UK Atomic Energy Authority

UKAEA benchmarking of the Serpent-2 Monte-Carlo code for fusion applications

Serpent User Group Meeting 2019, Georgia Institute of Technology

Alex Valentine

Contents

Organisation overview

UK Atomic Energy Authority

UK Atomic Energy Authority

CCFE CULHAM CENTRE FOR FUSION ENERGY

RACE

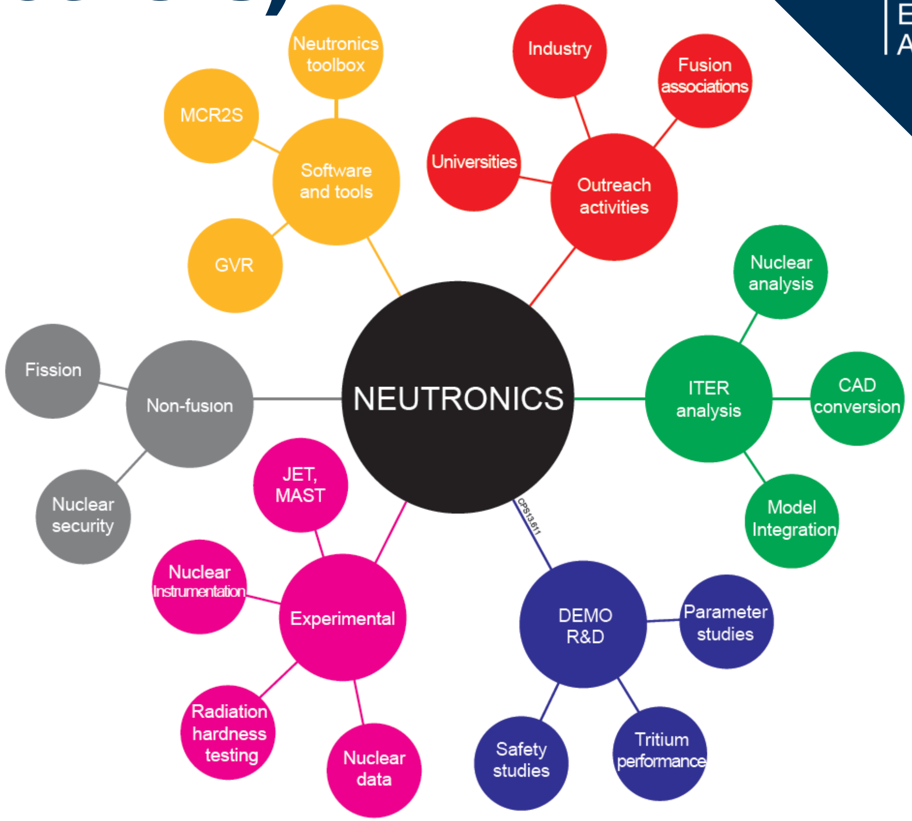
MATERIALS RESEARCH FACILITY

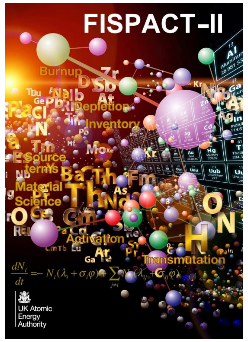
AS

Lead the commercial development of fusion power and related technology, and position the UK as a leader in sustainable nuclear energy

Applied Radiation Technology (and others)

- ART is part of the Technology Department
- ART currently has 10 members of staff
- Work closely with members the Materials Modelling & Validation Group





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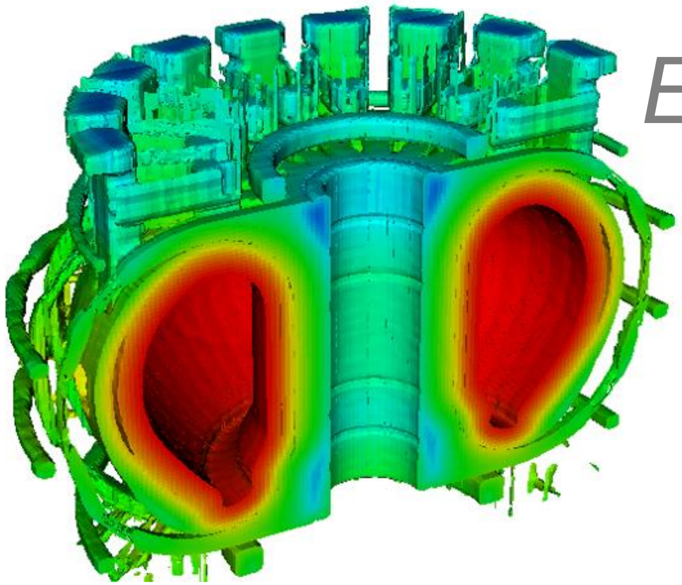
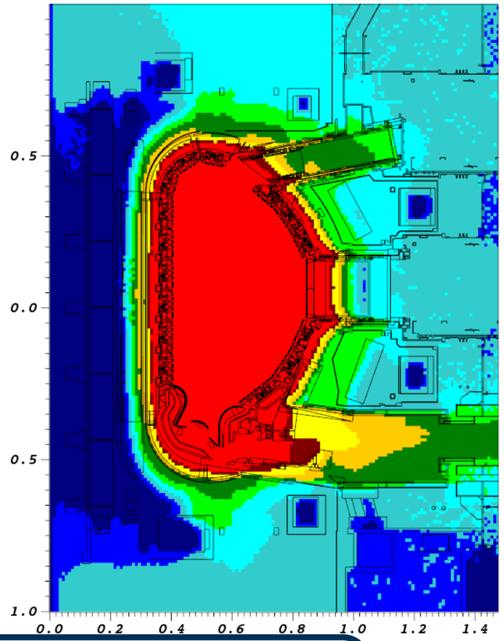


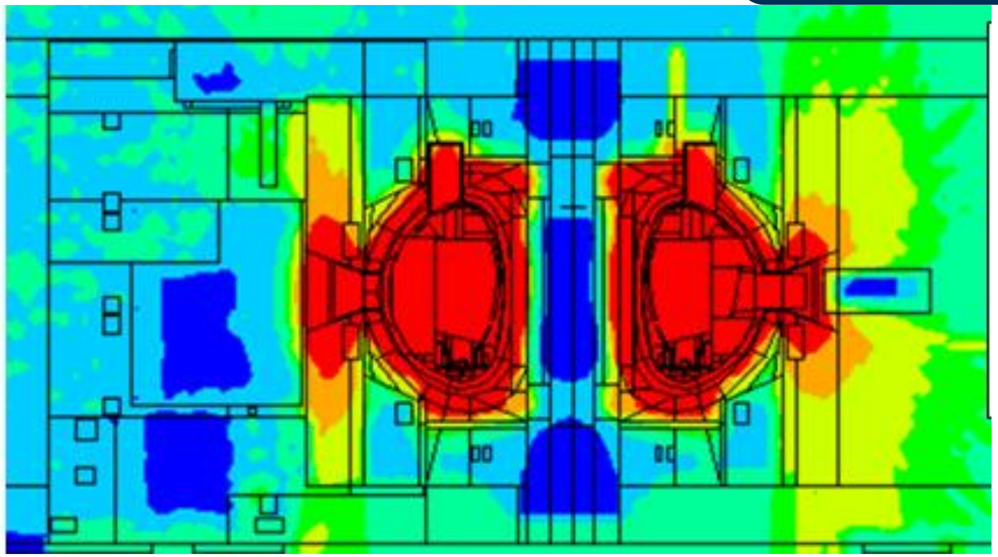
EU DEMO



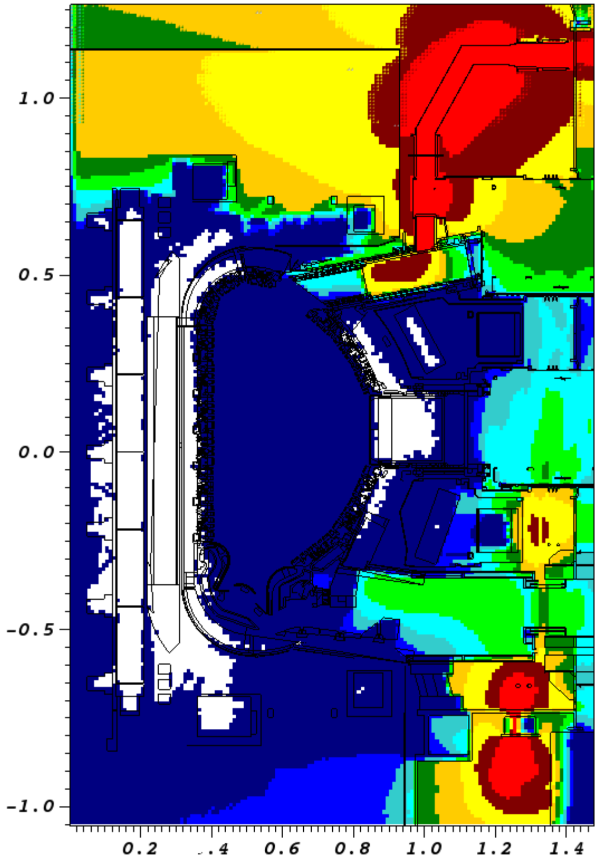
Plasma Source

ITER

Radiation field mapping for fusion reactors



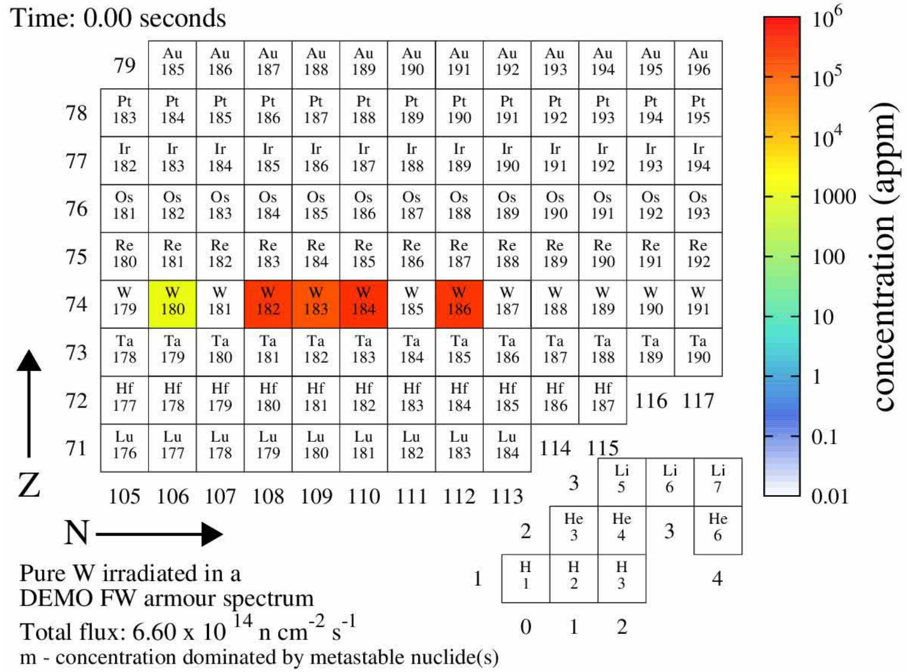
JET

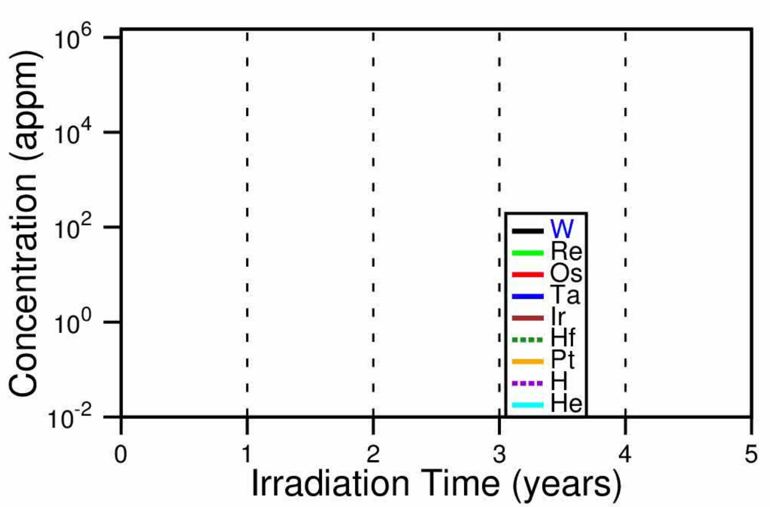


Cooling Water System Source

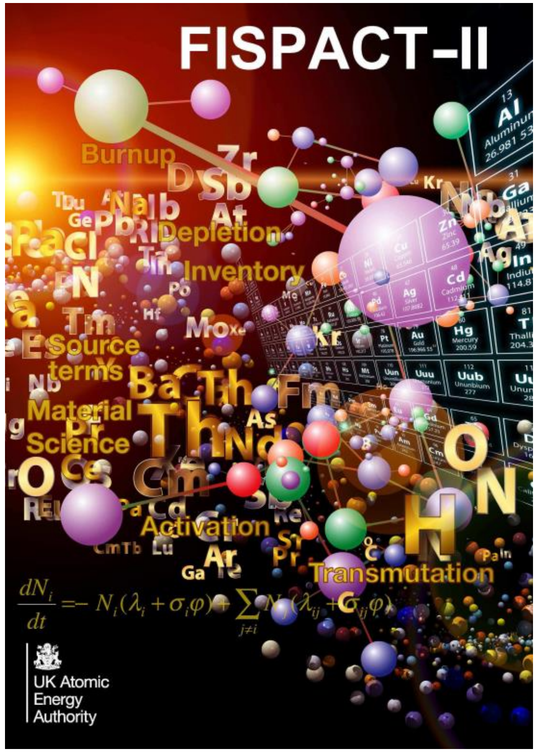
Nuclear Inventory Simulation

- 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 2017, ENDF/B-VIII.0, JEFF 3.3, JENDL-4.0 etc…



