UK Atomic Energy Authority

Use of SINBAD in validation of emergent radiation transport codes

Alex Valentine

33rd WPEC Meeting, Subgroup 47, 11th May 2021

Contents

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Nuclear Analysis and Modelling at UKAEA

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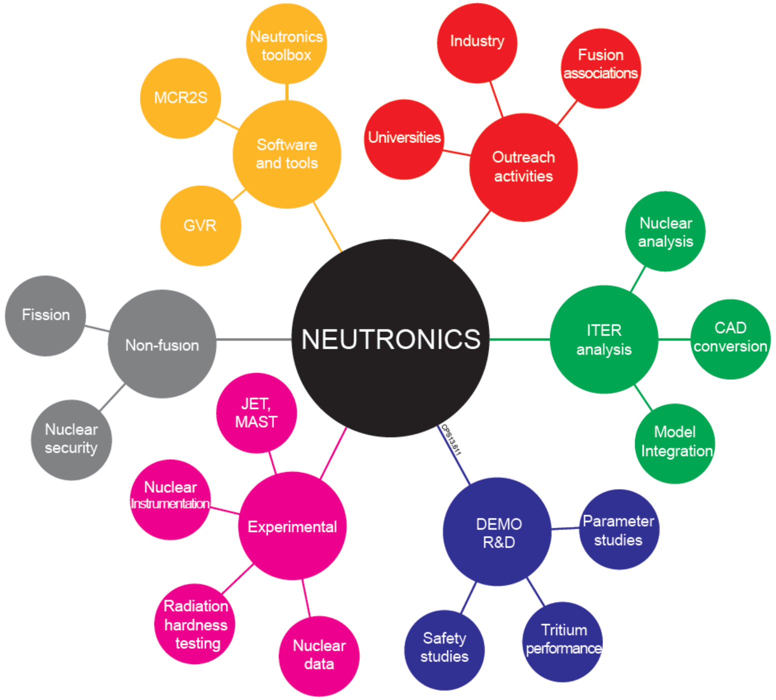
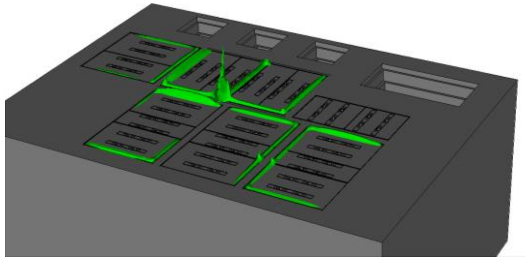
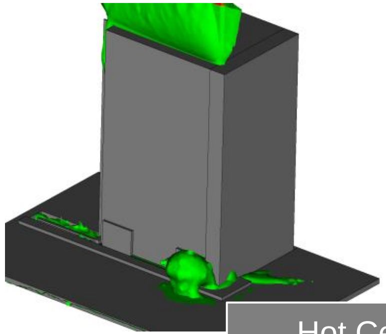


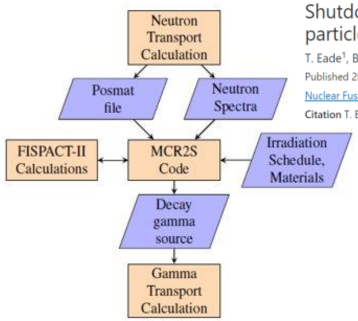
SPACECLAIM CORPORATION · VisIt · OpenMC · MIRION TECHNOLOGIES · McCad · SuperMC · OAK RIDGE National Laboratory · ORTEC · AMETEK · MCNP6 · DAGMC · Serpent · CAEN Tools for Discovery

ESS Active Cells Assessment

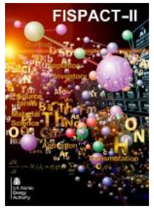




Hot Cell commissioning



PAPER
Shutdown dose rate benchmarking using modern particle transport codes
T. Eade[1], B. Colling[1], J. Naish[1], L.W. Packer[1] and A. Valentine[1]
Published 20 April 2020 • © 2020 Crown copyright
Nuclear Fusion, Volume 60, Number 5
Citation T. Eade et al 2020 Nucl. Fusion 60 056024



Code development

README.md

SpaceClaim API Neutronics Tools — GitHub

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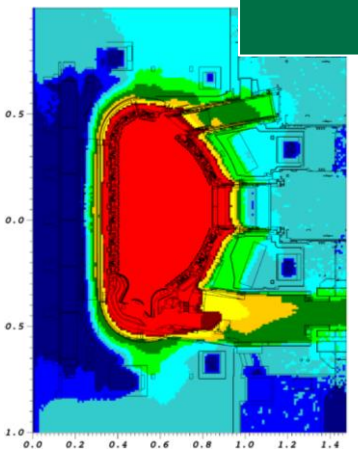
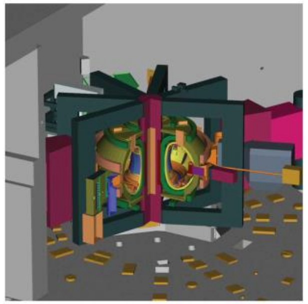
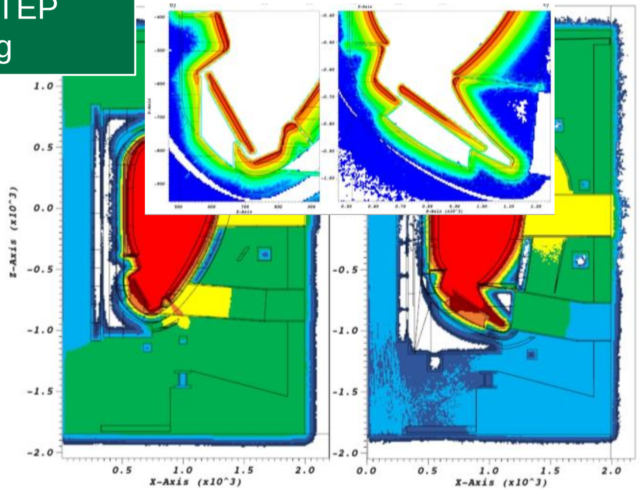
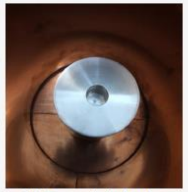
JET, ITER, DEMO and STEP radiation field mapping







