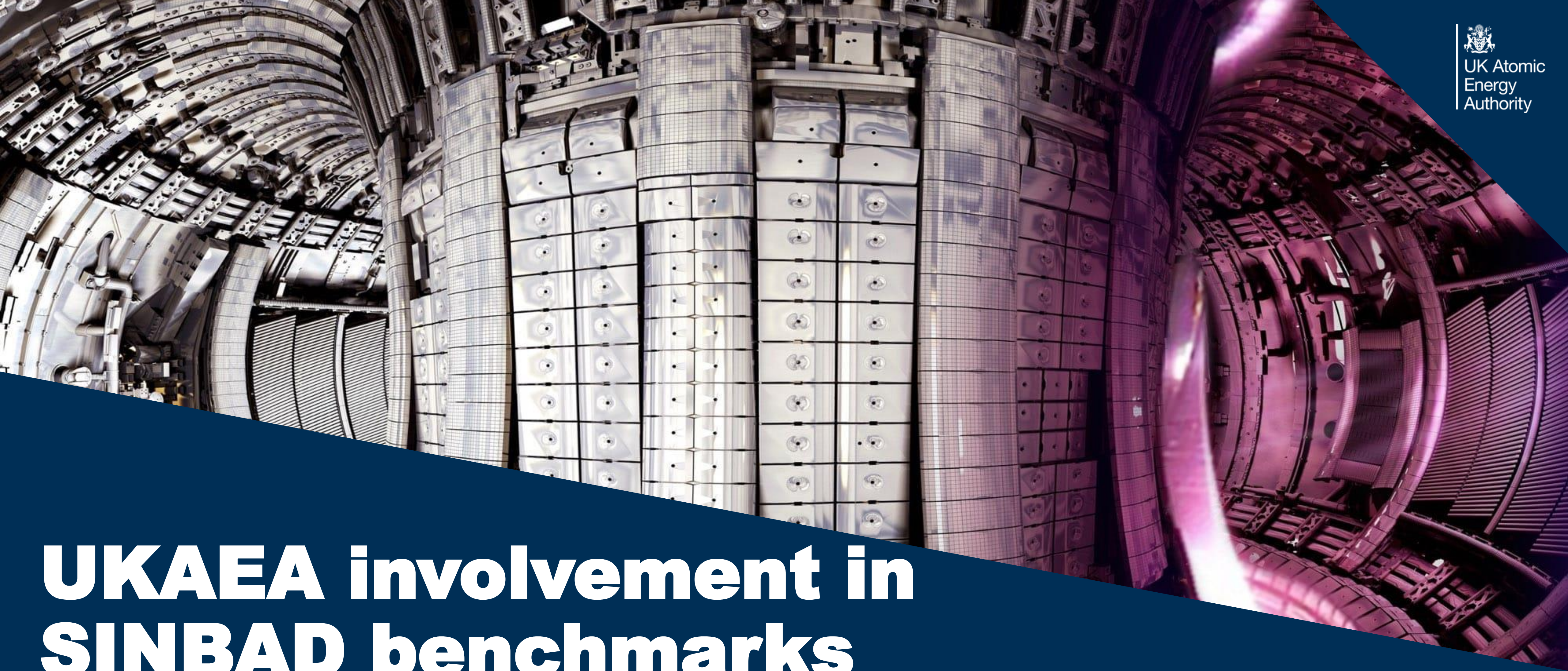

UK Atomic Energy Authority

# UKAEA involvement in SINBAD benchmarks

**Alex Valentine**, Greg Bailey, Thomas Berry, Steven Bradnam, Bethany Colling, Andrew Davis, Tim Eade, Mark Gilbert, Jonathan Naish, Chantal Nobs, Lee Packer, Olga Vilkhivskaya, Chris Wilson, Ross Worrall

**32nd WPEC Meeting, Subgroup 47, 12th May 2020**

# Contents

1. Overview of United Kingdom Atomic Energy Authority (UKAEA) and the Applied Radiation Technology (ART) group
2. Experience with SINBAD for neutronics code benchmarking
   I. Serpent 2 Monte Carlo code benchmarking
   II. Comments on user experience
3. UKAEA involvement in future SINBAD benchmarks

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# Organisation overview

UK Atomic Energy Authority

UK Atomic Energy Authority


CCFE
CULHAM CENTRE FOR FUSION ENERGY

RACE

MATERIALS RESEARCH FACILITY

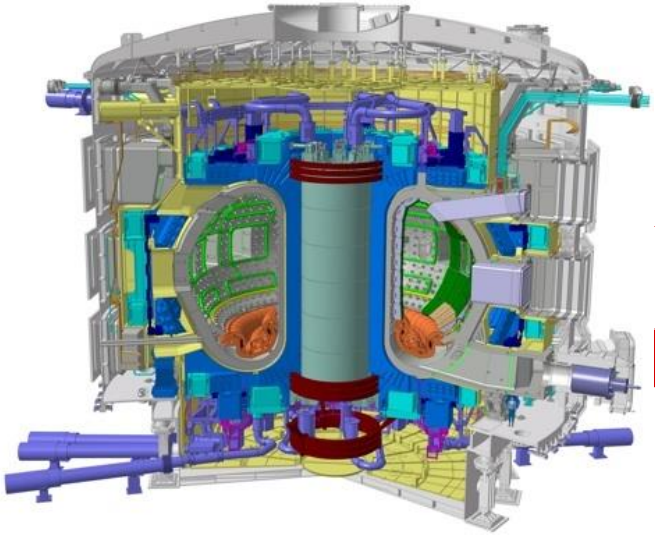
CAS

**Deliver sustainable fusion energy and maximise scientific and economic impact**

# Goals on the path to delivering fusion power

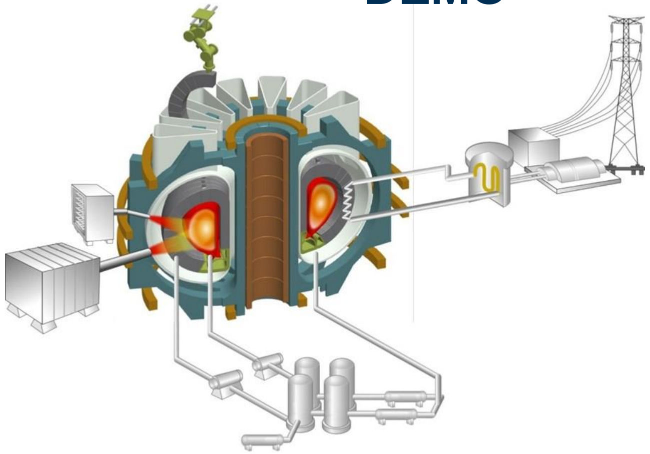
UK Atomic Energy Authority

ITER



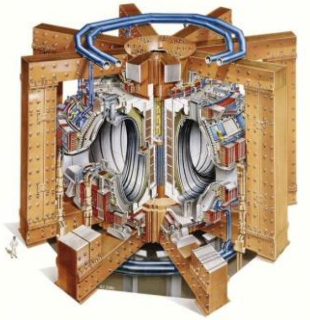
Enable the delivery of sustainable fusion power plants

DEMO

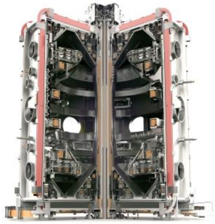


Be a world leader in fusion research and development

JET



MAST-U



Drive economic growth and high tech jobs in the UK in fusion and related technologies

STEP

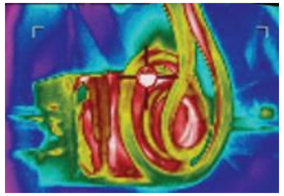
Create places that accelerate innovation and develop skilled people for industry to thrive

