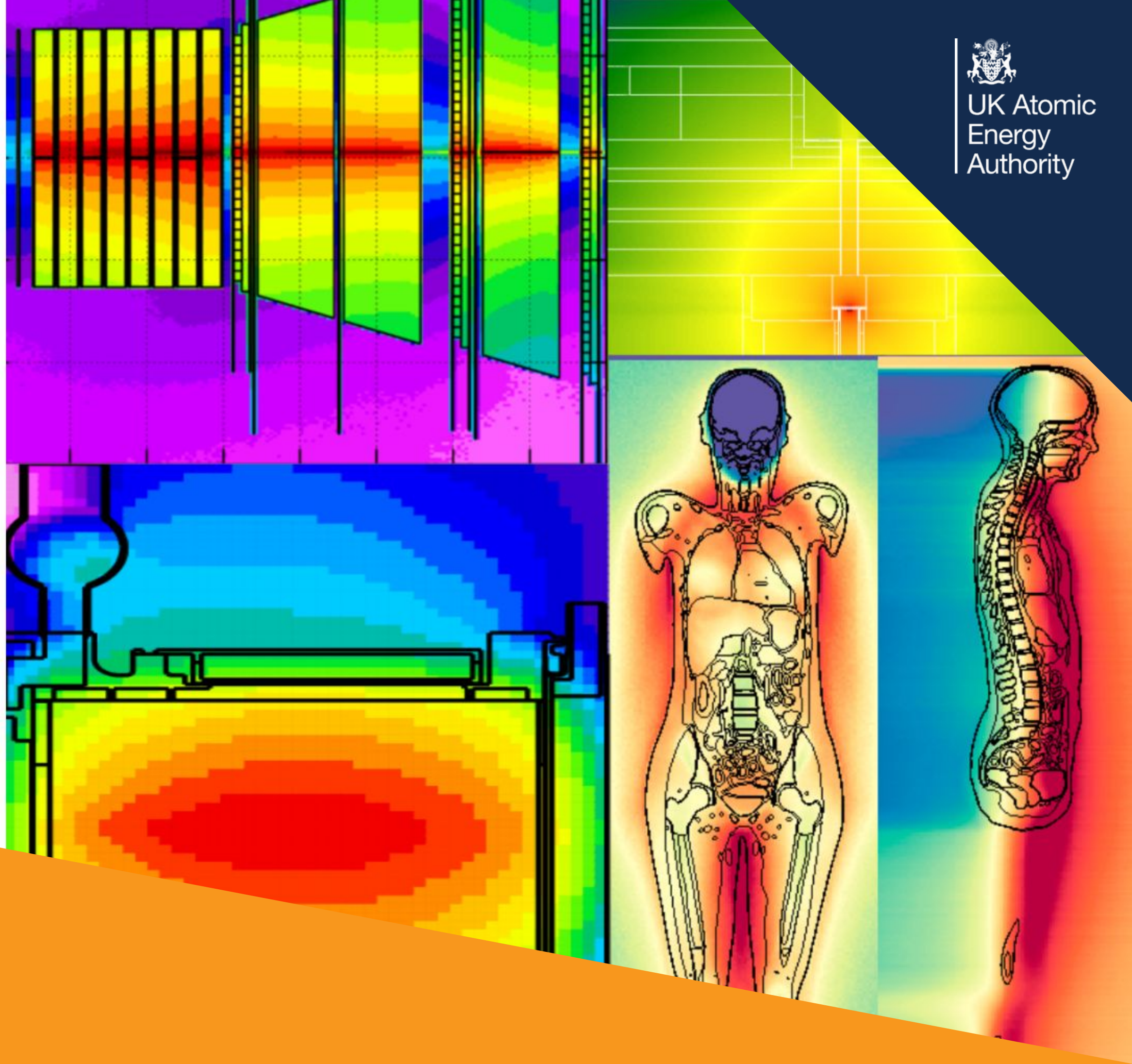

Andrew Davis

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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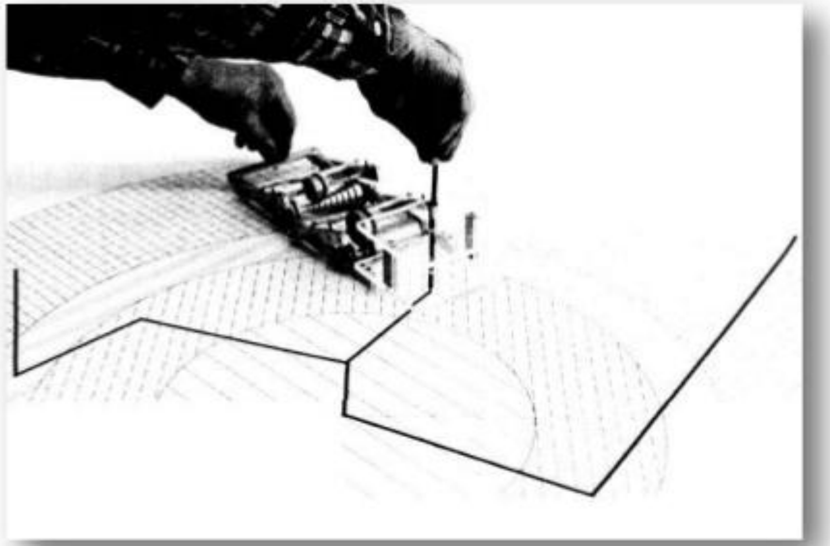
CULHAM CENTRE FOR FUSION ENERGY

Contents

Monte Carlo Analysis

- Monte Carlo analysis was born in the Manhattan Project
- Von Neuman, 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



33

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 (provenence)
  - User friendly, easier to fix and modify than CSG (effort)
  - Faster analysis turn around (efficiency)
- CAD model integrity - “cleanliness”
- Several routes for use:
  - Translation - MCAM, McCAD, FastRAD, CATIA-GDML
  - Directly - DAGMC
  - Hybrid - OiNK

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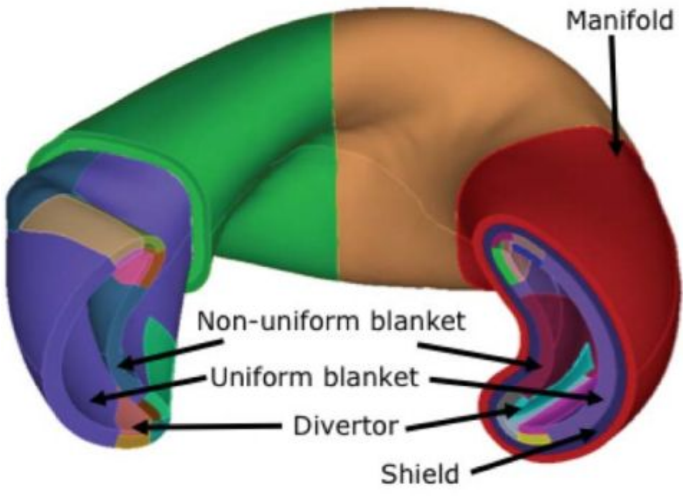
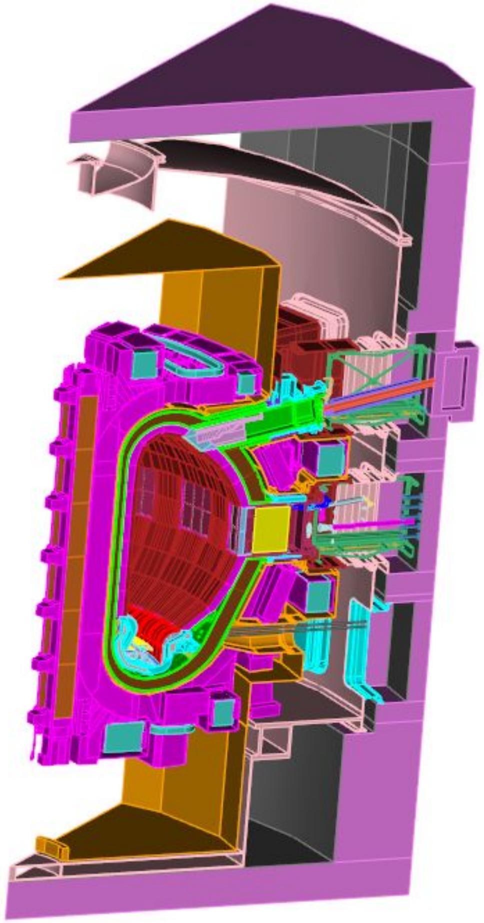
CAD Based Workflows

- 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





The Problem

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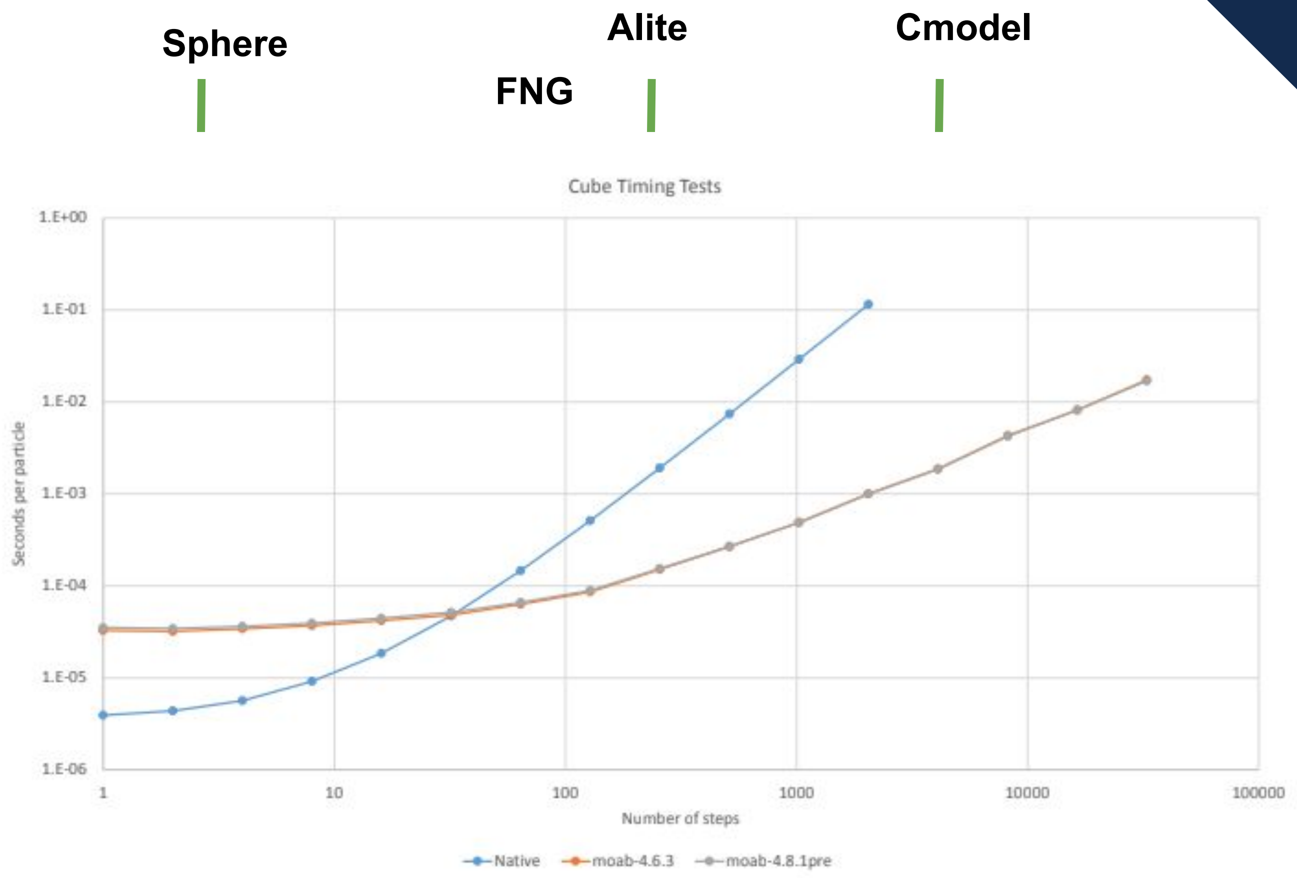
- Traditional CSG geometries are limited in absolute throughput due to the linear nature in which MC codes search through the surfaces to hit
- Hence MCNP advice of regarding avoiding unions
- DAGMC attempts to overcome this by using OBB Trees to speed ray queries, preprocessing to force the valence (connectivity) of surfaces to be 1<V<= 2



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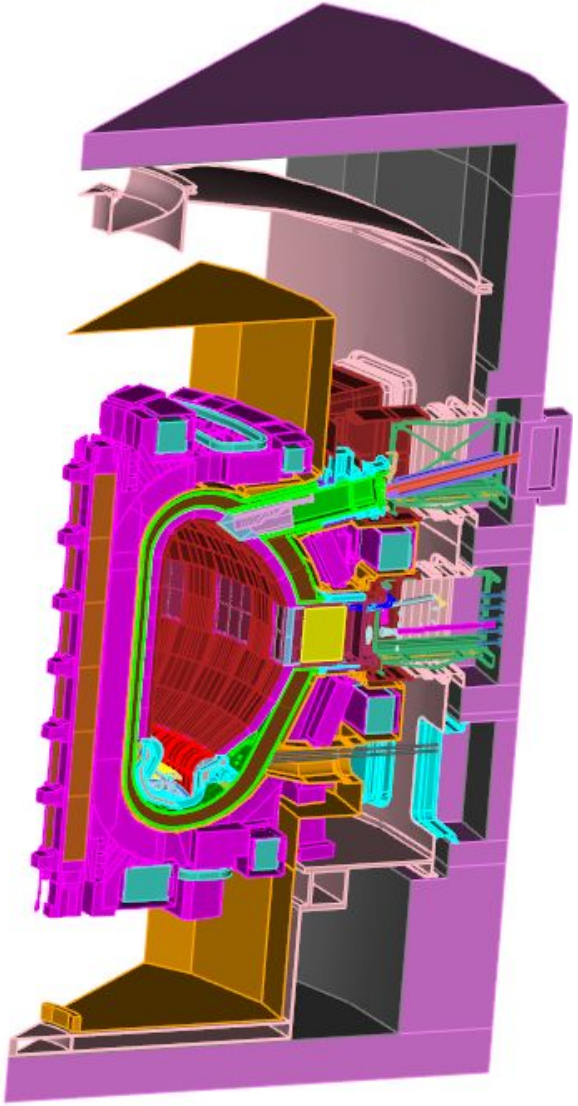
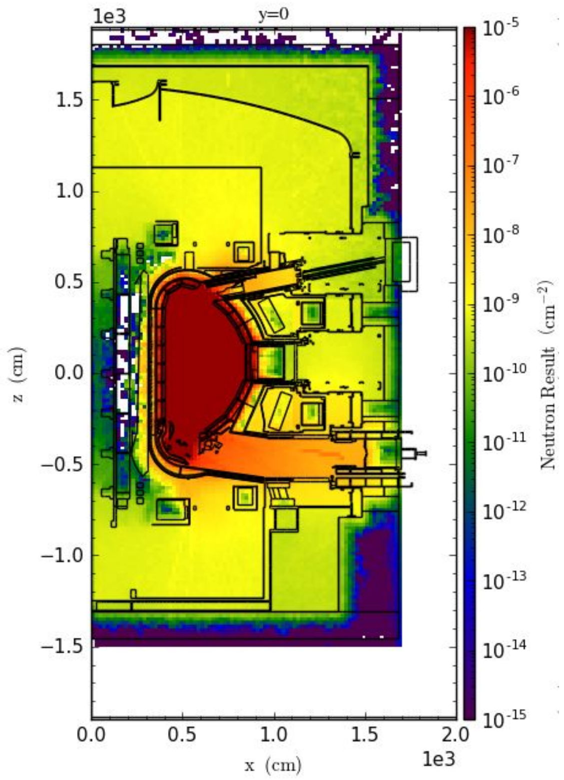
What is DAGMC?

- 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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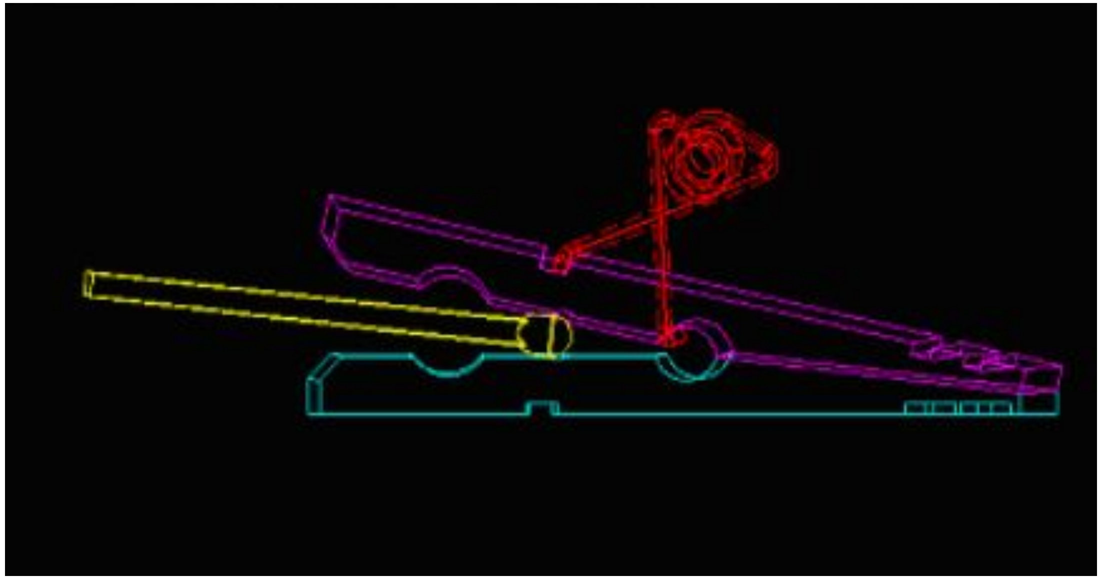
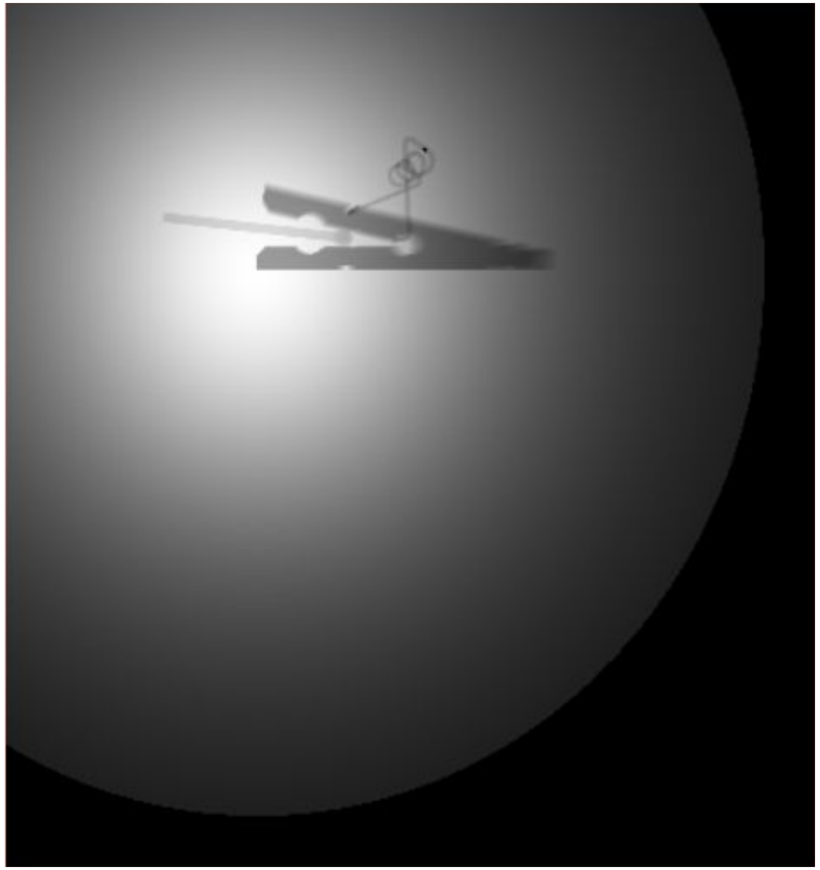
What is DAGMC?

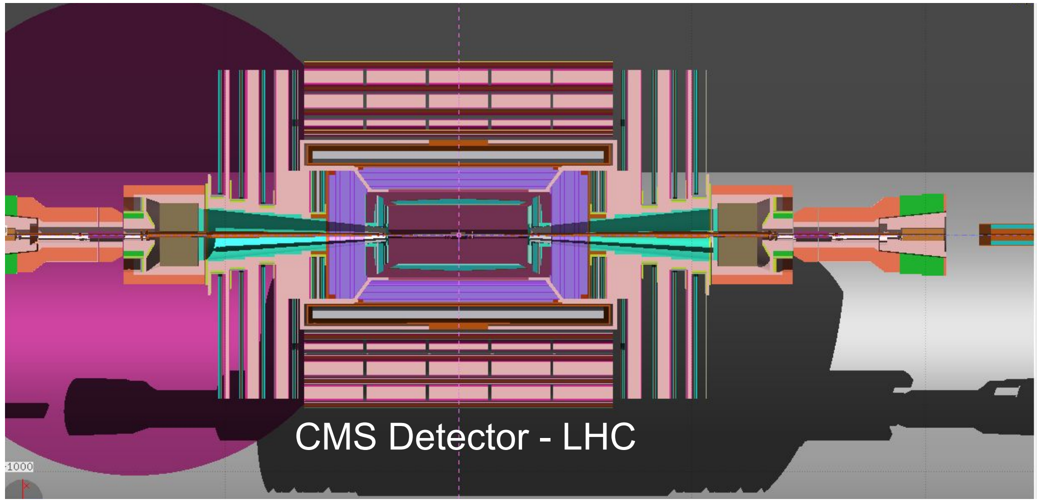
- Direct Accelerated Geometry Monte Carlo (DAGMC) started in 2001 (proof of principle by 2004) integrated directly into MCNP/X and tied directly into a CAD engine



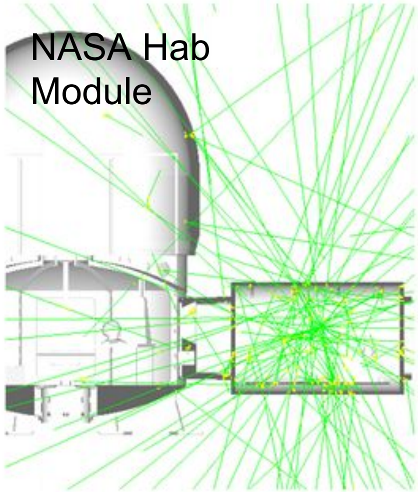


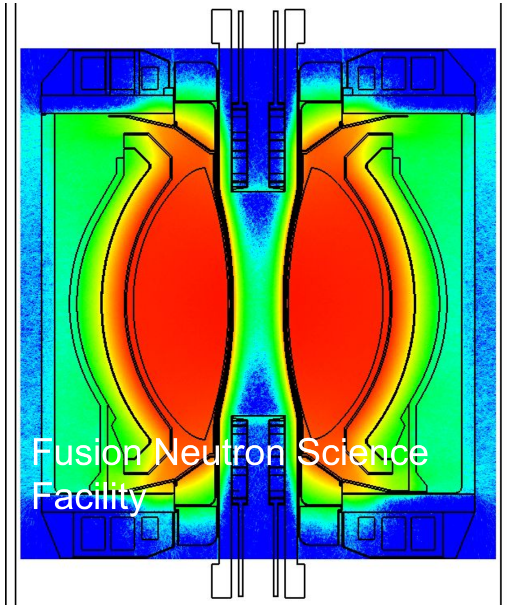
Example use, Clothes peg defined in CAD with spiral winding in clasp, Right MCNP/X radiograph