Trans-SPEC Portable HPGe detector



SAGe well detector

Experimental Activities

BEGe detector with NaI Compton suppression

190% RE coaxial HPGe detector

Serpent 2 benchmarking and SINBAD

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- As part of the efforts to validate Serpent 2 Monte Carlo code for deployment on fusion neutronics problems, several of the 31 fusion benchmarks present in SINBAD.
- Some effort has been made in automating the running of the benchmarks available to allow faster validation of emergent radiation transport codes. See later.
- This has been performed in parallel with using computational benchmarks such as ITER and DEMO models.
- FNG ITER dose rate benchmarking MCR2S methodology for the evaluation of shutdown does rates, see paper by T. Eade et al.

SINBAD

Fusion Neutronics Shielding (31)

Osaka Nickel Sphere (OKTAVIAN)
Osaka Iron Sphere (OKTAVIAN)
Osaka Aluminium Sphere (OKTAVIAN)
Osaka Silicon Sphere (OKTAVIAN)
Osaka Tungsten Sphere (OKTAVIAN)
FNS Experimental data for fusion neutronics benchmark
FNS Clean Experiment on Graphite Cylindrical Assembly
FNS Liquid Oxygen
FNS Vanadium Cube
FNS Tungsten
FNS Skyshine
FNS Dogleg Duct Streaming
FNG-SS Shield (integral measurements)
FNG-ITER Blanket Bulk Shield (integral measurements)
FNG/TUD ITER Blanket Bulk Shield (spectra measurements)
FNG-ITER Neutron Streaming (integral measurements)
FNG-ITER Dose Rate Experiment
FNG Silicon Carbide (integral measurements)
FNG/TUD Silicon Carbide (spectra measurements)
FNG Tungsten (integral measurements)
FNG HCPB Tritium Breeder Module (integral measurements)
FNG/TUD Tungsten (spectra measurements)
TUD Iron Slab Experiment
IPPE Vanadium Shells
IPPE Iron Shells
ORNL 14-MeV Neutron SS/Borated Poly Slab
University of Illinois Iron Sphere (D-T)
KANT Spherical Beryllium Shells
MEPhI empty slits streaming experiment
Juelich Li Metal Blanket Experiment
Osaka Manganese Sphere (OKTAVIAN)

Valentine, A., et al (2020), "*Benchmarking of Serpent 2 for Fusion neutronics applications*". PHYSOR conference.
Turner, A., (2017). "*Investigations into Alternative Radiation Transport Codes for ITER Neutronics Analysis*". ANS meeting.
Turner, A., (2018). ***"****Applications of Serpent 2 Monte Carlo Code to ITER Neutronics Analysis*", Fusion Science and Technology.
Eade, T., (2020) et al. *"Shutdown dose rate benchmarking of emergent radiation transport codes".* Nuclear Fusion.

Serpent 2 Monte Carlo code

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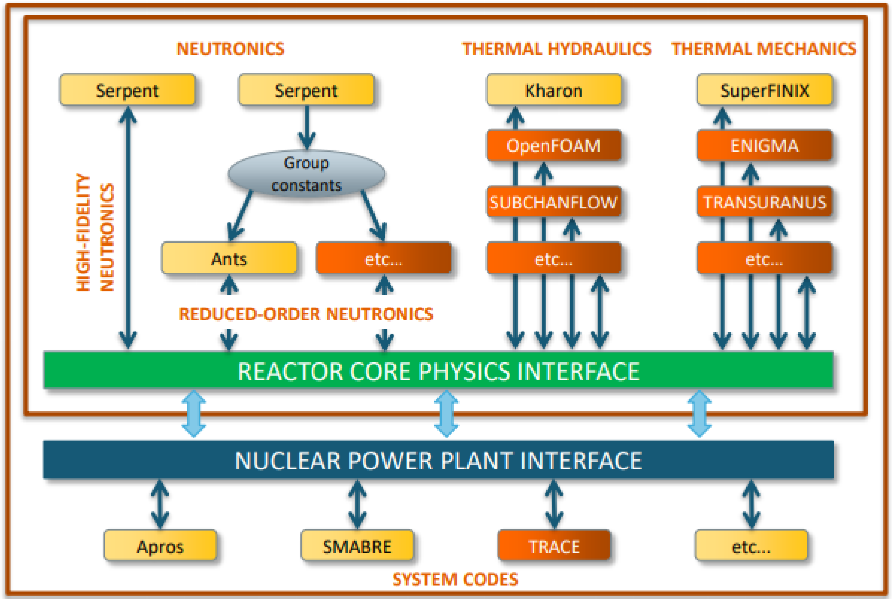
- Developed and maintained by VTT technical research
- Serpent v2.1.32 is current code version. This will be the base version of Serpent v2.2, the first official release of the code (some time this year).
- Now >1000 users worldwide. >810 peer reviews conference papers since 2005.
- Available through NEA databank and RSICC since 2009.
- Majority of users work in fission applications however since development of neutron – photon coupled transport [2] and CAD based geometry transport (STL)in 2016 the scope of the code has extended to applications in nuclear fusion.
- Serpent also now includes powerful Multi-physics framework (KRAKEN).
- Recently, a built-in variance reduction capability has been developed for Serpent. Being a fundamental requirement for fusion neutronics, this feature has been the focus of more recent validation efforts at UKAEA. See [1]



Leppänen, J., et al. (2015) *"The Serpent Monte Carlo code: Status, development and applications in 2013."* Ann. Nucl. Energy, 82 (2015) 142-150.