OAS

RACE

MRF

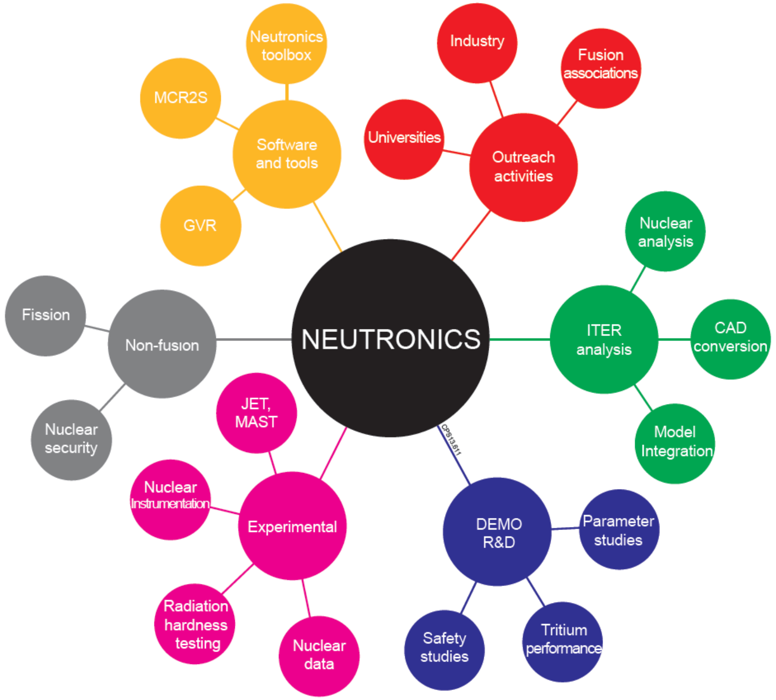
H3AT



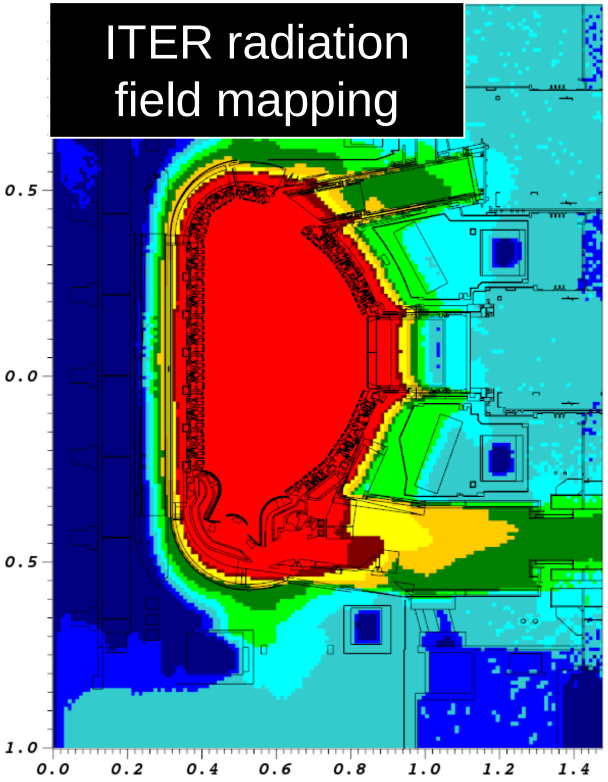
FTF

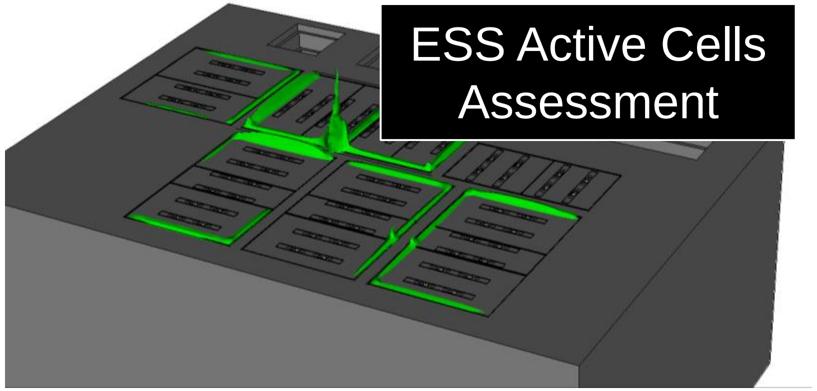
# Nuclear Analysis and Modelling at UKAEA

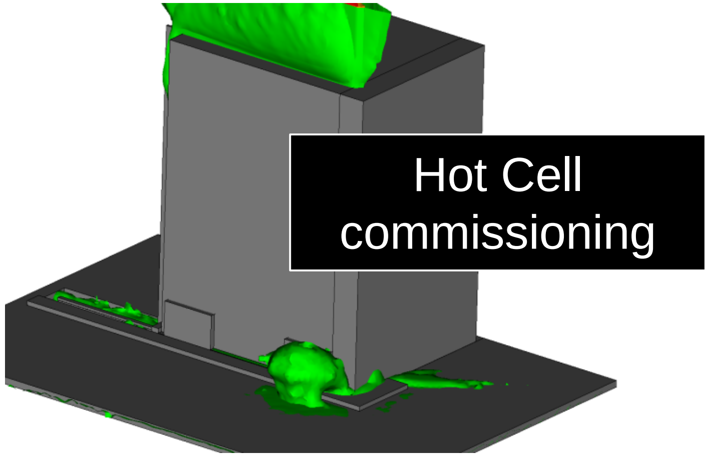
UK Atomic Energy Authority




SPACECLAIM CORPORATION
MCNP6
SuperMC
VisIt
OpenMC
DAGMC
McCad
Serpent
Oak Ridge

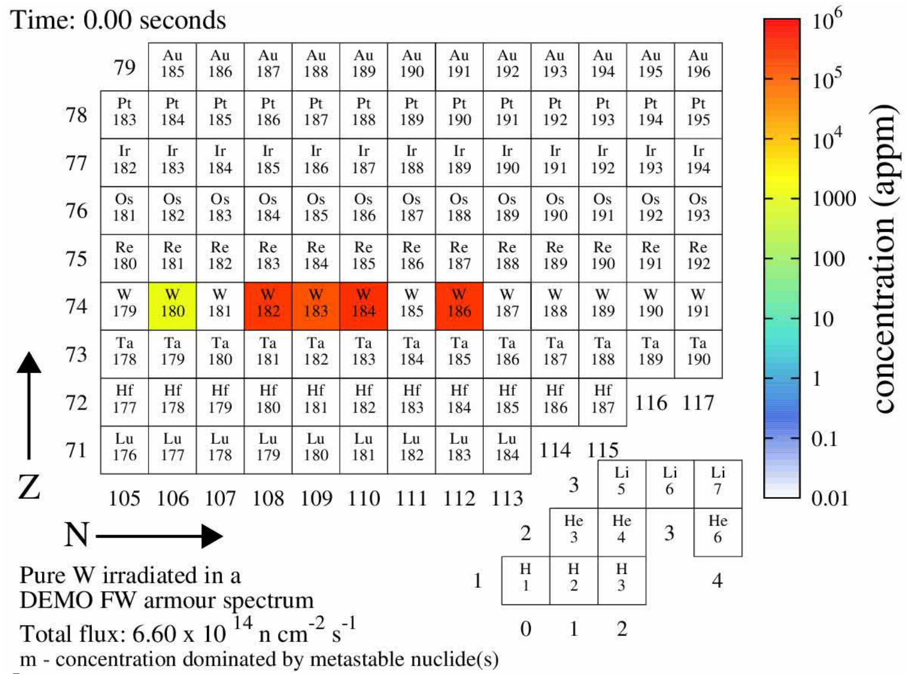


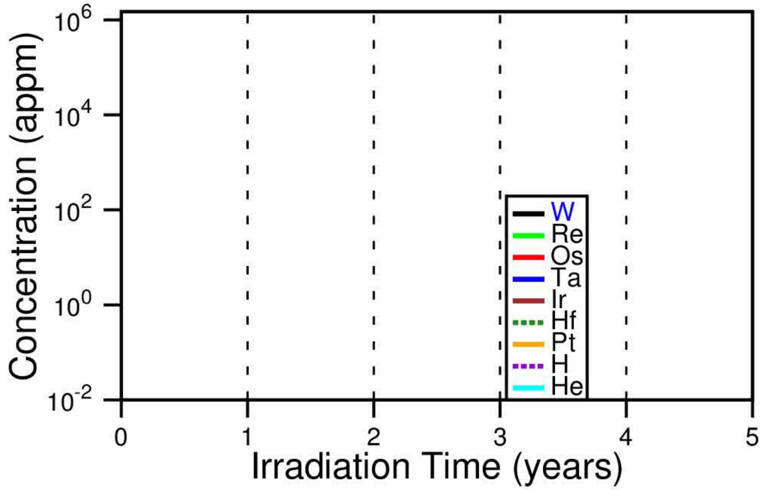



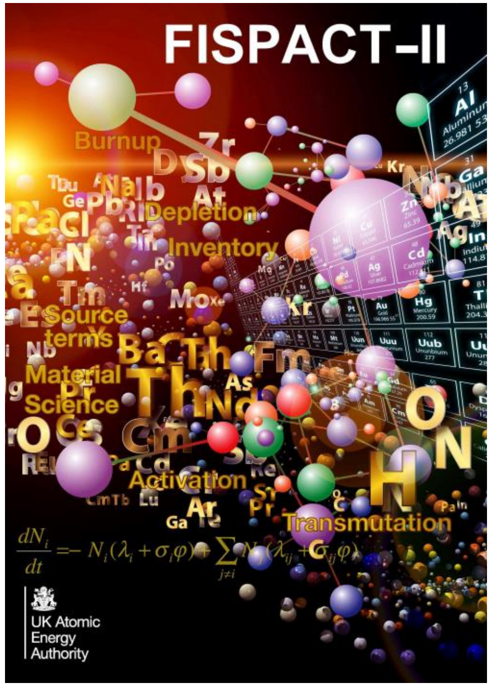
# Nuclear Inventory Simulation

- FISPACT-II is a multi-physics platform for predicting the inventory changes in materials under both neutron and charged particle irradiations
  - Calculates the activation, burn-up, dpa, PKAs, gas production, etc.
- Can read data from the most up to date international nuclear data libraries including TENDL 2019, ENDF/B-VIII.0, JEFF 3.3, JENDL-4.0 etc…
- New features include a fully integrated API, JSON output for easy parsing and PYPACT utility for straightforward manipulation of output files
- Available from the NEA databank (v4.0)