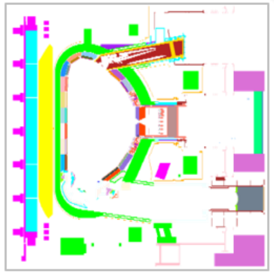


M. R. Gilbert et al., *Nucl. Sci. Eng* **171** (2014) 291-306



Neutronics workflow

Neutronics model

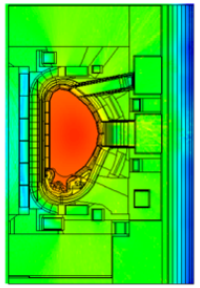


CAD conversion

ANSYS SpaceClaim

FDS SuperMC

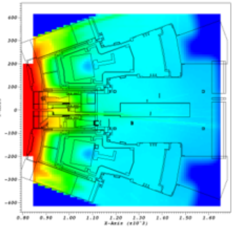
Global variance reduction (GVR)

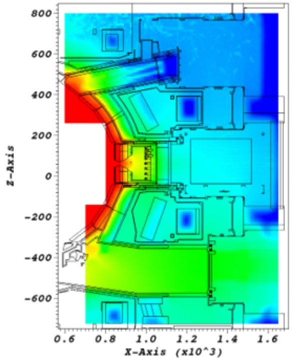


WWITER

ADVANTG

Oak Ridge National Laboratory





MCNP6

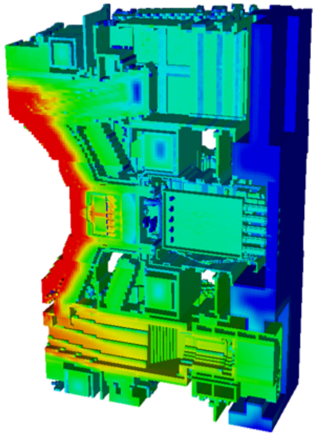
Coupled neutron-photon transport with GVR

Primary responses:

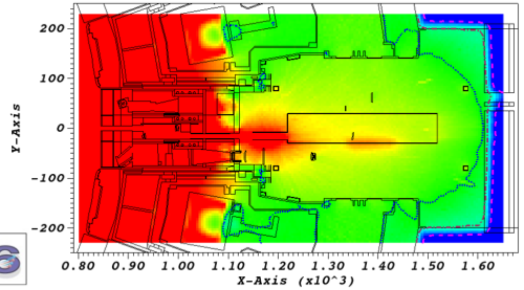
- High resolution neutron/ photon flux maps
- Gas production
- Heating
- Material dose/dpa rates

MCR2S

Decay gamma source from MCR2S



Photon Transport (SDDR)



MCNP6

Secondary responses:

- Nuclide inventory
- Radioactive waste
- Shutdown dose rates

Serpent 2 Benchmarking: Summary

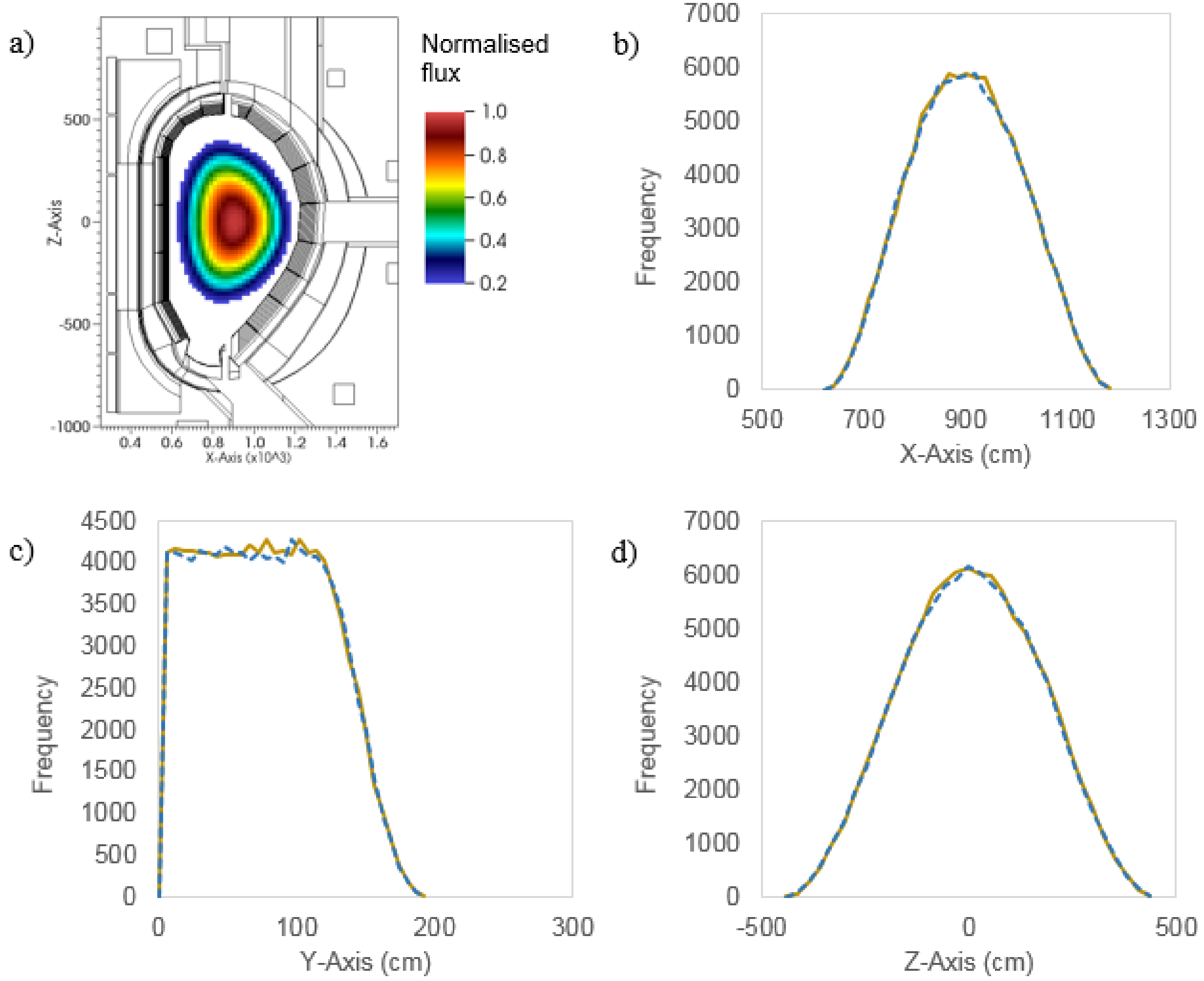
UK Atomic Energy Authority

- UKAEA started looking into Serpent for fusion applications ~3 years ago
- Ongoing benchmarking of the code under EUROfusion PMI-3.3 T042 (current) with focus on the following:
  - Produce a source term for the Frascati Neutron Generator (FNG)
  - Generate a Serpent model of the FNG HCPB mock up experiment and perform calculations to compare with MCNP and Experiment.
  - Investigate other SINBAD experiments and report on their usability and relevance to code benchmarking
  - Generation of a Serpent model of DEMO Helium Cooled Pebble Bed (HCPB) blanket concept. Calculate in – vessel nuclear responses including **neutron/photon flux, tritium production rate** (TPR), **displacements per atom** (dpa) and the neutron/ photon **nuclear heating**- compare these results against MCNP
  - Produce a document as guidance for Serpent users (interested in performing fusion calculations) including a description of useful key words, run parameters, errors, relevant theory etc …
- The results of the above were presented at a recent WPEC meeting at the NEA which prompted in depth discussion on the existence of erroneous cross section data. This topic was revisited at the FENDL meeting in Vienna where UKAEA also reported results from Serpent.
- A paper is in preparation for PHYSOR 2020 with focus on HCPB mock up and DEMO HCPB analysis

Source creation

- **Parameterised plasma source**
- MCR2S source (under development)
- Frascati Neutron Generator Source (14 MeV neutrons from T(d,n)α)

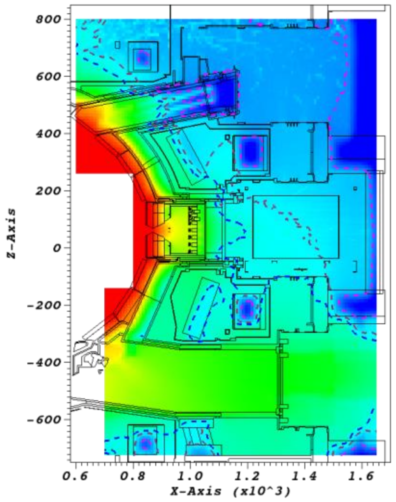
- Fortran parametric plasma source rewritten in C and used as a Serpent user defined source.
- A comparison of the starting particle location and energy between the two codes carried out to check the Serpent user source implementation.



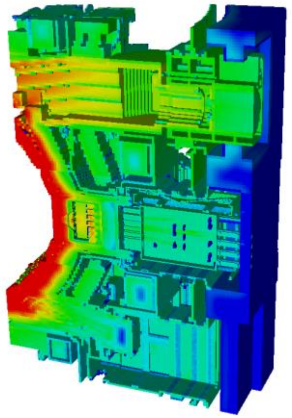
Source creation

- Parameterised plasma source
- **MCR2S source (under development)**
- Frascati Neutron Generator Source (14 MeV neutrons from T(d,n)α)

- Inventory analysis (FISPACT-II)
- MCR2S couples shutdown inventory with space and time
- Full 3D activation and shutdown dose analysis tool
- Serpent2 MCR2S source for shutdown photon calculations