[1] Valentine A., et al (2021) *"Investigation of novel weight window methods in Serpent 2 for fusion neutronics applications"*. In-review. Fusion Engineering and Design

VTT

FNG HCPB mock-up experiment (NEA-1553/71)

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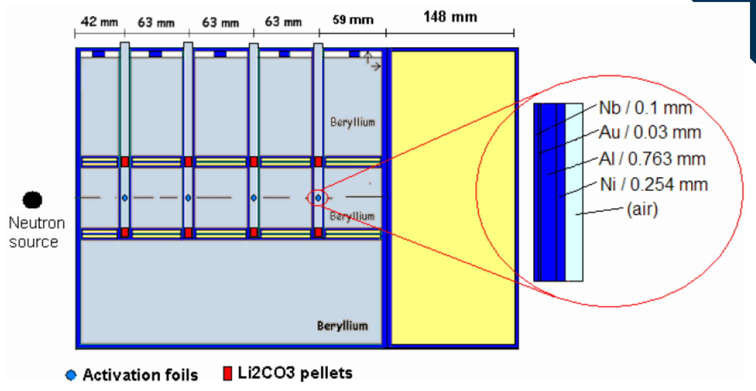
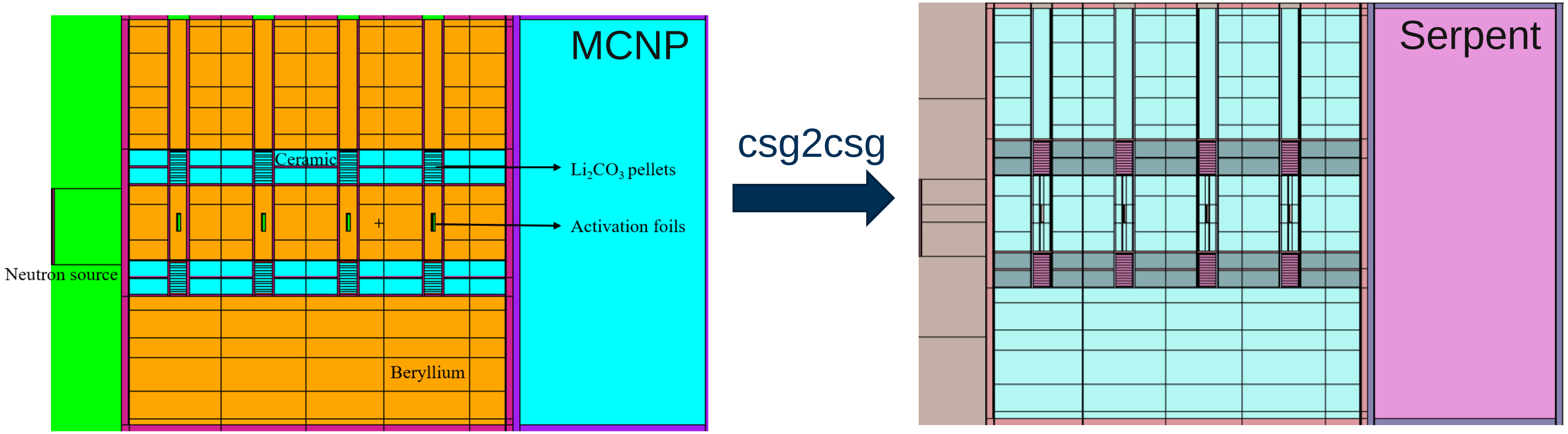
- Experiment performed in 2005. Experimental data available for the reaction rates in activation foils; **Nb(n,2n)** ; **Au(n,γ)**; **Al(n,α)**; **Ni(n,p)** and the tritium activity in **Li_2CO_3** pellets.
- Serpent 2 model created using automated conversion tool from MCNP input, csg2csg [1] – Most of the SINBAD benchmarks are distributed with an MCNP model – this tool provides a robust method for the first step in distributing SINBAD with several MC code inputs
- 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.