M. R. Gilbert et al., *Nucl. Sci. Eng* **171** (2014) 291-306



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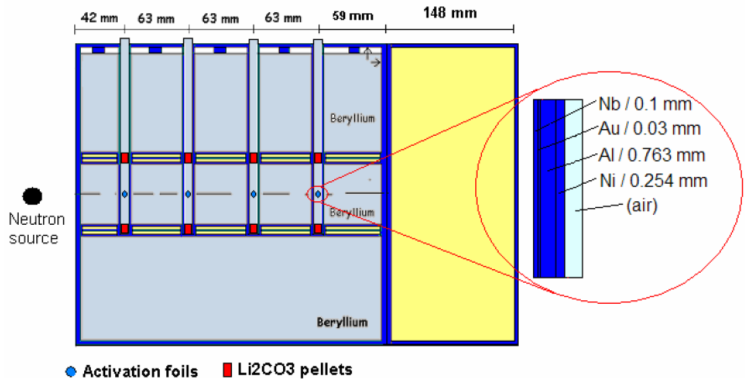
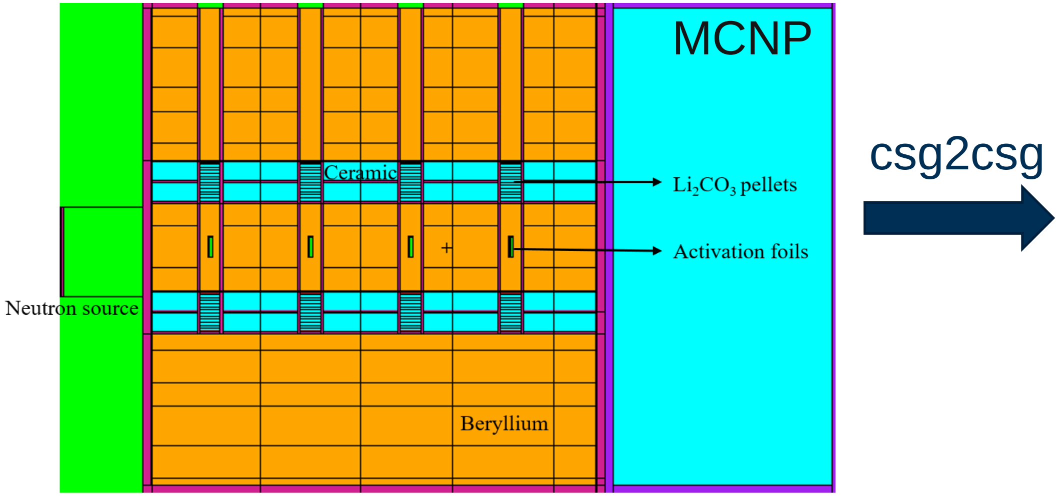
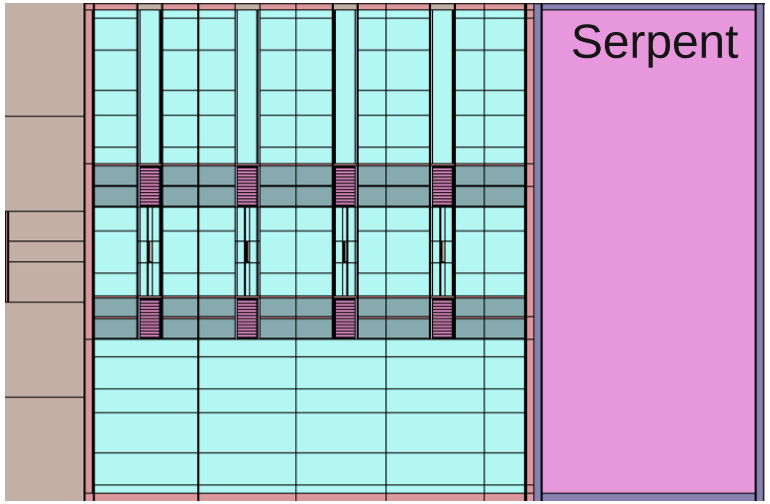
# Serpent 2 Benchmarking: FNG HCPB mock-up experiment

- Experiment performed in 2005. Experimental data available for the reaction rates in activation foils; Nb(n,2n) ; Au(n,γ); Al(n,α);Ni(n,p) and the tritium activity in $Li_2CO_3$ pellets.
- Serpent 2 model created using automated conversion tool from MCNP input, CSG2CSG – Most of the SINBAD benchmarks are distributed with an MCNP model – there is a strong interest to include other codes (inc. Serpent 2) with the distribution.
- As calculational results are provided using FENDL-2.1 library, this library was used for MCNP and SERPENT calculations in this task. For the reaction rates in activation foils, LLDOS, IRDFF2002 and IRDFFv1.05 have been used.

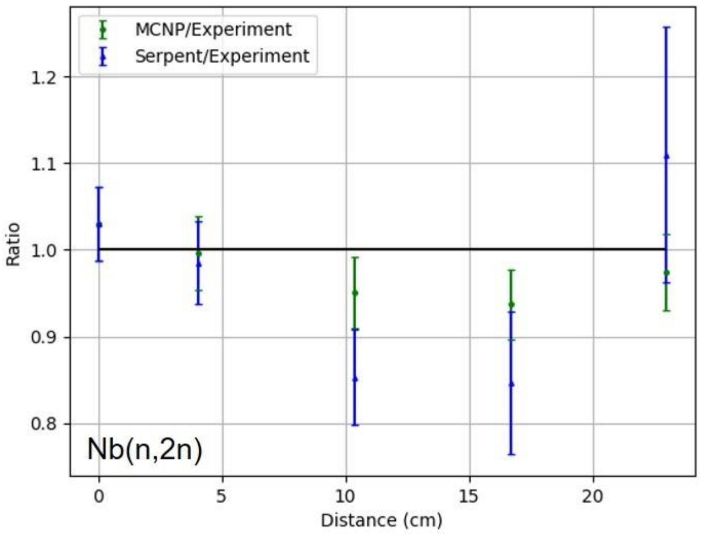


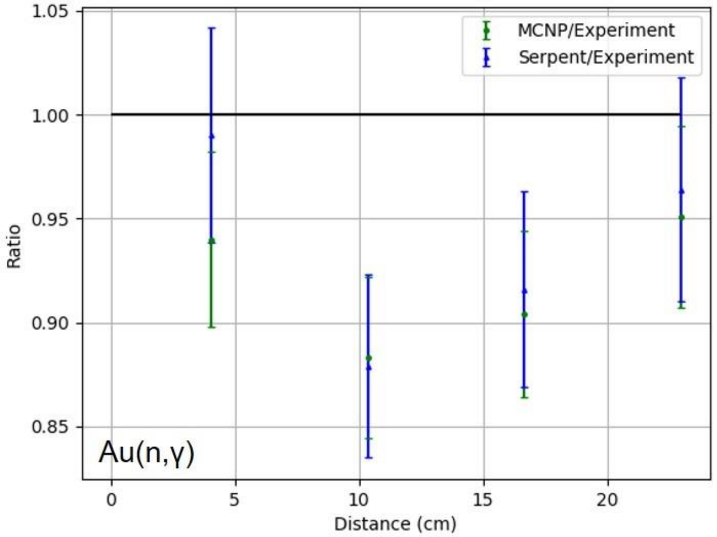



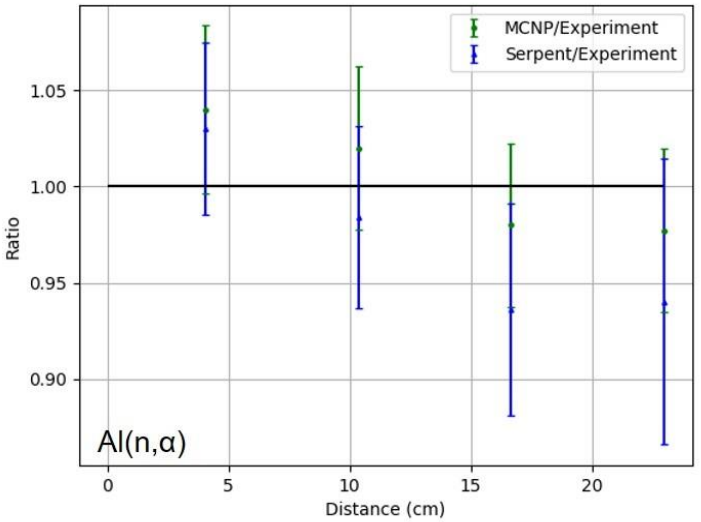



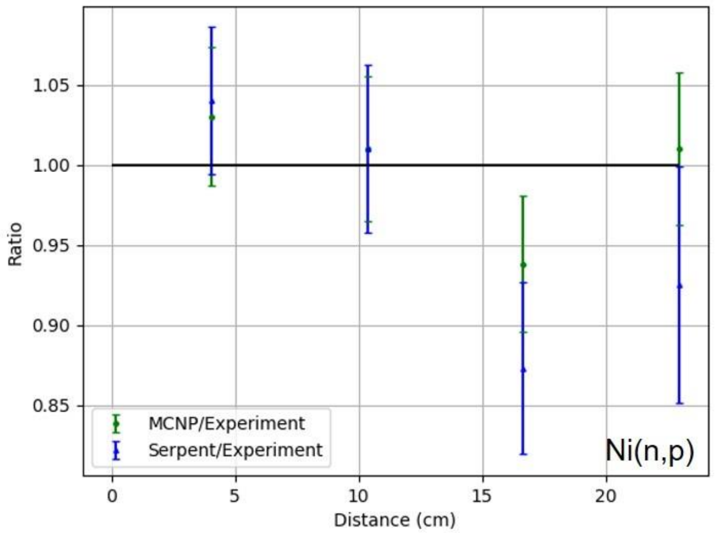
# Serpent 2 Benchmarking: FNG HCPB mock-up experiment