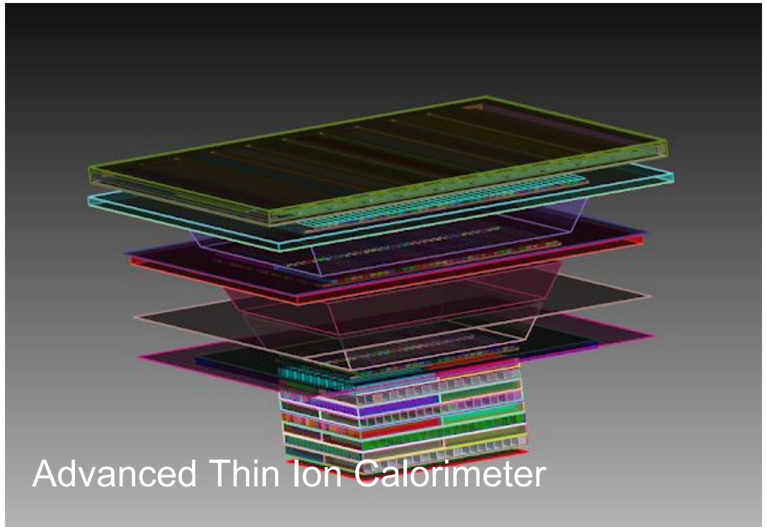
Examples of DAGMC Use


CMS Detector - LHC

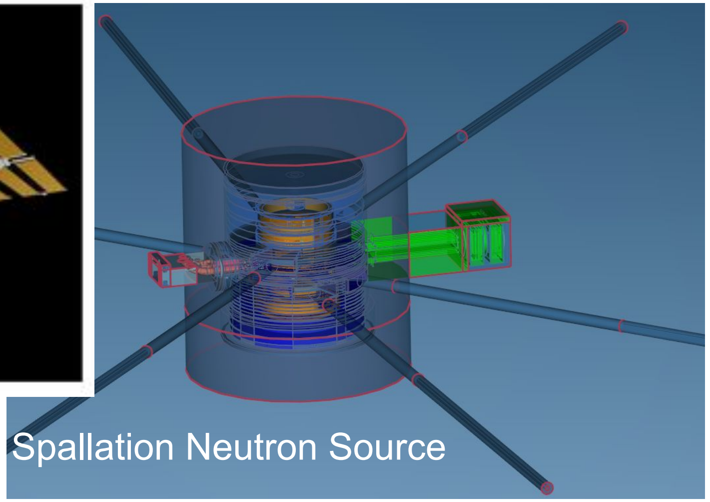

ATR


NASA Hab Module


Fusion Neutron Science Facility


Advanced Thin Ion Calorimeter


ISS


Spallation Neutron Source

DAGMC Theory

UK Atomic Energy Authority

- 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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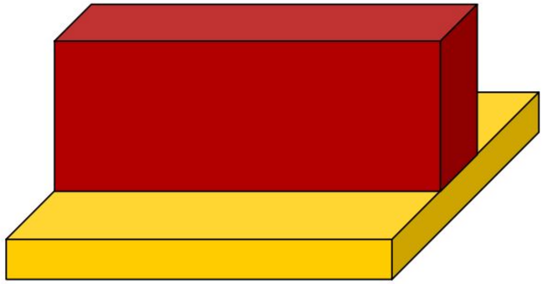
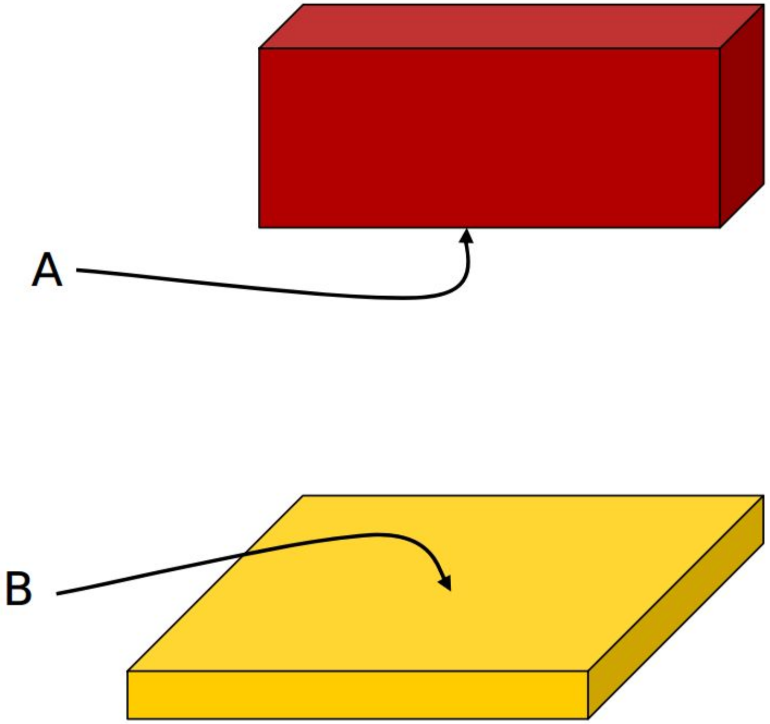
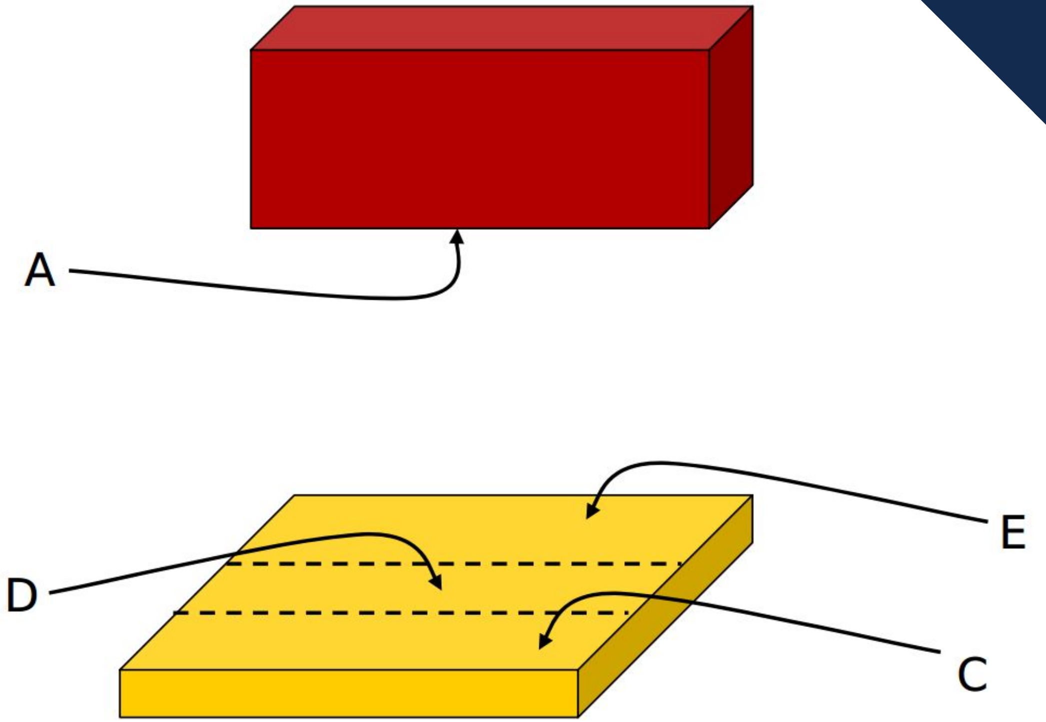
DAGMC Accelerations - Imprinting



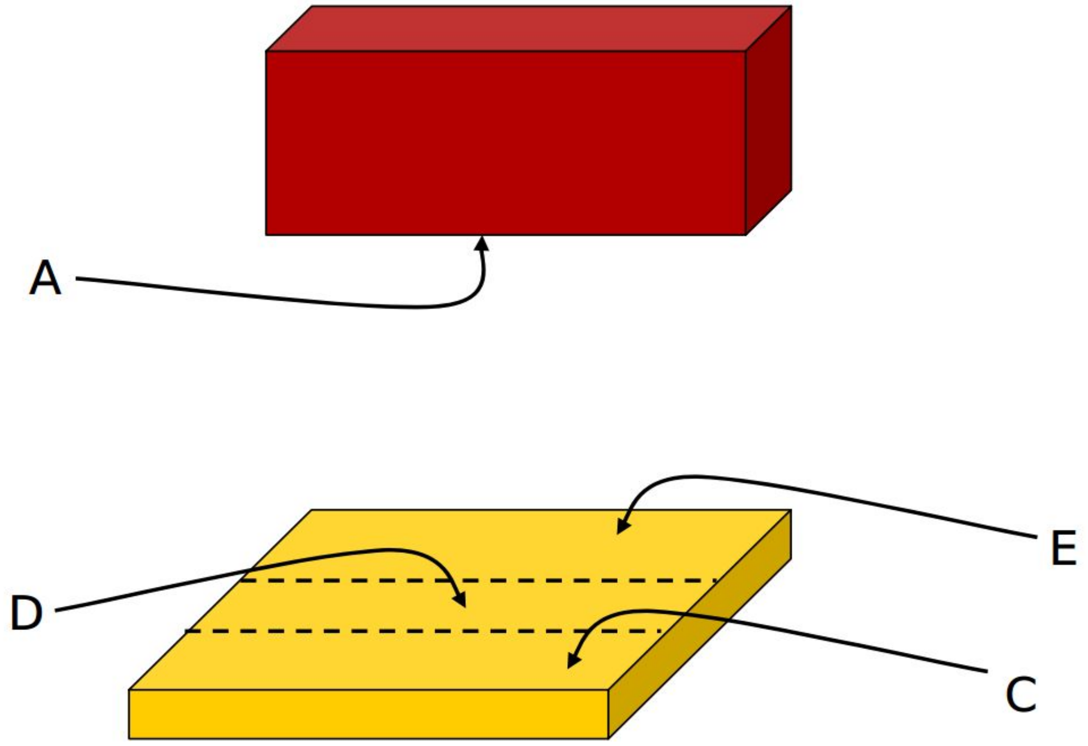
Reduces the complexity in determining neighboring regions of space

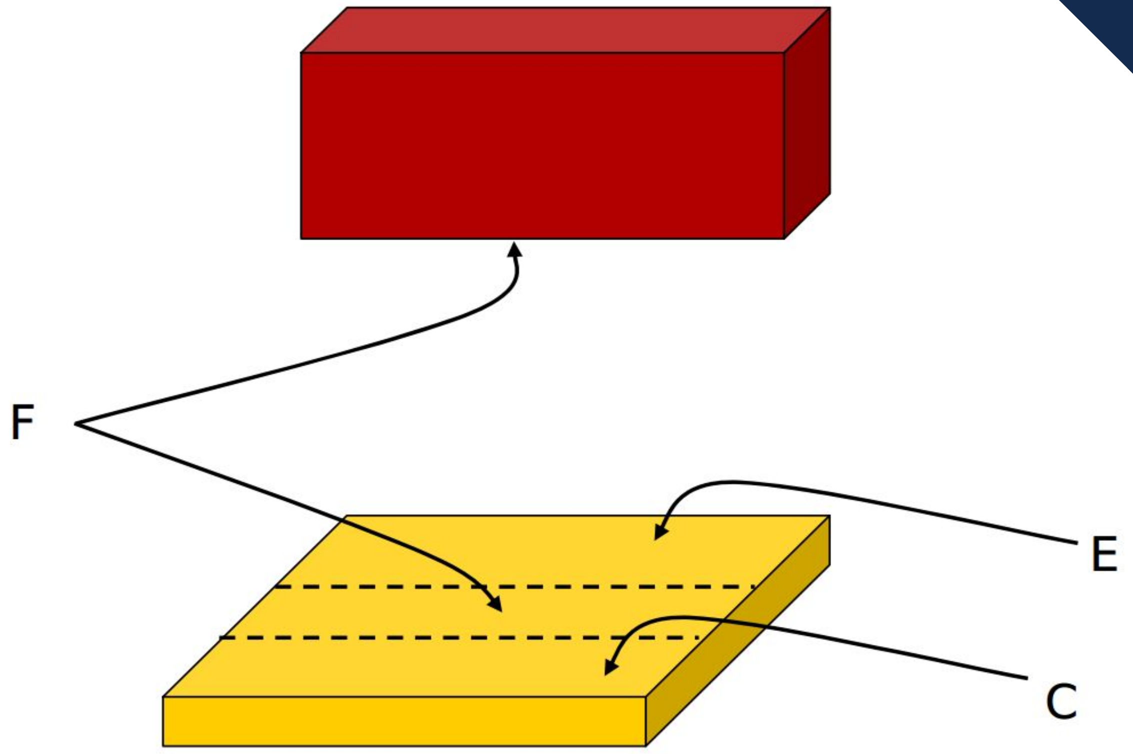




Surfaces A & B shared between the volumes

DAGMC Accelerations - Merging



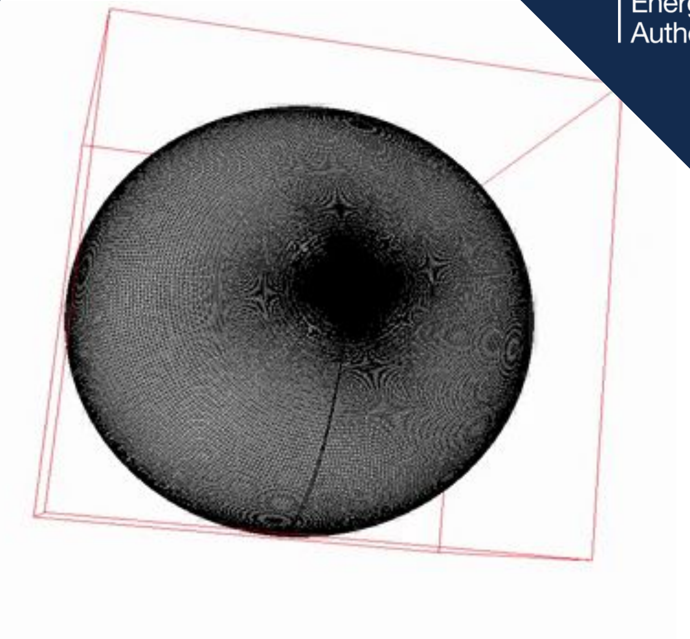


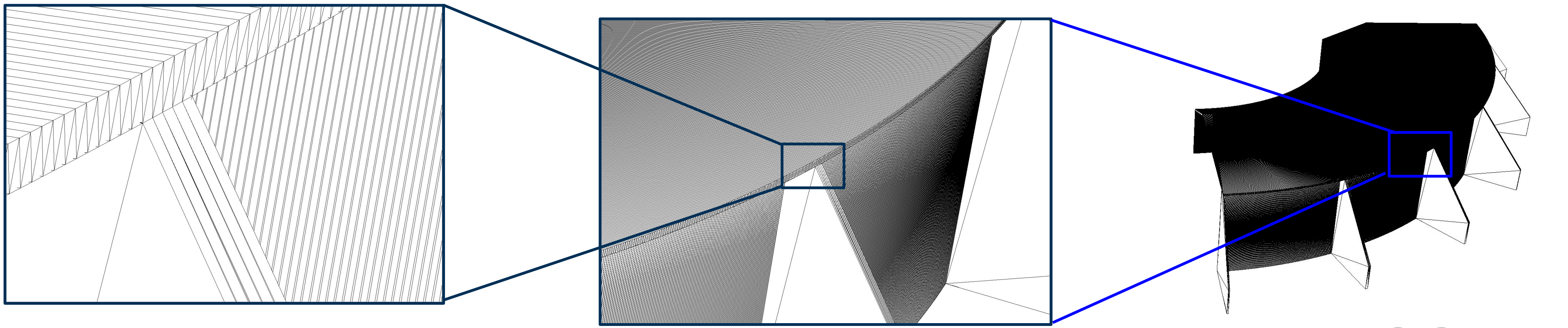
4 surfaces (3 new ones created during imprint), surface A imprinted upon surface B to create C,D,E

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

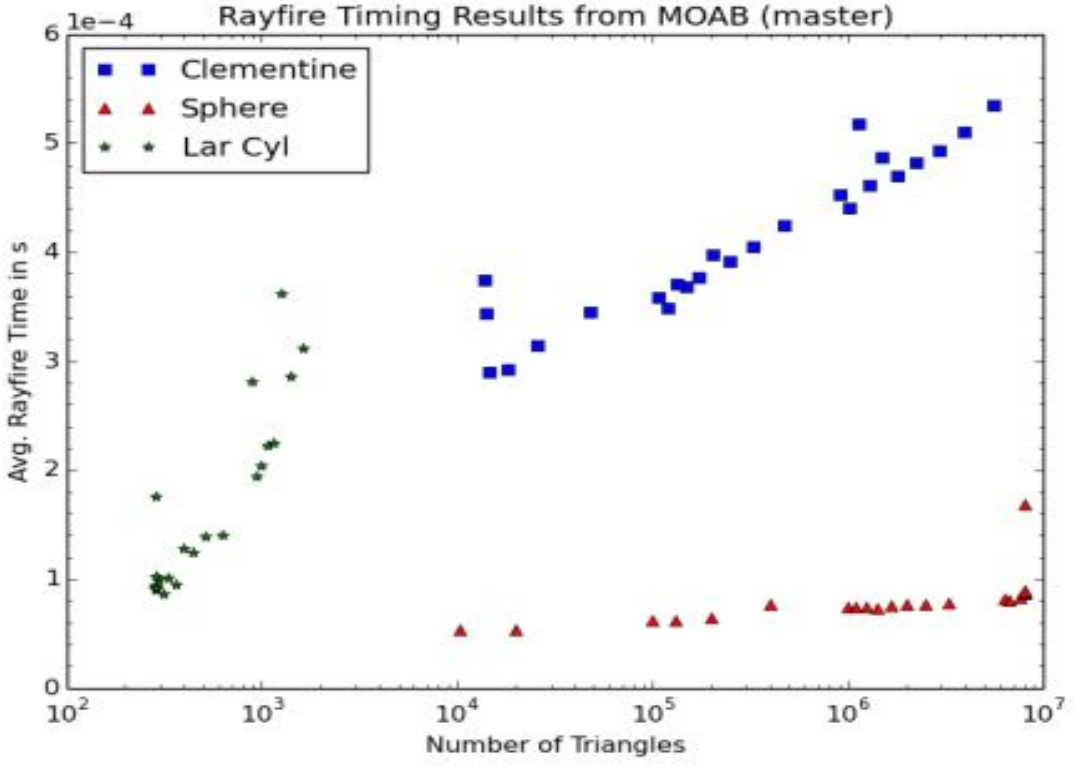
DAGMC Accelerations - Faceting

- 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

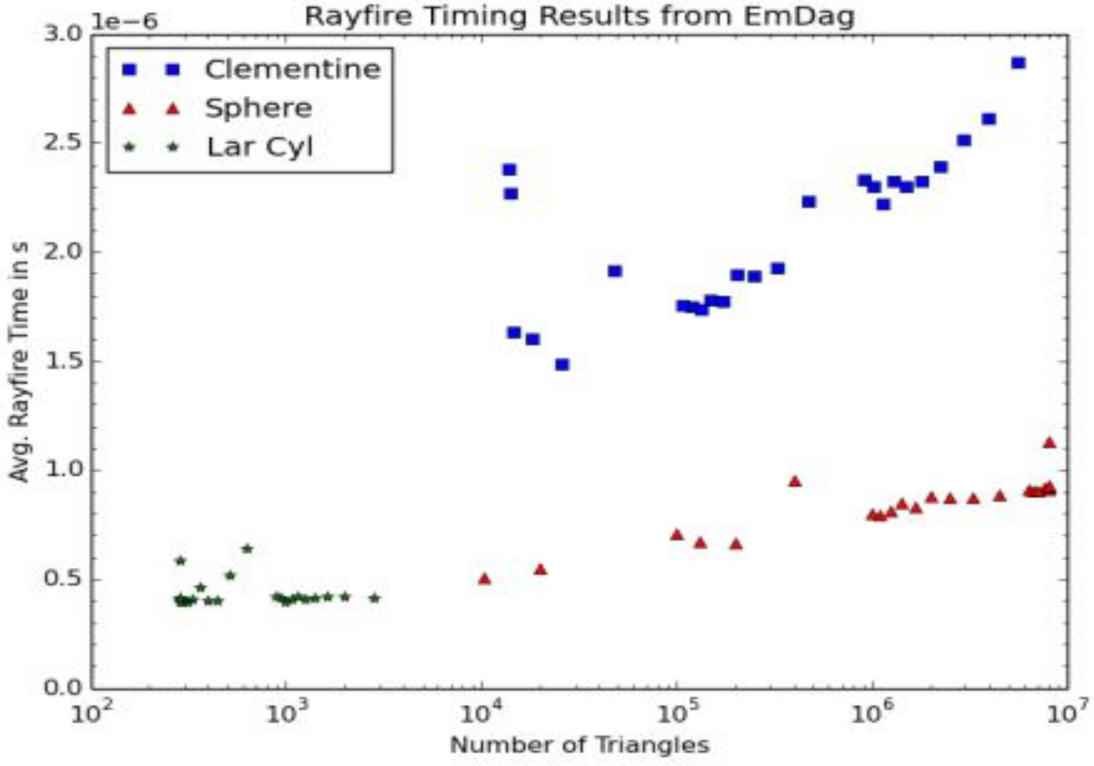




DAGMC Accelerations - BVH Trees



MOAB OBBs



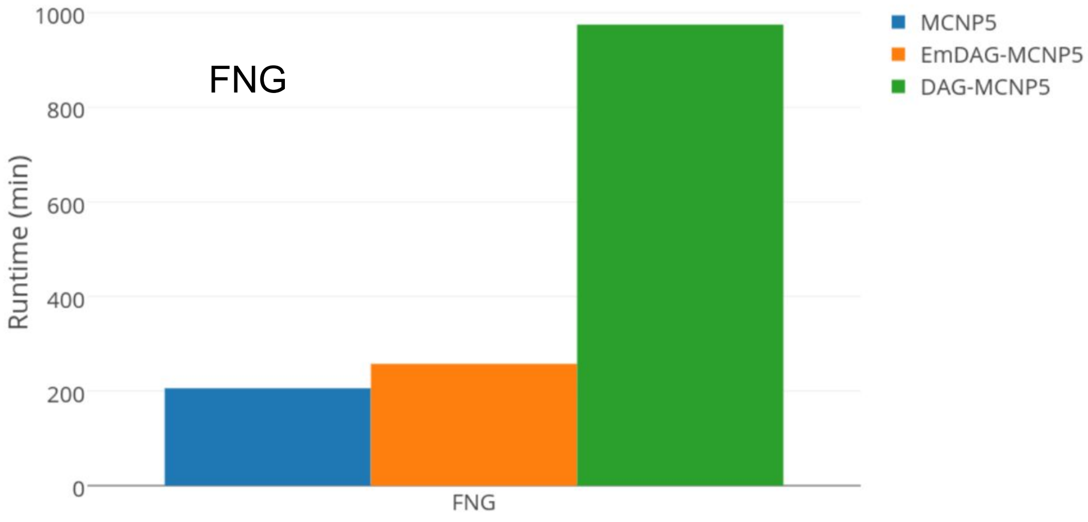
Embree AABB

News fresh off the press

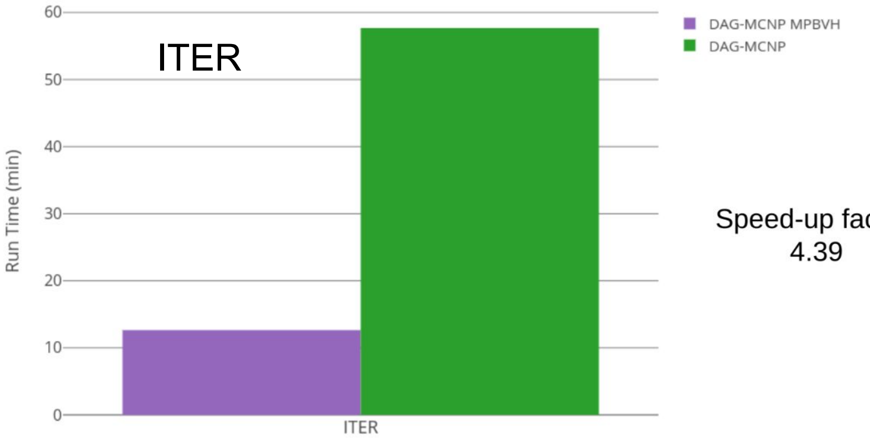
Patrick Shriwise (some of you may have met) is doing his viva (defence) tomorrow, his work has focussed on performance improvements of DAGMC

- Signed Distance Field
- High valence Vertices
- Mixed Precision Bounding Volume Hierarchy (MPBVH)

ITER geometries should now run ~ 2x faster with DAGMC than with MCNP

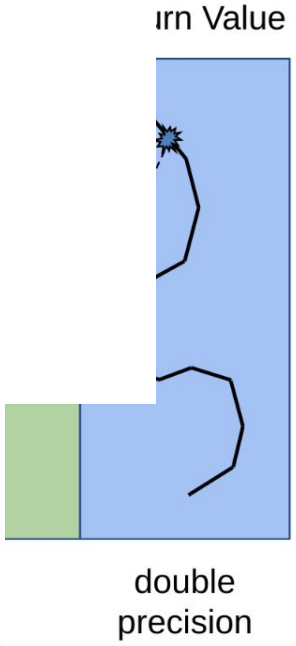


Native & DAGMC: zero lost particles
EmDAG: 240 lost particles in 100M



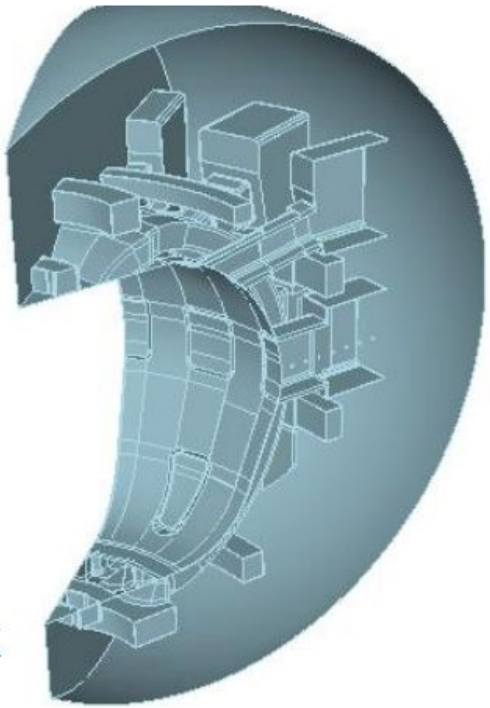
10M Particles
zero lost particles, same numerical answer

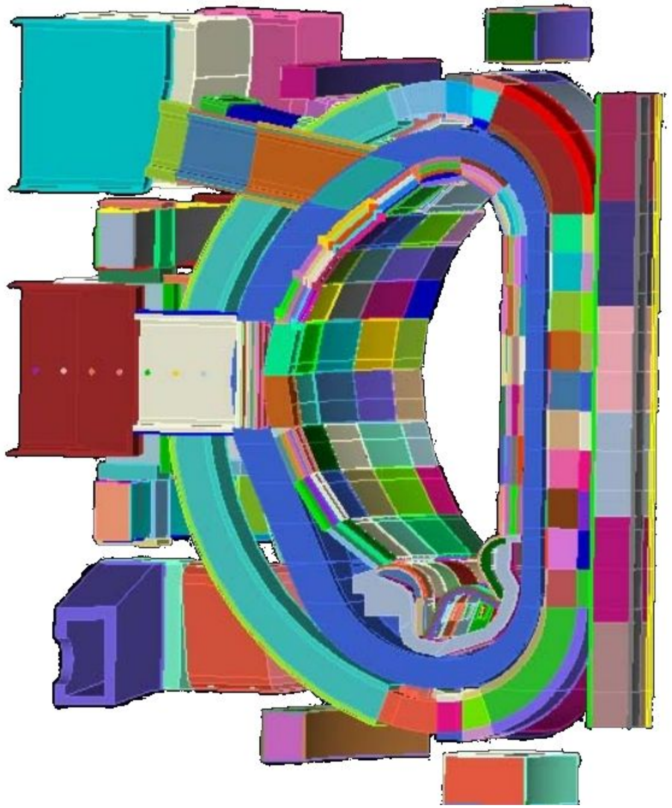
Speed-up factor:
4.39



DAGMC Convenience - Implicit Compliment

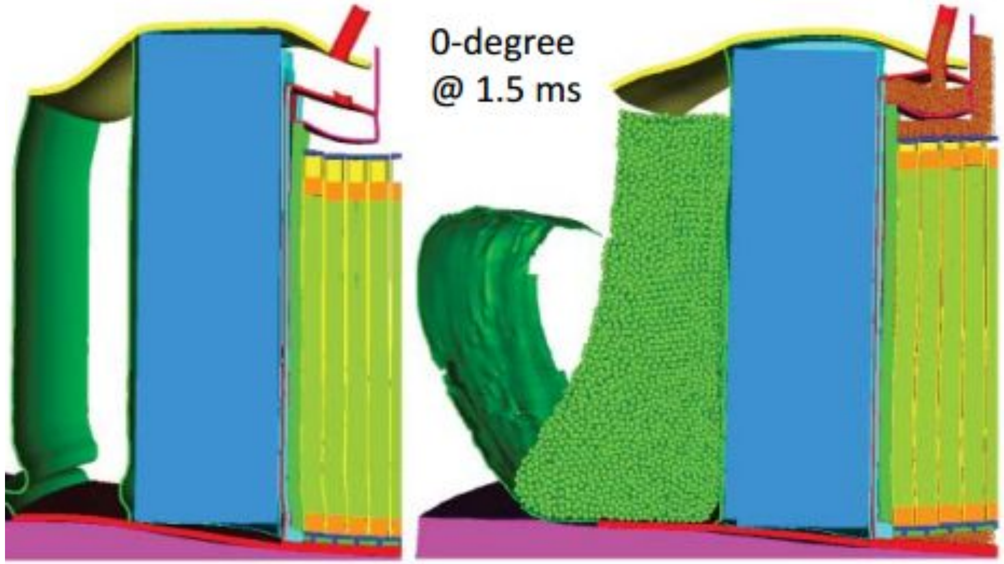
- CAD models generally do not define “void space”, including:
  - Coolants
  - Vacuum
  - Air
- DAGMC
  - Any surface that does not associate with 2 volumes must bound this compliment space (due to imprinting a surface can only be associated with 1 or 2 volumes)
- Is **automatically** generated
- On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