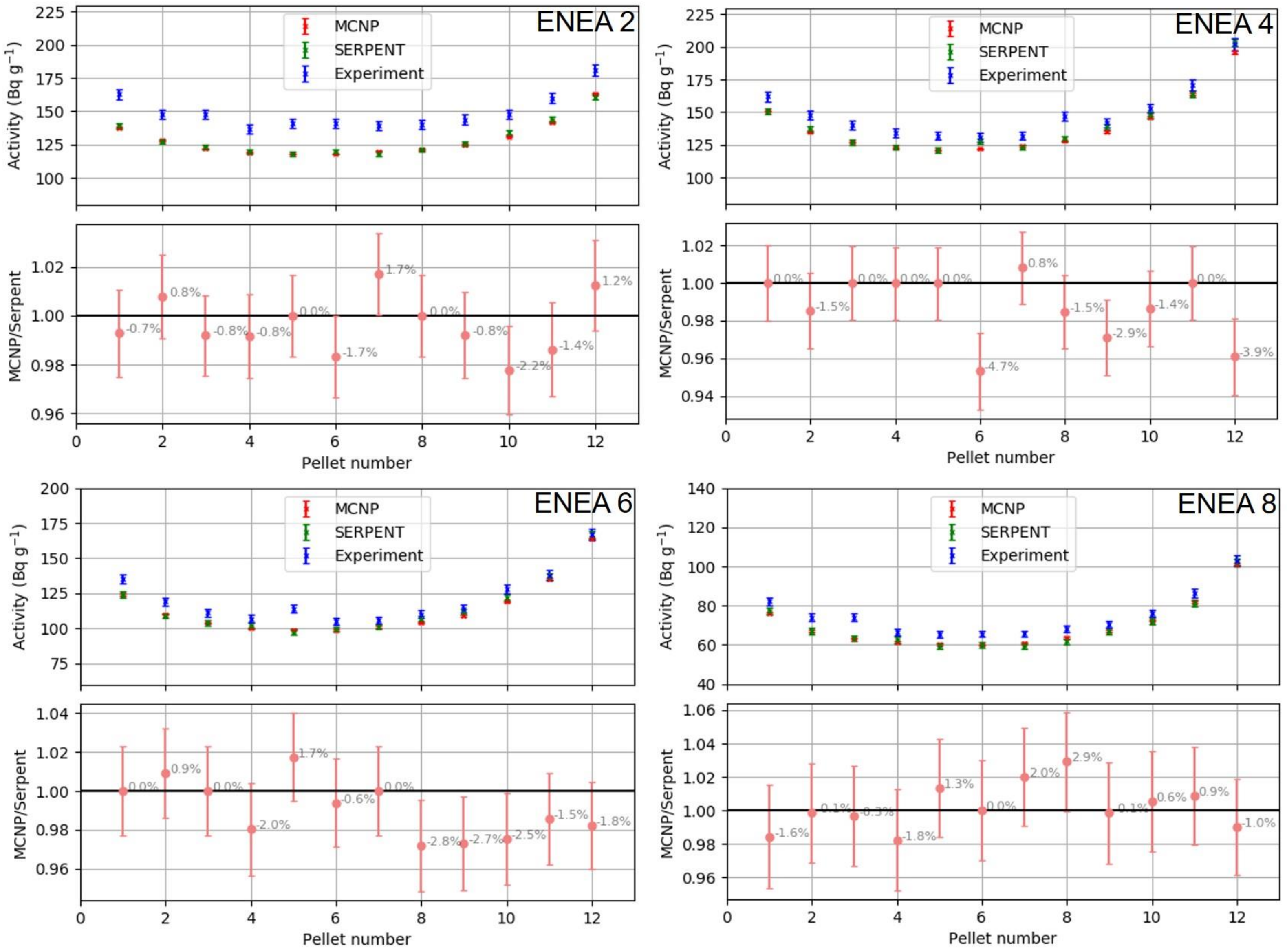


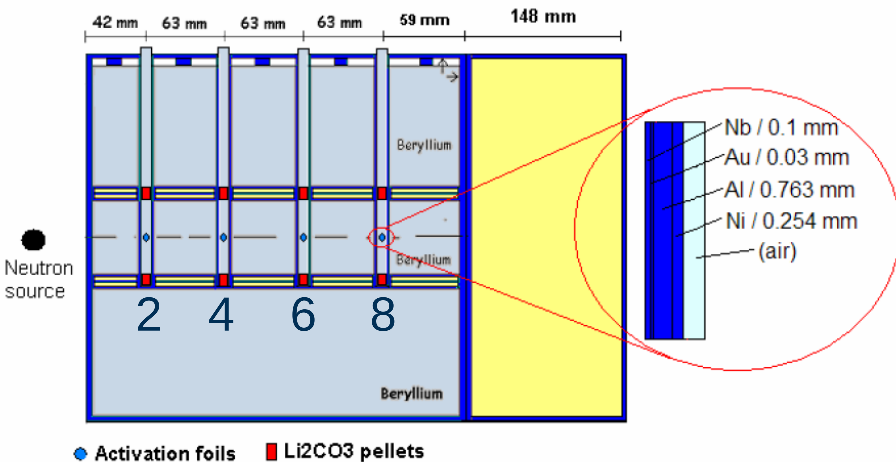


[1] Davis, A., https://github.com/makeclean/csg2csg

Serpent 2 Benchmarking: FNG HCPB mock-up experiment

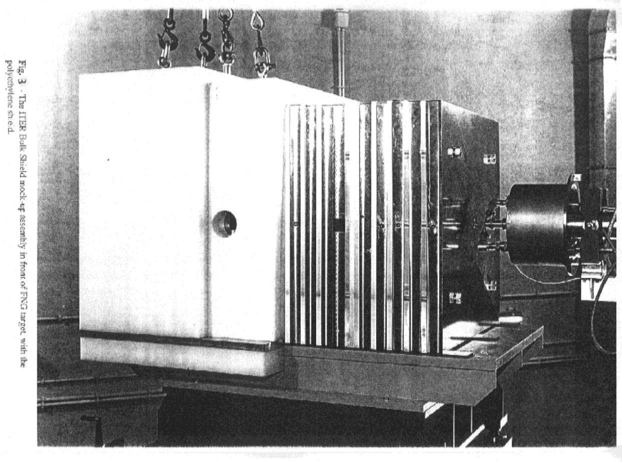
Activity of tritium in Li_2CO_3 pellets

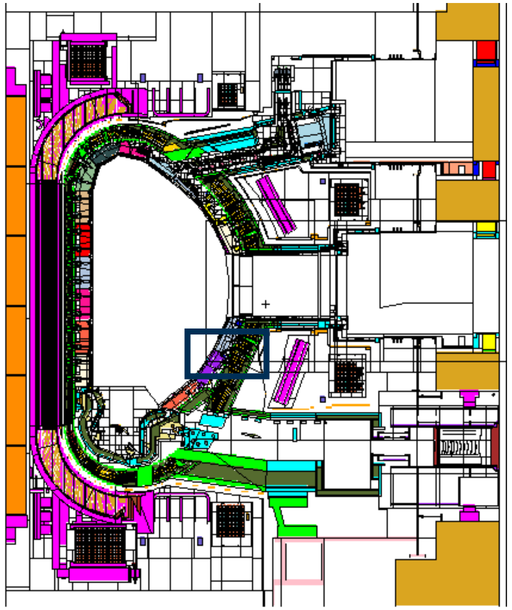




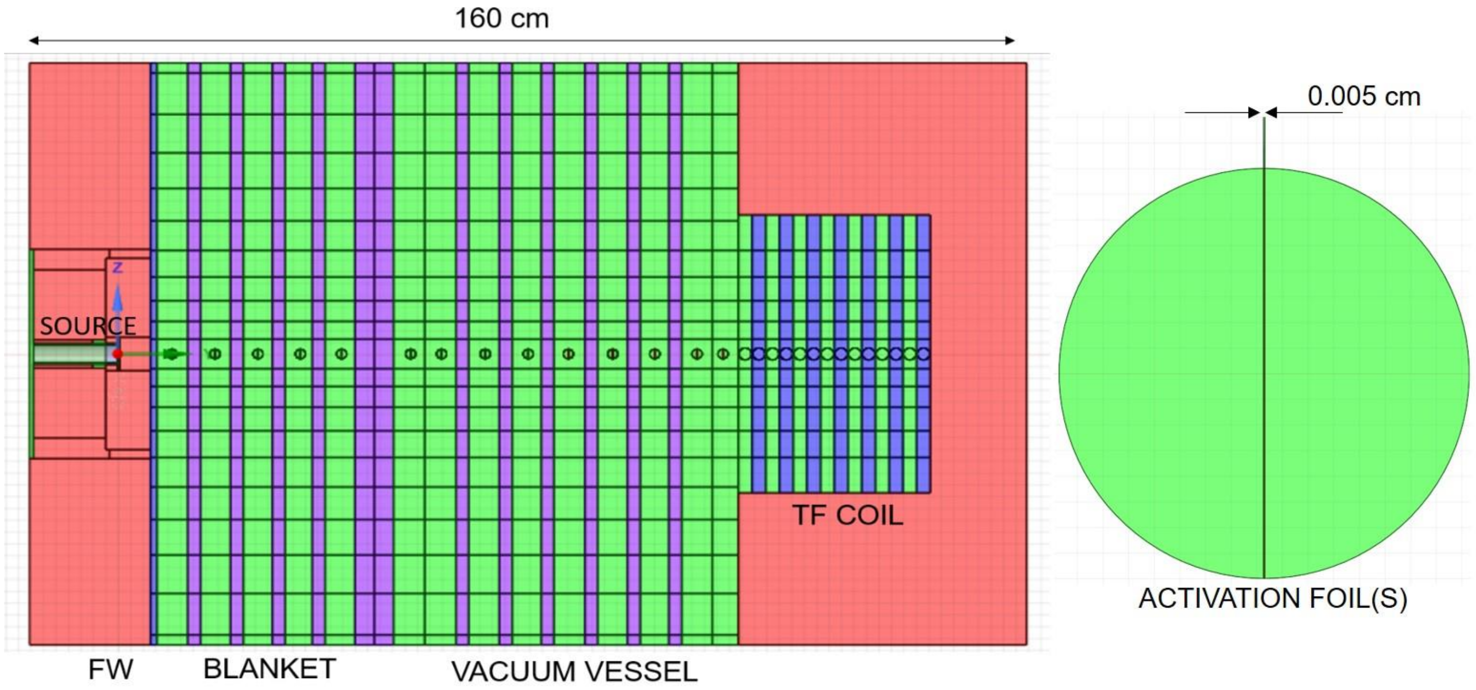
FNG ITER bulk shielding benchmark

SINBAD ABSTRACT NEA-1553/69 *: Mock-up designed in 1995 for validation of ITER in-board shielding. Includes a description of the first wall, blanket, vacuum vessel and the toroidal field coils. Consists of a copper, stainless steel/perpex sandwich, with a smaller block at the rear of the mock-up comprising alternating layers of copper and stainless steel to represent the magnet.*





ITER C-model R181031 MCNP slice at PY=0



ITER bulk shield mock up at PX=0 with activation foils at increasing distance from source