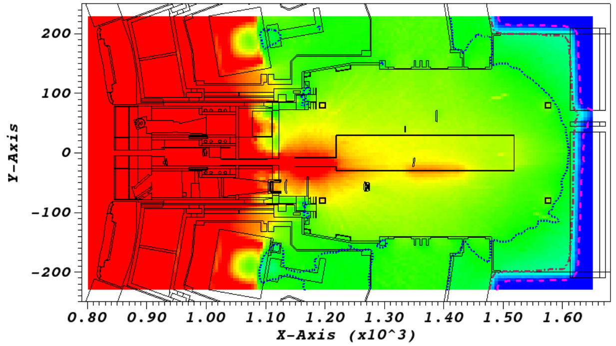


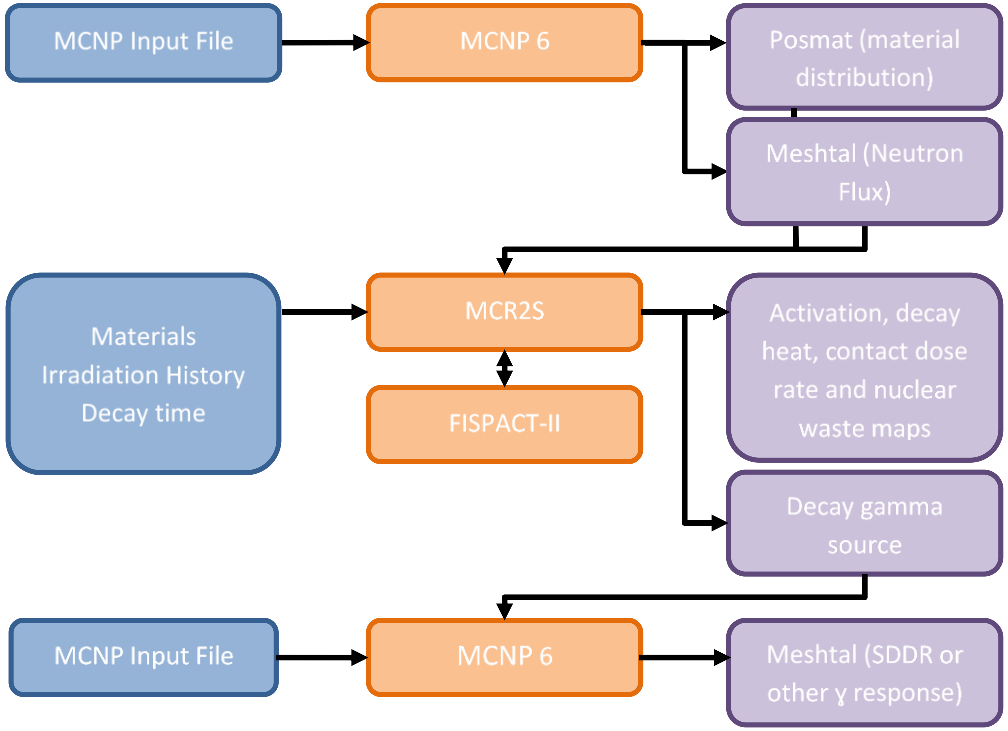
Neutron Flux



Gamma Source

Shutdown Dose



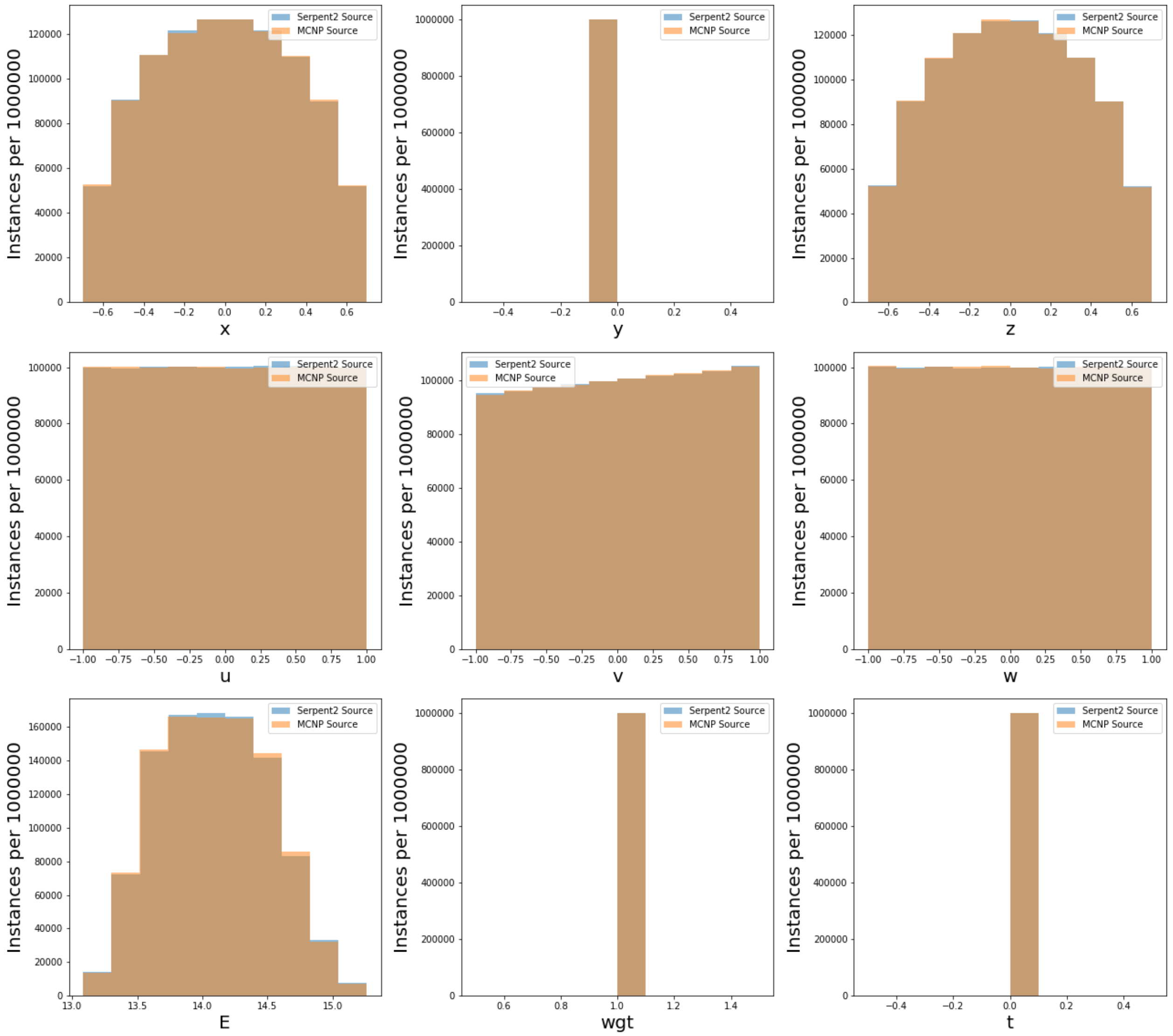


Source creation

- Parameterised plasma source
- MCR2S source (under development)
- **Frascati Neutron Generator Source (14 MeV neutrons from T(d,n)α)**

- Fortran FNG Source wrapped in C and called from user defined source in the Serpent input
- A comparison of the starting particle location and energy between the two codes carried out to check the Serpent user source implementation.

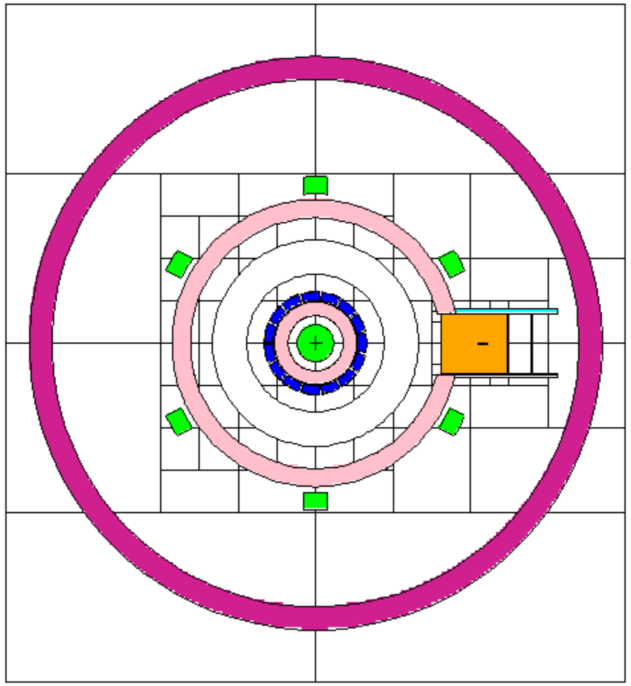
Probability distribution
Blue = Serpent 2
Orange = MCNP
Brown = overlap with both Serpent2 and MCNP



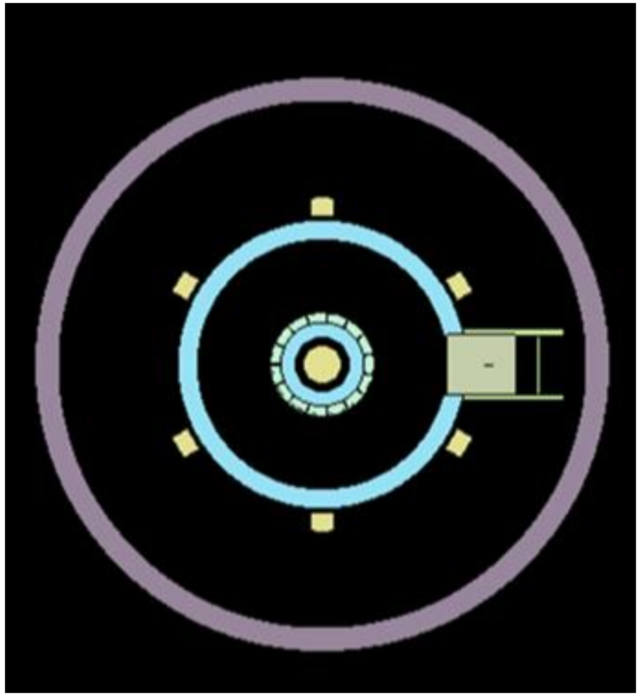
Serpent 2 tool development

- Python neutronics toolkit
  - Serpent 2 output reader (basic tally extraction plotting) and converter to VTK format
  - MCNP to Serpent 2 conversion tool
- ‘csg2csg’ (https://github.com/makeclean/csg2csg)
  - Currently supports converting MCNP files to Serpent, OpenMC and Fluka

MCNP

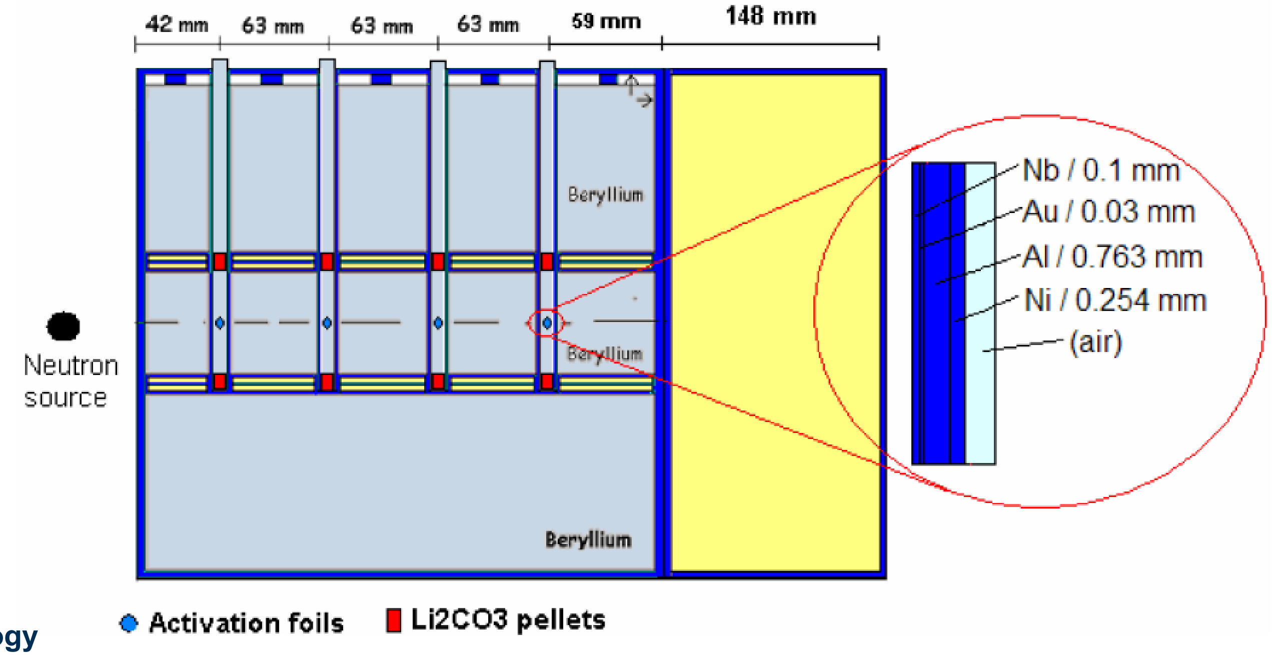


Serpent



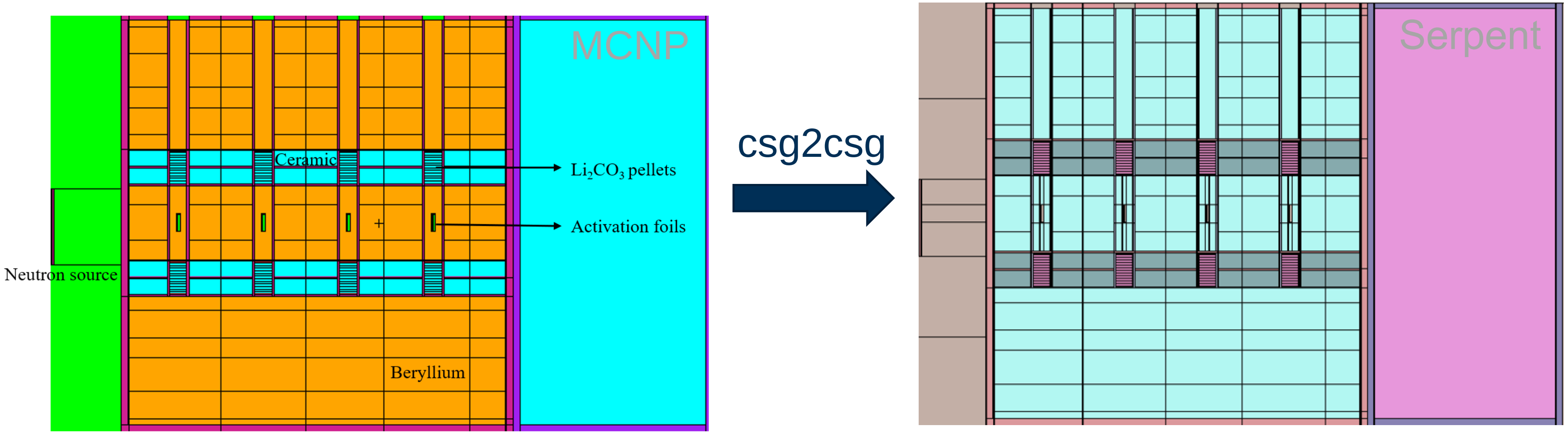
Serpent 2 Benchmarking: FNG HCPB mock-up experiment

- The SINBAD distribution includes experimental results with uncertainties, various reports on the experiment and results calculated by MCNP
- This experiment was performed in April 2005 with total neutron yield of 5.834×10^{15} and is part of the SINBAD database
- The reaction rates in a set of activation foils were measured including the following reactions: Nb(n,2n) ; Au(n,γ); Al(n,α);Ni(n,p).
- The tritium production rate was also experimentally determined in stacks of Li_2CO_3 pellets through the mock up.