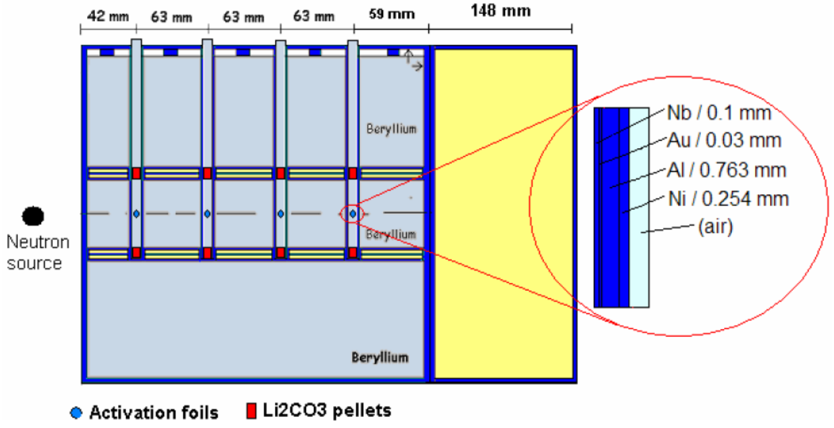


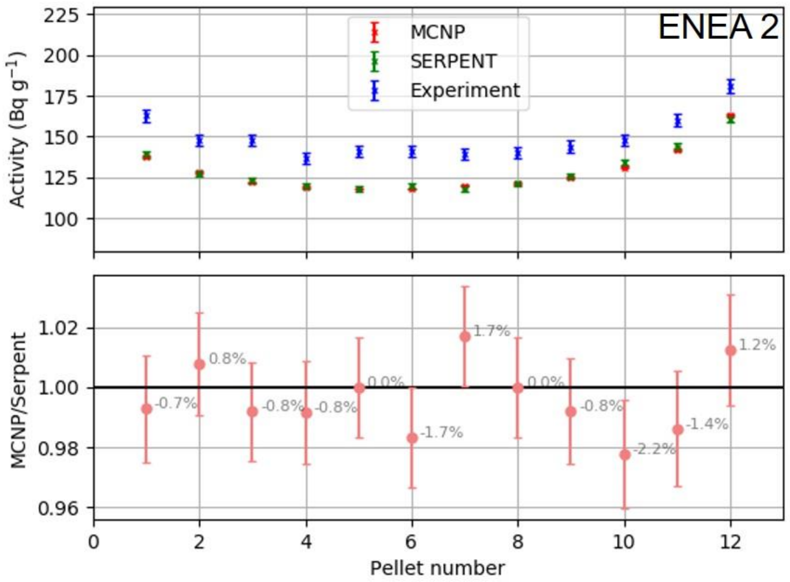



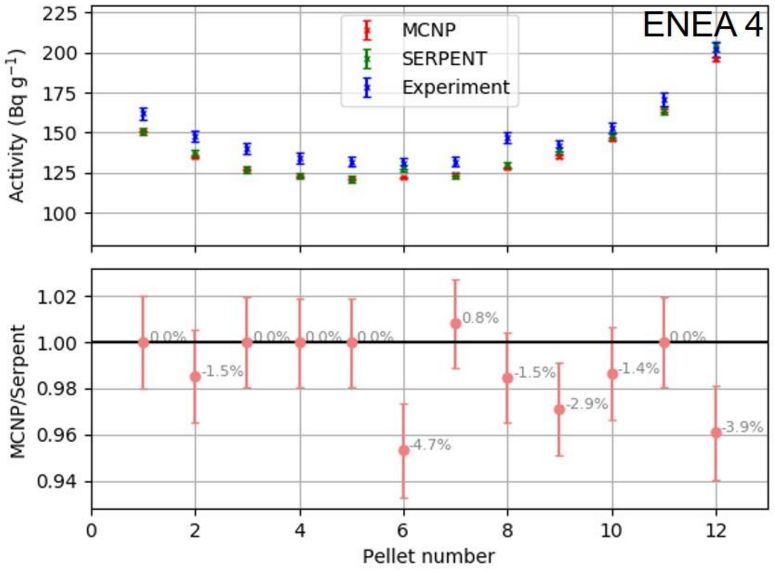

Reaction rates in a series of activation foils through the mock up.

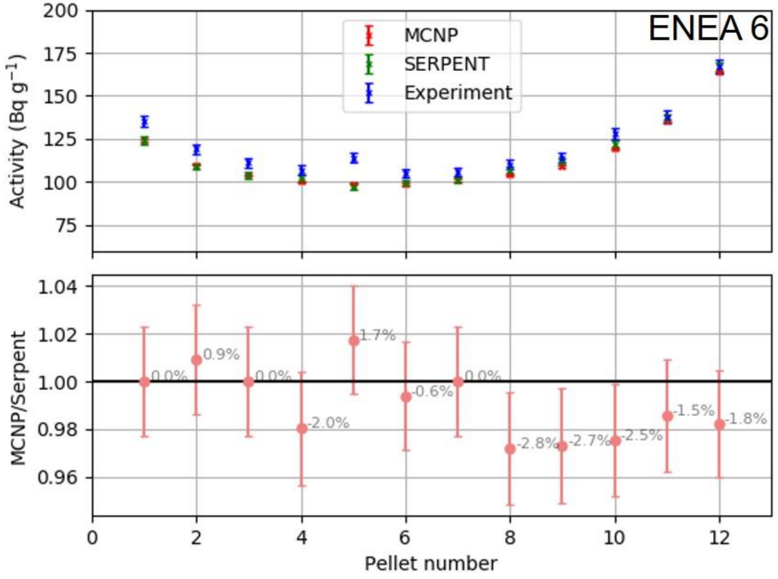


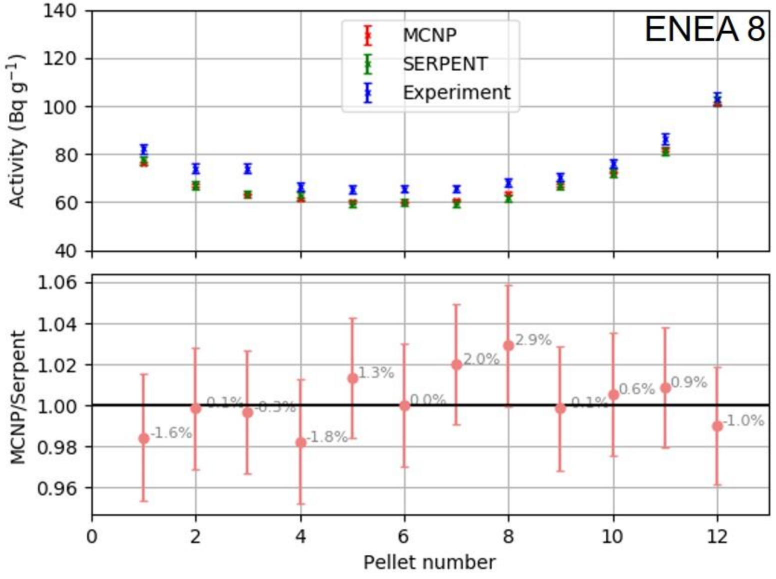
# Serpent 2 Benchmarking: FNG HCPB mock-up experiment