Serpent input file production

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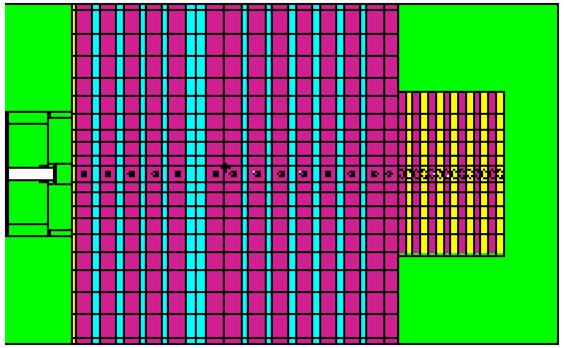
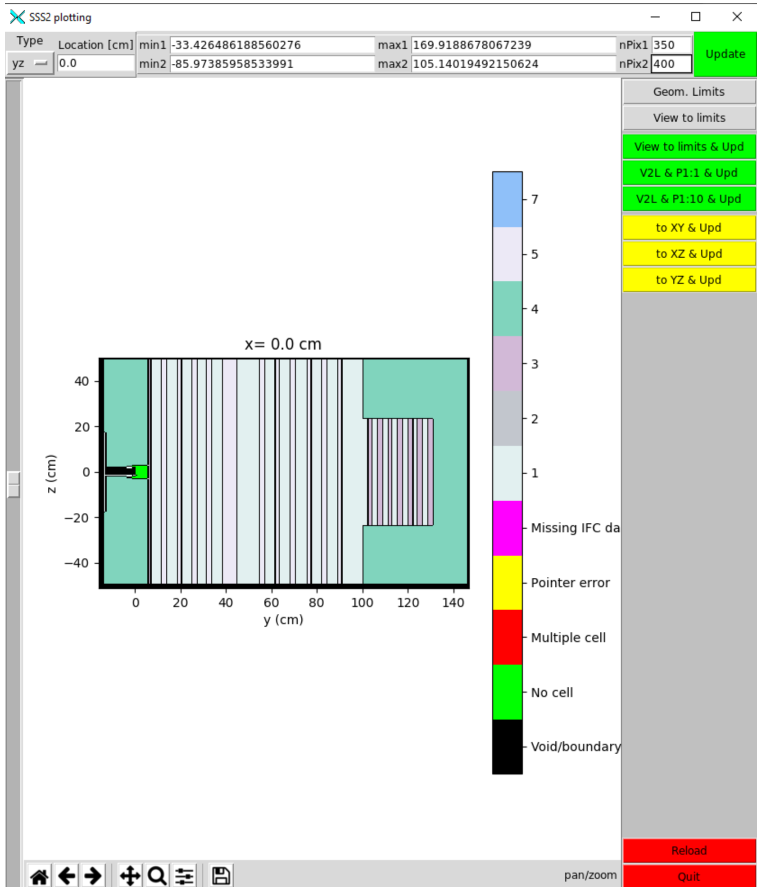


MCNP

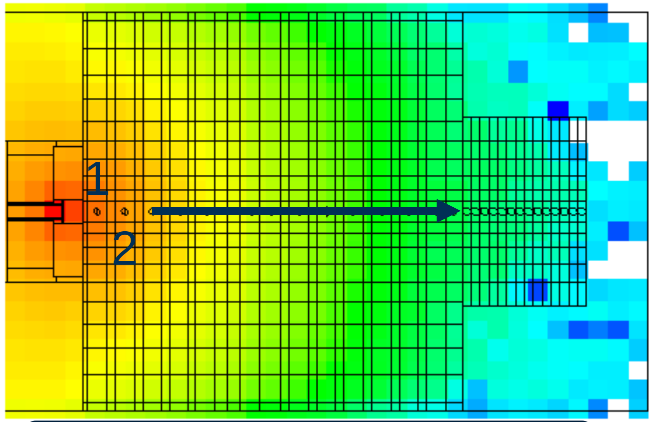
csgcsg



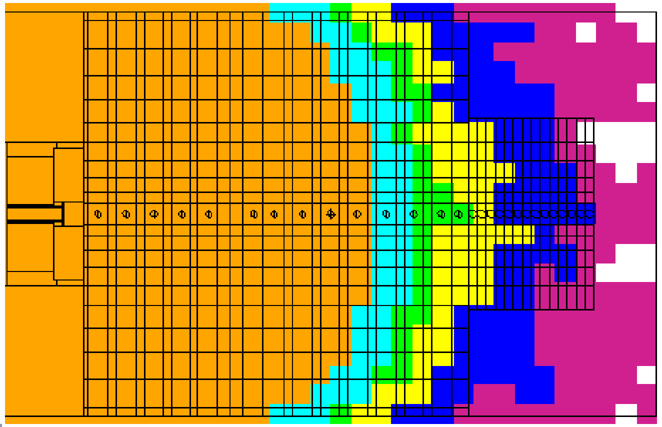
SERPENT

FNG ITER bulk shielding benchmark

- The experimental data is available in the SINBAD database. Activation foils are placed at increasing depth from the source. Reaction rate determined for ^{197}**Au(n,g)**.
- Frascati Neutron Generator (14 MeV neutron source) rewritten in C (native Serpent language).