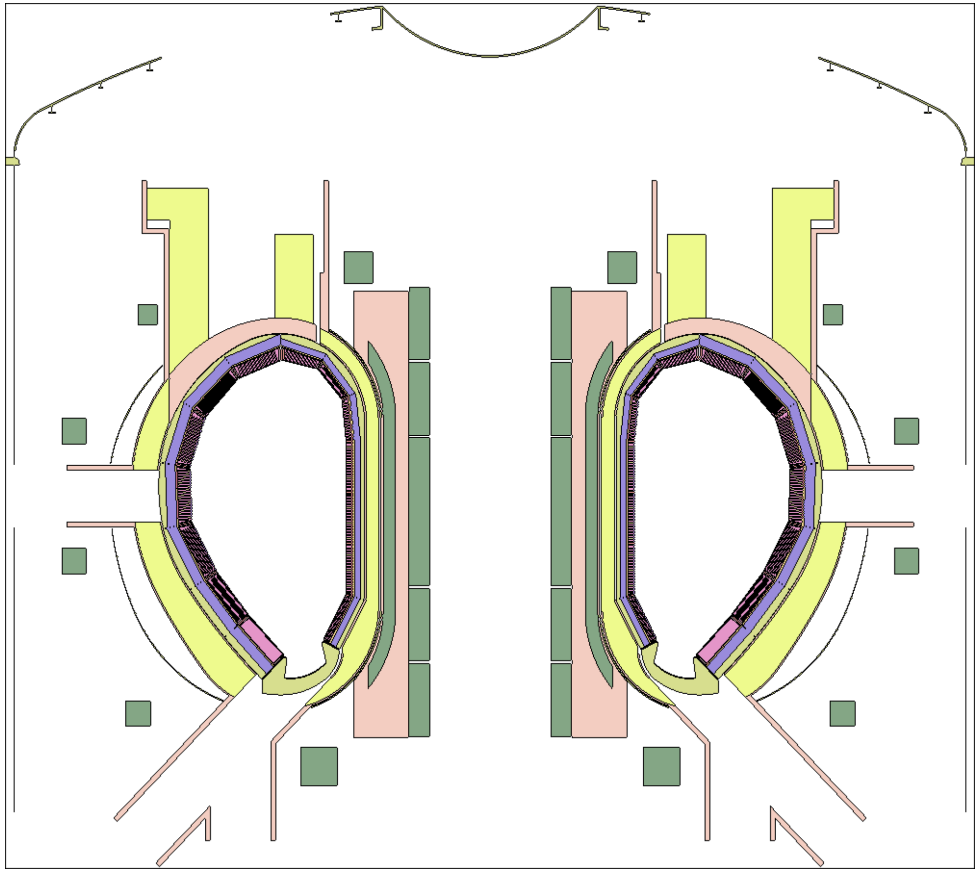
Serpent 2 Benchmarking: FNG HCPB mock-up experiment

- Serpent 2 model created using automated conversion tool from MCNP input – 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 calculations in this task. For the reaction rates in activation foils, LLDOS, IRDFF2002 and IRDFFv1.05 have been used.
- As the interface source was not yet complete we used MCNP to generate a list of x,y,z weight and direction for x number of source particles and pointed to this in Serpent.
- We point to exactly the same ACE files for Serpent and MCNP.

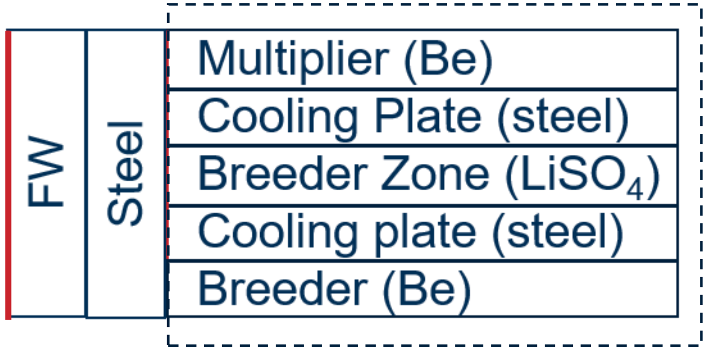


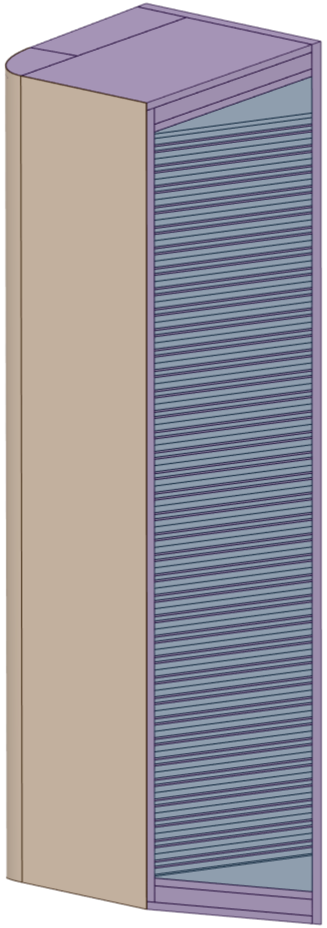
Serpent 2 Benchmarking: DEMO HCPB model

- To model the 360° tokamak, we use reflecting boundary conditions on the lateral bounding planes of the sector – In Serpent this is achieved through unfolding the model into a 360 degree model using *usym* option
- The lattice implementation is quite different to MCNP when using Fill transforms



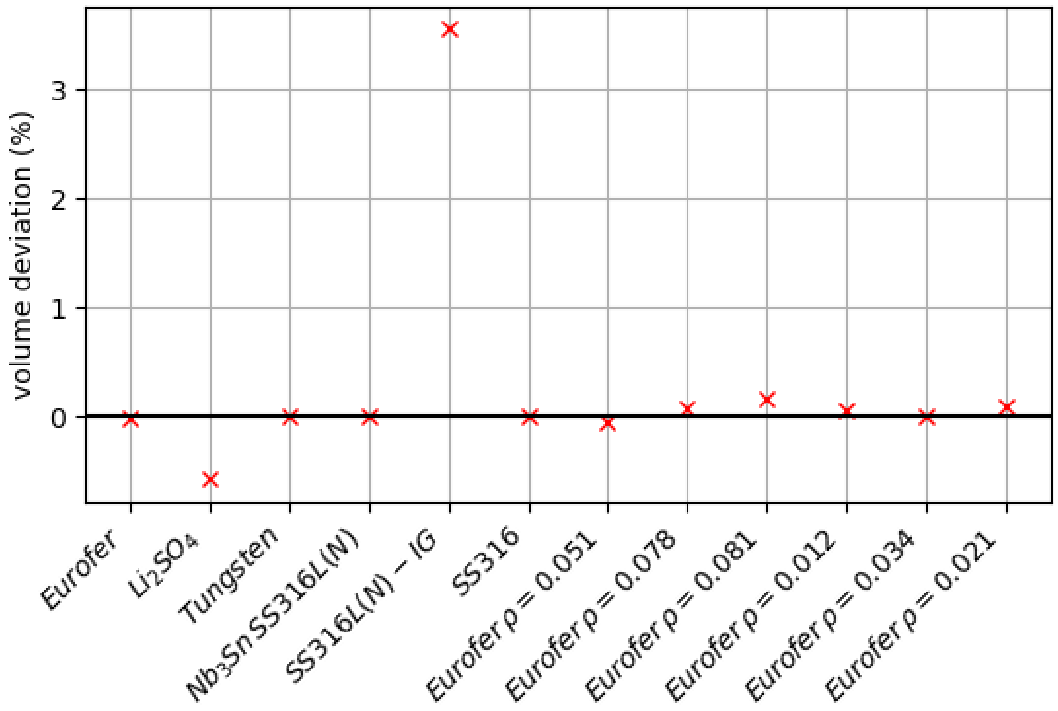
Repeating lattice:



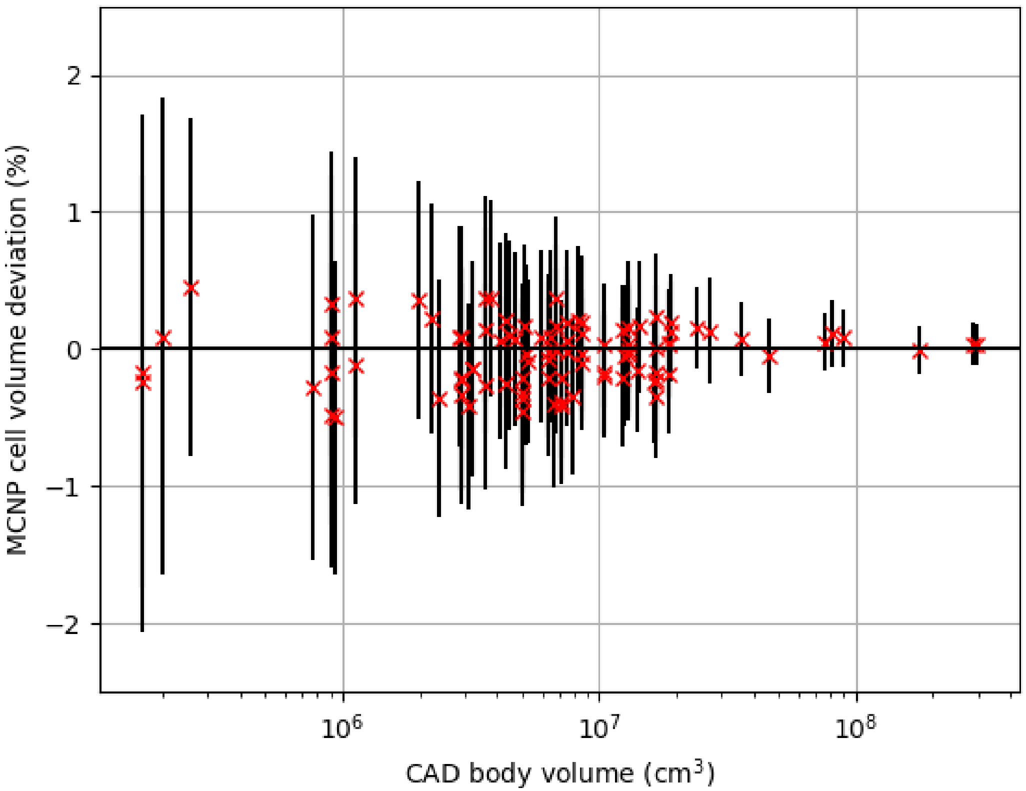


Serpent 2 Benchmarking: DEMO HCPB model validation

- In a typical neutronics workflow we would validate the conservation of mass in the simplification and conversion (SuperMC) process by performing a stochastic volume calculation -> Spherical source surrounding geometry with inward biased cosine distribution and starting *wgt* equal to πr^2
- Can perform either material wise or cell wise validation