UK Atomic Energy Authority

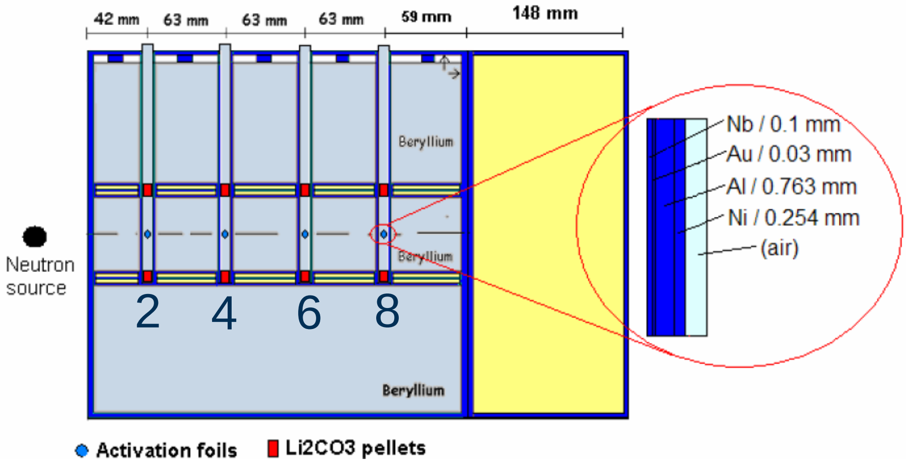


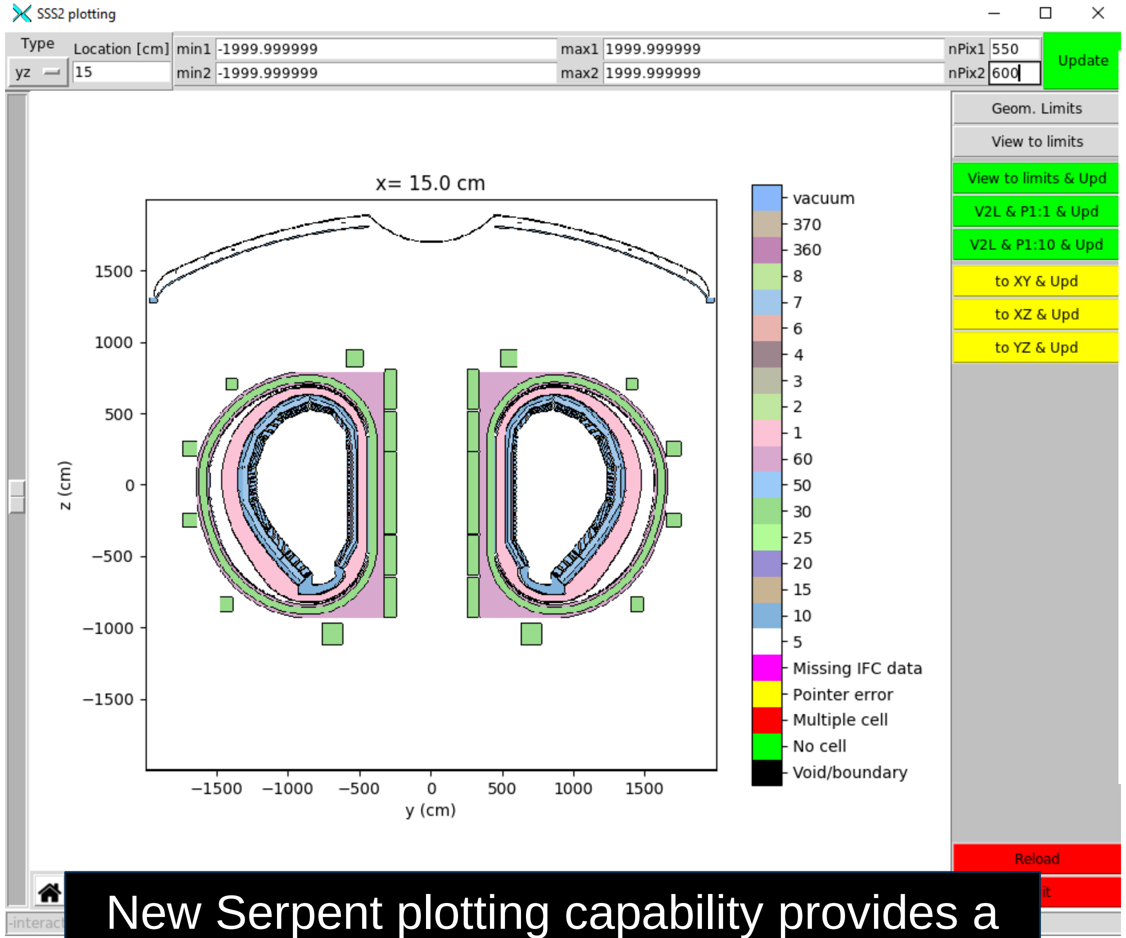




Activity of tritium in $Li_2CO_3$ pellets

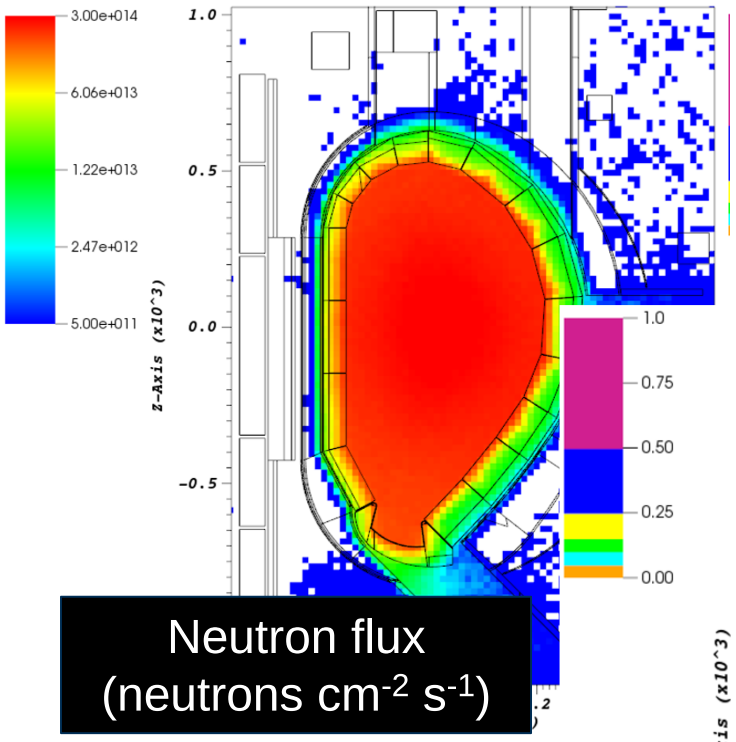


# Serpent 2 Benchmarking: EU DEMO with Helium Cooled Pebble Bed (HCPB) blanket concept

UK Atomic Energy Authority

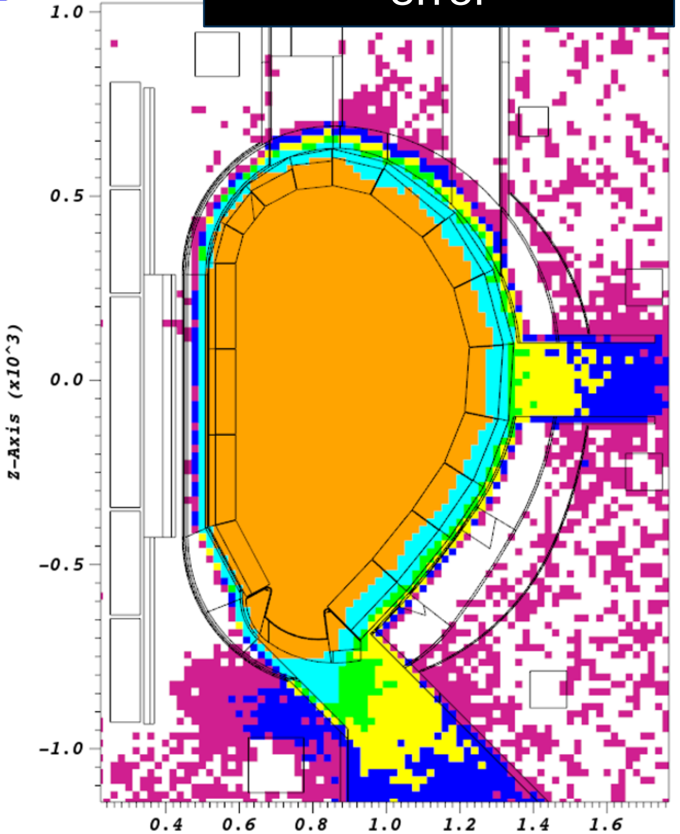



New Serpent plotting capability provides a straightforward to use GUI.



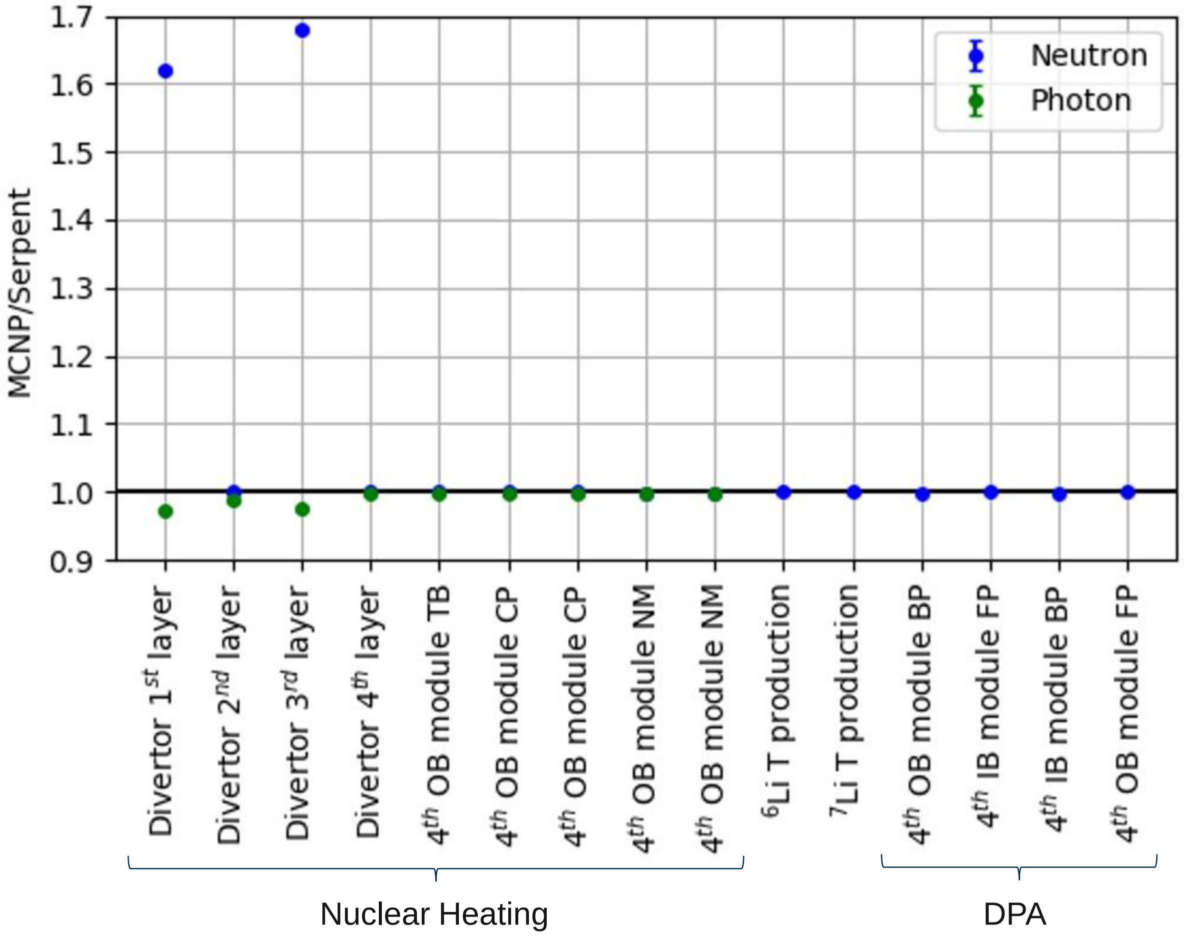

Neutron flux (neutrons cm$^{-2}$ s$^{-1}$)