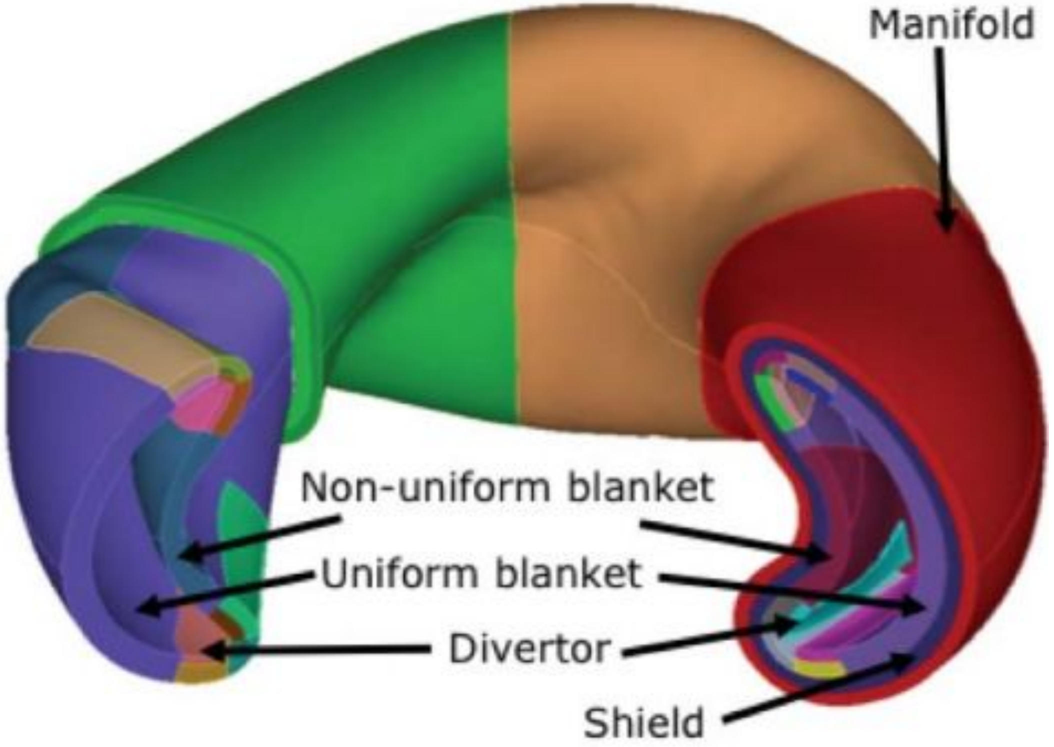




DAGMC Advantages

- 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

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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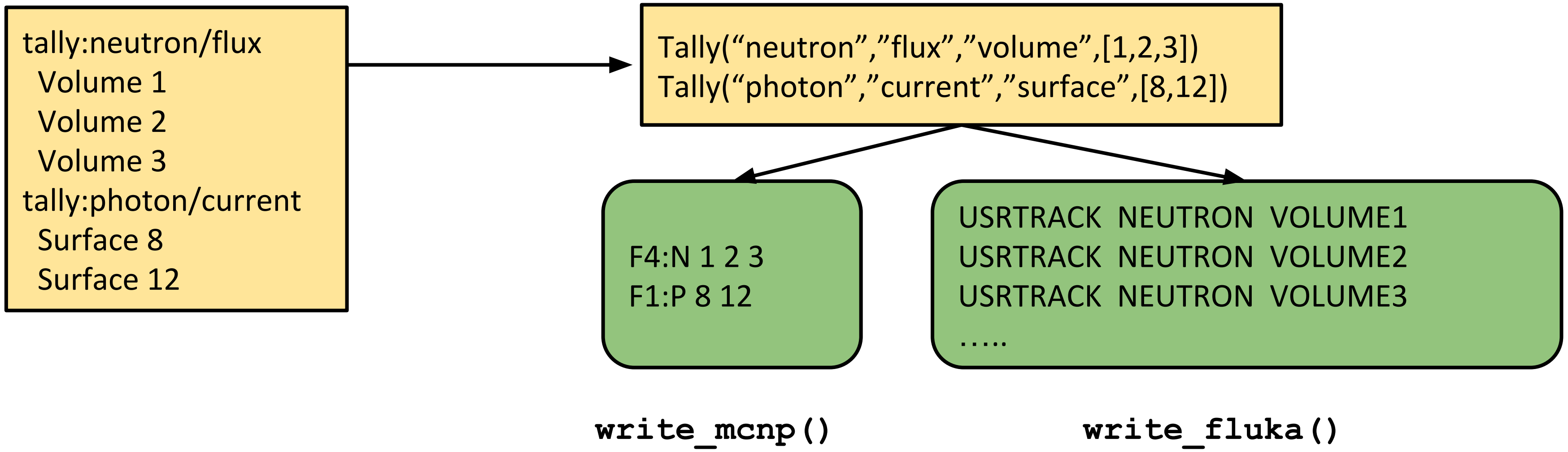
Unified Workflow

- Growth in the number of DAG enabled codes (MCNP, Fluka, GEANT4, Shift, etc)
  - Needed to create a *Lingua Franca* to describe geometry metadata
    - Describe materials information, tally descriptions, *etc*
  - Canonical form that we translate to native form when required.
- Store metadata information beside the geometric form in generic form
  - Geometry, tallies & materials are bound together for
    - Provenance
    - Reproducibility
    - Comparison
- Translate & write out tally, material data for each code at runtime
  - Impossible to misinterpret or make mistake
- Recommended method if you want MC code geometry independence

Unified Workflow - Tallies



- Groups assigned according to metadata syntax <particle_name>/<tally_type>
- Tagged into DAG geometry, alongside geometry & materials
- Written out by MCNP, Fluka at runtime when required, write_mcnp(), write_fluka(), etc

Unified Workflow - Materials

DAG Geometry

mat:Stainless Steel
mat:Blanket Mix 1
mat:Divertor copper
mat:H2O&SS

Material Library

Stainless Steel
Density = 7.98 g/cc
Composition:
Fe56: 0.23
Fe58: ....

Pyne

`material.write_mcnp();`

C Material Composition from
C Density is 7.98 g/cc
C Reference to Material
M1 26056.70c -0.23
26058.70c ....

- Using human readable naming scheme for material groups
- We then lookup into a PyNE material library
- When each MC needs to know the composition, we call the appropriate method
  - **material.write_mcnp()**
  - **material.write_fluka()**

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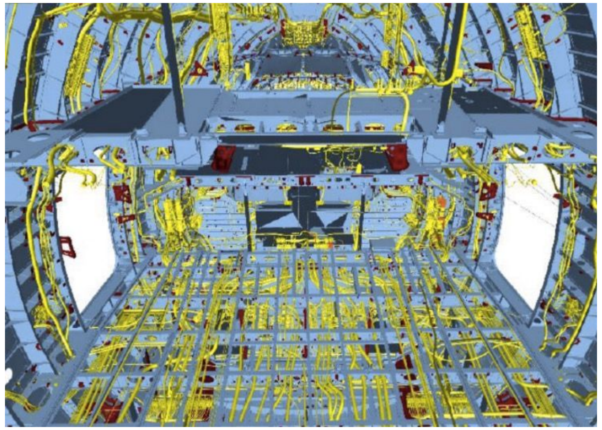
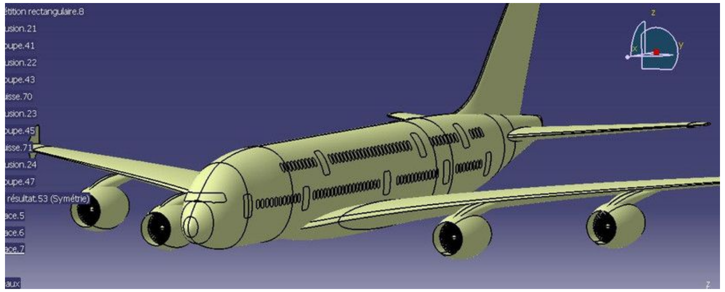
Example CAD Based Workflow Airbus A380

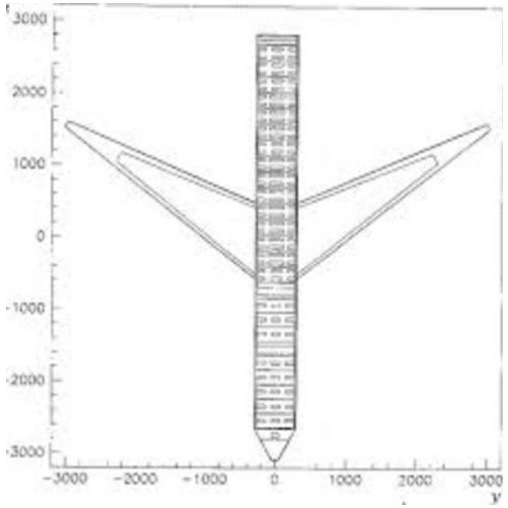
Defeaturing



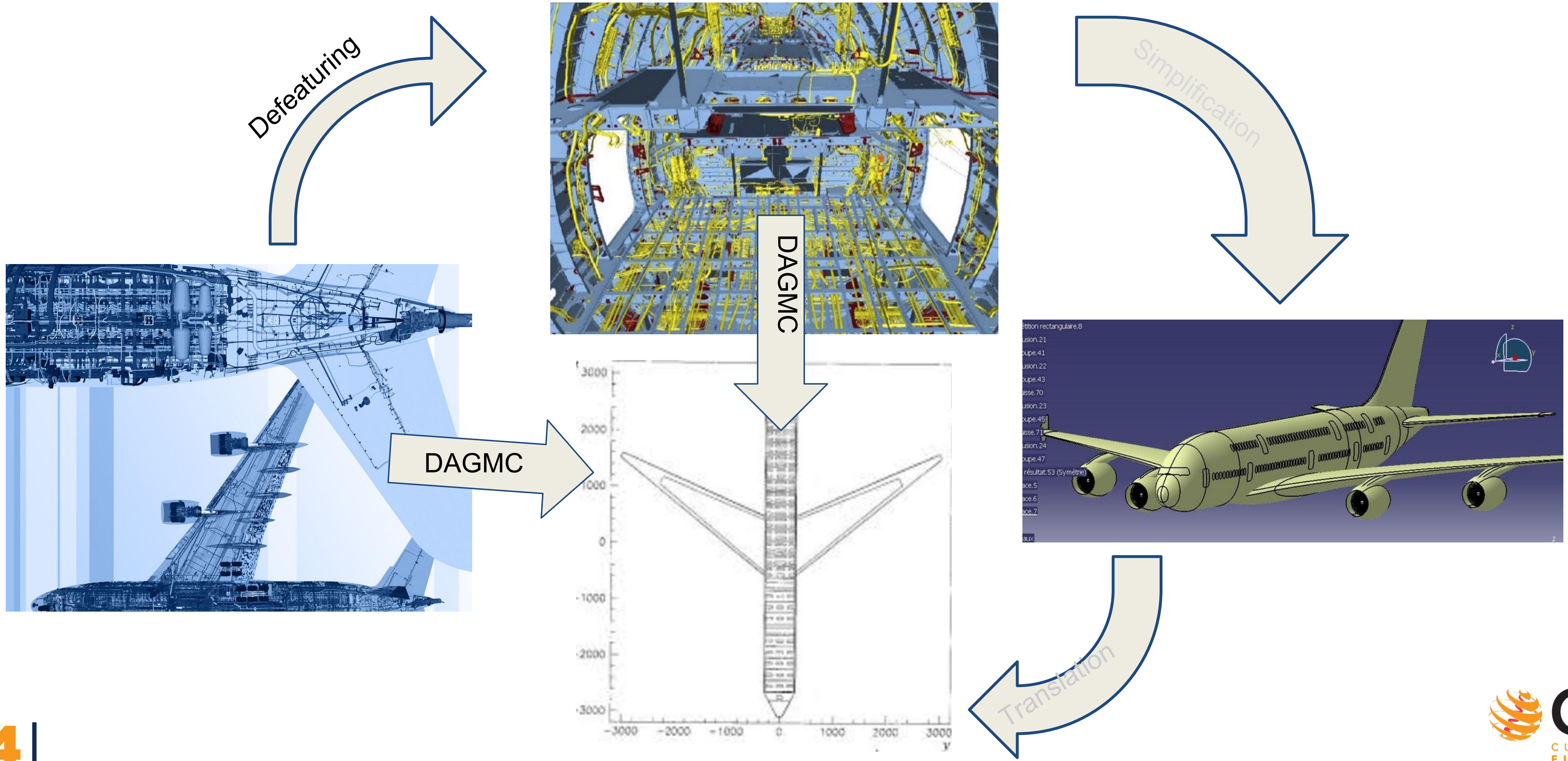
Simplification



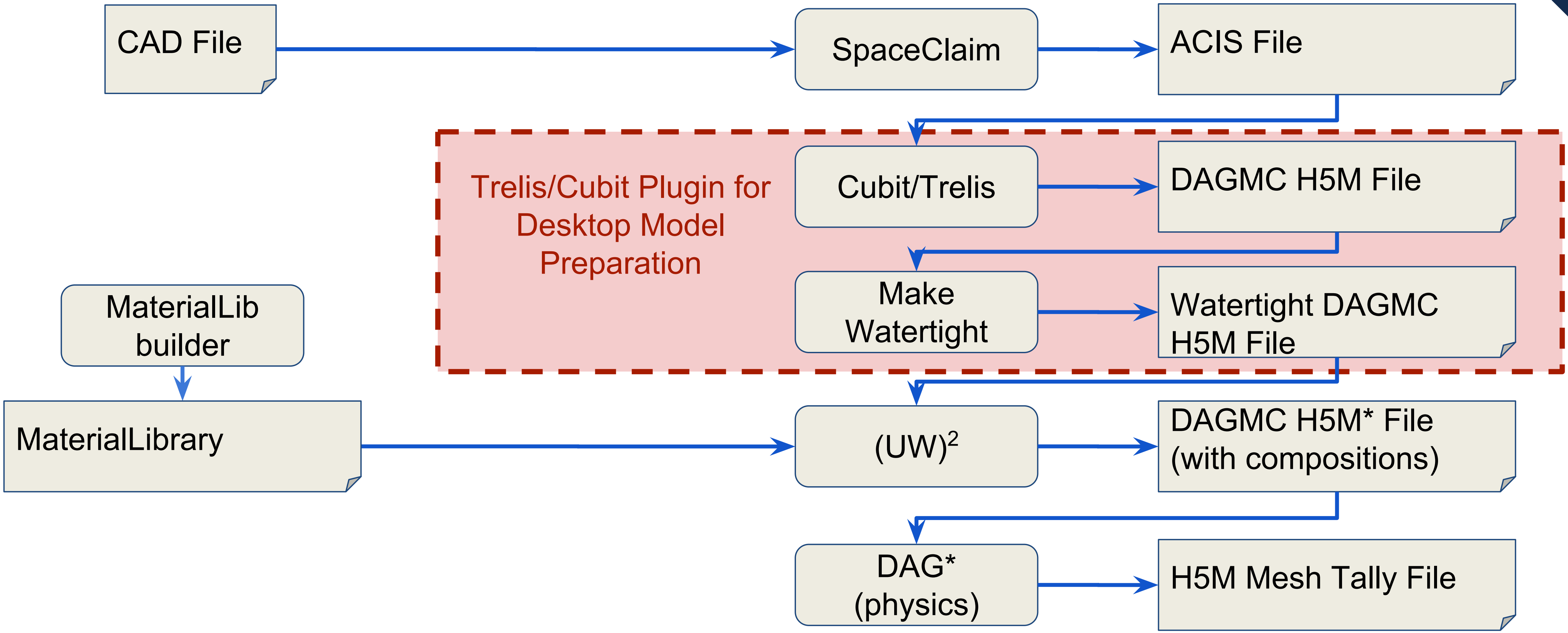
Translation



Example CAD Based Workflow Airbus A380

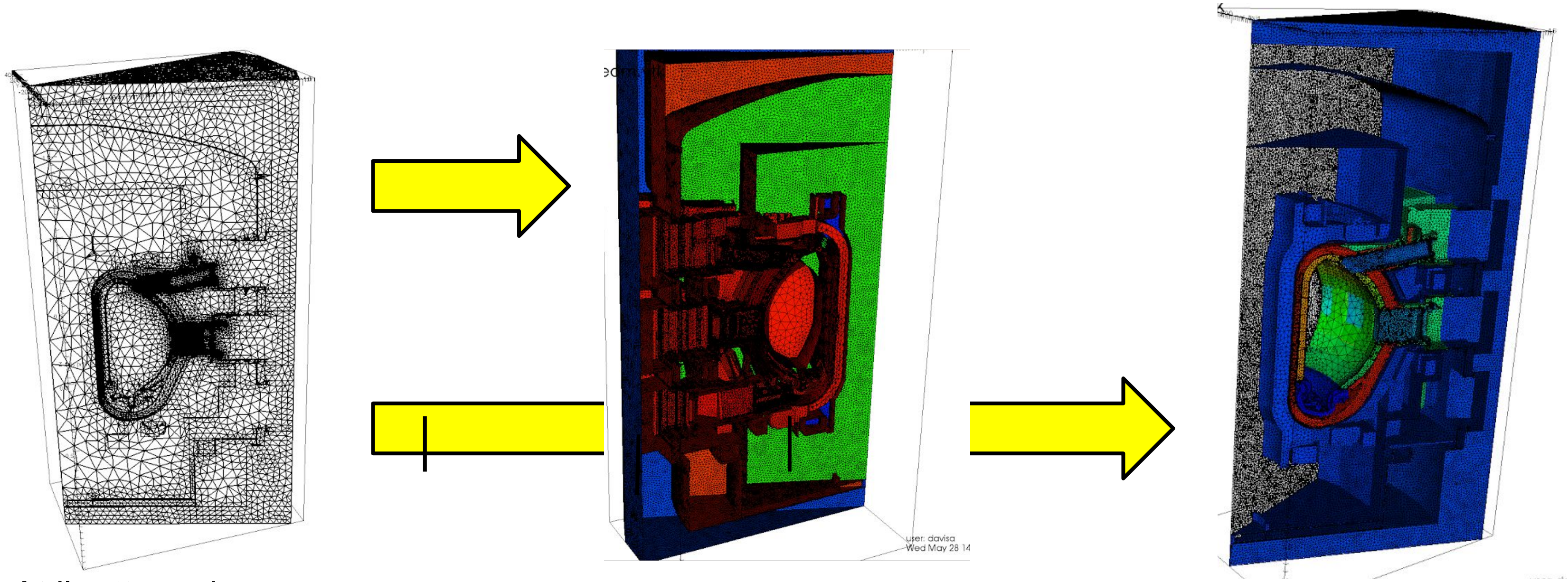


DAGMC Workflow



DAGMC Workflow (2)

- DAGMC file format is specific enough that many other formats can easily be translated to it, simply a matter of assigning correct topological relationships



Attila rtt mesh DAGMC Geometry DAGMC Tally Mesh

- Boundary information can be brought across along with id numbers, material assignments done via "`lcad` file" - see examples later

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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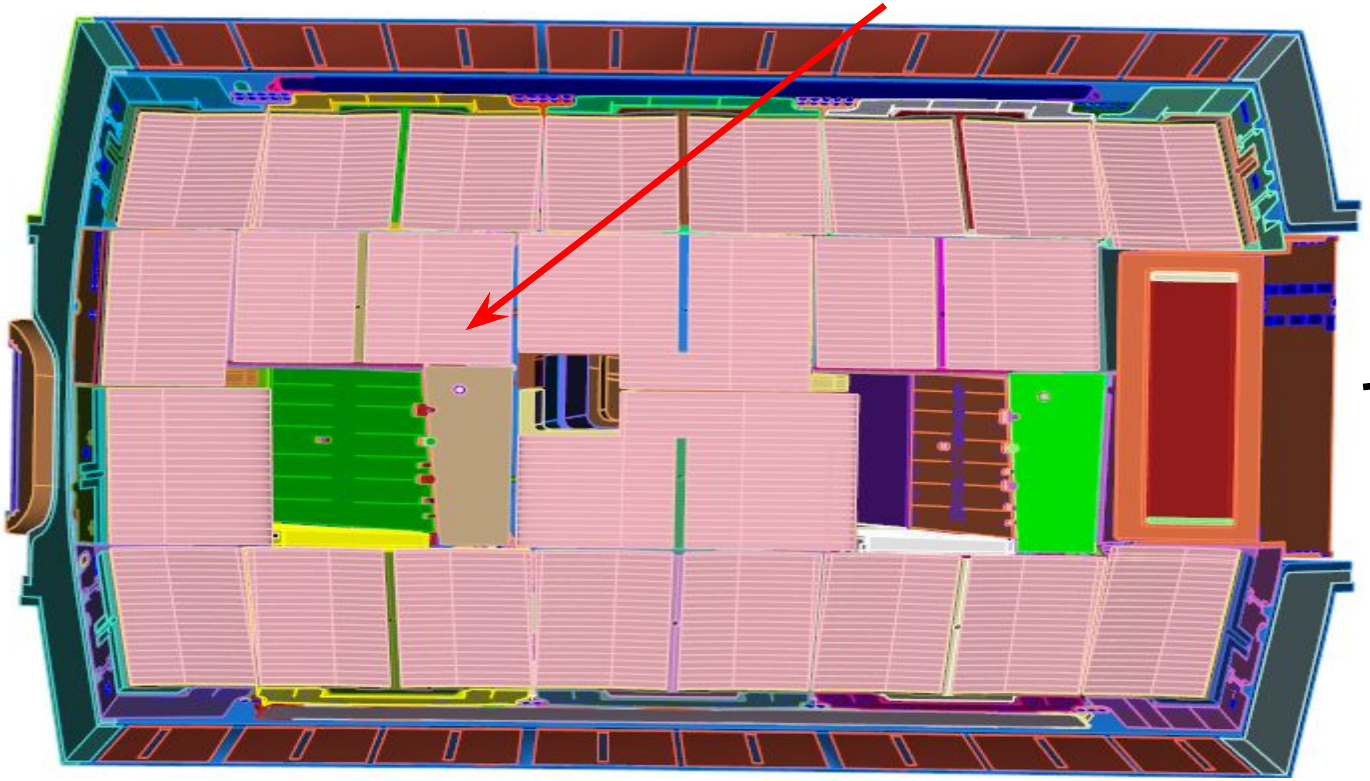
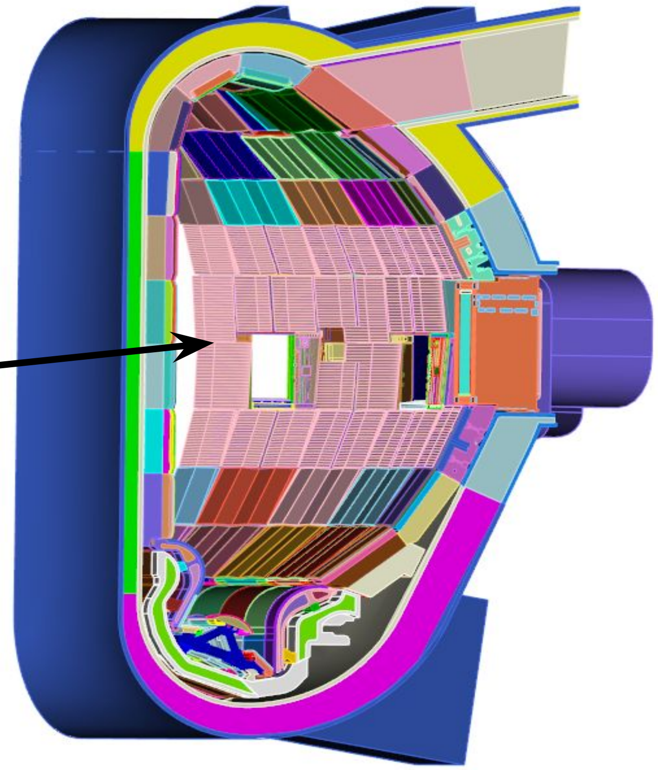
DAGMC Examples - ITER NBI Sector