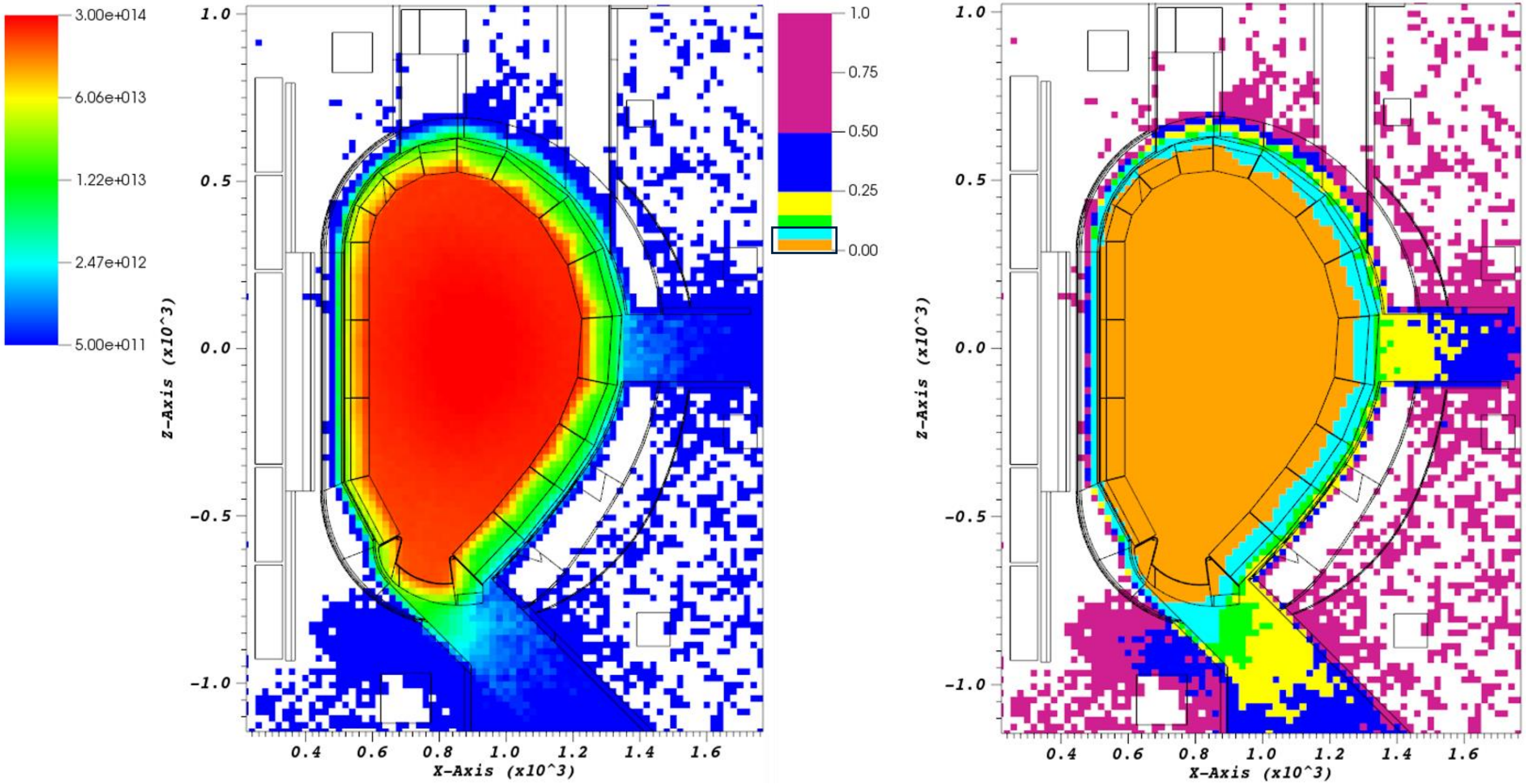
Material - wise



Cell - wise

Serpent 2 Benchmarking: DEMO HCPB model flux

- Parametric plasma source called as ‘user defined source’ [CCFE modification]
- 1E8 histories gives good convergence in Blanket.

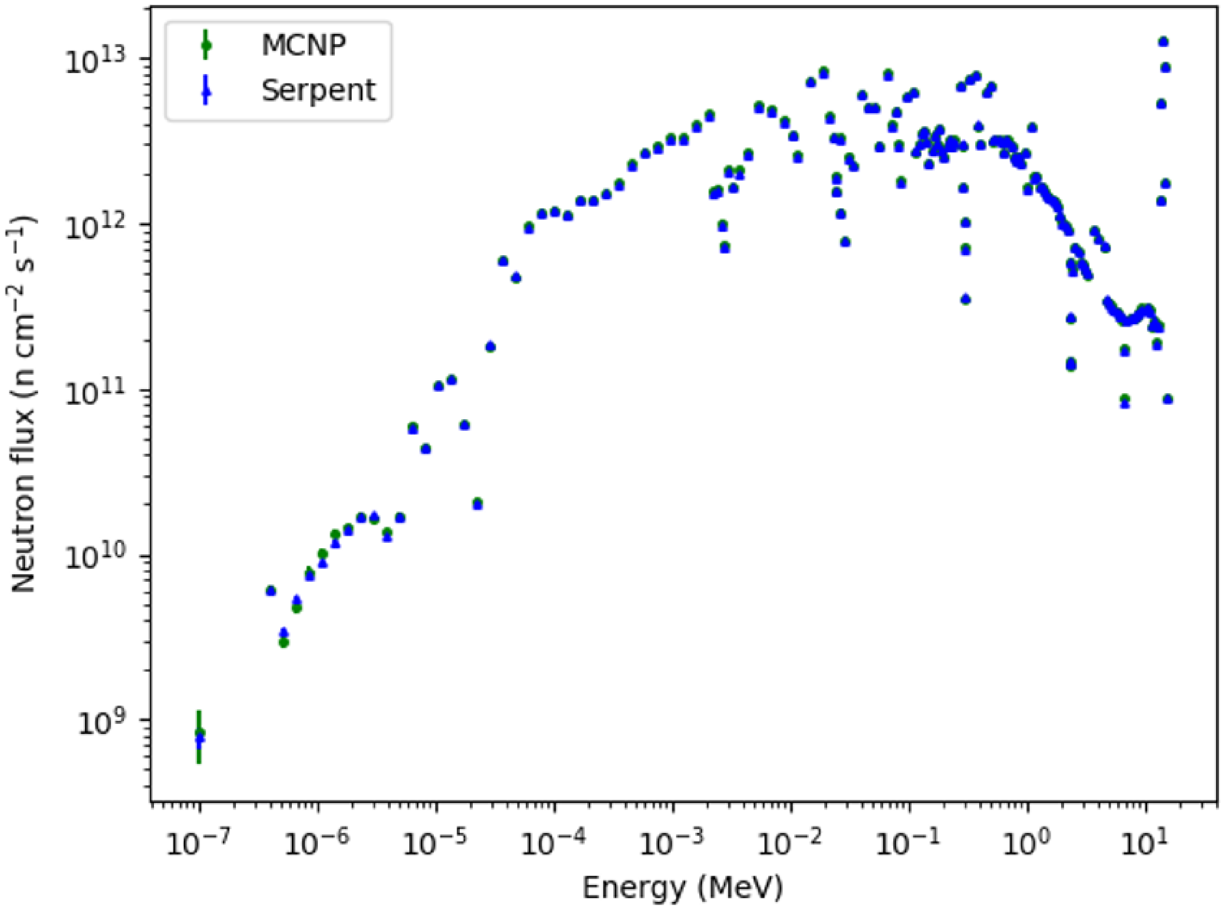


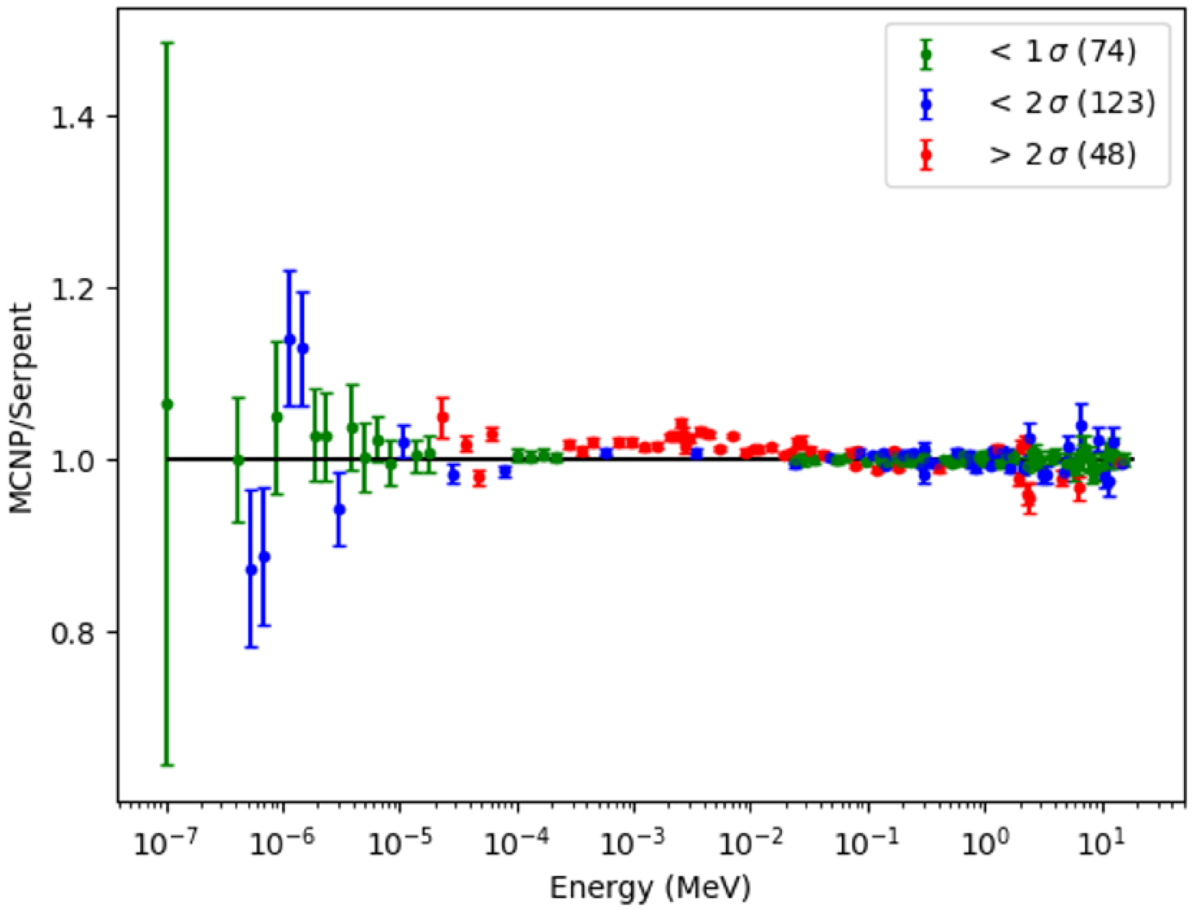
Neutron flux (n cm^{-2} s^{-1}) and error map

All plots with Visit software

Serpent 2 Benchmarking: DEMO HCPB model flux

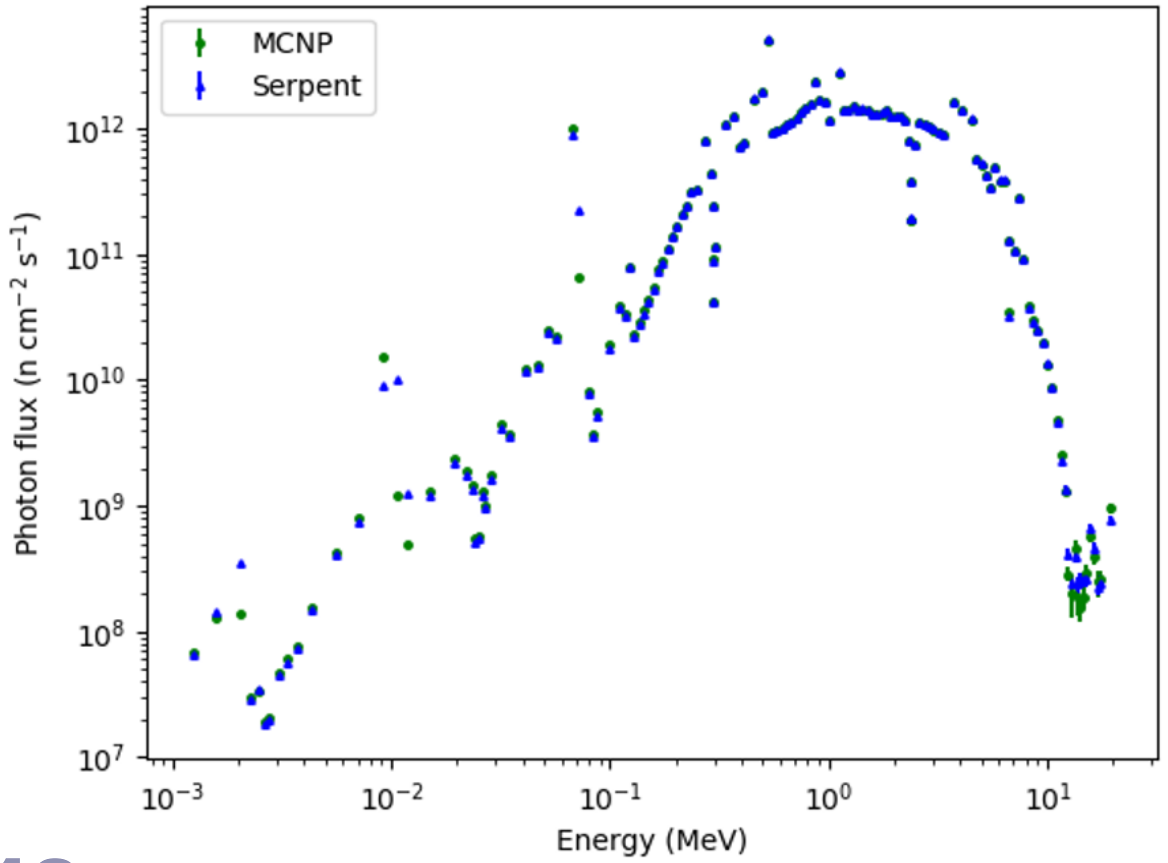
- Neutron flux tallied in a single cell first wall, plasma facing layer of divertor. (Tungsten)
- Generally, very good agreement. Note all Serpent results are multiplied by 1/36 to capture sector.