Map of statistical error

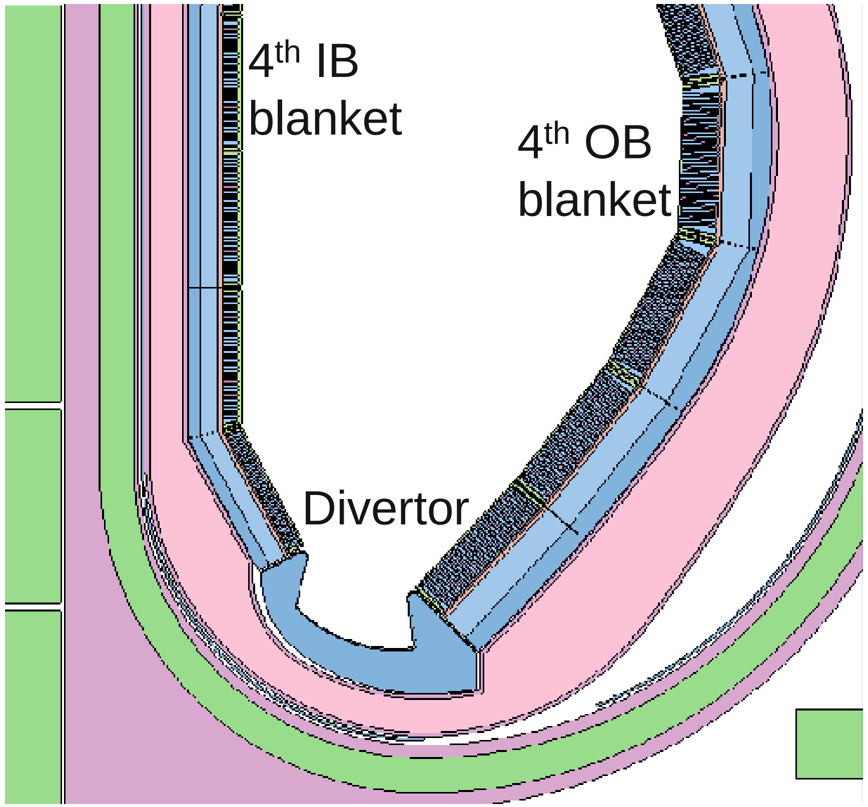


# Serpent 2 Benchmarking: DEMO HCPB model nuclear responses

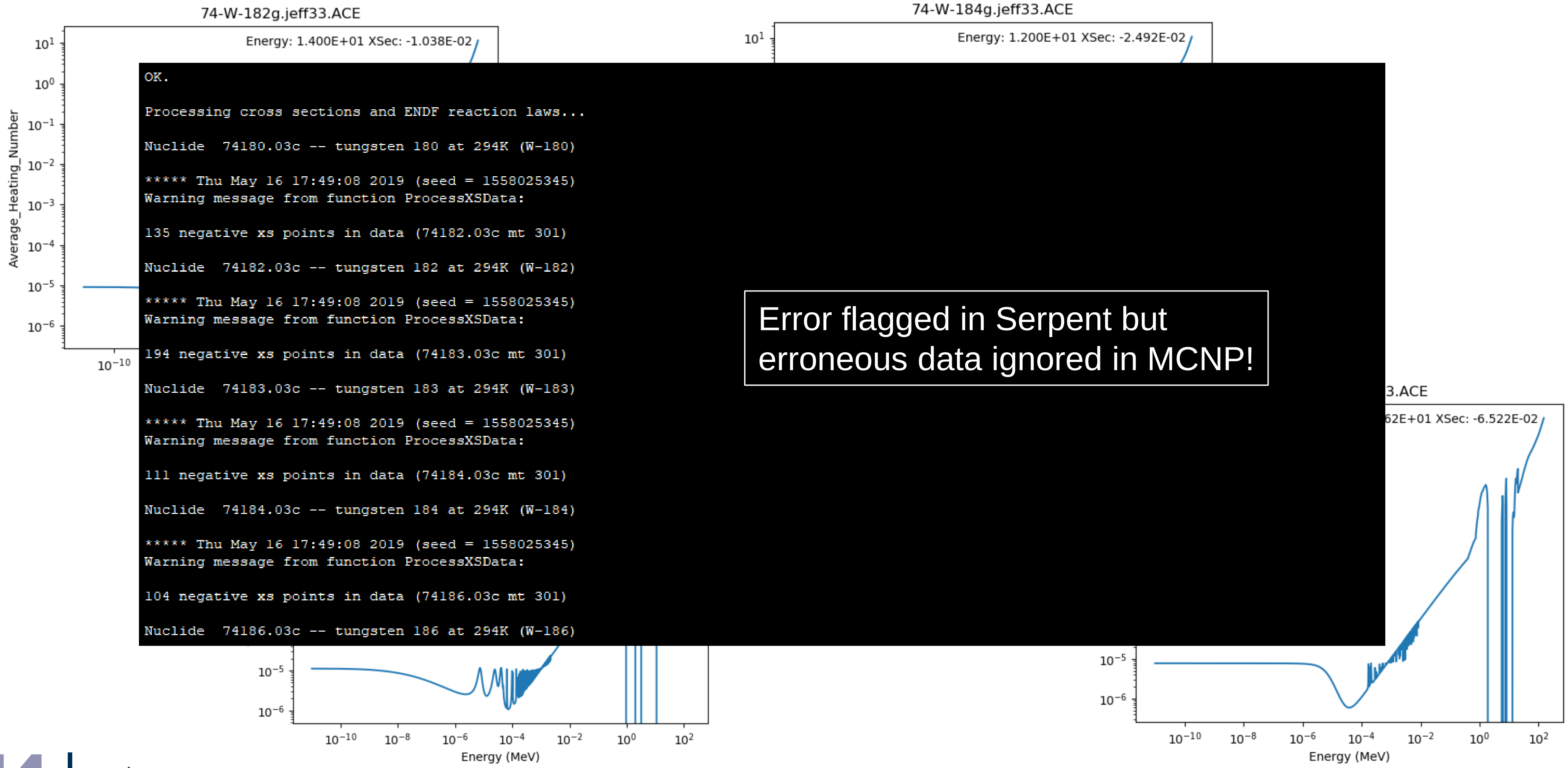
- Only major discrepancy is in the nuclear heating, particularly for neutrons.
- Traced back to erroneous nuclear data and differences in how the code handles this.




TB: Tritium Breeder
CP: Cooling Plate
NM: Neutron Multiplier
OB: Outboard
IB: Inboard
T: Tritium
BP: Back plate (blanket)
FP: Front plate (blanket)



# Serpent 2 Benchmarking: DEMO HCPB model negative cross sections




```
OK.

Processing cross sections and ENDF reaction laws...

Nuclide  74180.03c -- tungsten 180 at 294K (W-180)

***** Thu May 16 17:49:08 2019 (seed = 1558025345)
Warning message from function ProcessXSData:

135 negative xs points in data (74182.03c mt 301)

Nuclide  74182.03c -- tungsten 182 at 294K (W-182)

***** Thu May 16 17:49:08 2019 (seed = 1558025345)
Warning message from function ProcessXSData:

194 negative xs points in data (74183.03c mt 301)

Nuclide  74183.03c -- tungsten 183 at 294K (W-183)

***** Thu May 16 17:49:08 2019 (seed = 1558025345)
Warning message from function ProcessXSData:

111 negative xs points in data (74184.03c mt 301)

Nuclide  74184.03c -- tungsten 184 at 294K (W-184)

***** Thu May 16 17:49:08 2019 (seed = 1558025345)
Warning message from function ProcessXSData:

104 negative xs points in data (74186.03c mt 301)

Nuclide  74186.03c -- tungsten 186 at 294K (W-186)
```

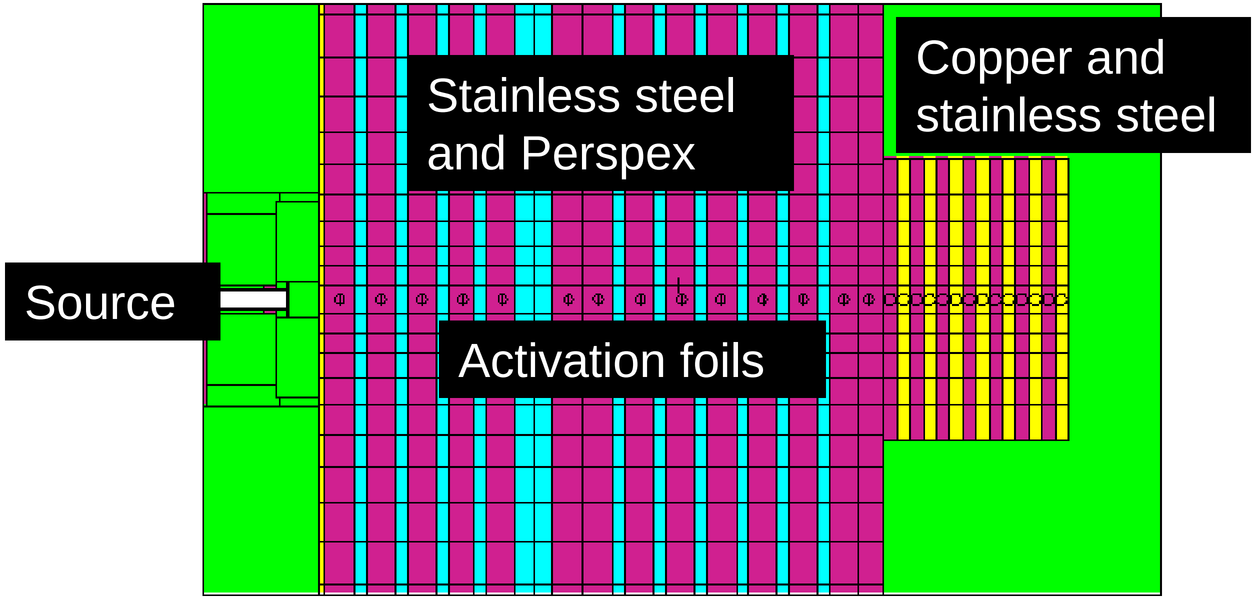
Error flagged in Serpent but erroneous data ignored in MCNP!

# Serpent 2 benchmarking 2020

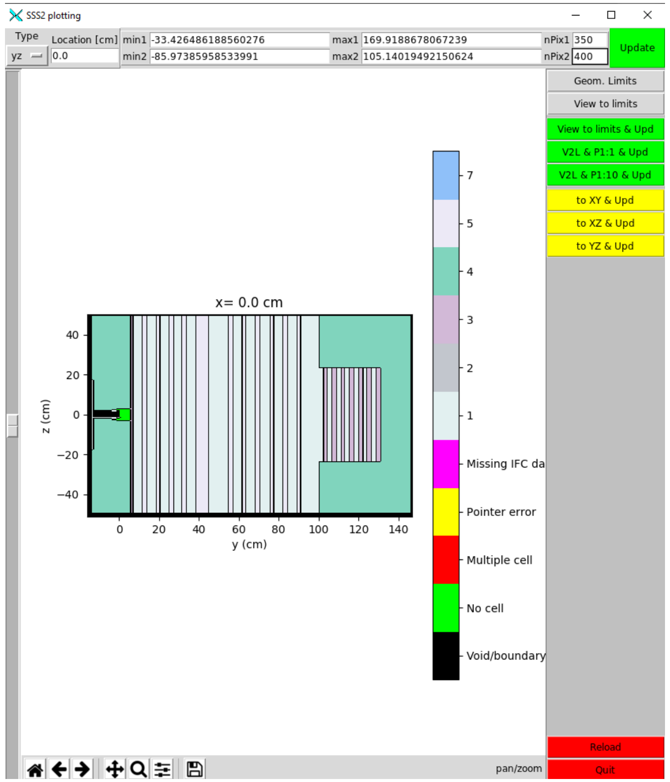
UK Atomic Energy Authority

The following tasks will be undertaken in 2020:

- Investigate use of variance reduction with Serpent, including methods for weight window generation, for a potential robust workflow. Define a simple model to test the variance reduction and compare with current methods adopted in MCNP (see next slide)
- Perform computational comparison of nuclear responses beyond the vacuum vessel in the DEMO HCPB model, including TF and PF coil responses.
- Develop model of the FNG bulk shield mock-up experiment and perform Serpent comparison.
- Recent paper by T.Eade et al. on the benchmarking of shutdown dose rate calculations using different transport codes with MCR2S (https://dx.doi.org/10.1088/1741-4326/ab8181).