Analogue transport calculation

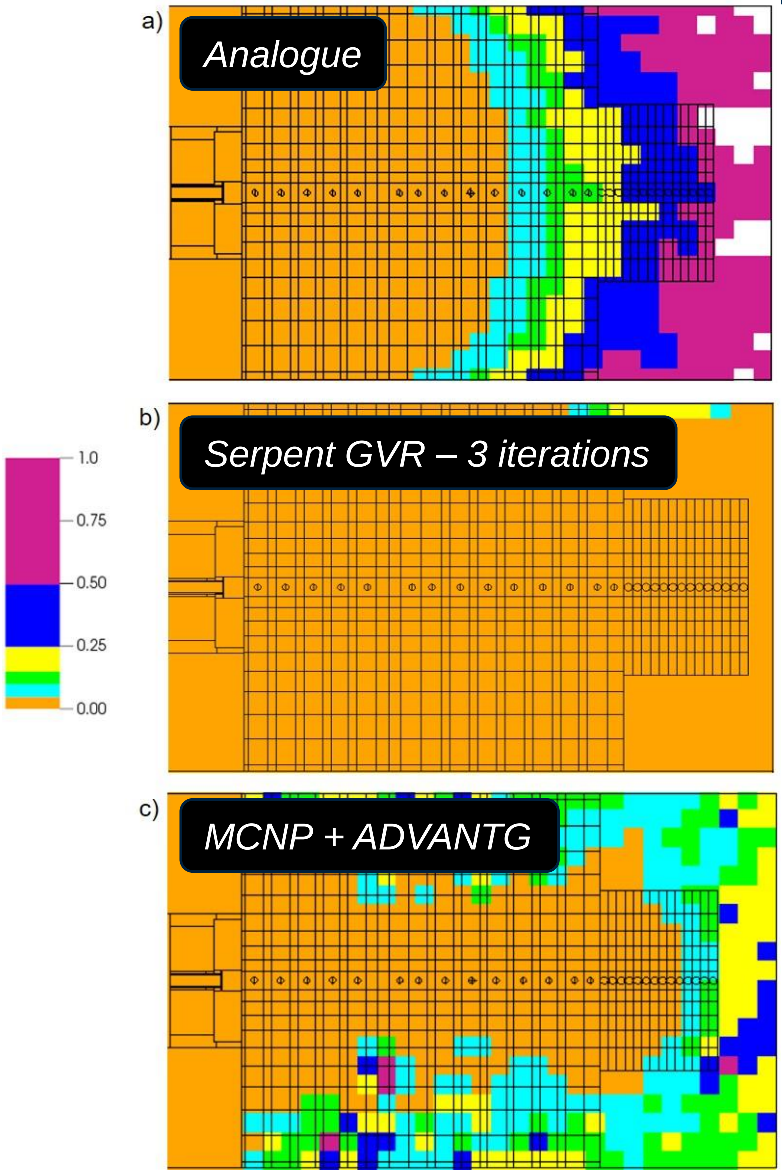


Detector	Depth (cm)	Experiment	Reactions	Error	C/E
1	3.43	6.37E-03	5.97E-03	6.70%	9.38E-01
2	10.32	9.72E-03	9.47E-03	5.22%	9.74E-01
3	17.15	5.50E-03	5.41E-03	6.66%	9.83E-01
4	23.95	2.44E-03	2.62E-03	9.66%	1.07E+00
5	30.8	9.47E-04	7.55E-04	16.8%	7.97E-01
6	41.85	1.65E-04	1.60E-04	31.7%	9.73E-01
7	46.85	6.64E-05	6.60E-05	68.1%	9.93E-01
8	53.8	3.76E-05	5.57E-05	57.0%	1.48E+00
9	60.55	1.71E-05	-	error high	-
10	67.4	6.82E-06	-	error high	-
11	74.4	2.68E-06	-	error high	-
12	81.1	1.12E-06	-	error high	-
13	87.75	3.66E-07	-	error high	-
14	92.15	1.71E-07	-	error high	-

Analogue calculation: 1E8 histories. Only to the 4th detector (from the source) is the relative error reasonably small and the results comparable to experiment

Application of variance reduction

- MCNP has built in methods for weight window generation that can be time consuming. Other methods far more esoteric taking ~days to optimise.
- ADVANTG has become a common method for automation of generating variance reduction (VR) parameters in fusion (complex geometries). Weight window generation is now on the order of hours.
- Serpent uses a Response matrix method-based solver to derive the importance map and in turn generate weight window bounds on a user defined spatial mesh. Proceeds iteratively to populate geometry. Optimised weight window in minutes – hours.
- All above methods were trialled with the FNG ITER bulk shielding mock up. ADVANTG and Serpent weight windows produced in ~2 minutes.
- ADVANTG most effective when specifying single response at rear of the mock up.



Statistical error map on 2 x 2 x 2 cm voxel mesh at PX=0

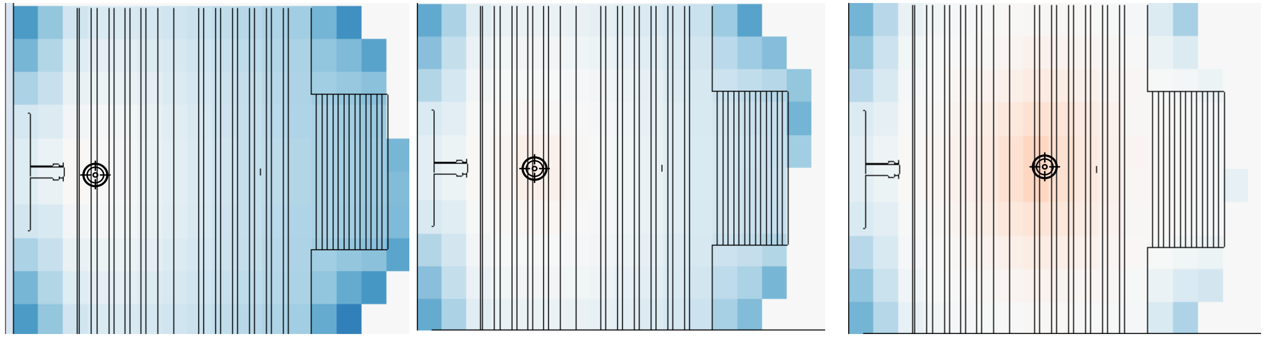
Serpent global and targeted response

- Both global variance reduction (mesh target), GVR, and target of single response is possible in Serpent.
- When targeting specific detectors only the specified response should be considered valid (contributions to other detectors are killed). This method also effective but less so for heavily shielded regions of the mock-up.