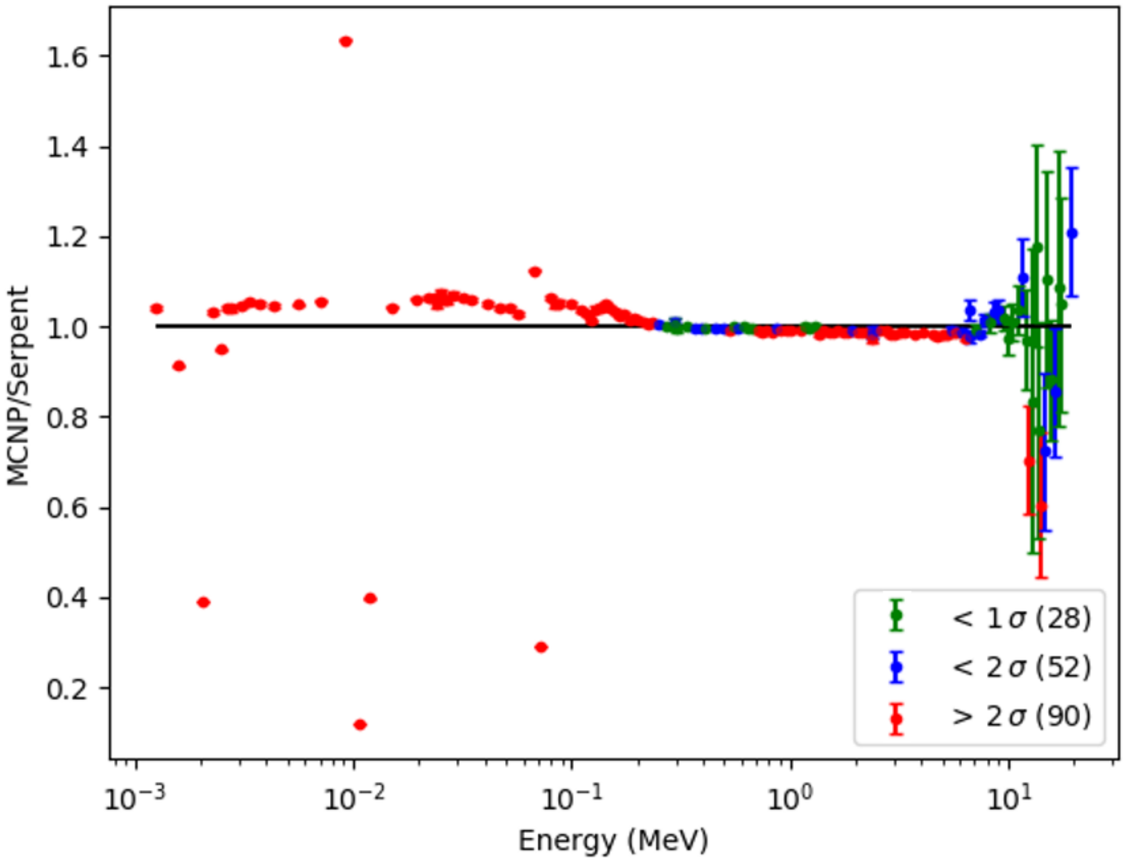




Serpent 2 Benchmarking: DEMO HCPB model flux

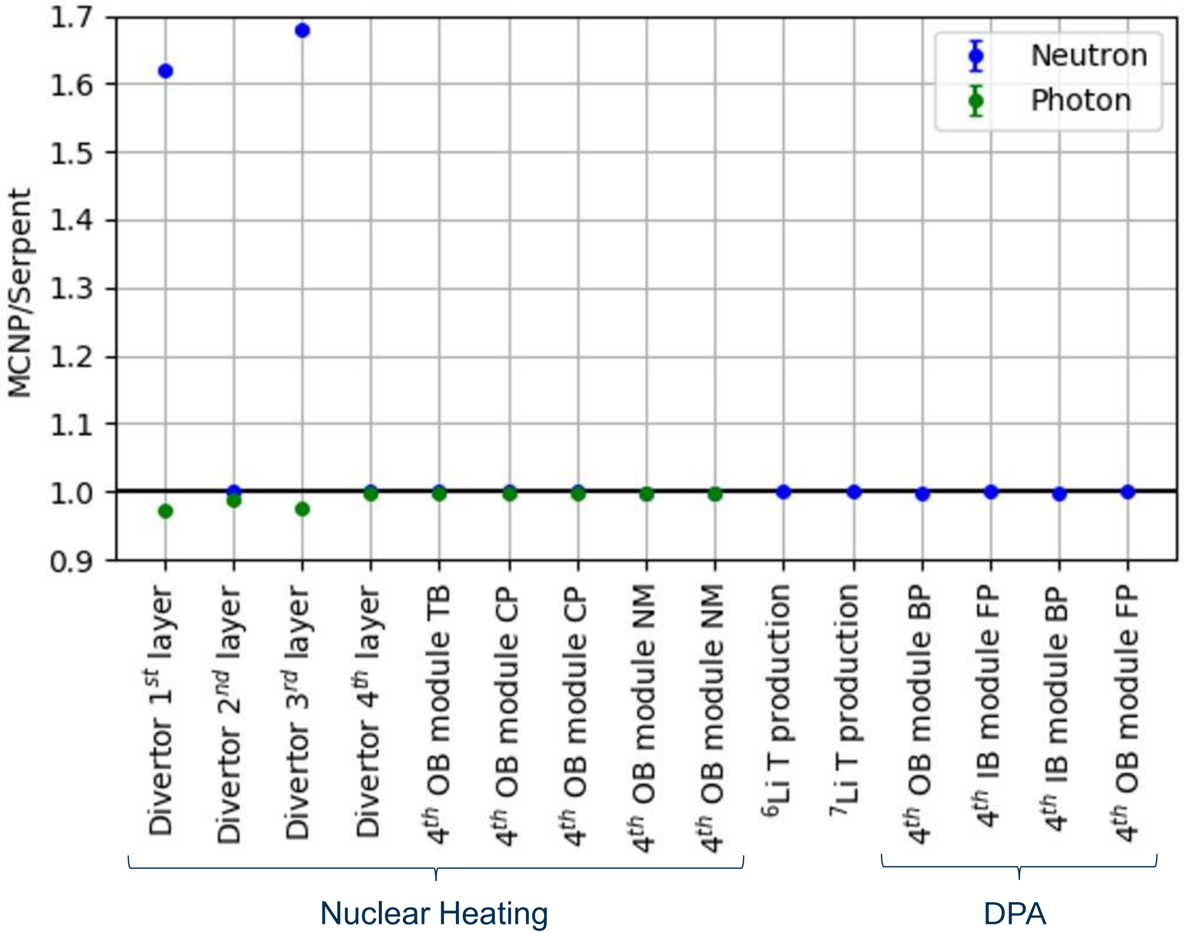
- Photon flux tallied in a single cell first wall of divertor. (Tungsten)
- General shape is captured once more but deviations more significant – different physics models



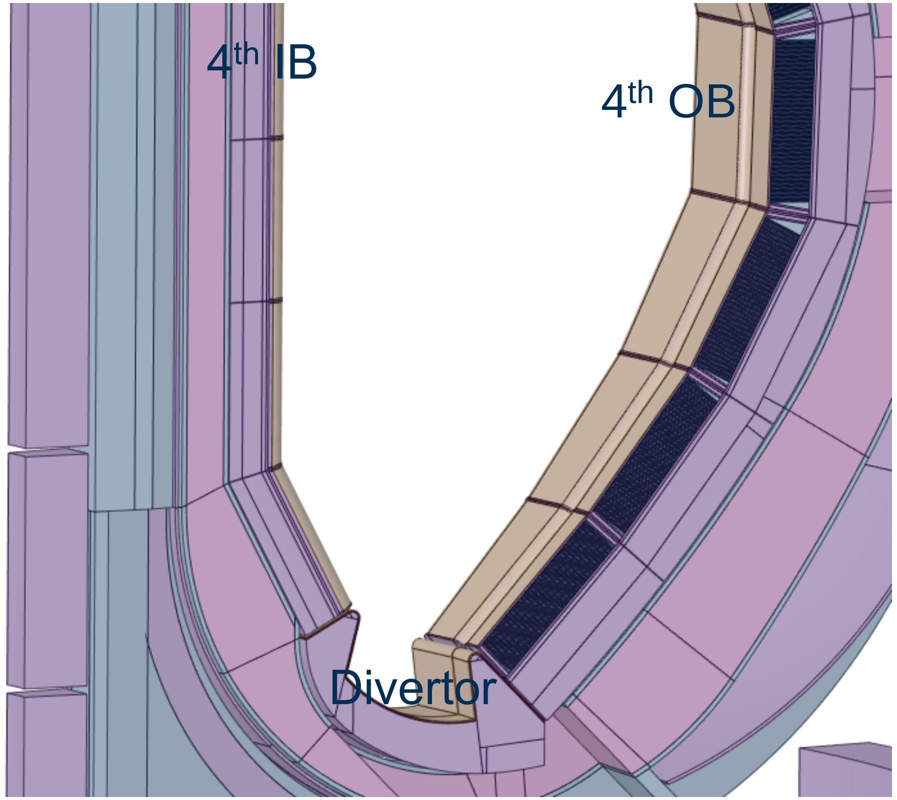


Serpent 2 Benchmarking: DEMO HCPB model nuclear responses

- Only major discrepancy is in the nuclear heating, particularly for neutrons.
- Traced back to erroneous nuclear data and how both codes handle this.



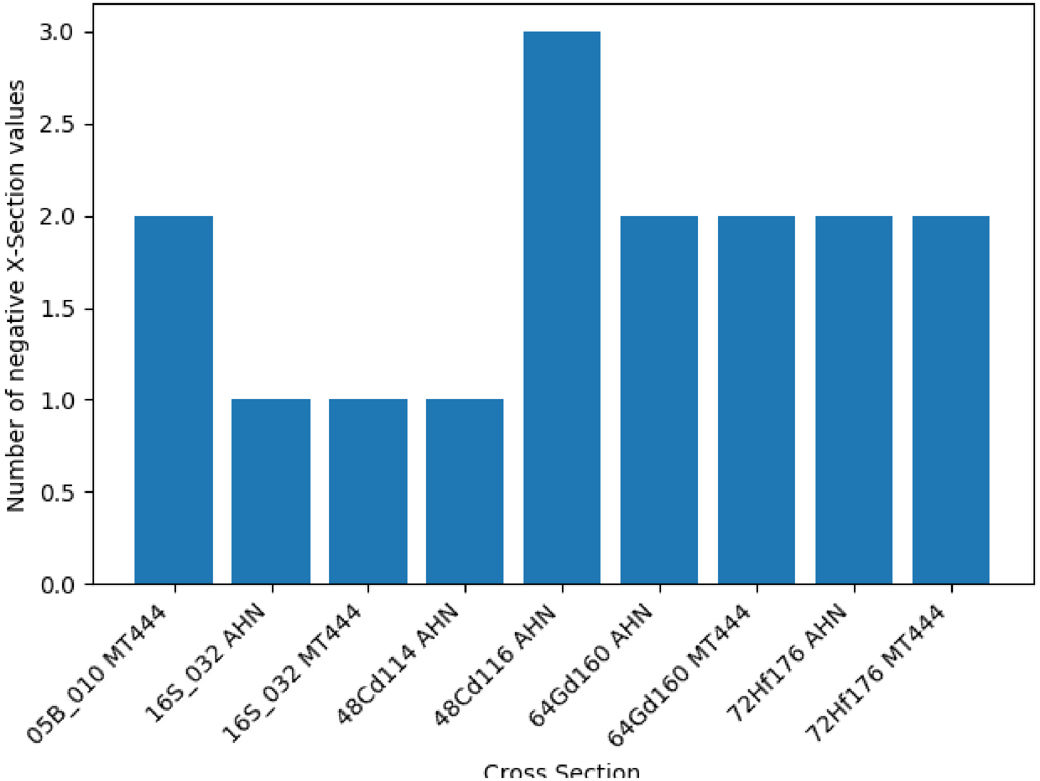
TB: Tritium Breeder
CP: Cooling Plate
NM: Neutron Multiplier
OB: Outboard
IB: Inboard
T: Tritium
BP: Back plate (blanket)
FP: Front plate (blanket)