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

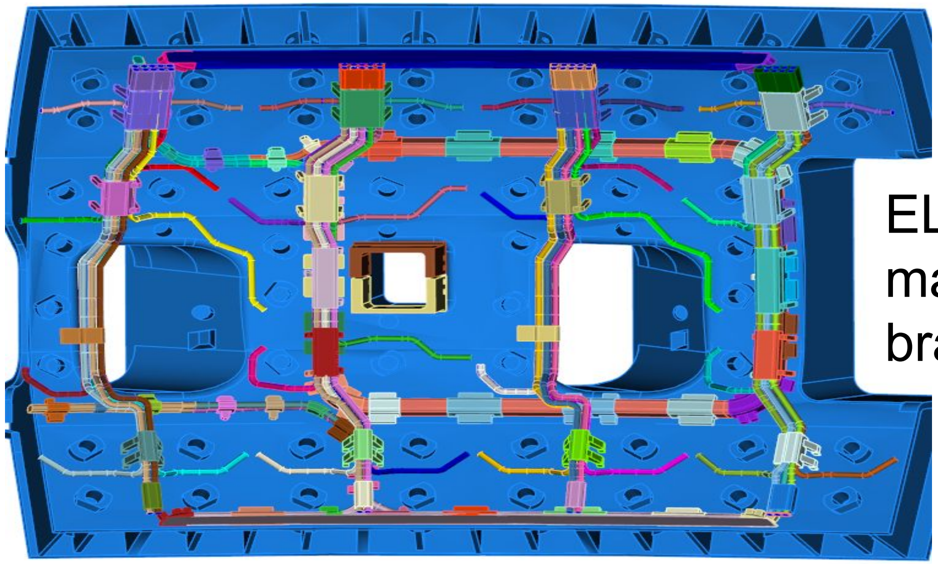




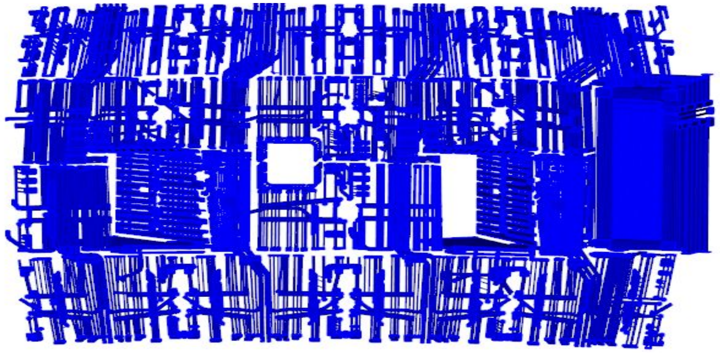
Calculations run using DAG-MCNP5 and FENDL-2.1 cross section library

DAGMC Examples - ITER NBI Sector

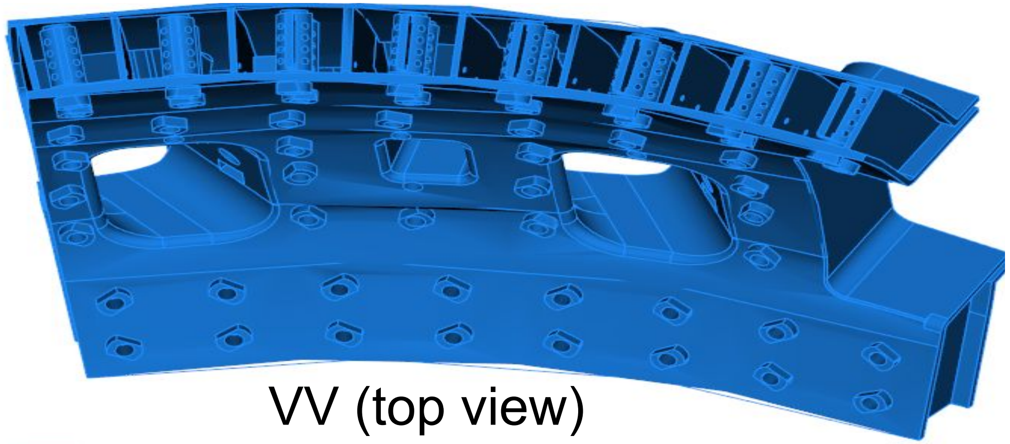
- A lot of detail in the BM13-16 region:



ELM coils, manifolds, brackets



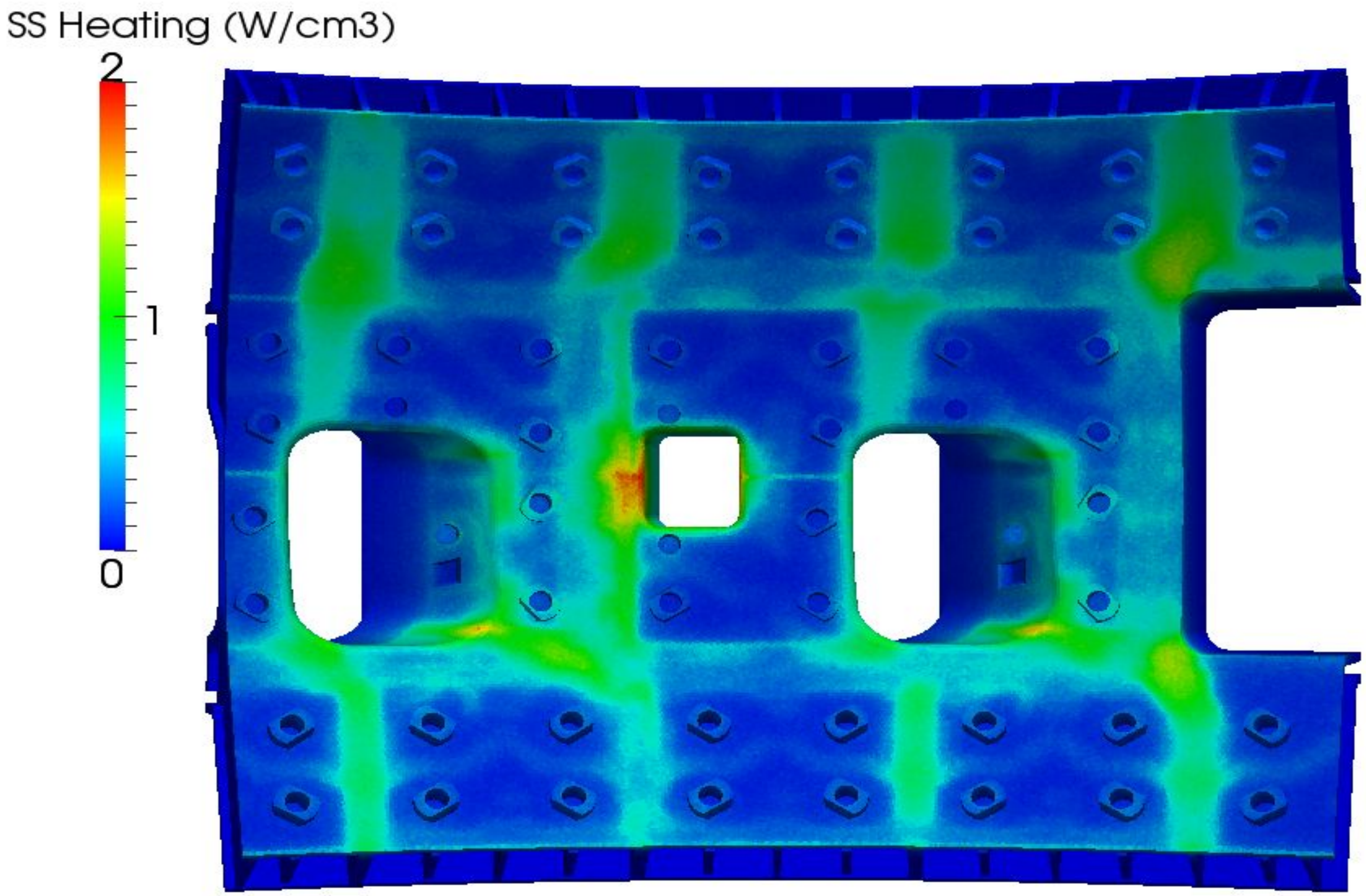
Water coolant channels

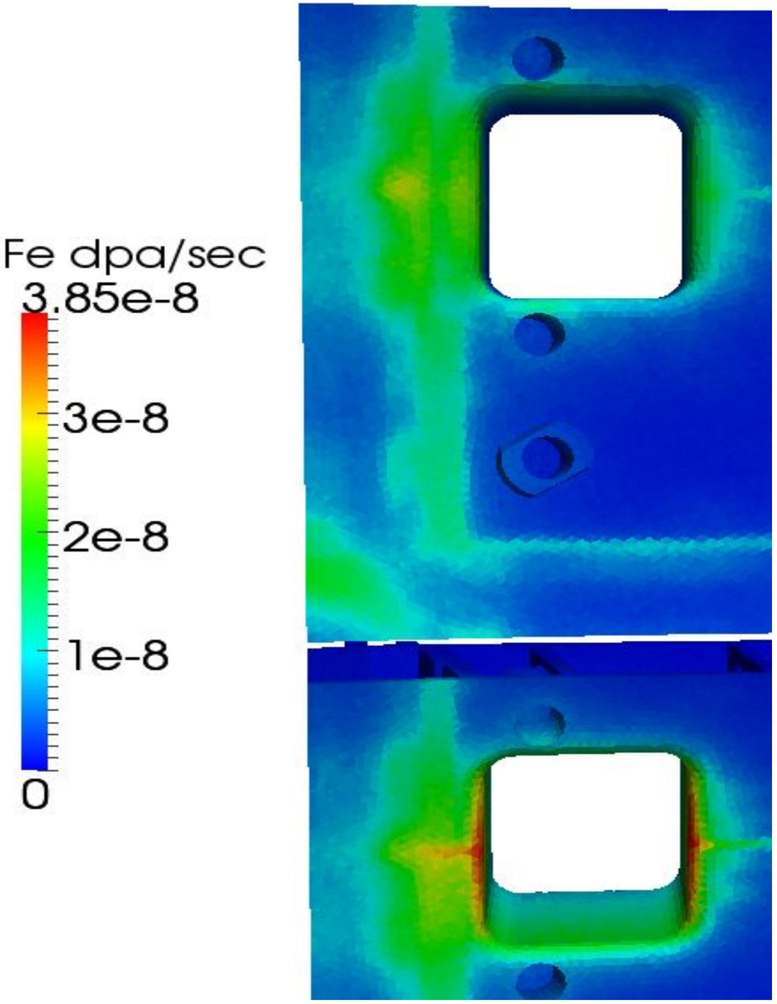


VV (top view)

SB (rear view)

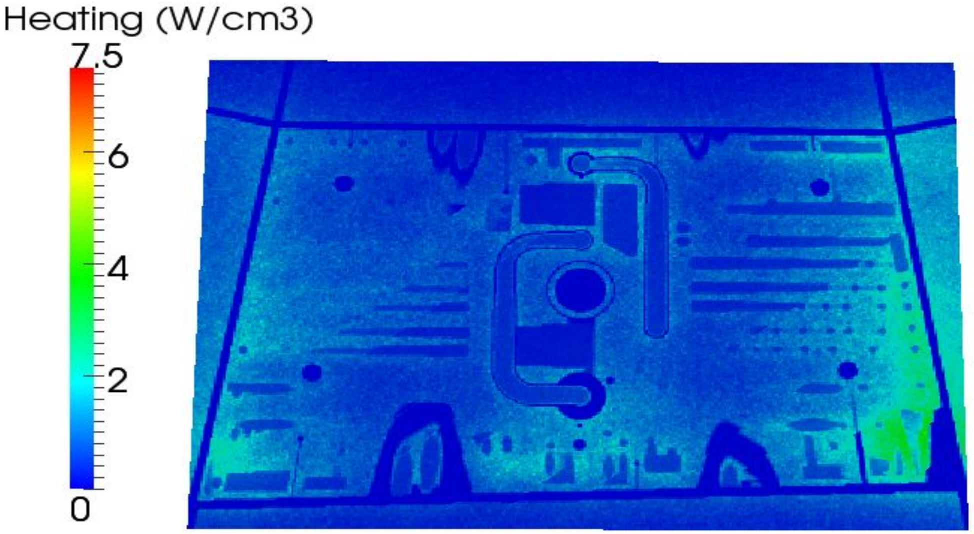
DAGMC Examples - ITER NBI Sector





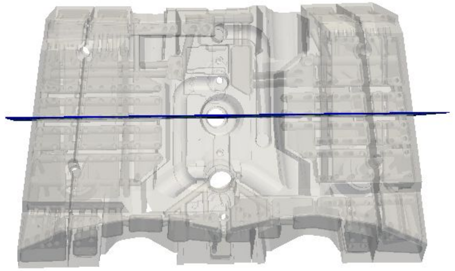
ITER lifetime is 0.54 FPY (1.7e7 sec) so 2.94e-8 dpa/sec corresponds to 0.5 dp

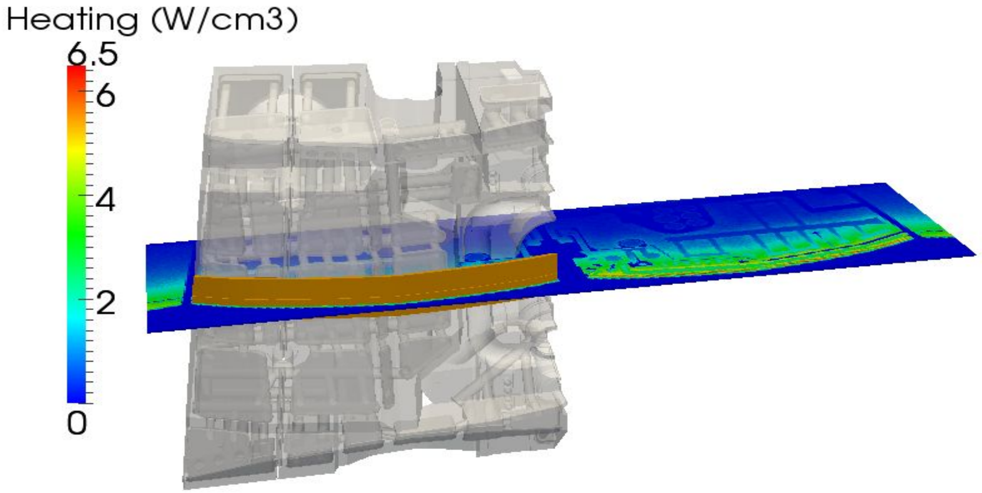
Detailed Blanket Module Heating

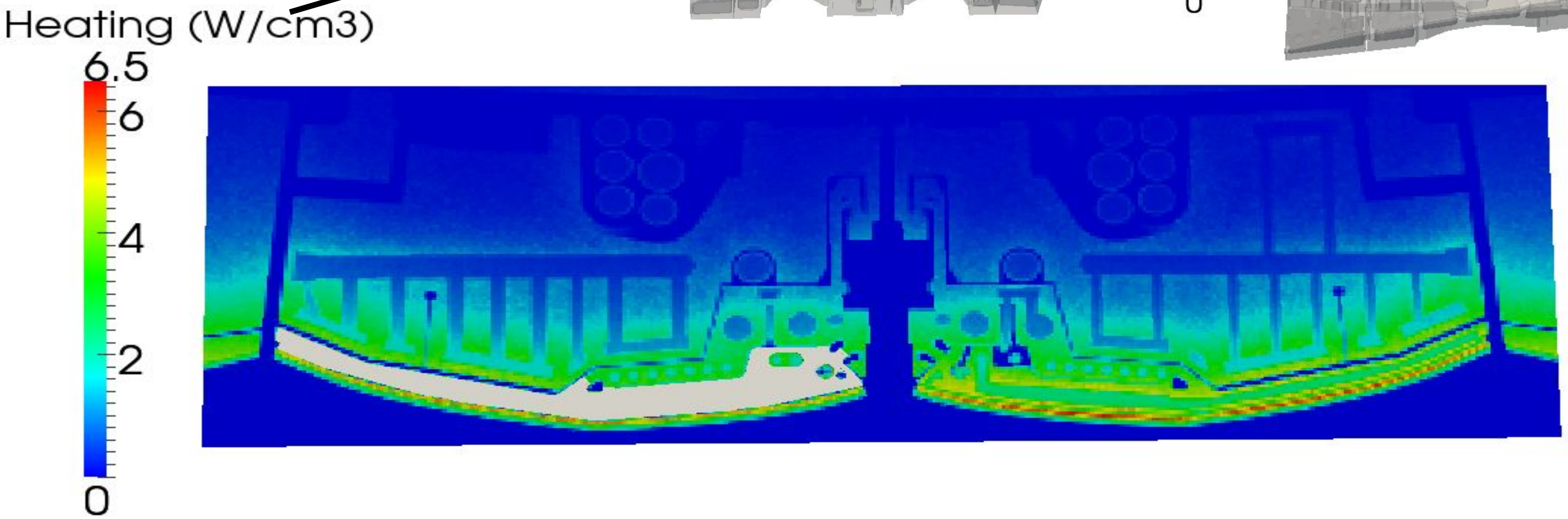


Slice through mid-plane

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

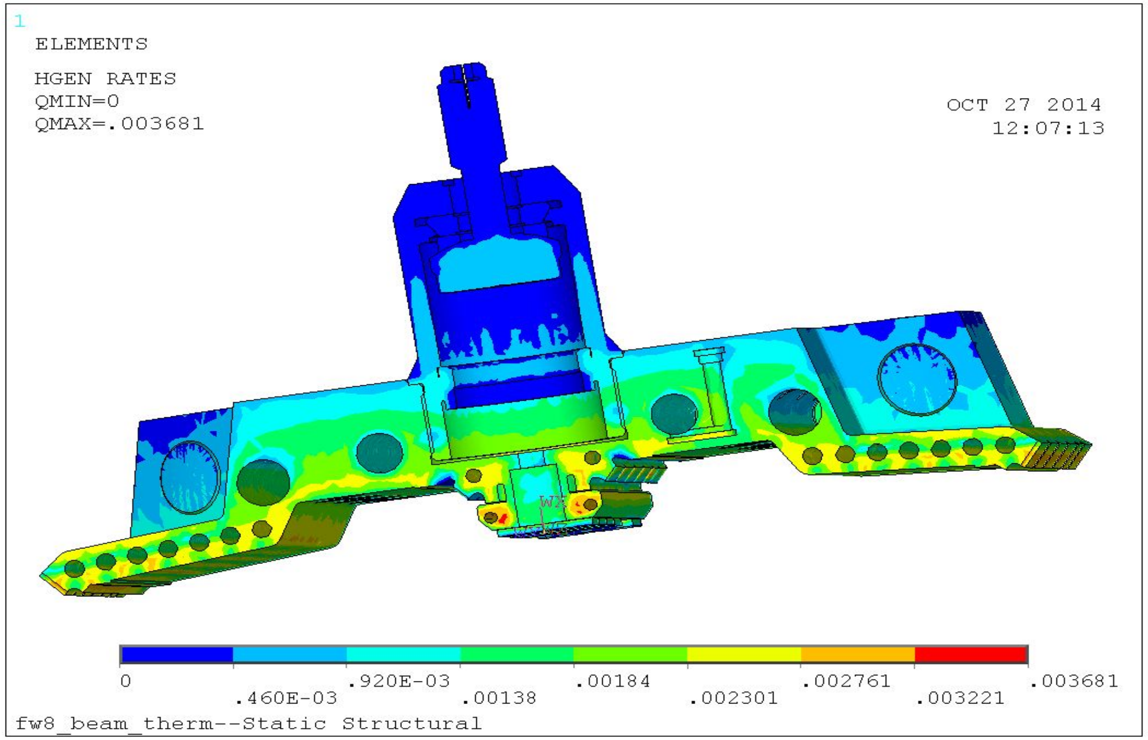


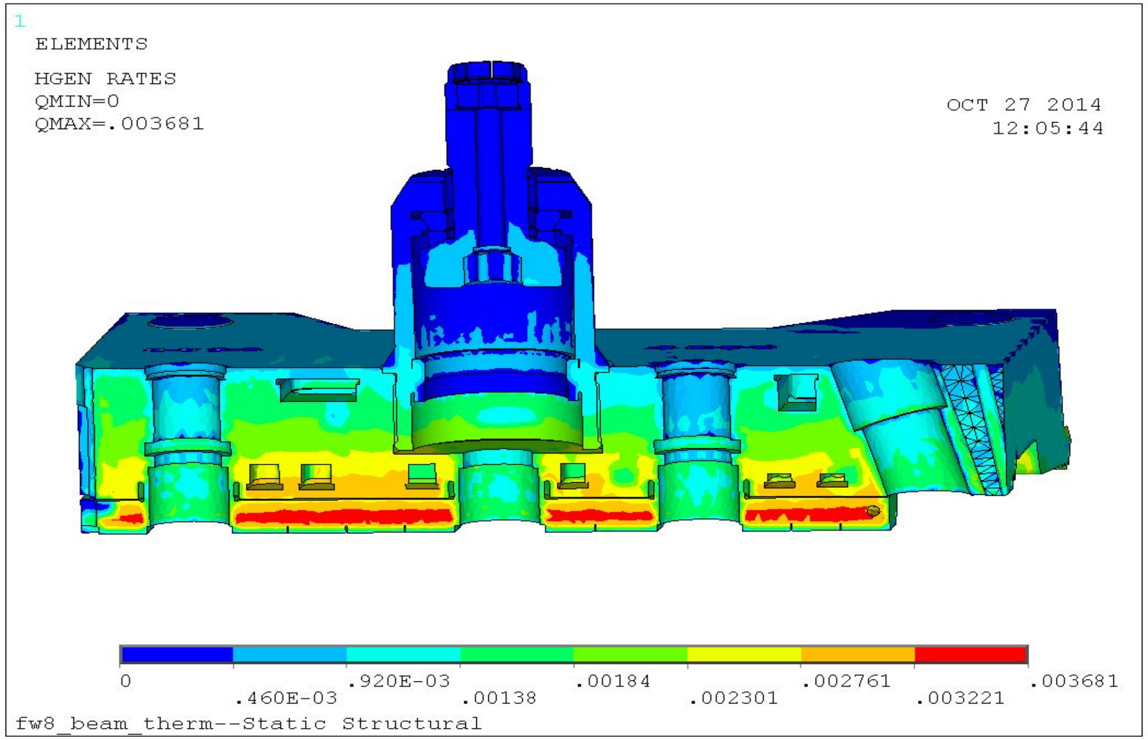




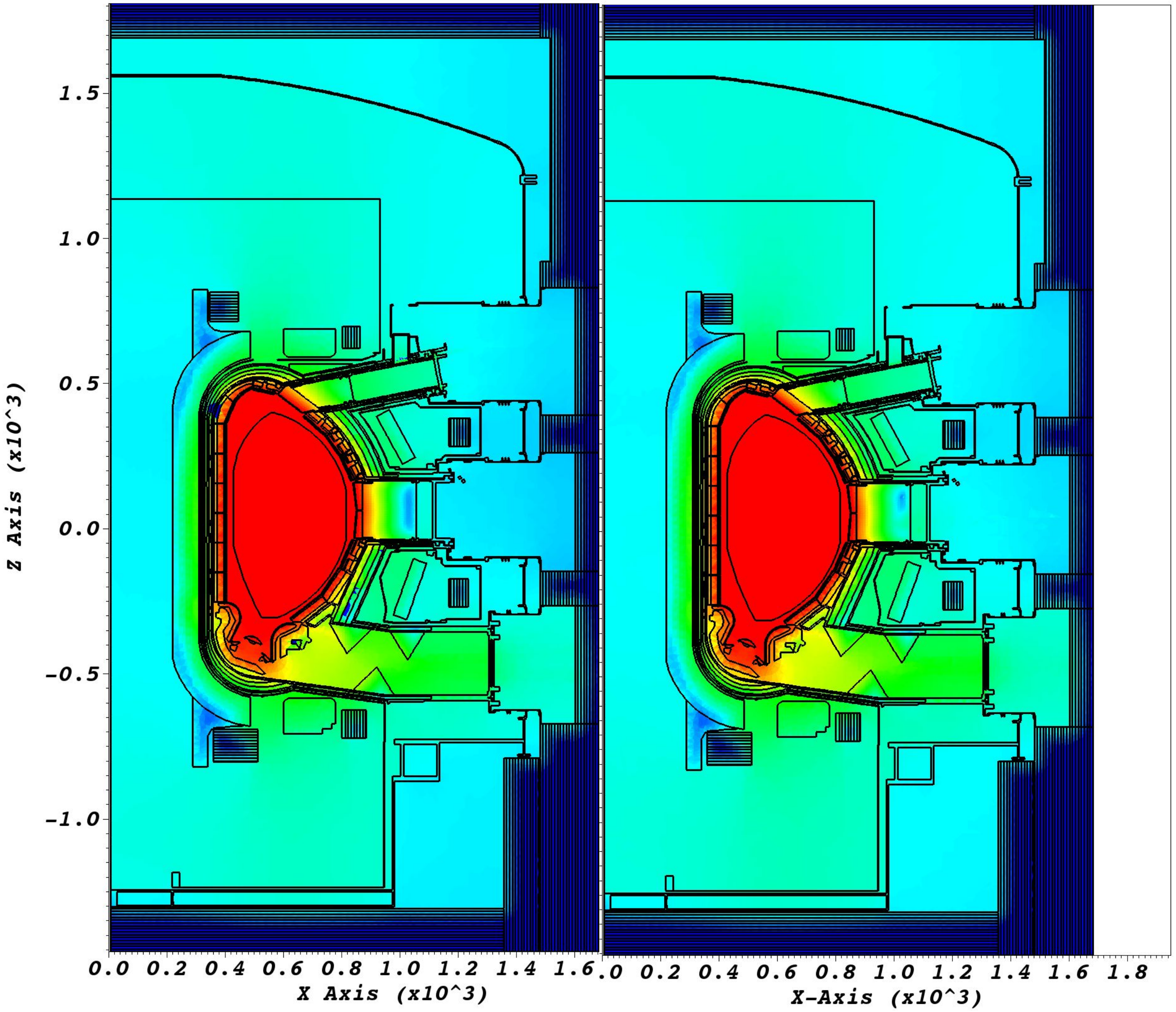
Detailed Blanket Module Heating

- 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:





DAGMC Attila Comparison

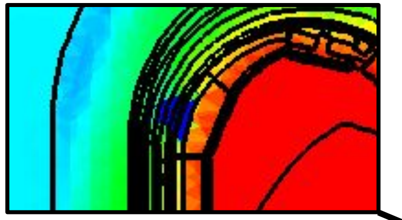


While at UW we did some benchmarking work for US Iter to compare the two main codes used in US for fusion neutronics, Attila and DAGMC

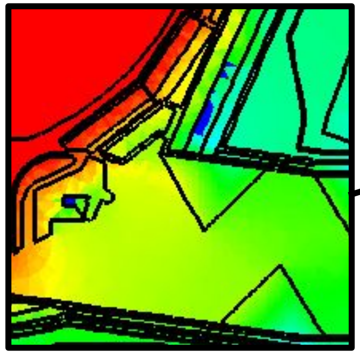
Found pretty good agreement between the codes, except in the standard problem areas