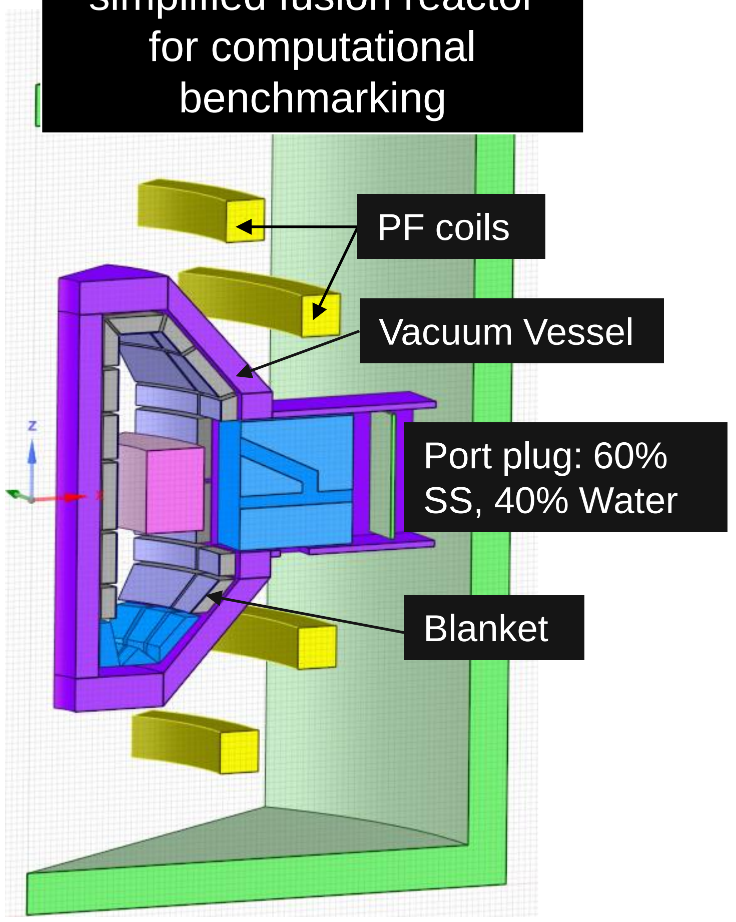

CSG2CSG
MCNP Serpent

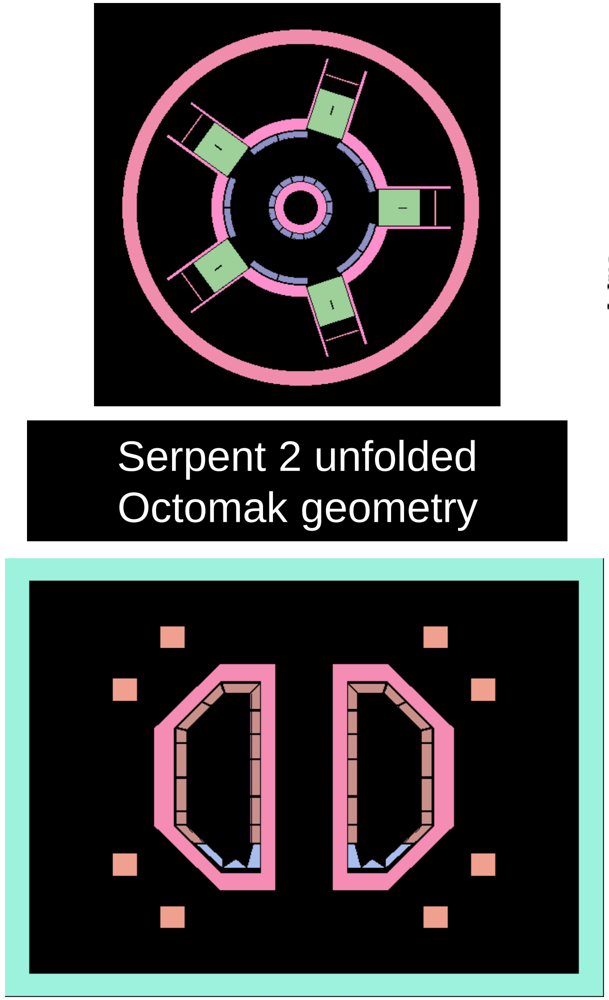



ITER bulk shield experiment

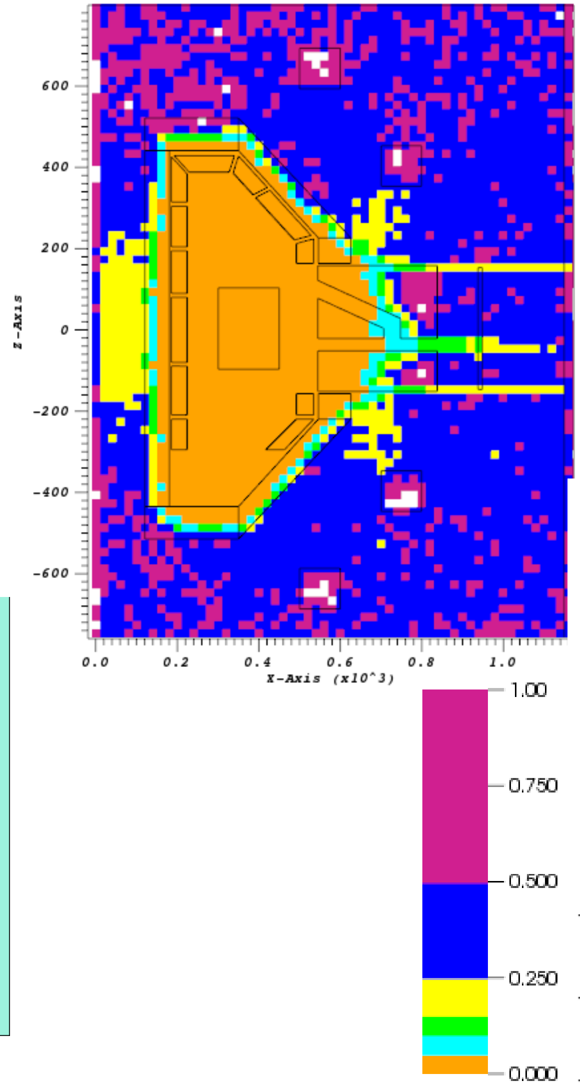
# Serpent 2 Variance Reduction

CAD model of Octomak simplified fusion reactor for computational benchmarking

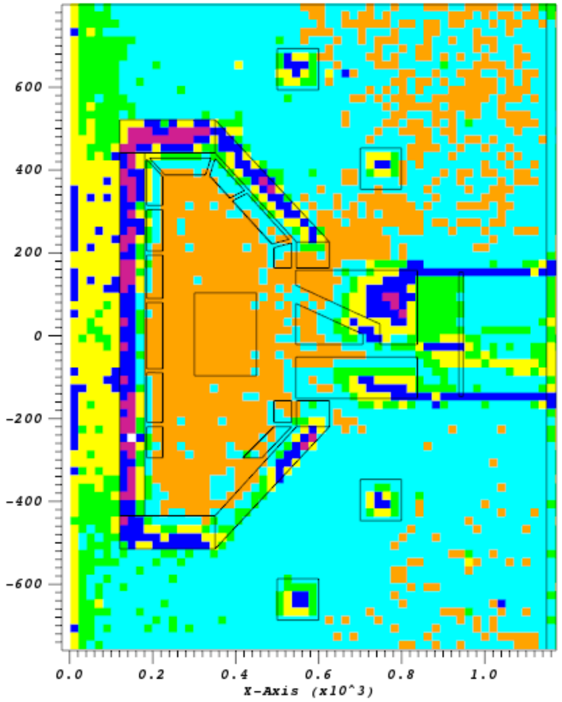


Serpent 2 unfolded Octomak geometry




Use global WW mesh generated in Serpent




*Further information: Jaakko Leppänen (2019): Response Matrix Method–Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code, Nuclear Technology*

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# General comments on SINBAD

UK Atomic Energy Authority

**Quality**

- Quality control is relatively poor with current benchmarks. For example, several MCNP input decks are not valid and can not be ran without modification to input file.
- Some input decks / variance reduction methods in the distributed models may now be obsolete.

**Repeatability**

- All documentation is orientated towards journal publication. This leaves out certain details. In many cases, the origin of normalisations convolved with the calculational results is not clear. Reproduction of original calculational results is difficult
- HTML format is OK, however may benefit with additional report on the calculational model distributed with each benchmark

**Availability**

- Benchmarks available through NEA data bank and RSICC. Can we transition to a more open, traceable and robust method of distribution such as a Git repository.