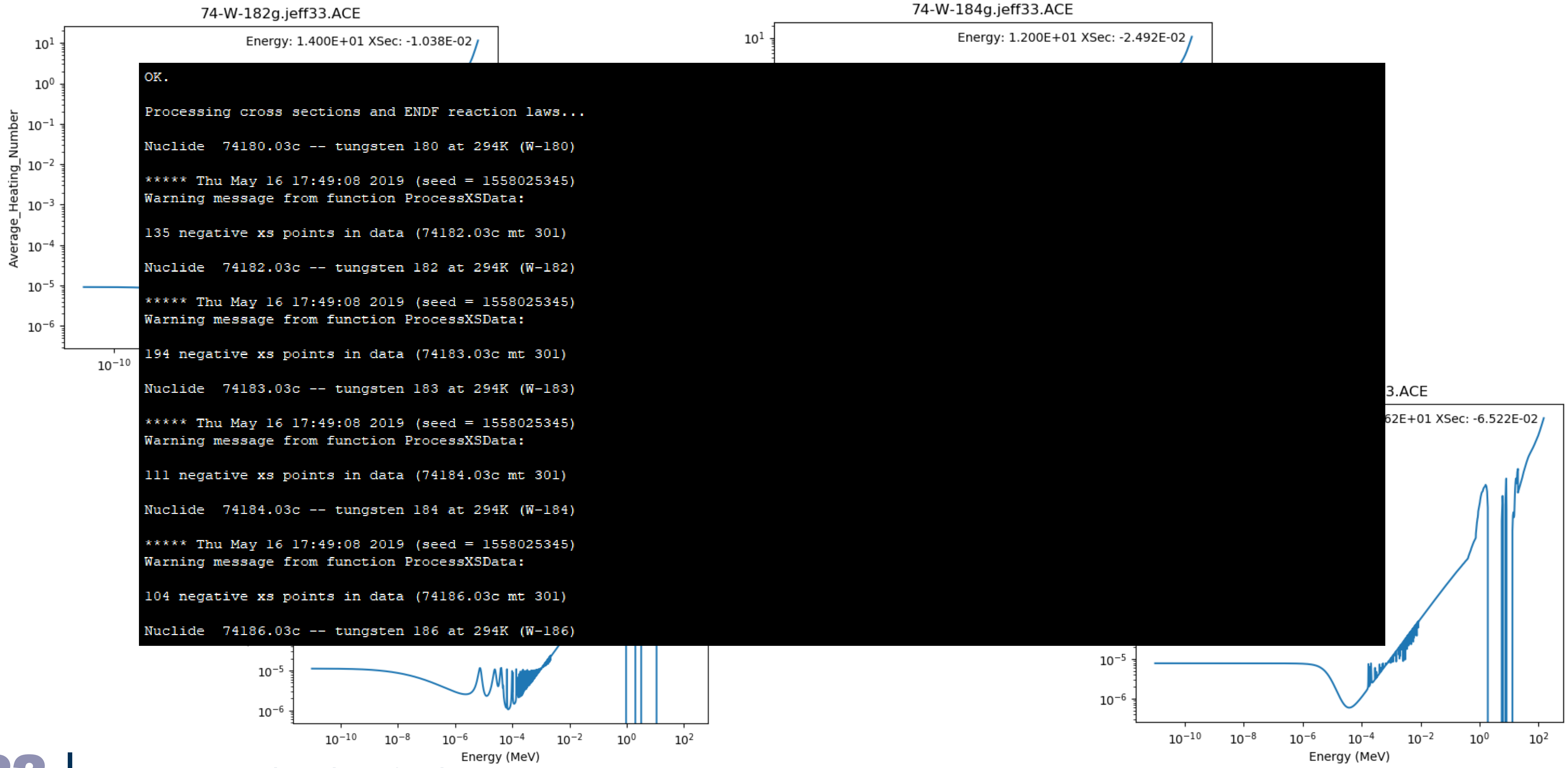
Looking at FENDL ACE files

- 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



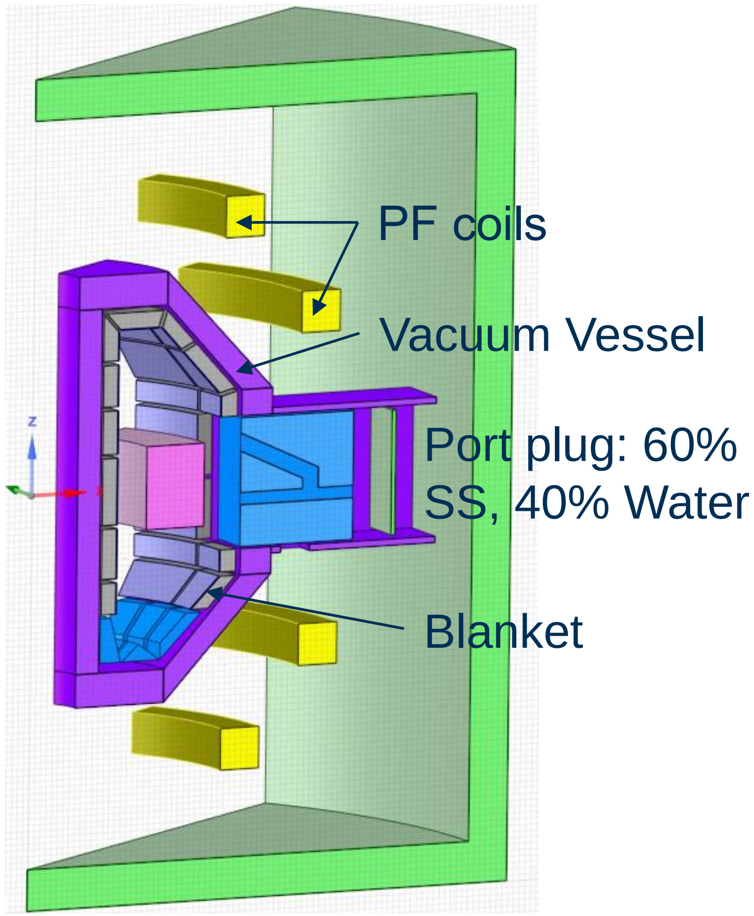
Serpent 2 Benchmarking: DEMO HCPB model negative cross sections



Variance Reduction

- Serpent implements two different variance reduction methods:
  - Weight-window mesh generated using the built-in response matrix method-based solver *
  - MCNP WWINP format weight window-mesh – Generally, generated using ADVANTG

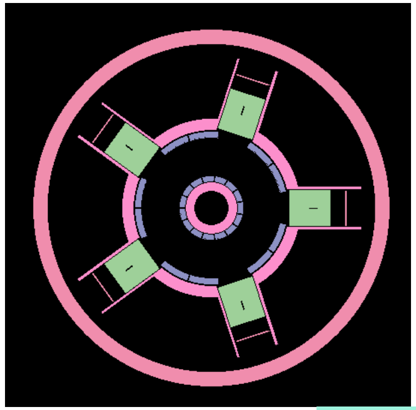
- Mixed success with the second implementation.
- The built in response matrix method based solver is relatively new and in testing for fusion tokamak models – A test case has been set up – the 'Octamak' (eight fold symmetry) with homogenised ITER-like materials. A 72° sector of this has been modelled.
- The Global Variance Reduction (GVR) scheme which is implemented in this method can be used to improve statistics in the ex-vessel region. This would give convergence in the PF coils and port interspace for shut down dose rate (SDDR) assessments. (For example, in ITER, the SDDR should be kept below 100μSv hr^{-1} following 12 days cooling)

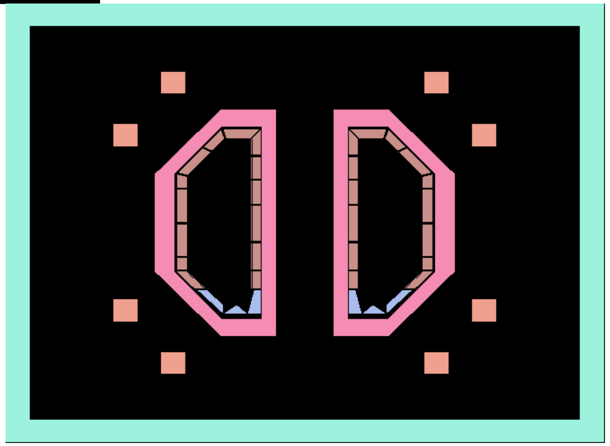


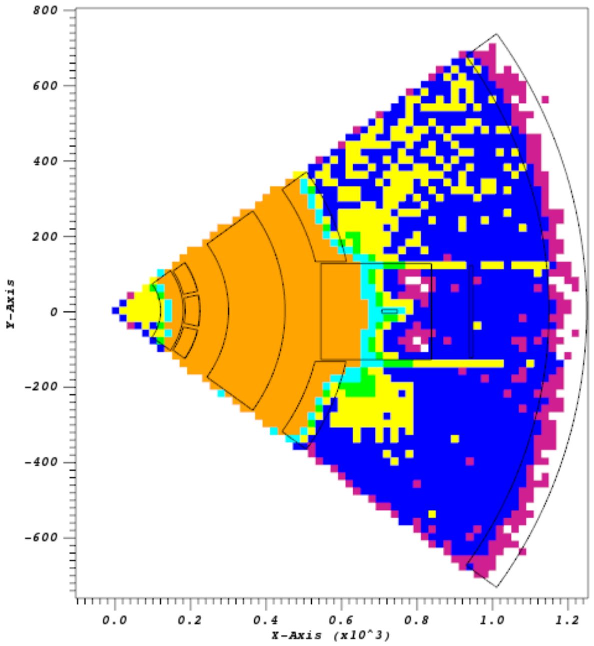
Jaakko Leppänen (2019): Response Matrix Method–Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code, Nuclear Technology

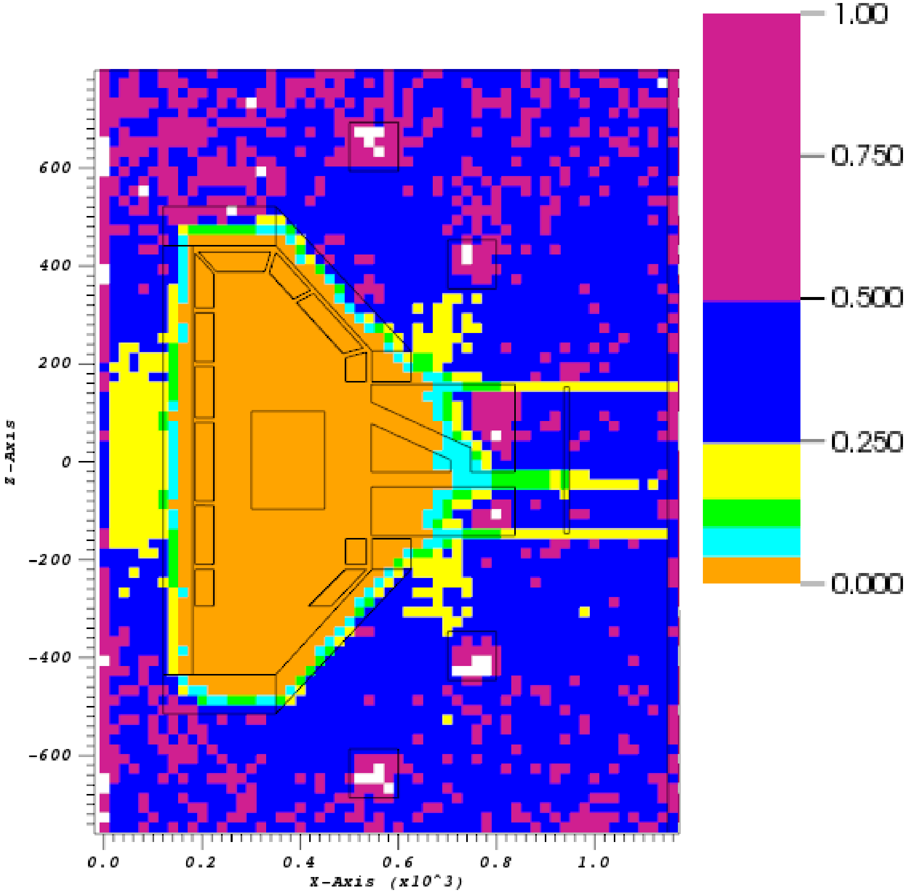
Variance Reduction

- ‘Literal’ reflecting boundaries have been implemented using the final option on the *usym* card. Geometry still unfolded but transport only in sector.
- Analogue calculation, 1E8 particle histories. Constrained to in-vessel responses