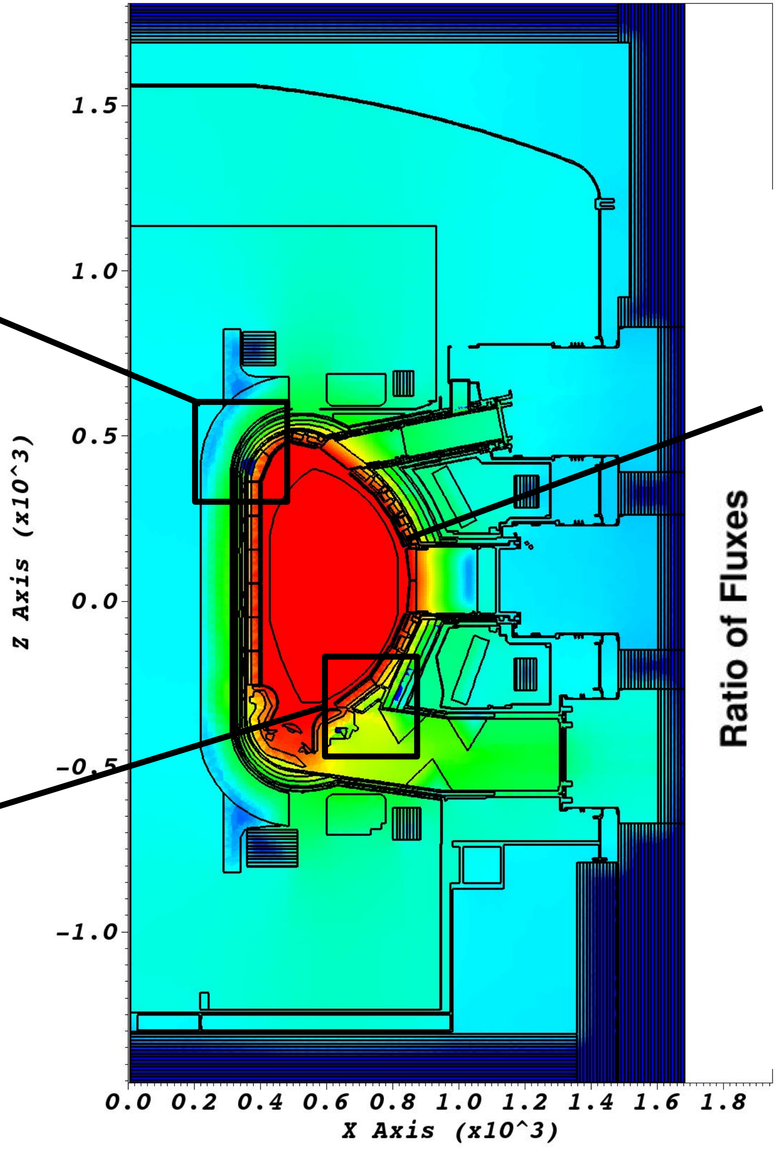
- Over Biased Variance Reduction
- Negative Fluxes

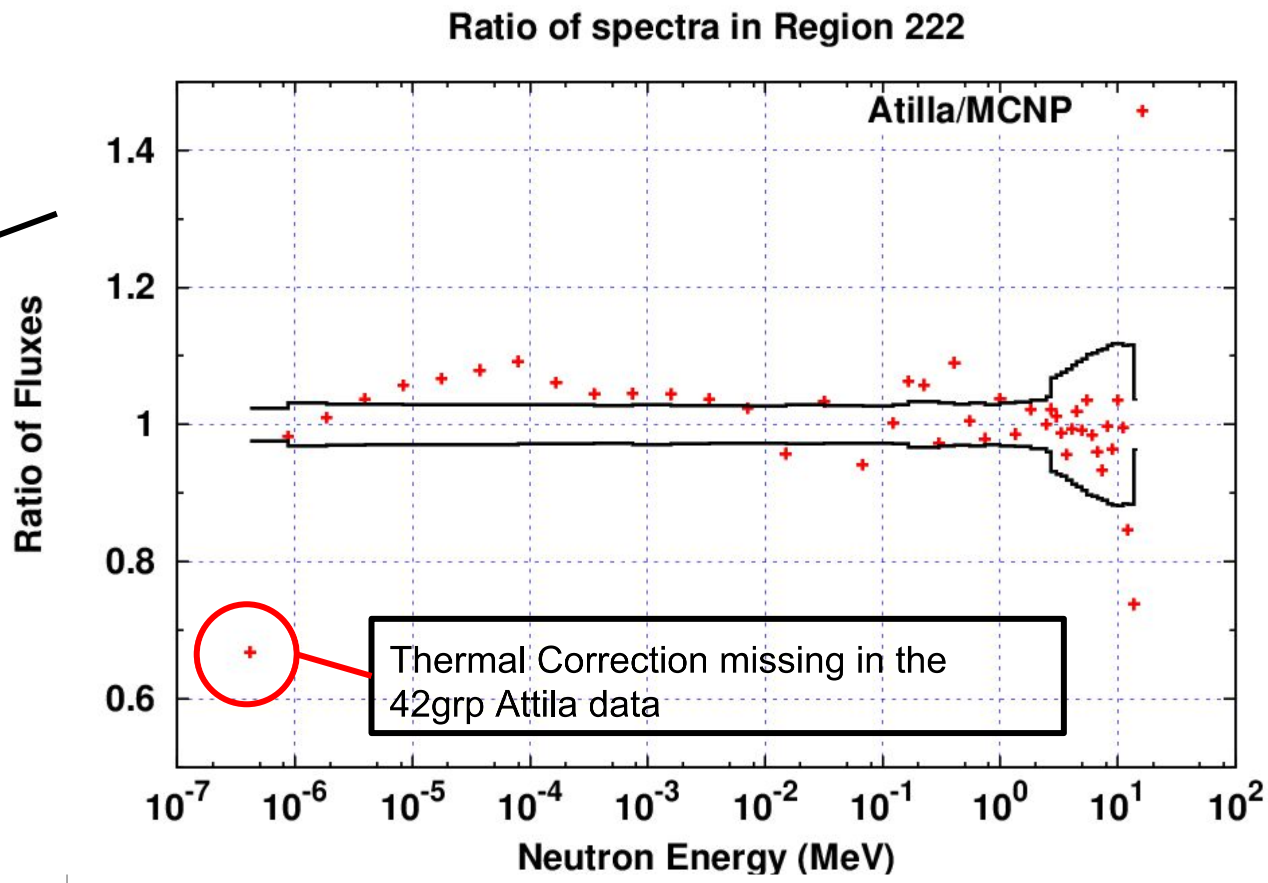
DAGMC Attila Comparison



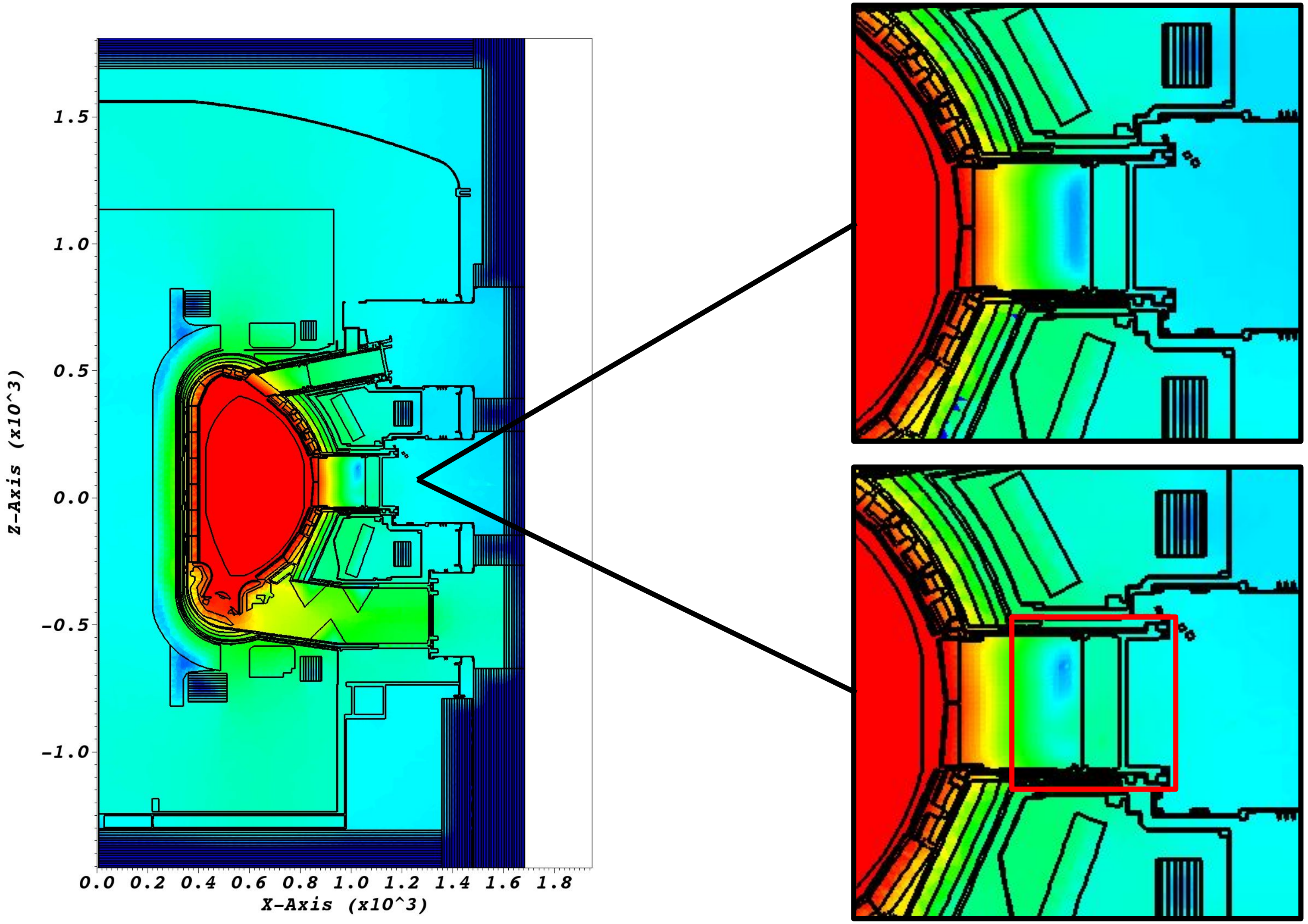
Negative fluxes, regions of poor convergence in the deterministic solution







DAGMC Attila Comparison



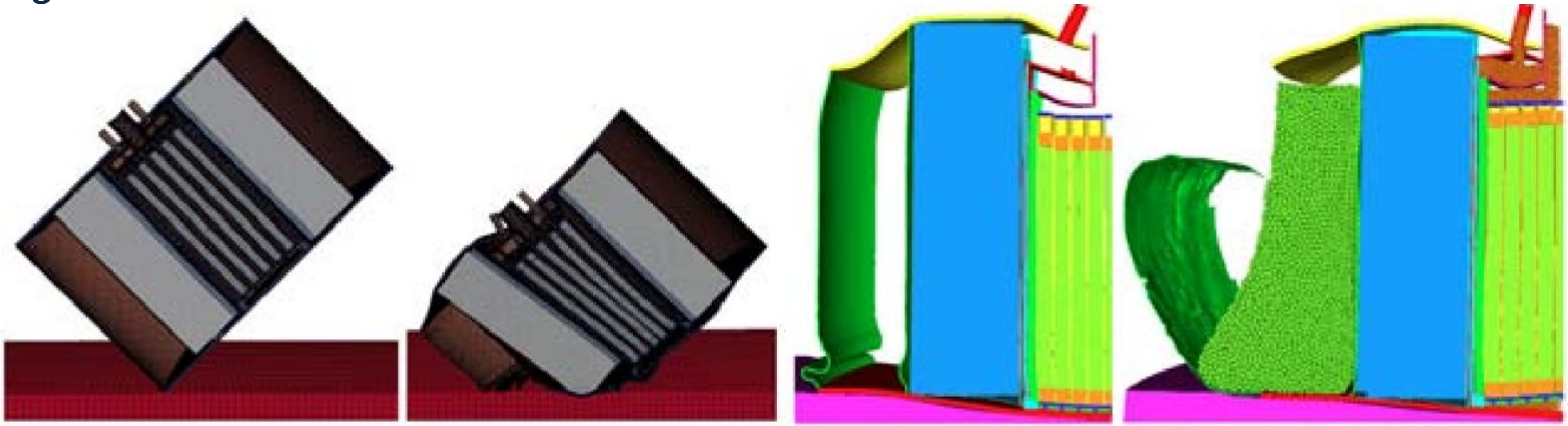
Attila

DAG-MCNP5

Large statistical error in local region

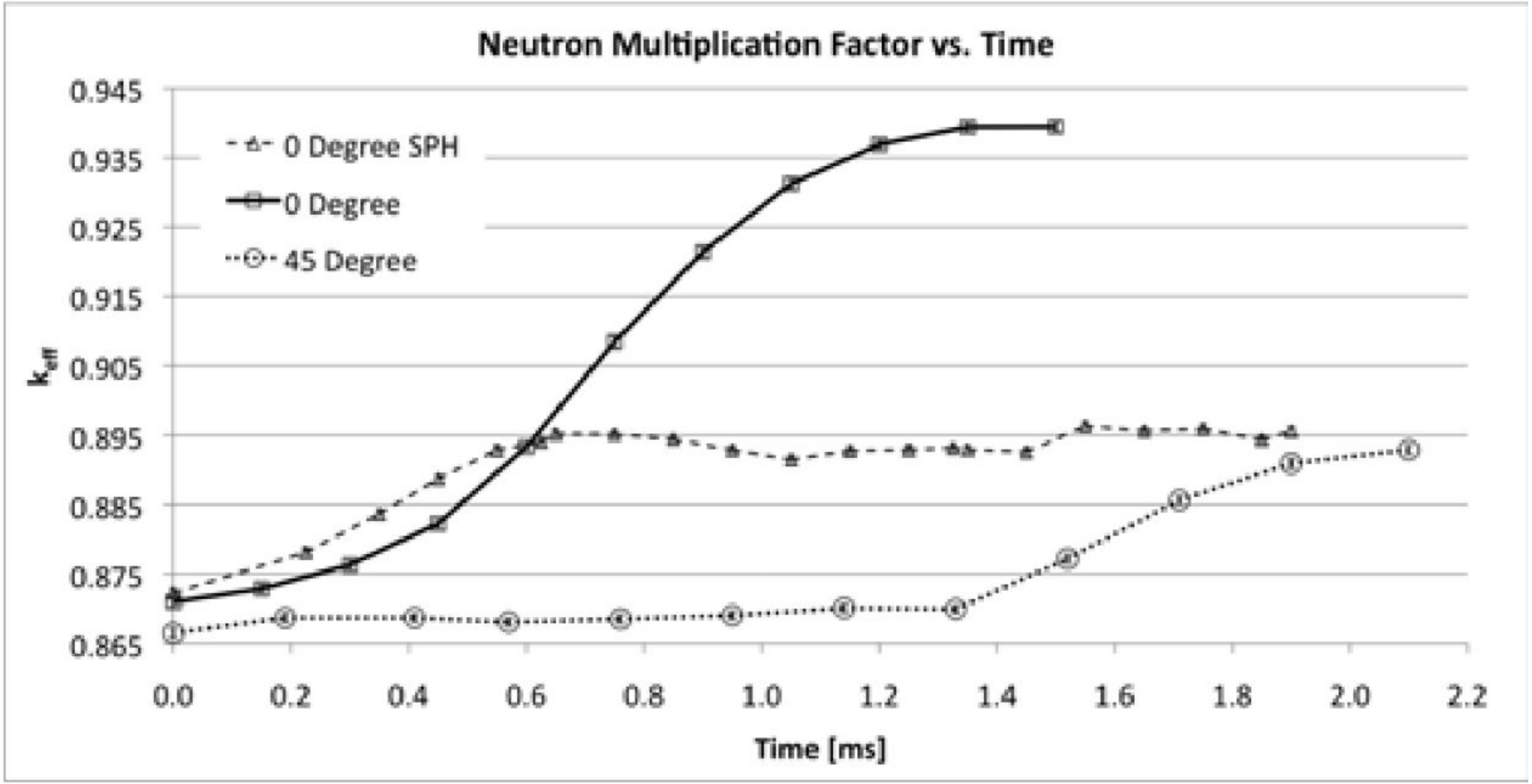
SNL Space Reactor

- 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



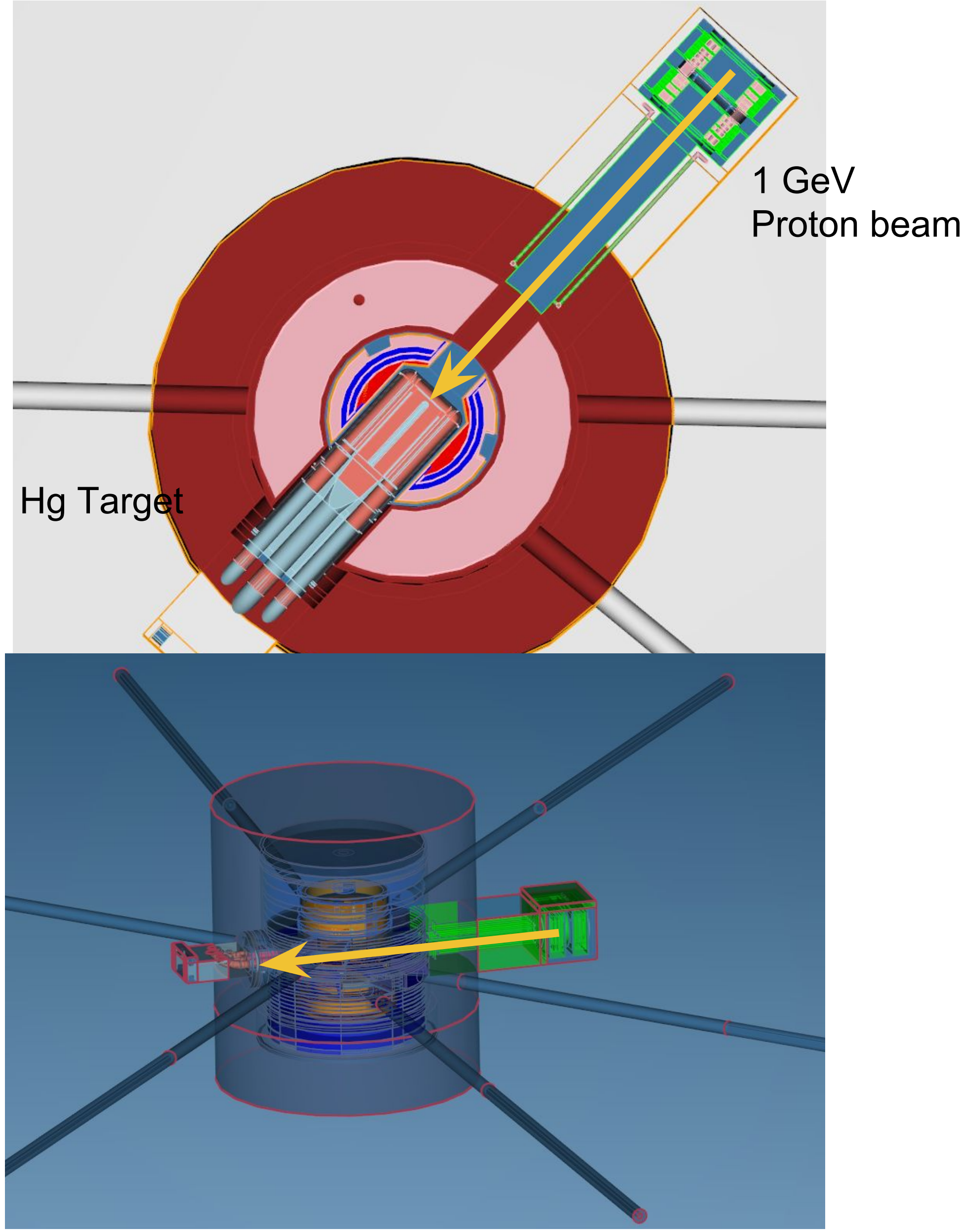
45-degree 0 ms | 45-degree 2.1 ms | 0-degree 1.5 ms | 0-degree SPH 1.5 ms

SNL Space Reactor

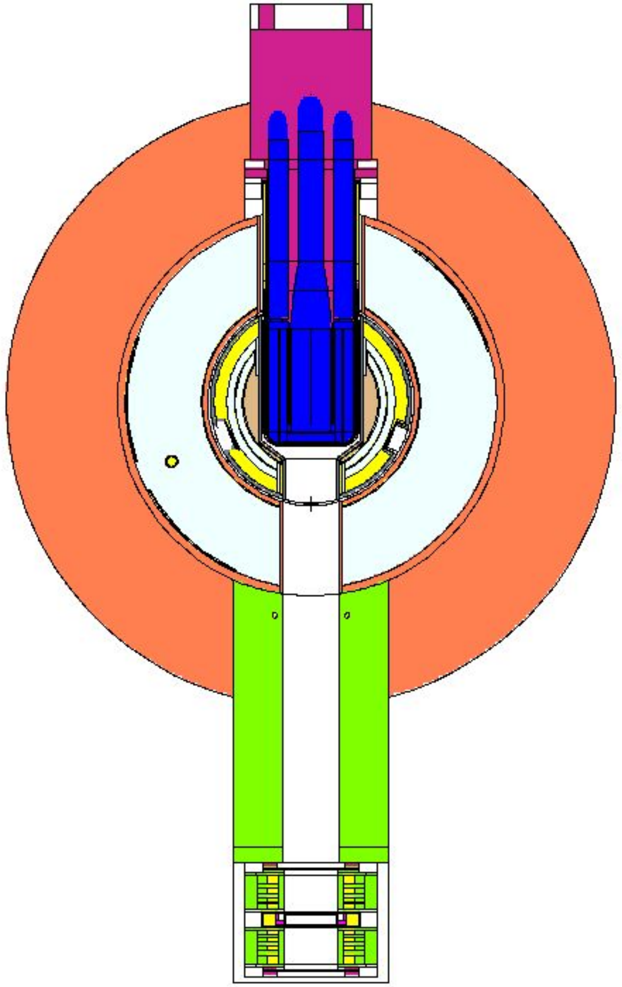


DAG-MCNP6 SNS

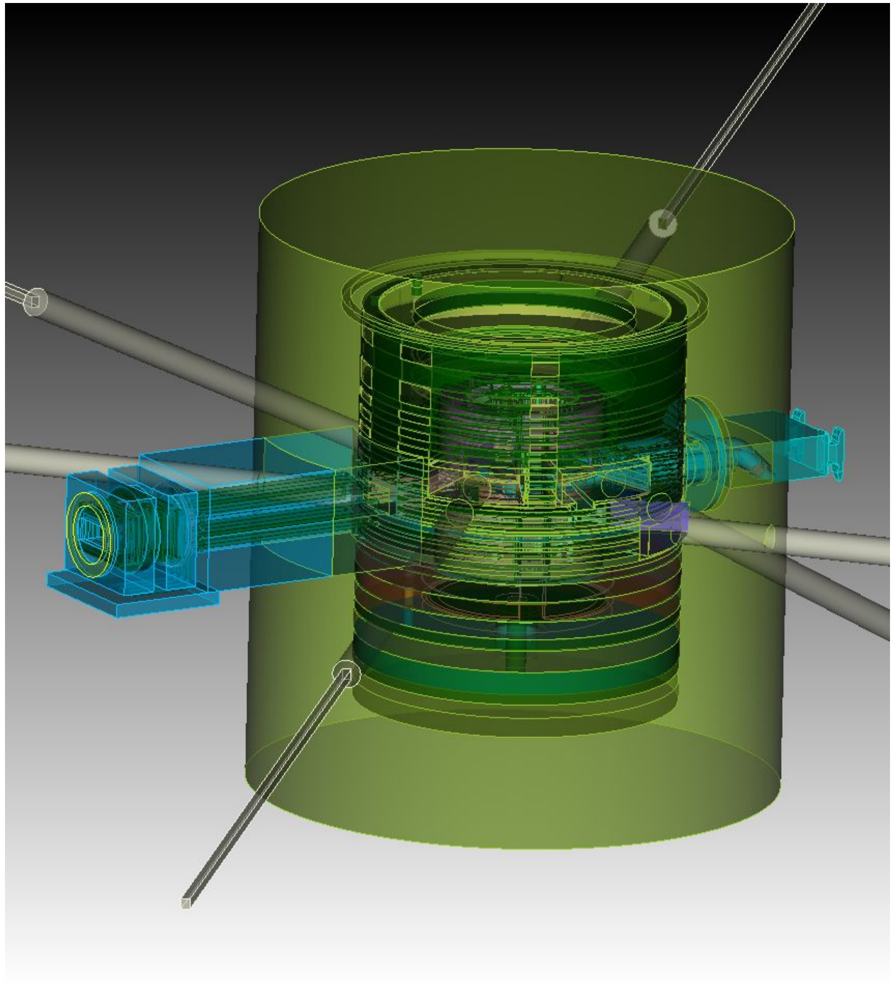
- Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS) are interested in shifting to a complete CAD based workflow
  - They have extensive CAD models of the facility and a planned upgrade
- SNS 1 GeV proton beam impinges on liquid mercury target delivering 1 MW of heat into the target,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