**Usability**

- Certain inputs lack clear commenting/ comments require translation. Good practice, as with writing any code should be implemented and should be an integral part of the review stage

**Completeness**

- There is a lack of solely photon and photonuclear benchmarks
- Neutron and photon heating benchmarks are also of high relevance in fusion
- Should the benchmarks be distributed in other MC code formats as well as MCNP?
- Many of the older benchmarks are not distributed with MCNP models

UK Atomic Energy Authority

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# UKAEA Perspective: Future Benchmarks

UK Atomic Energy Authority

- Government announced £220 million of funding last year for UKAEA to create a concept design of a spherical tokamak for energy production (STEP).
- This highly ambitious research program draws on the experience of industry and academia in the UK and aims to identify a pathway to supply net energy by the 2040s.
- STEP would greatly benefit from further specific shielding benchmarks, for example, a dedicated mock up of the inboard plasma facing components where extremely high heat density will necessitate strict optimisation of the design.
- Fusion pushes the scientific and technological boundaries of materials research. Materials of strong interest to STEP programme and in to the fusion community include:

  **W, Mo, Cr, Y, Ti, C, Zr, Li, Pb, Be, Si, Nb, La, Cu, Fe, Vn**

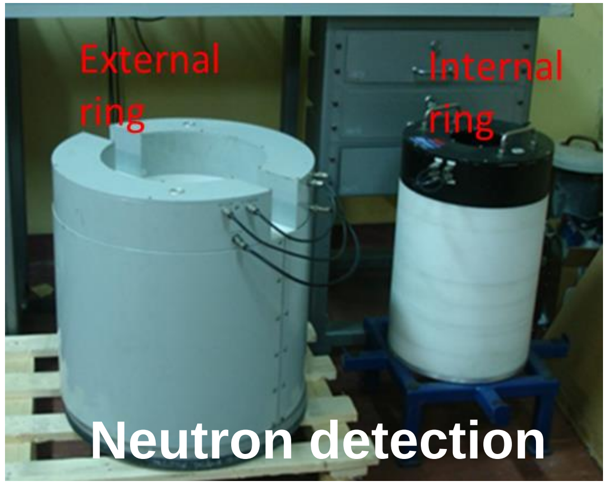
# Fusion experiments: Measurement of $^{16/17}N$ during irradiation of First Wall mock-ups

- The collaboration measured $^{16}N$ and $^{17}N$ production in water activated by DT neutrons and compared with calculations validate the methodology for water activation assessment.
- The main sources of uncertainty currently being due to modelling and nuclear data, and hence safety factors between 8.2 and 4.7 are applied. The motivation of this experiment was to provide a scientific justification to reduce these safety factors.

$^{16}O(n, p)^{16}N$, $^{16}N$ ($T_{1/2}$=7.13s) $\rightarrow {}^{16}O + \gamma$ (67% @ 6.13 MeV, 5% @ 7.12 MeV),

$^{17}O(n, p)^{17}N$, $^{17}N$ ($T_{1/2}$=4.17s) $\rightarrow {}^{17}O \rightarrow {}^{16}O$ + n (37.7% @ 0.386 MeV, 0.6% @ 0.886 MeV, 49.8% @ 1.16 MeV, 6.9% @ 1.69 MeV), $\gamma$ (3.7% @ 0.87 MeV).

- The results provided good C/E agreement for $^{16}N$, and highlighted inconsistencies in the nuclear data for $^{17}N$ - with a factor of 5 difference for some libraries.
- Following this work the development of GammaFlow continues in the SAE 2.3 task, to identify the requirements of a common fluid activation code for use by the EUROfusion community in ITER and DEMO projects.



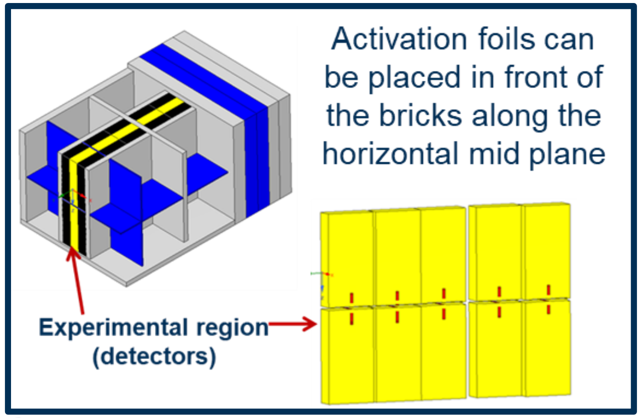


*C.R.Nobs, et al., Computational evaluation of N-16 measurements for a 14 MeV neutron irradiation of an ITER first wall component with water circuit, preprint submitted to ISFNT, 2019.*

# Fusion experiments: Water Cooled Lithium Lead (WCLL) neutronics mock-up experiment

UK Atomic Energy Authority

- The nuclear design and performance of breeder blankets fully rely on the results provided by neutronics calculations.
- An experimental campaign at ENEA is expected July/August 2020 aims to:
  - Provide a means to validate computational tools and nuclear data
  - Assess the prediction accuracy in providing fundamental data for the nuclear design, optimization and performance evaluation of DEMO, comprising safety, licensing, waste management and decommissioning issues.
- CCFE have been tasked with diagnostic activities to support the experiments, primarily dosimetry foils
- The foils (Ta, Fe, Ni, Y and Sc) will be embedded in the experimental region and used to monitor the local flux.
- Following irradiation at ENEA, spectroscopy measurements will be performed at ADRIANA – UKAEA Gamma Spectroscopy laboratory.
- This experiment will be folded into SINBAD. Uncertainty/sensitivity analysis performed by I.Kodeli

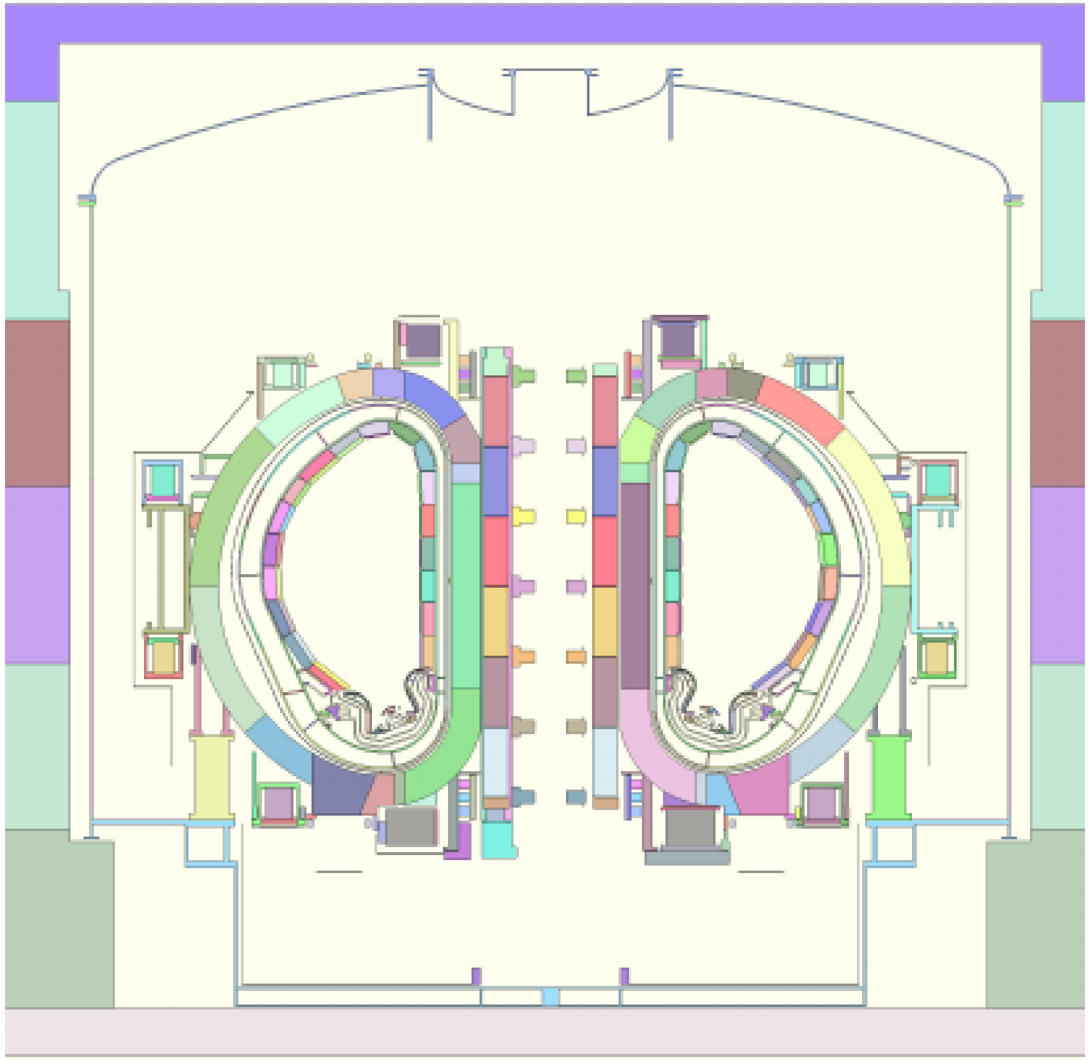

NNUF National Nuclear User Facility
http://www.nnuf.ac.uk
EUROfusion ENEA

# Conclusions

UK Atomic Energy Authority

- UKAEA is the UK's national fusion laboratory aiming to deliver sustainable fusion energy and maximise scientific and economic impact.
- The neutronics group is performing significant benchmarking of the Serpent 2 Monte-Carlo code for this application. This years efforts are focussed towards its in built variance reduction scheme.
- The SINBAD database provides valuable experimental data which is used in the benchmarking of new codes used for radiation transport calculations in fusion systems.
- There is a strong interest from the fusion community to see additional materials included in the database that will become more prominent in future fusion reactors. These include: W, Mo, Cr, Y, Ti, C, Zr, Li, Pb, Be, Si, Nb, La

# Thank you for listening



*ITER C-lite SERPENT model described with STL geometry. 11 components, 1,548 solids, 1,842,576 points, 614,192 triangular facets*

# Back Slides

# Looking at FENDL ACE files

- Carried out examination of FENDL3.1d ACE files
- Automated tool written to checked cross-section in each file and plot if negative values found
- 9 cross section found to have negative values
- 4 x DPA cross sections and 5 x Average Heating Number

AHN – Average Heating Number