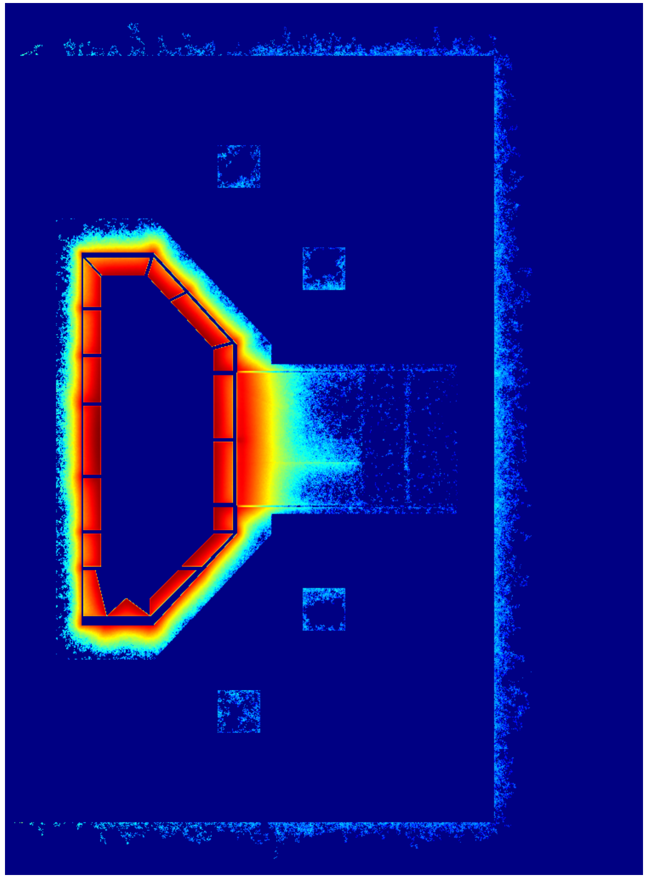




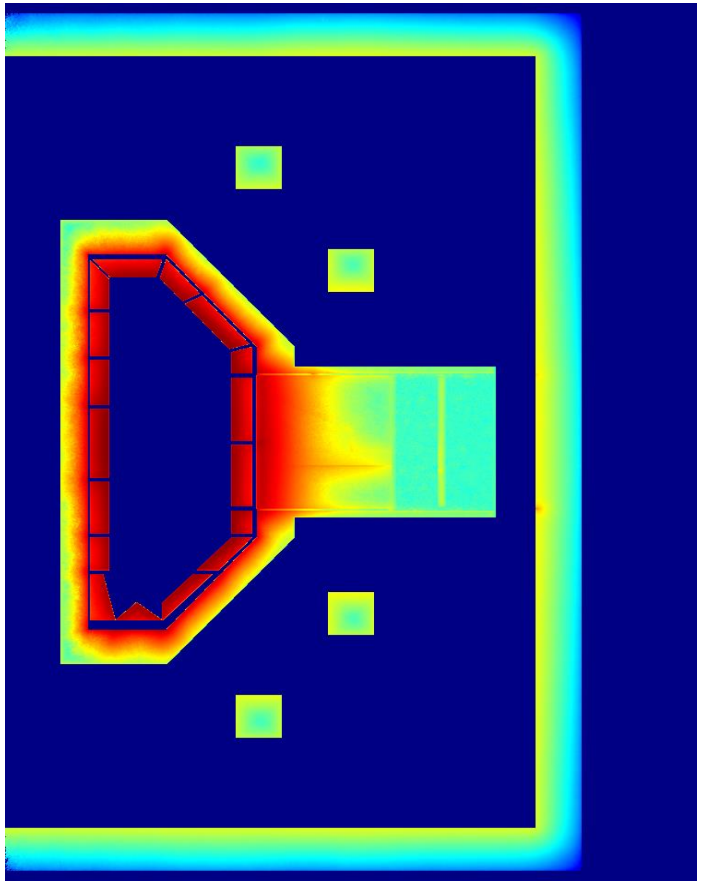


Variance reduction: Built in solver iterations

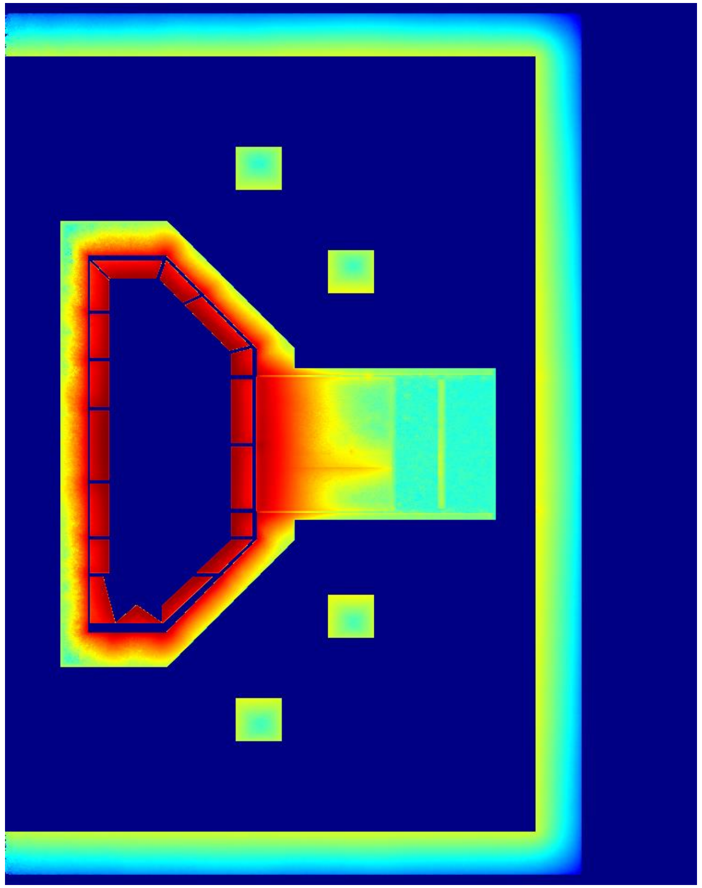
- Apply rectangular, adaptive mesh method with 9 iteration cycles. Single 32 CPU node- 1 hour run time.
- Weight window for neutrons only.



First iteration



Second Iteration

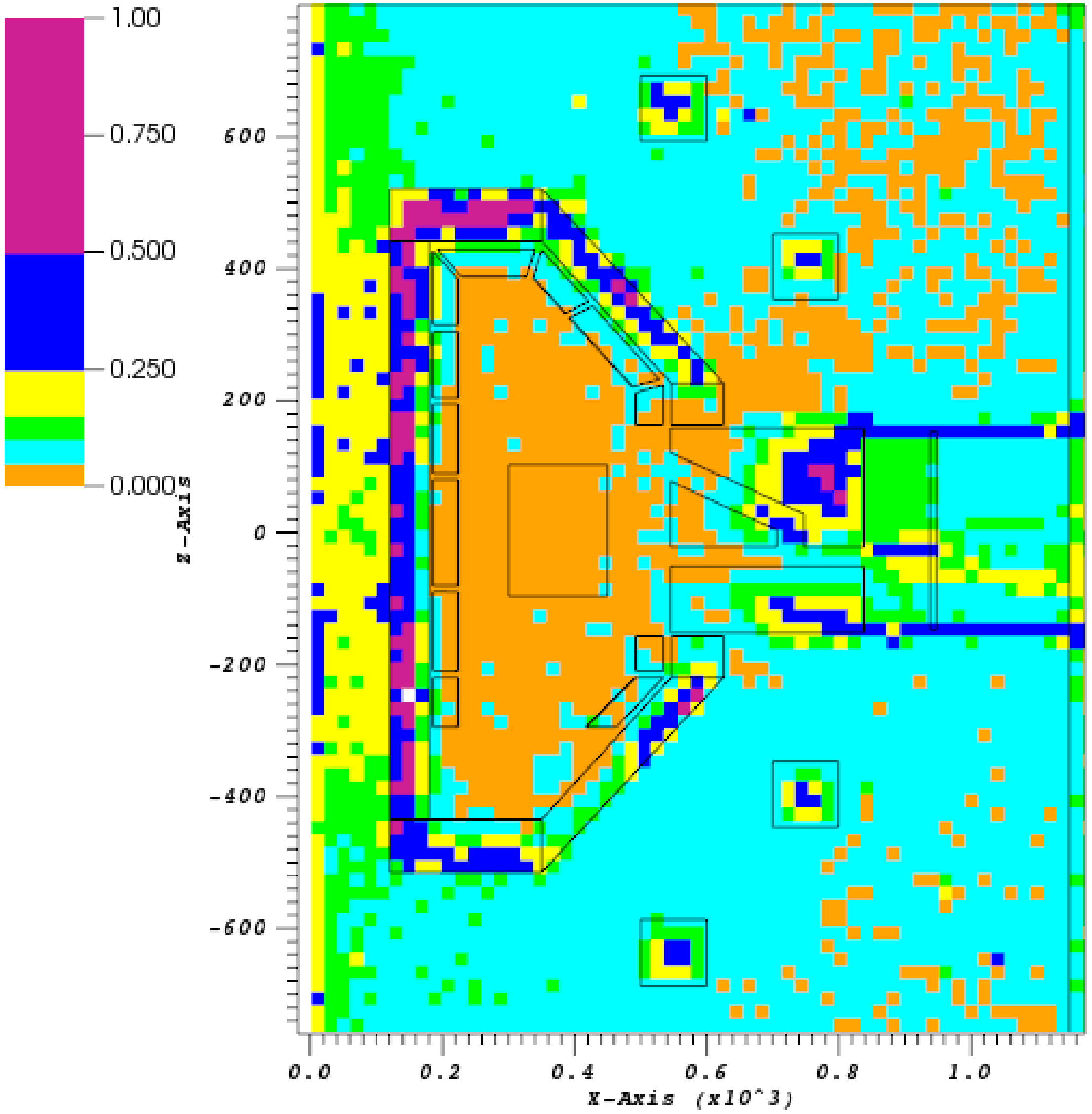


Final Iteration

Variance reduction: Built in solver error map

UK Atomic Energy Authority

- Testing was performed with a point source however now possible to use 360 degree source in sector models.
- 5×10^6 neutron histories
- Relative to generating weight windows in ADVANTG (conventional method) this is significantly more efficient and seemingly more effective for tokamak geometry.



Serpent User guide (Fusion)

UK Atomic Energy Authority

October 15, 2019

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Serpent User Guide for Fusion Applications

October 15, 2019

Serpent User Guide for Fusion Applications

Alex Valentine, Bethany Colling, Ross Worrall

October 15, 2019

UK Atomic Energy Authority
Culham Science Centre
Abingdon
Oxfordshire
OX14 3DB

October 15, 2019

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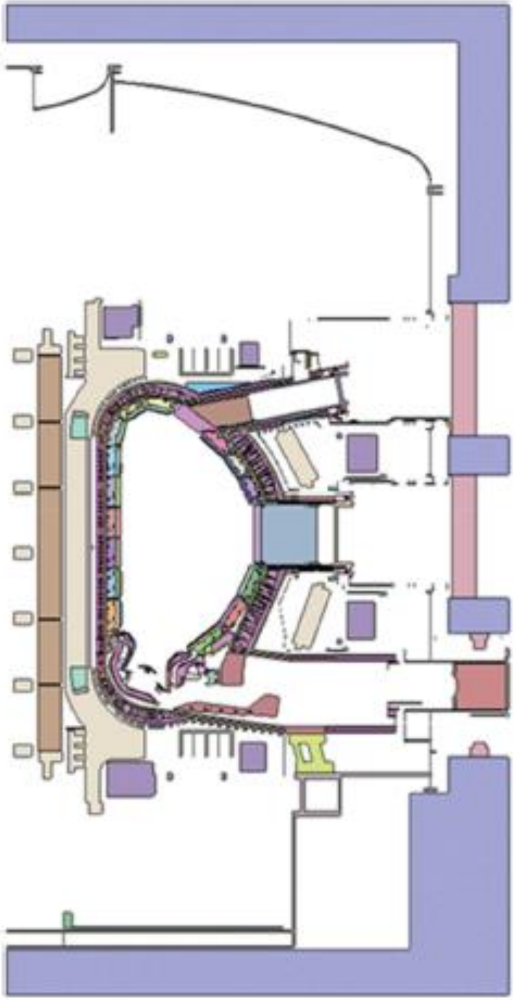
Contents

Summary

UK Atomic Energy Authority

- UKAEA has been actively looking into the Serpent code for almost 3 years
  - Many of the features needed in the fusion domain are now implemented in the code
- Collaboration is ongoing
  - A.Valentine and R.Worrall visit to VTT and Aalto University fusion group 30/09-04/10
  - PHYSOR 2020 paper
  - DEMO EUROfusion task PMI3.3-T042
- The priority in terms of applications in fusion remains variance reduction – with significant promise shown for the new GVR scheme we hope this can extended to ITER models (Serpent model on right)
- MCNP remains the most adopted code in fusion neutronics, however there is general acceptance among the community of the need for a transition at least in part, and currently Serpent shows the most promise for this.



Questions?

Alex.Valentine@ukaea.uk