DAG-MCNP6 SNS



MCNP geometry

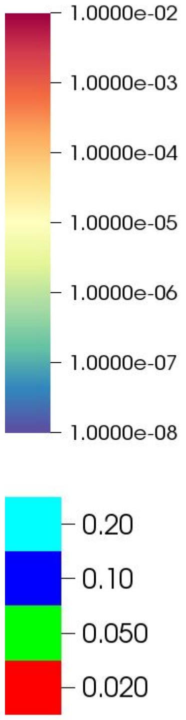


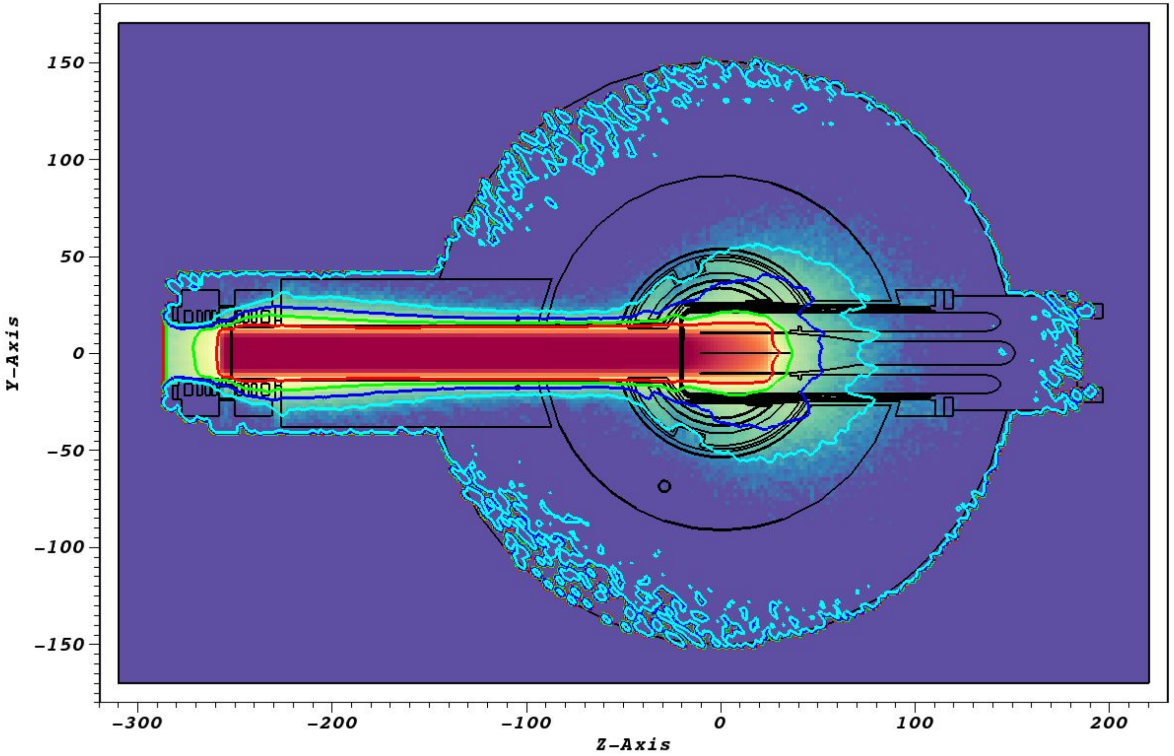
CAD model

- 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)

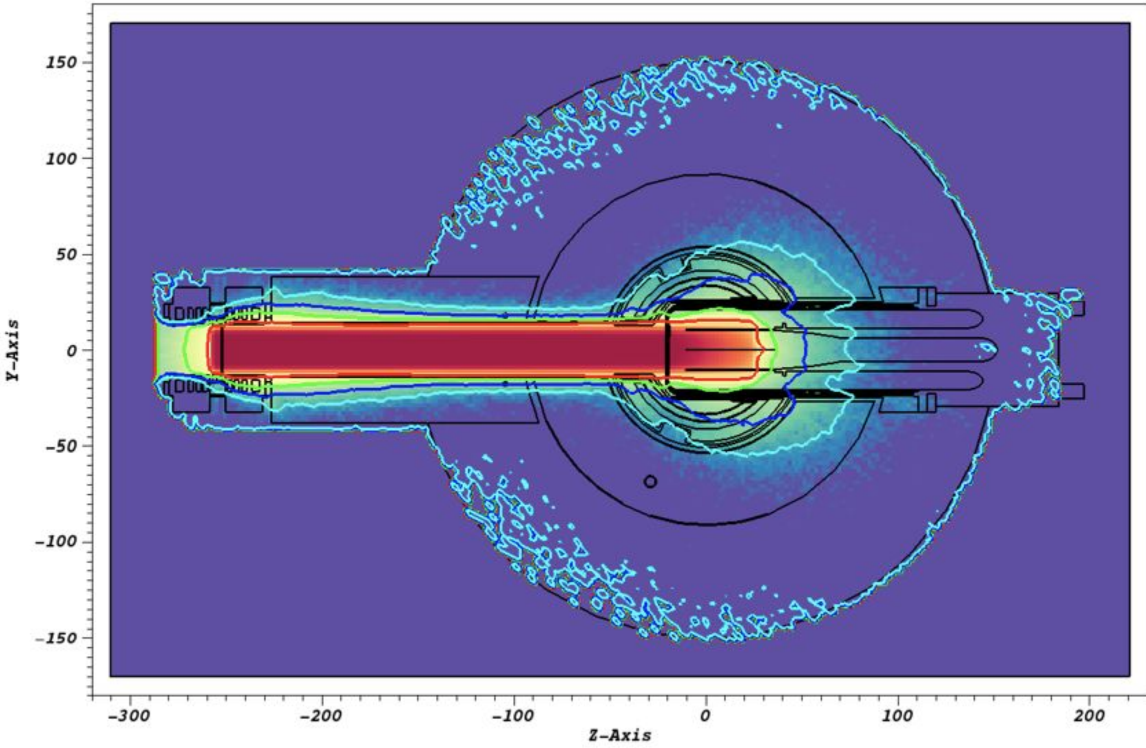
DAG-MCNP6 SNS

MCNP6





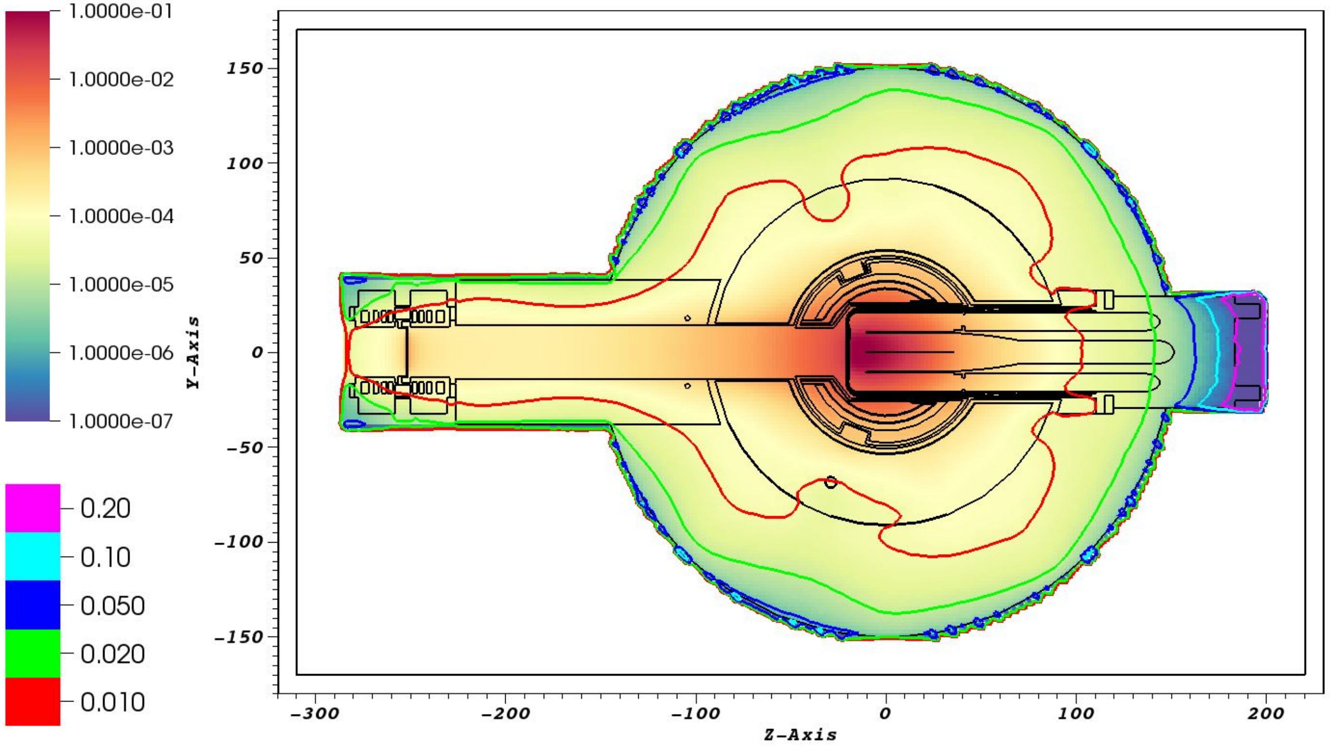
DAG-MCNP6



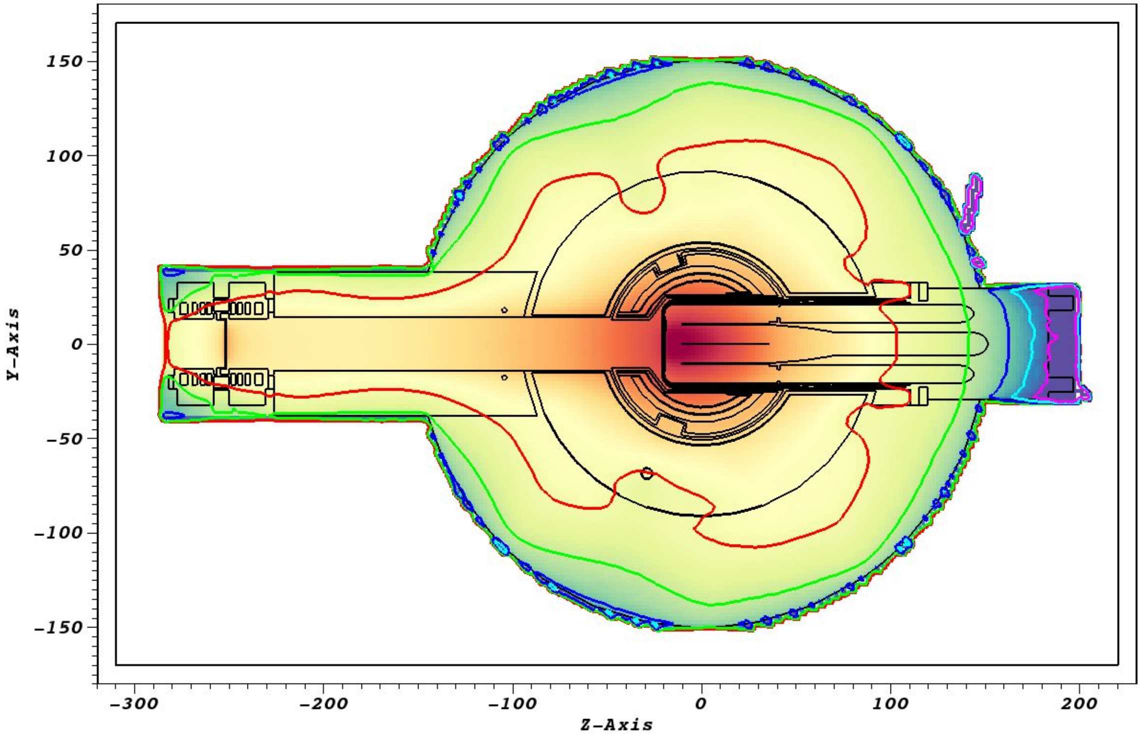
Proton Flux

DAG-MCNP6 SNS

MCNP6

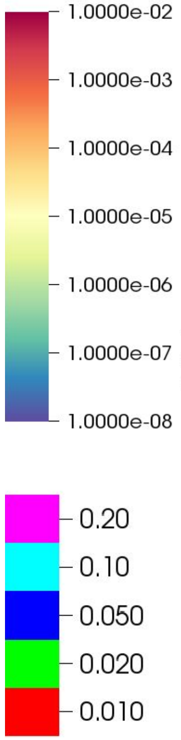


DAG-MCNP6

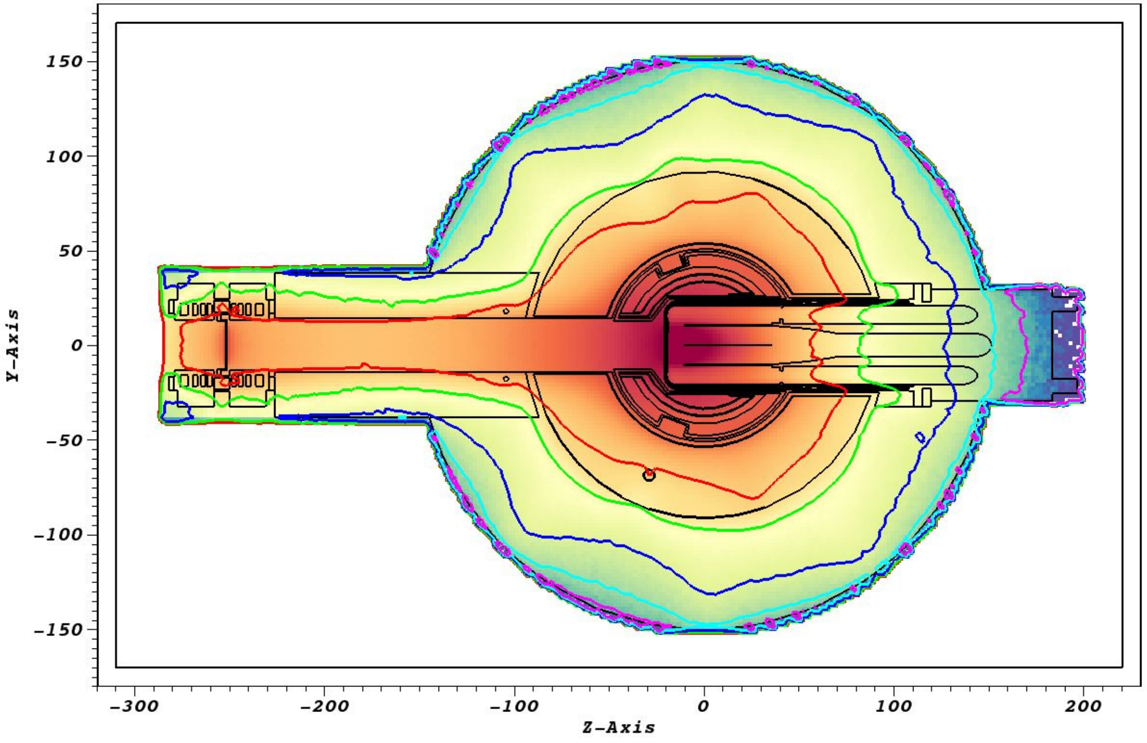


Neutron Flux

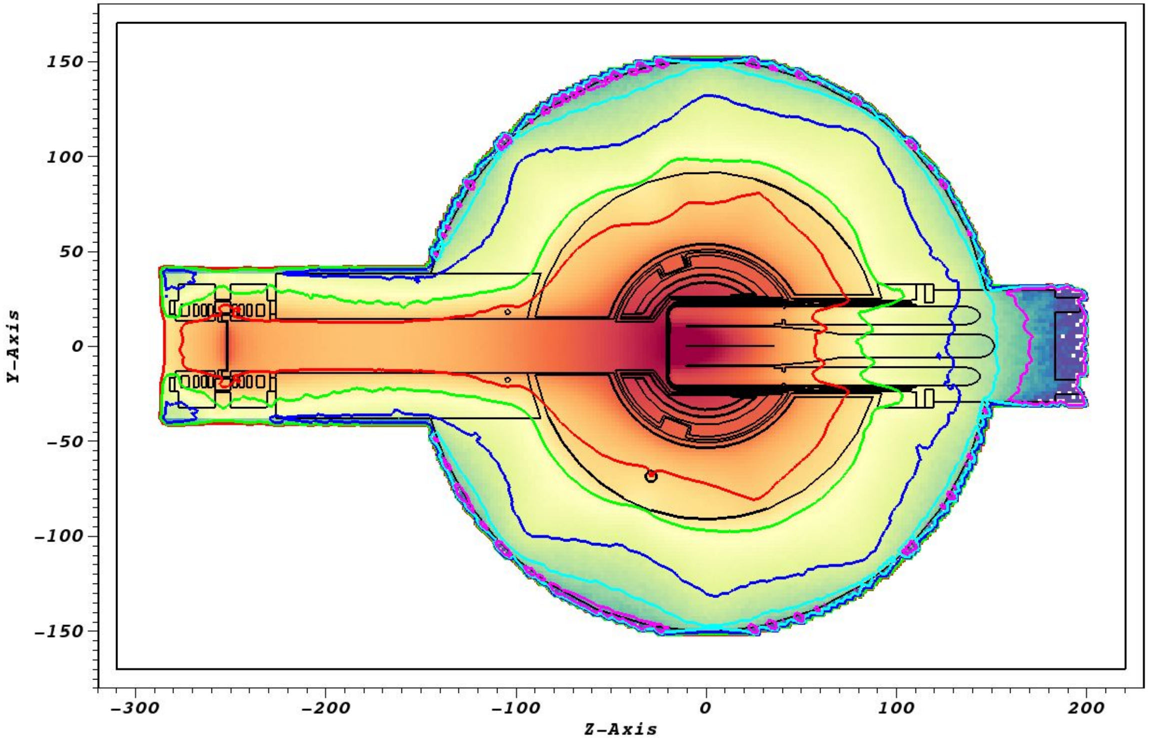
DAG-MCNP6 SNS



MCNP6

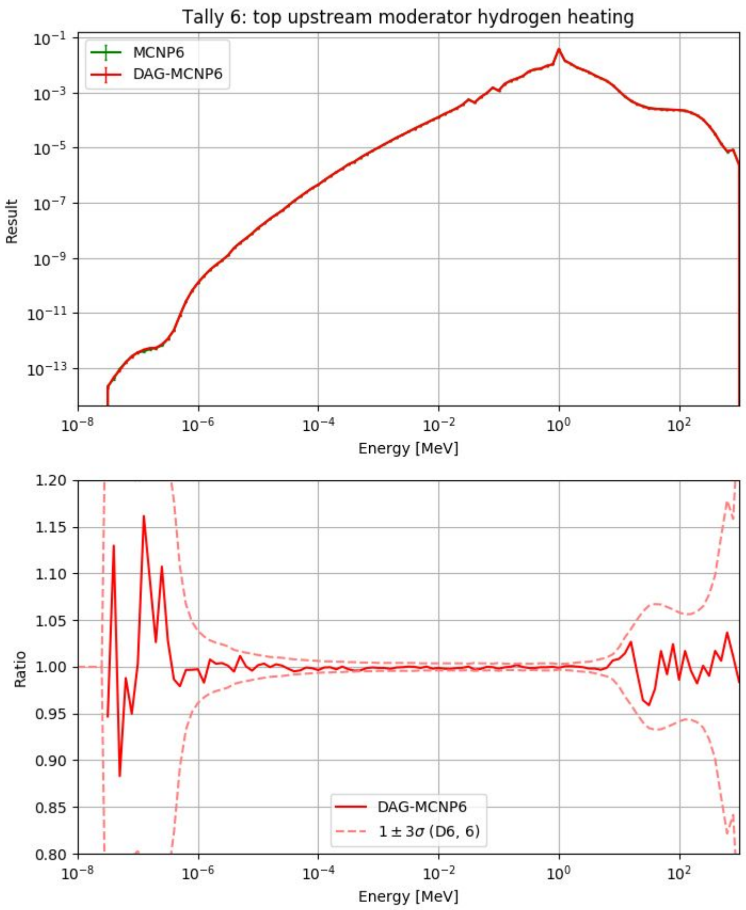


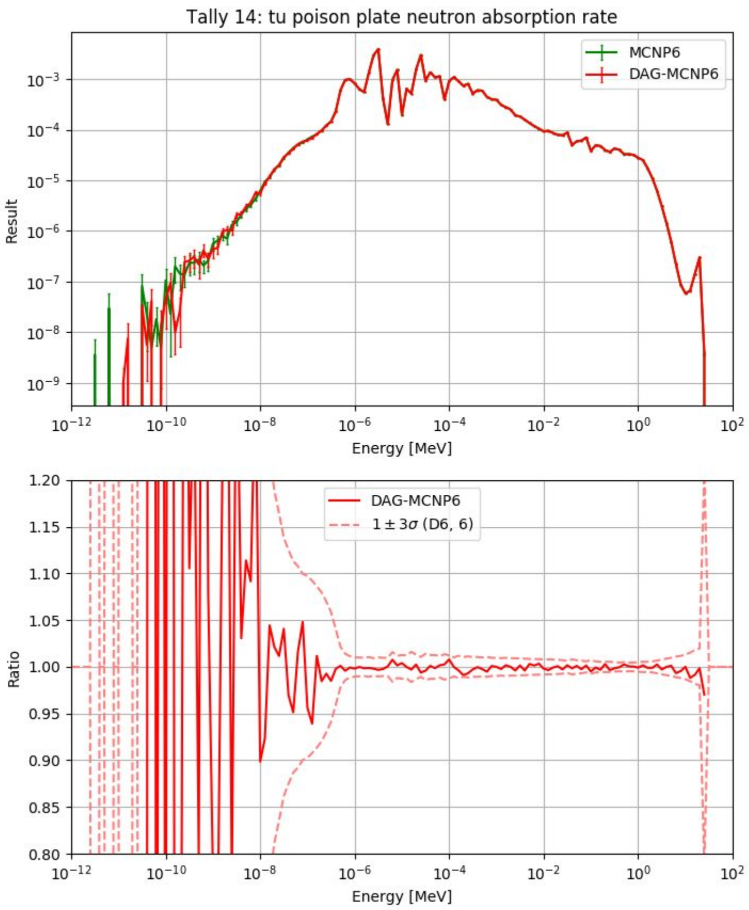
DAG-MCNP6

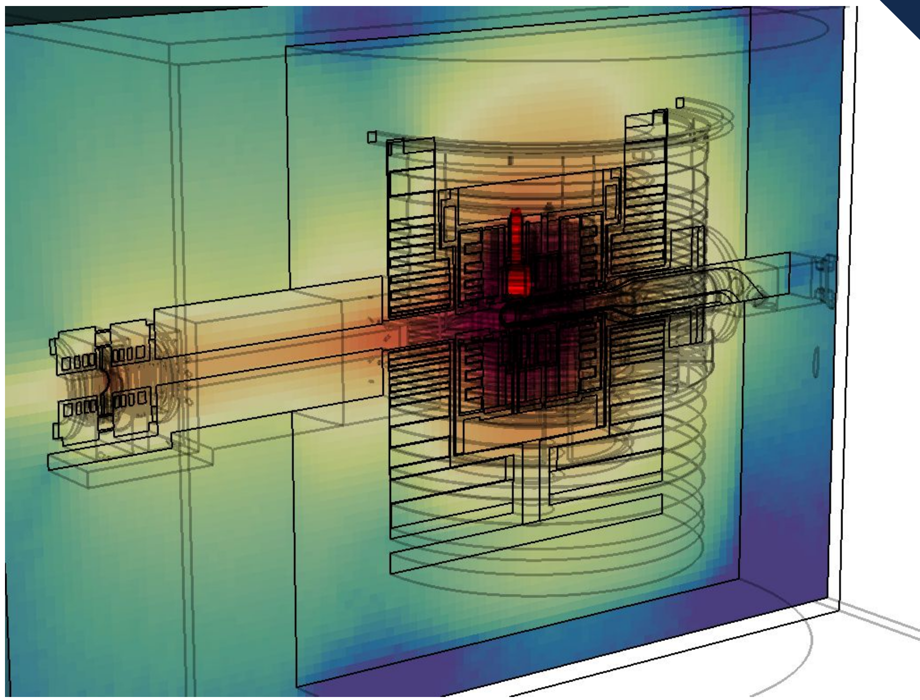


Photon Flux

Specific Tally Comparison in SNS



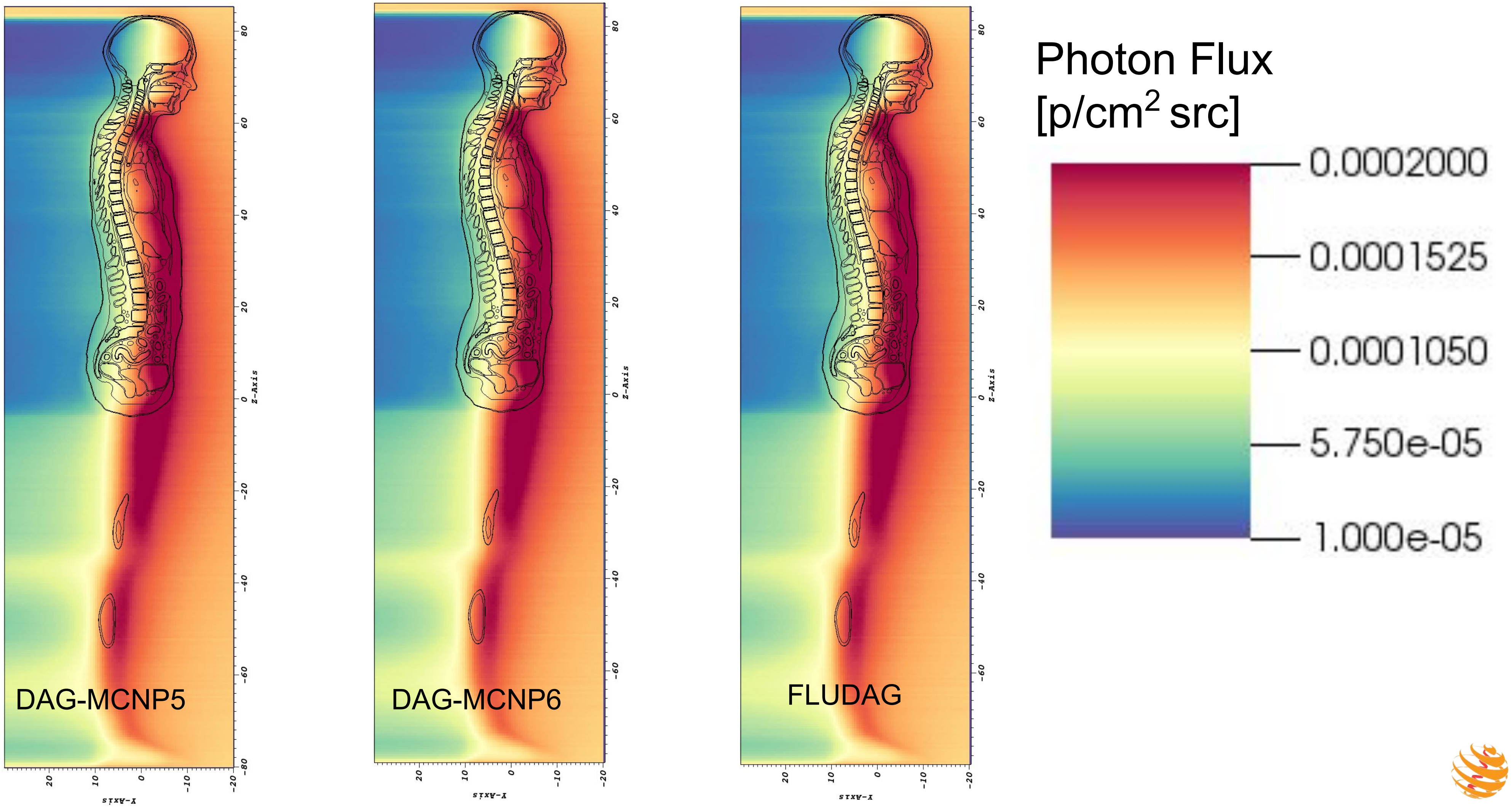




Human Mesh Phantom

UK Atomic Energy Authority

Results: 0.1 MeV Photon Source



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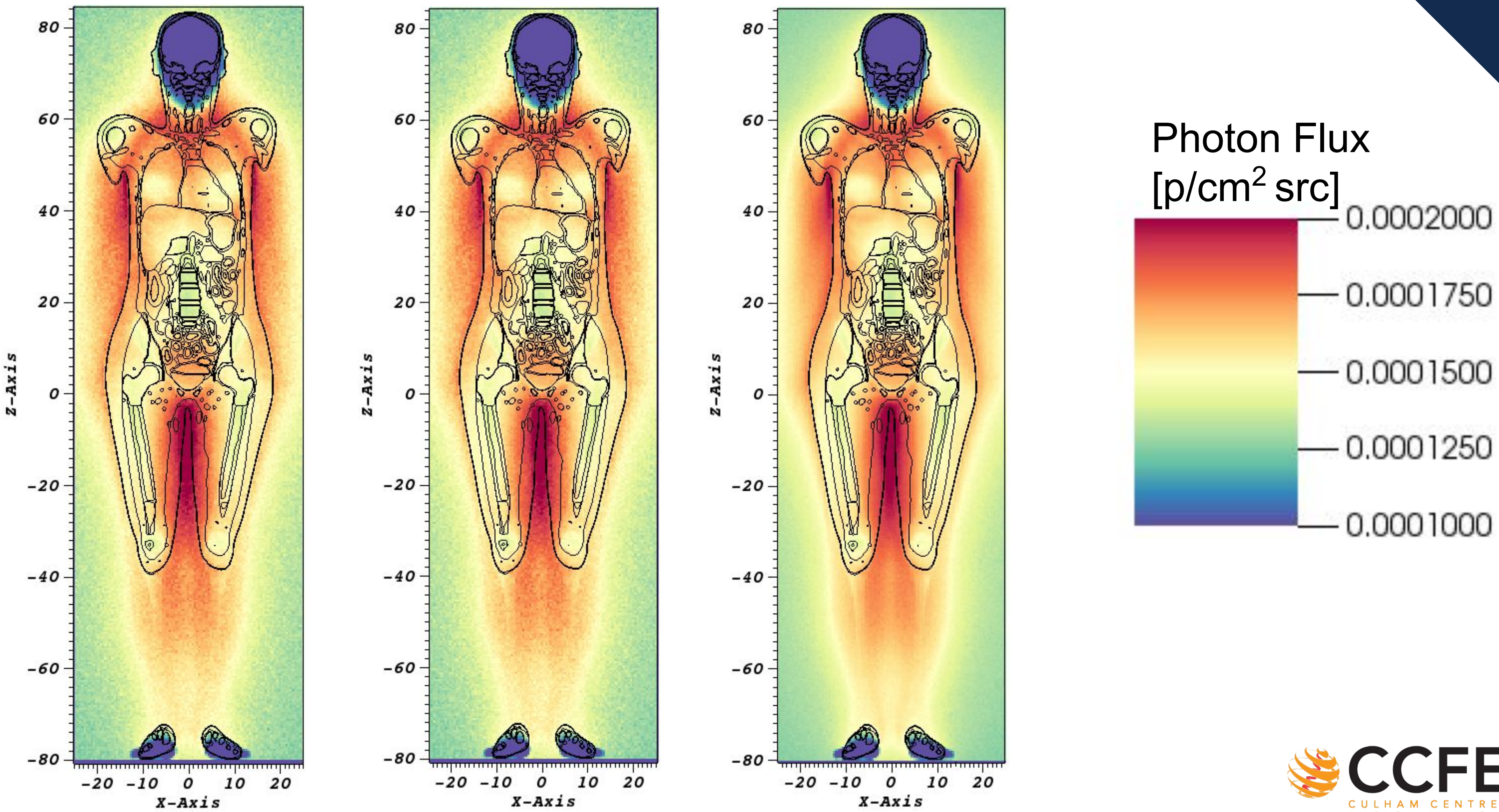
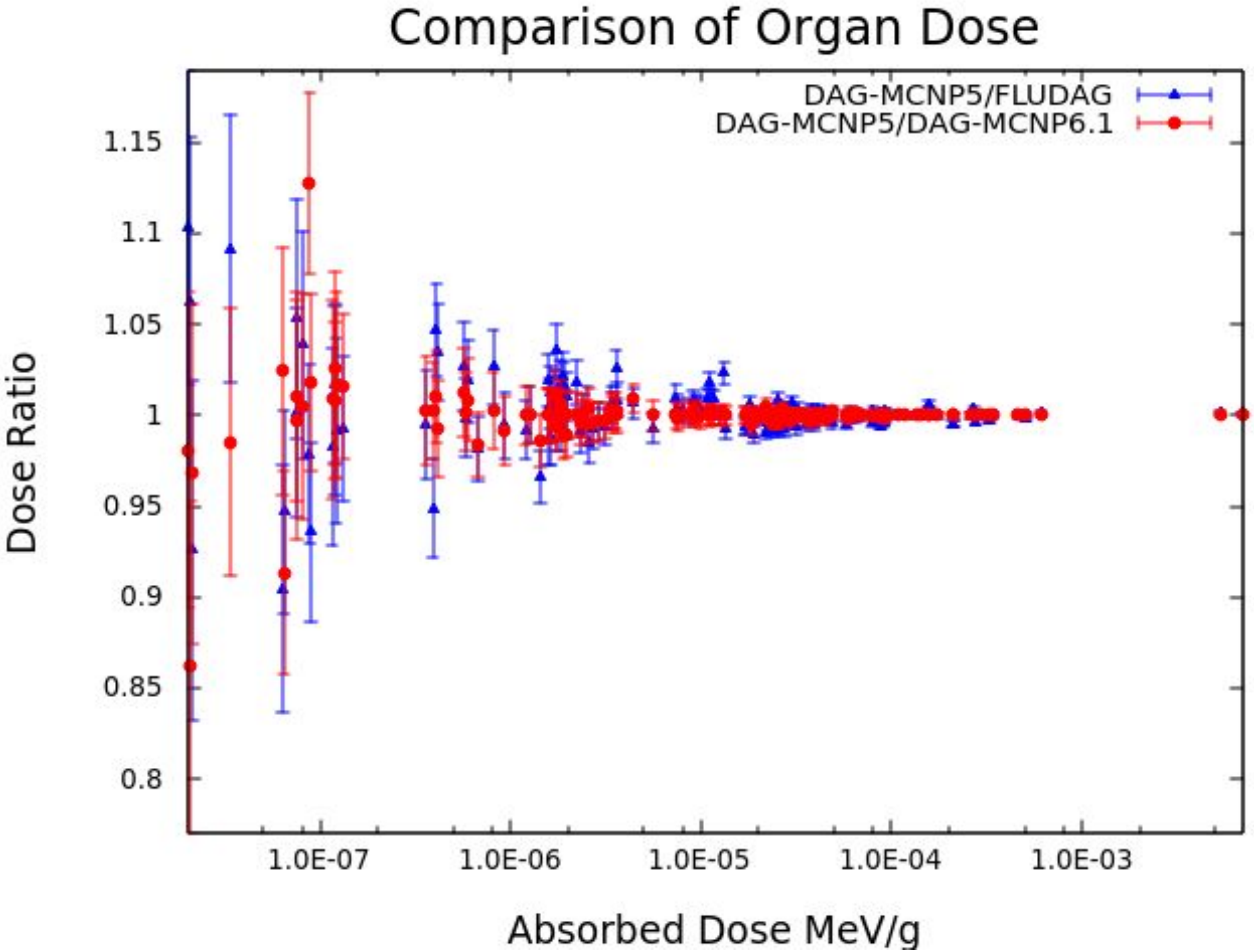
CULHAM CENTRE FOR FUSION ENERGY

Human Mesh Phantom



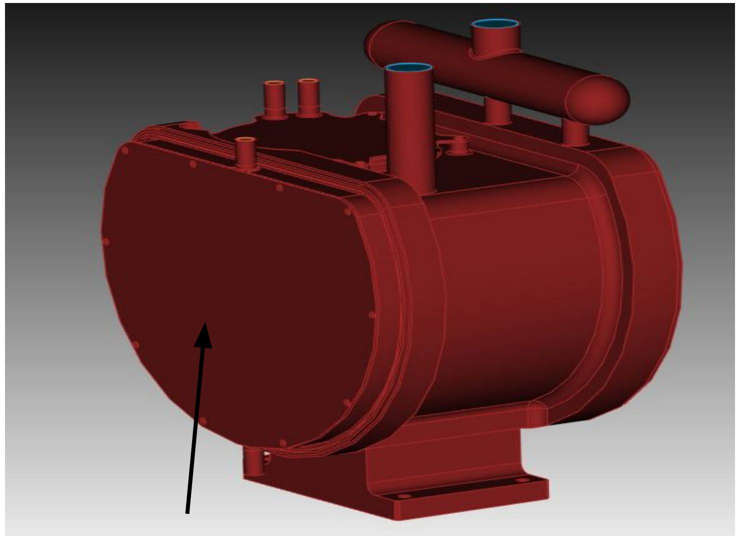
Human Mesh Phantom



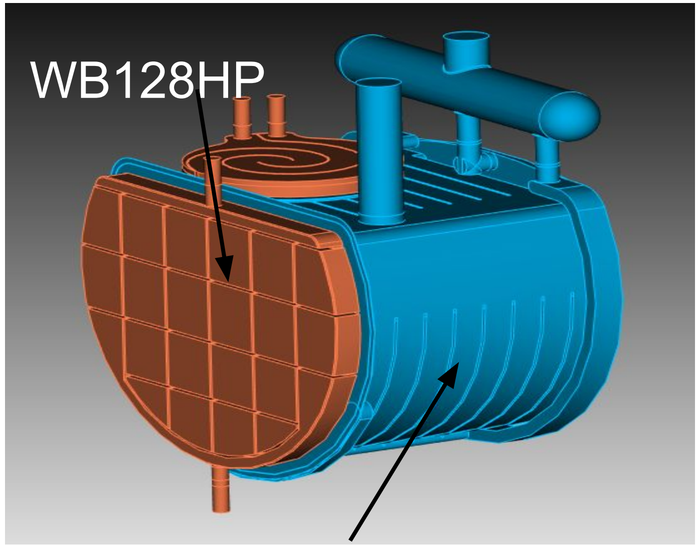
High Energy Physics Example

UK Atomic Energy Authority

- 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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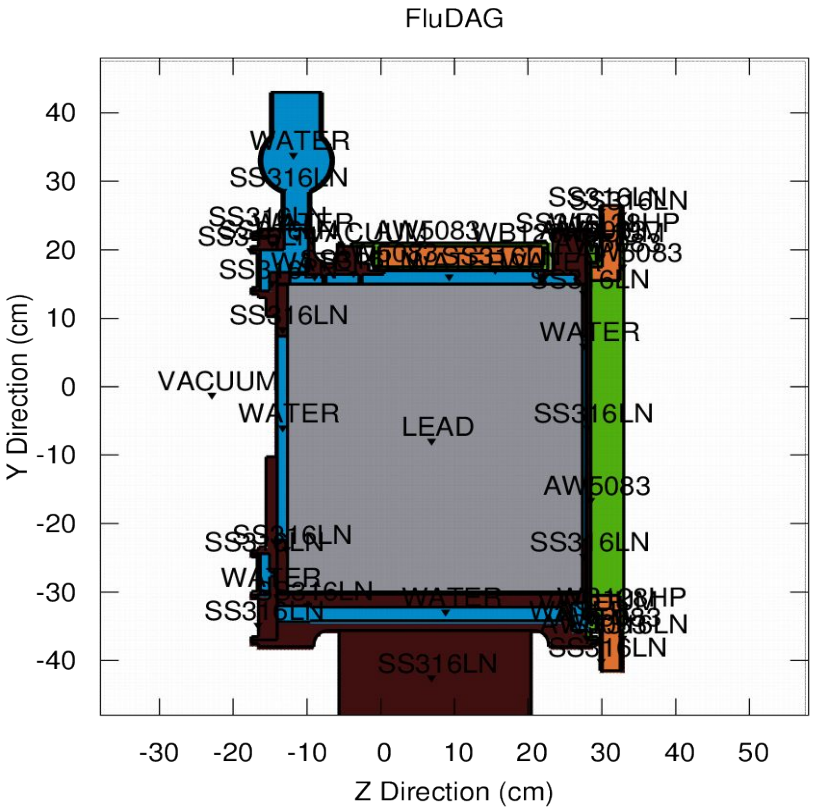
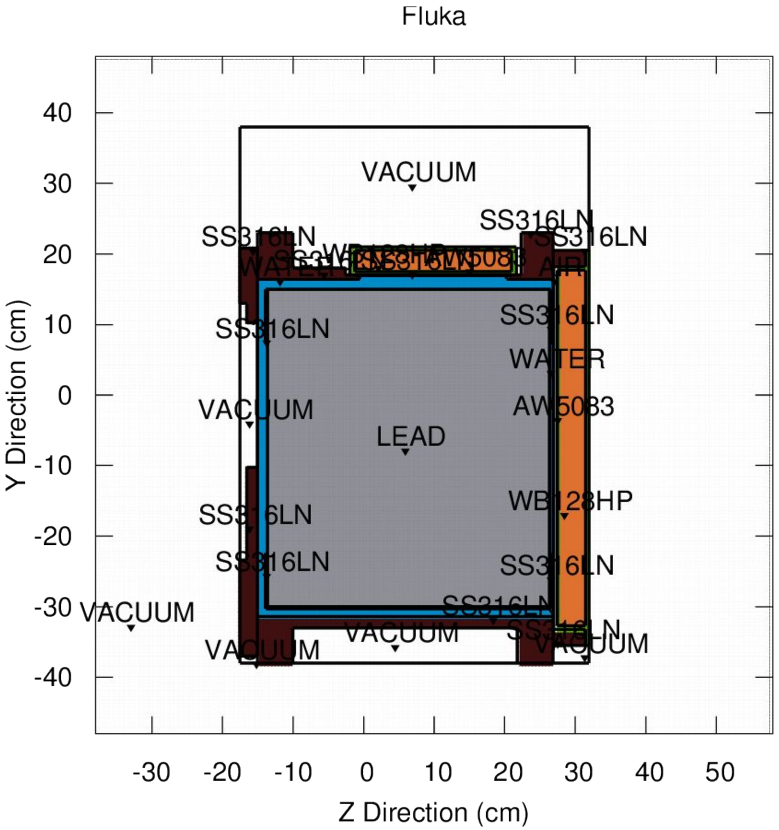
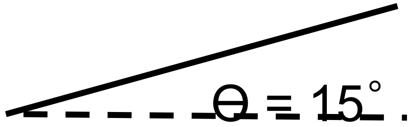
nTOF Geometry

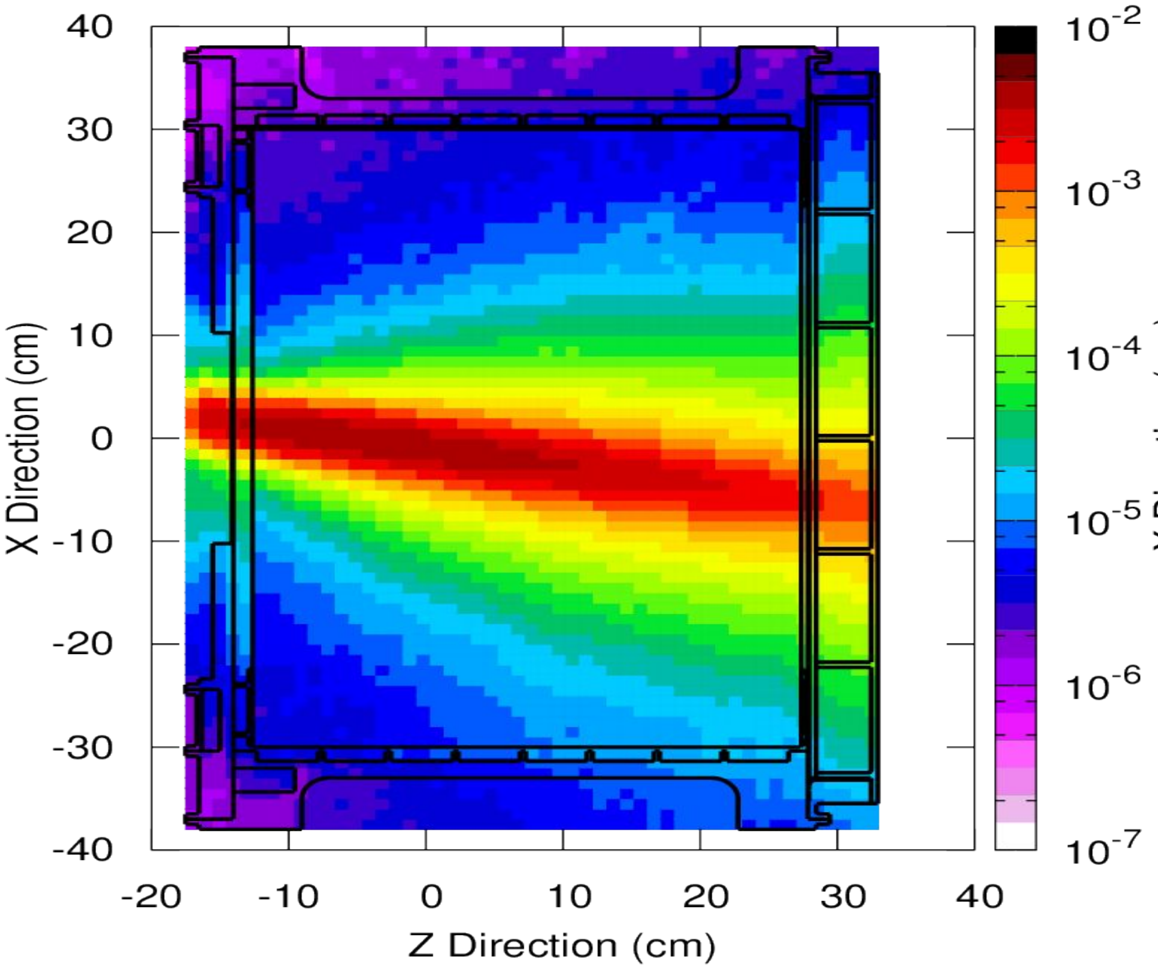


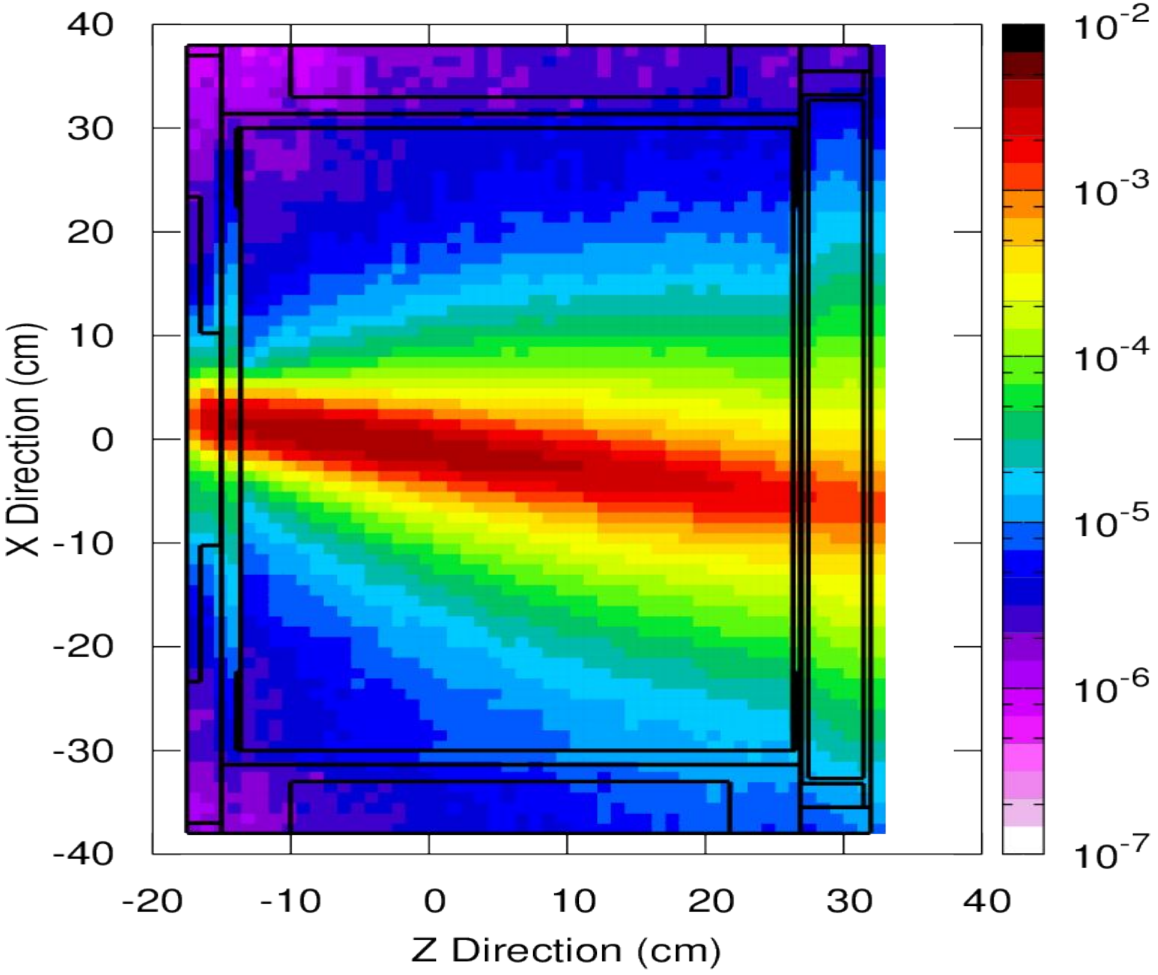




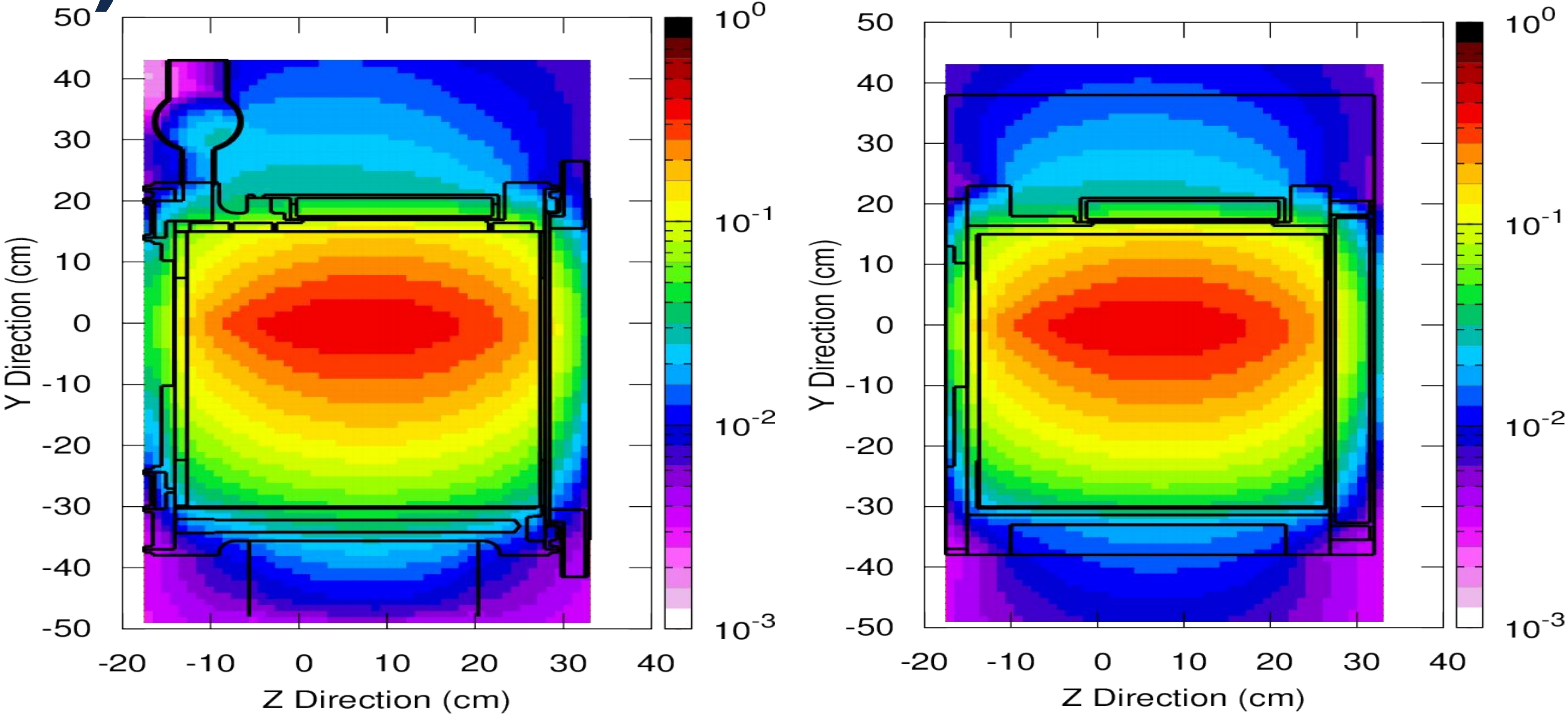
Slice through x=0

nTOF Comparisons - Proton Flux

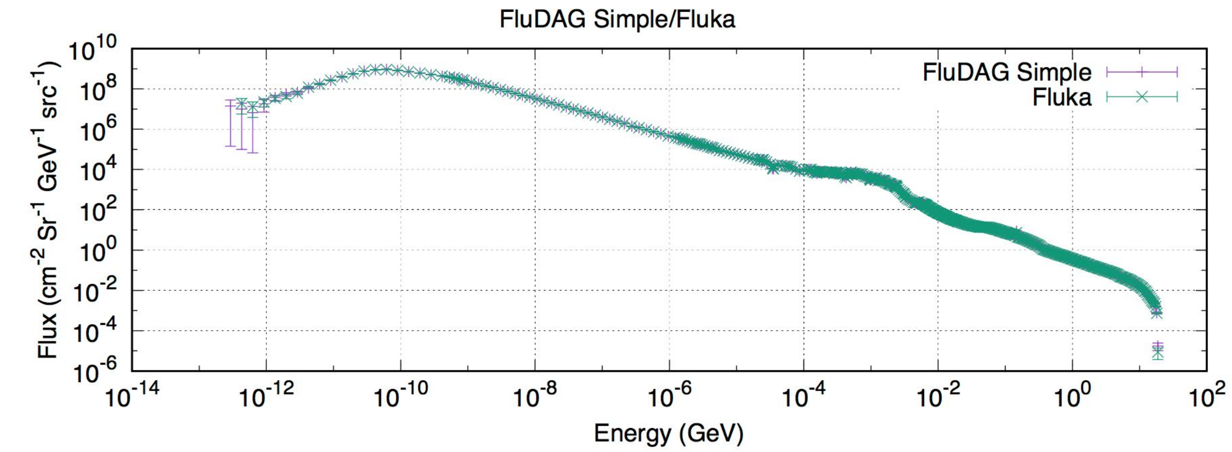


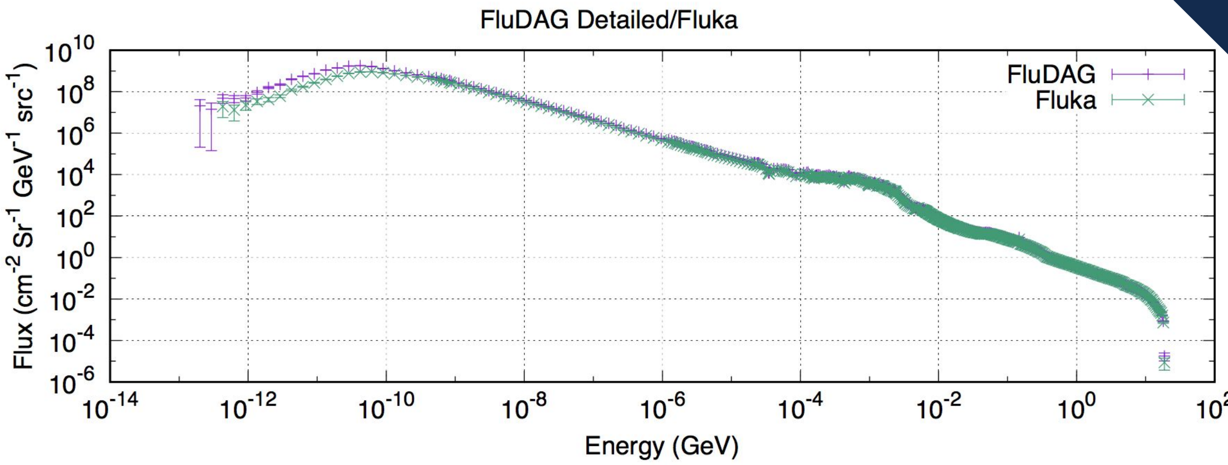


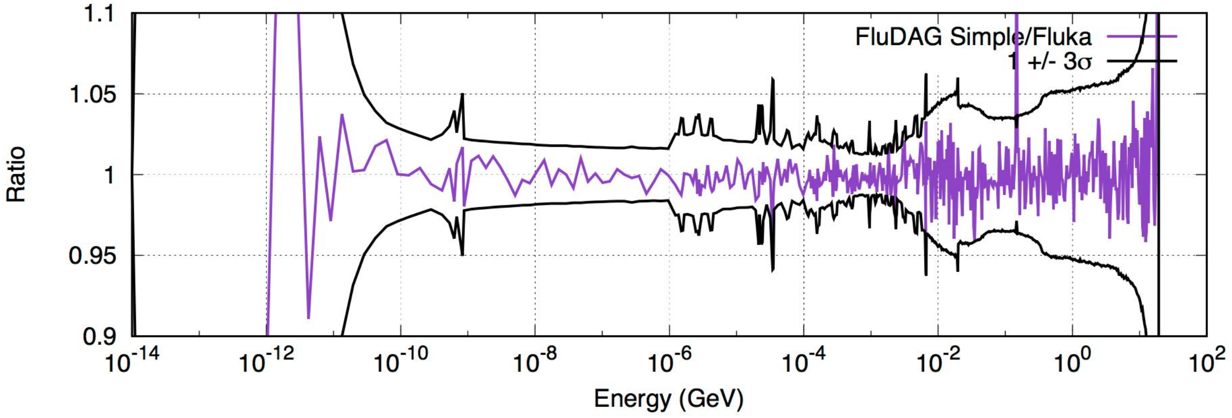
nTOF Comparisons - Neutron Flux (per src)

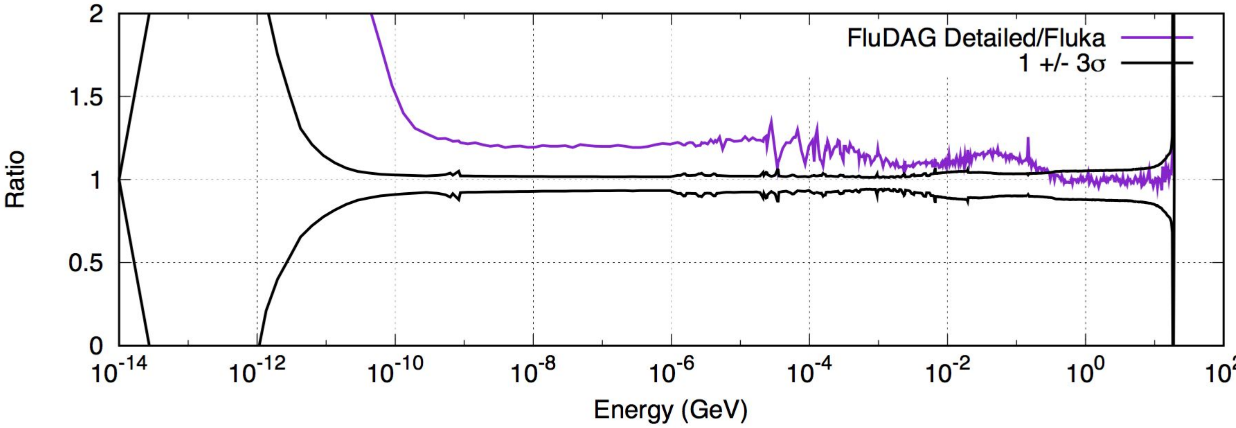


nTOF Comparisons - Neutron Spectrum



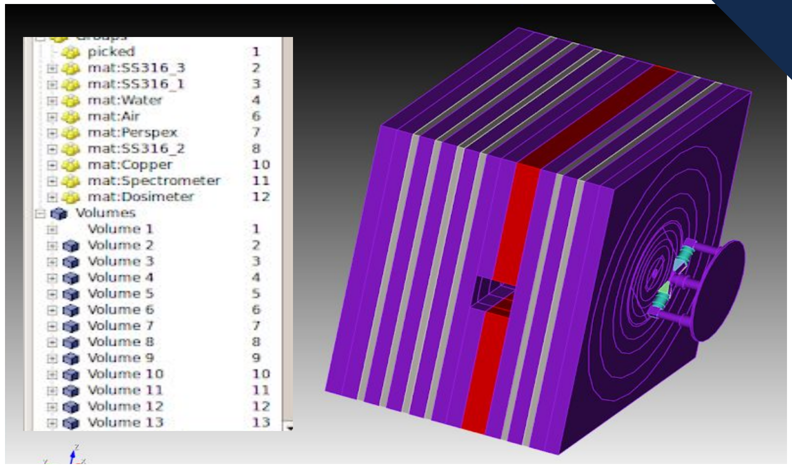




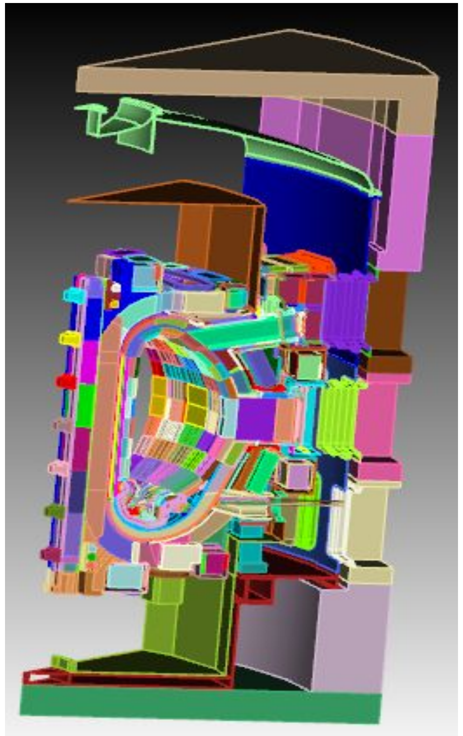


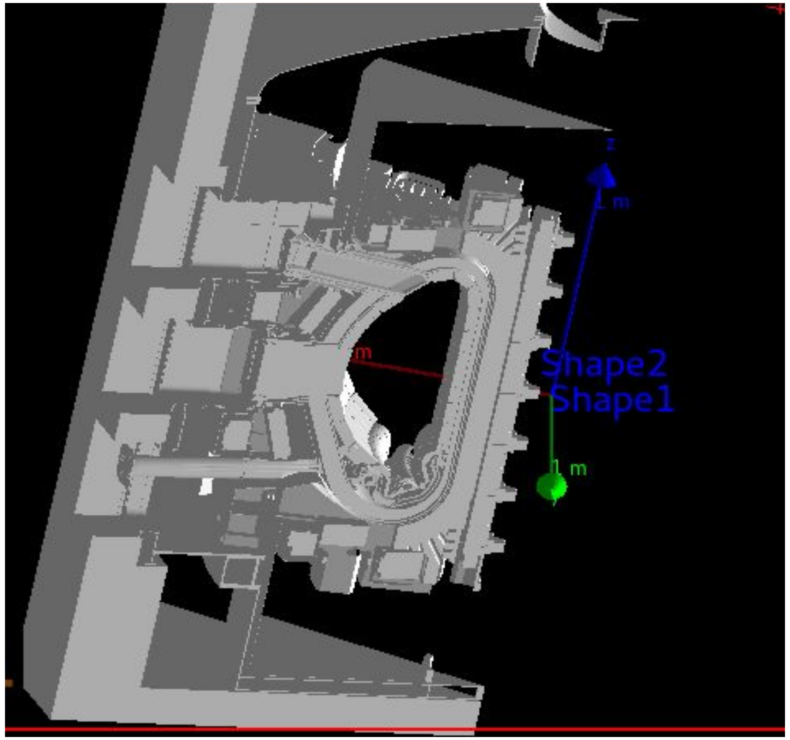
DagSolid + Geant4 = DAGGeant4

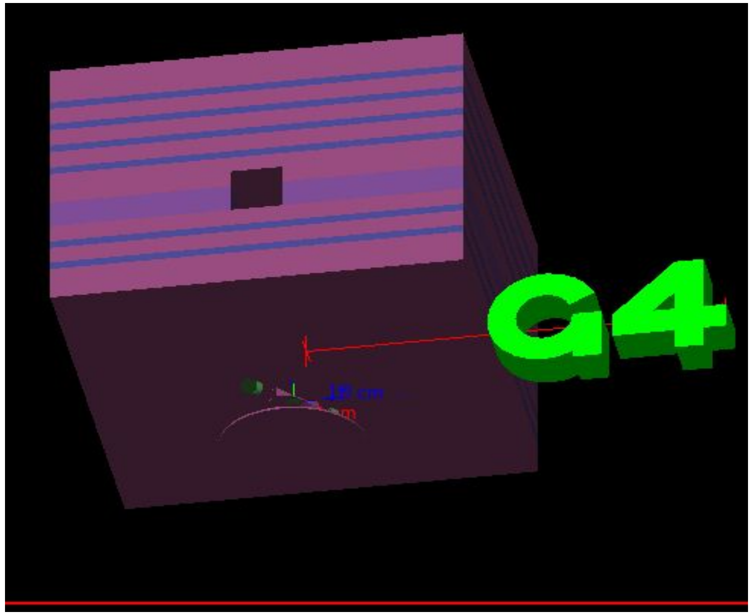
UK Atomic Energy Authority



- Implementation of single Geant4 executable
  - Takes models in UW^2
  - Including tallies & materials
  - Cartesian scoring meshes are output in MOAB mesh *h5m
  - Not optimized for any one application







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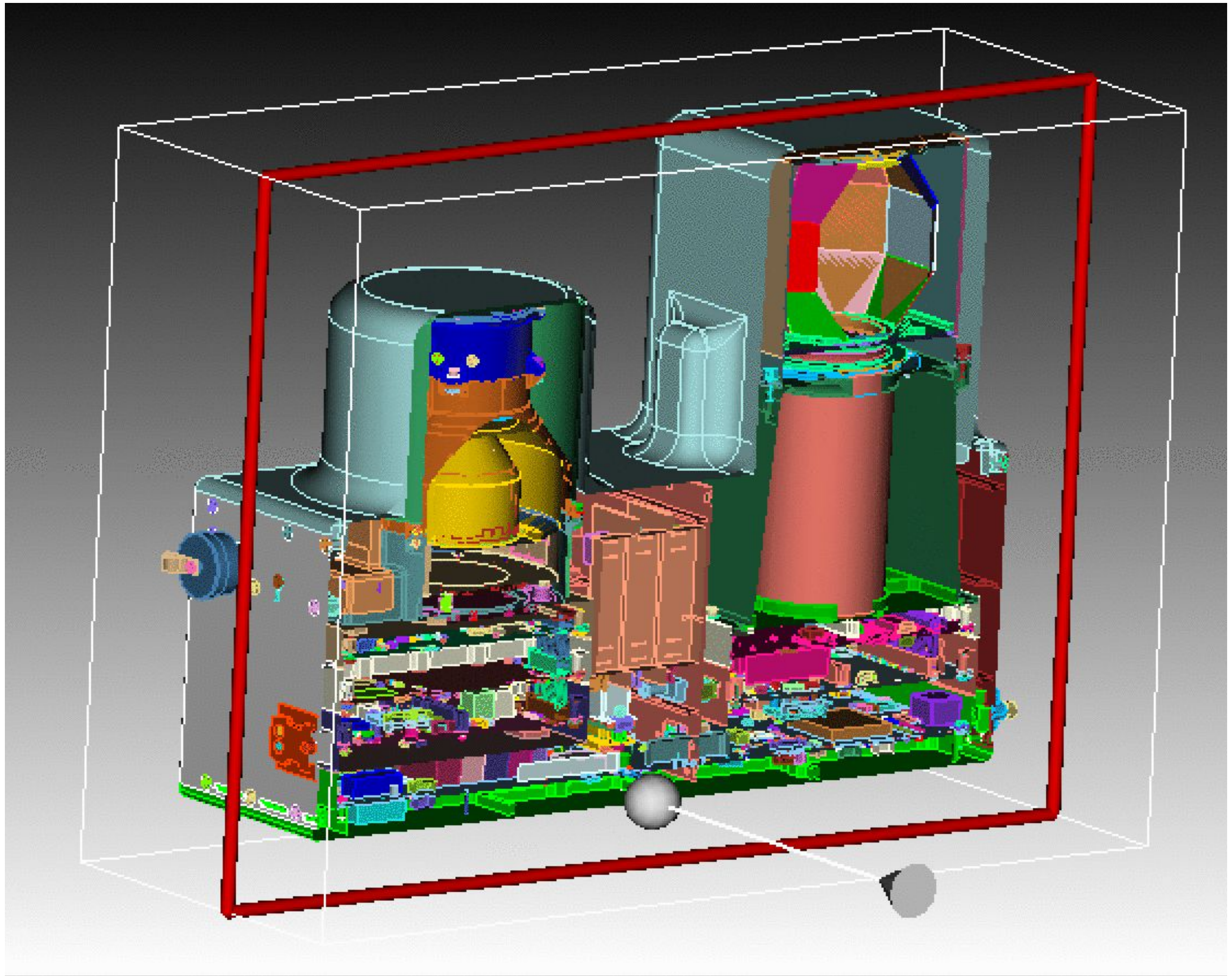
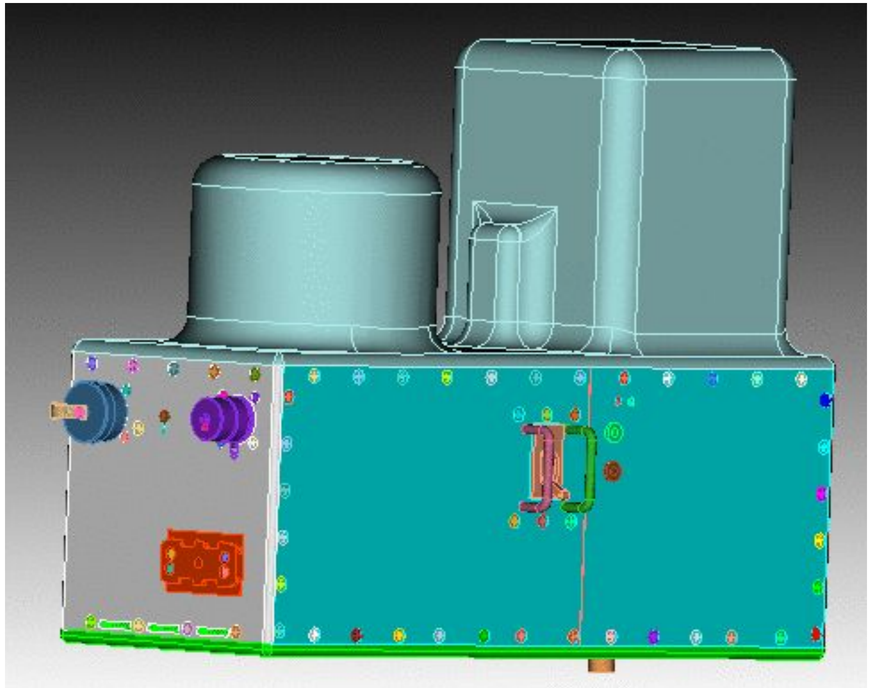
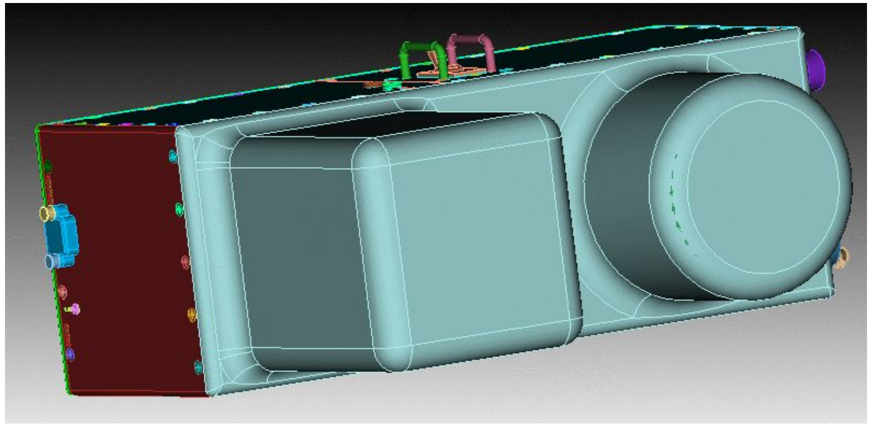
Space Radiation Example

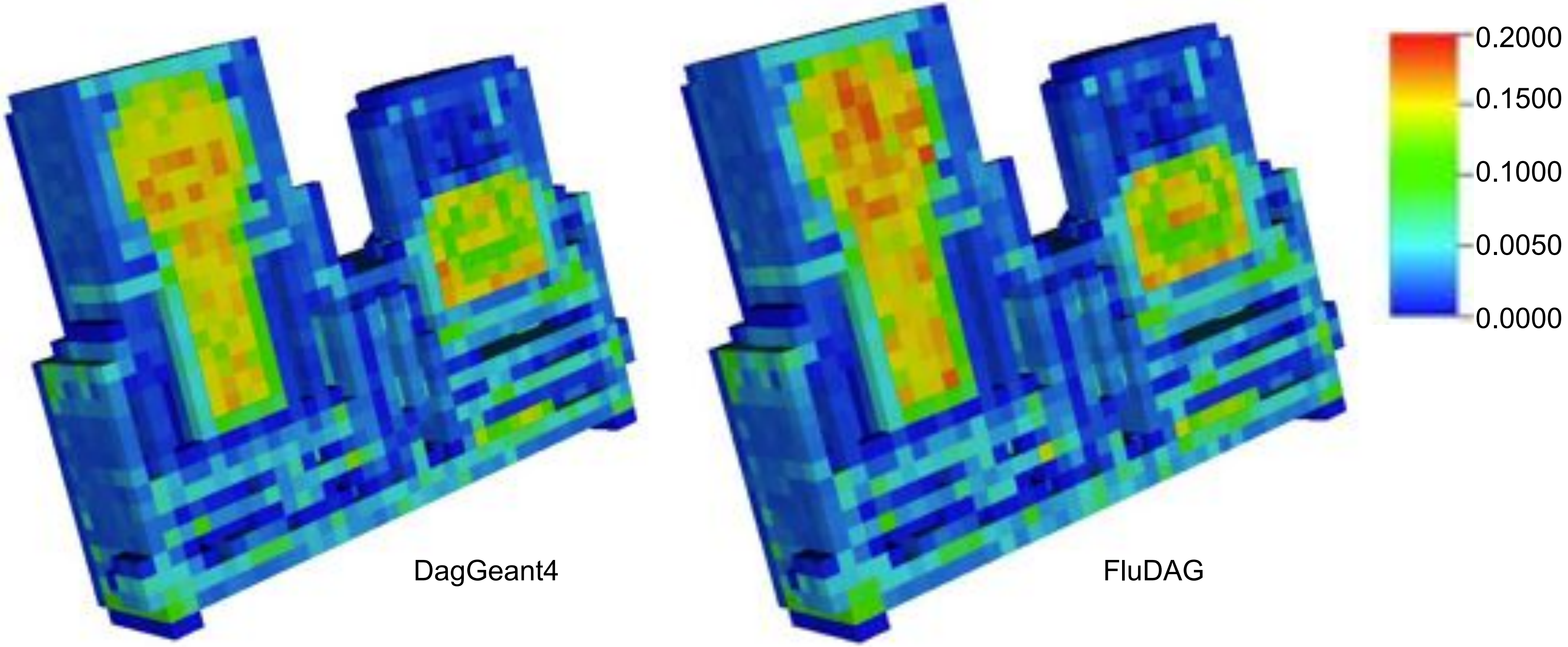






This work performed by SRAG - NASA

Space Radiation Example

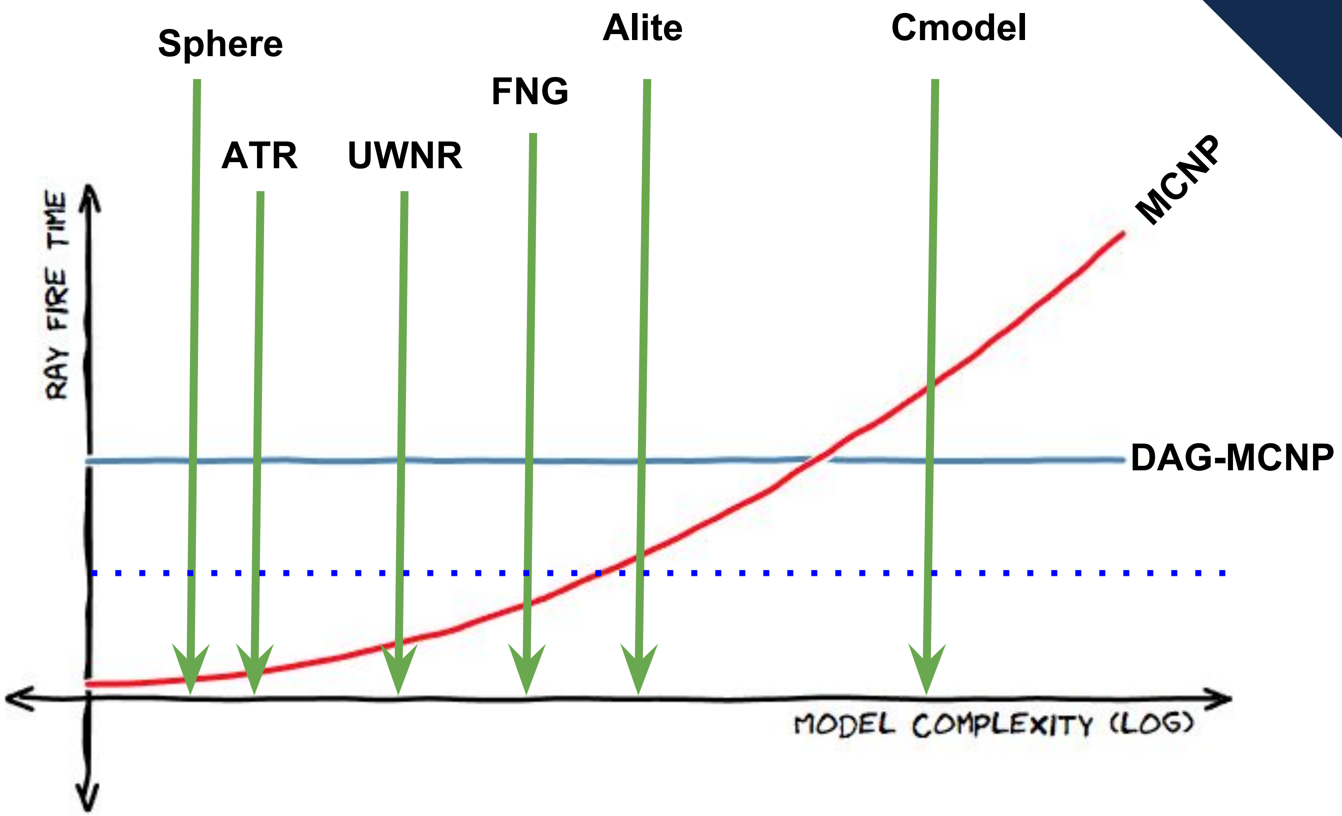


DagGeant4

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 workflow 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