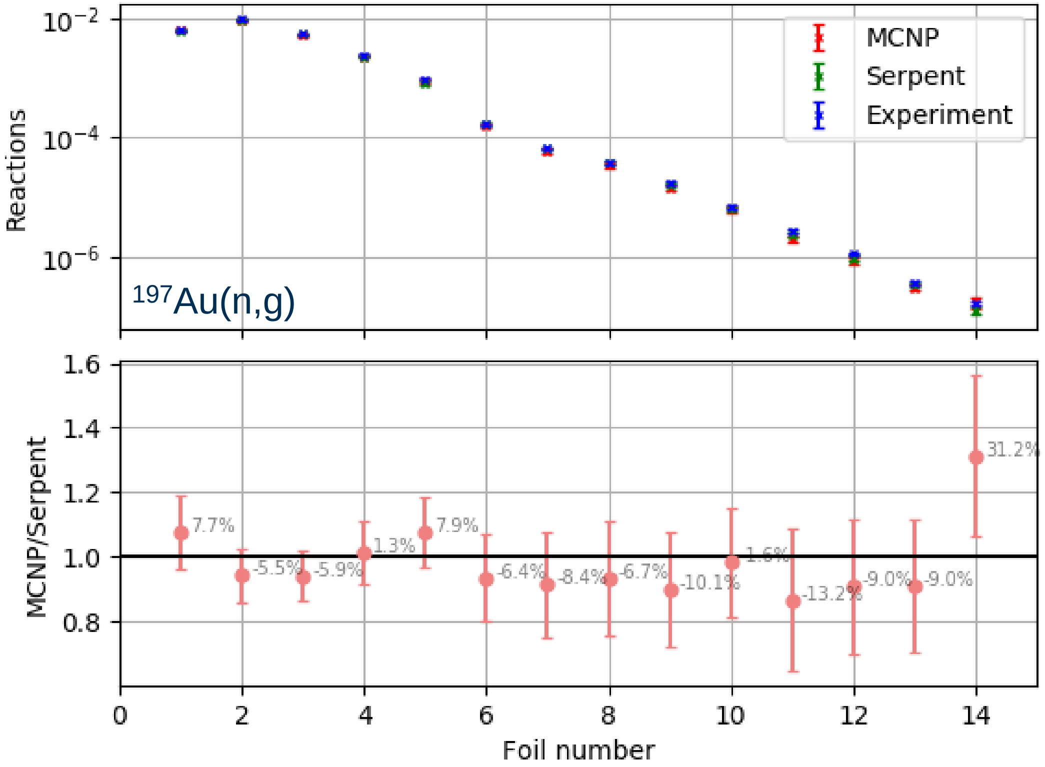
			GVR 3 iterations			Detector 1 target			Detector 5 target			Detector 7 target		
Detector	Depth (cm)	Experiment	Reactions	Error	C/E	Reactions	Error	C/E	Reactions	Error	C/E	Reactions	Error	C/E
1	3.43	6.37E-03	6.11E-03	4.63%	9.59E-01	6.33E-03	4.77%	9.94E-01	6.06E-03	3.19%	9.94E-01	6.51E-03	3.35%	1.02E+00
2	10.32	9.72E-03	9.41E-03	3.56%	9.68E-01	9.71E-03	4.15%	9.99E-01	9.35E-03	2.21%	9.91E-01	9.91E-03	2.54%	1.02E+00
3	17.15	5.50E-03	5.40E-03	3.57%	9.81E-01	5.40E-03	7.63%	9.81E-01	5.29E-03	1.62%	9.53E-01	5.44E-03	2.17%	9.89E-01
4	23.95	2.44E-03	2.24E-03	4.29%	9.17E-01	1.70E-03	22.61%	6.98E-01	2.40E-03	2.29%	9.98E-01	2.31E-03	2.86%	9.46E-01
5	30.8	9.47E-04	8.01E-04	5.30%	8.46E-01	7.67E-04	39.16%	8.10E-01	9.22E-04	4.13%	9.96E-01	9.57E-04	2.27%	1.01E+00
6	41.85	1.65E-04	1.71E-04	6.49%	1.03E+00	0.00E+00	0.00%	0.00E+00	1.98E-04	16.40%	1.02E+00	1.66E-04	2.21%	1.01E+00
7	46.85	6.64E-05	6.51E-05	5.85%	9.81E-01	0.00E+00	0.00%	0.00E+00	2.84E-05	62.60%	1.02E+00	6.30E-05	1.79%	9.49E-01
8	53.8	3.76E-05	3.72E-05	6.35%	9.90E-01	0.00E+00	0.00%	0.00E+00	1.39E-05	93.90%	1.08E+00	3.67E-05	2.35%	9.77E-01
9	60.55	1.71E-05	1.59E-05	6.56%	9.28E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	1.63E-05	4.91%	9.53E-01
10	67.4	6.82E-06	6.36E-06	6.11%	9.33E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	5.78E-06	14.72%	8.47E-01
11	74.4	2.68E-06	2.34E-06	7.21%	8.74E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	1.40E-06	44.97%	5.23E-01
12	81.1	1.12E-06	9.66E-07	7.54%	8.63E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	1.44E-06	55.62%	1.29E+00
13	87.75	3.66E-07	3.35E-07	7.16%	9.14E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00
14	92.15	1.71E-07	1.28E-07	11.46%	7.50E-01	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00	0.00E+00	0.00%	0.00E+00

Reaction rate convergence with VR

- Optimal case for deep shielding is GVR and subsequent targeted response using the statistics achieved ….
- Plots of importance can be automatically generated by Serpent as a useful metric of the effectiveness of the weight window.
- MCNP and Serpent are consistent in under-predicting the experimental results



Plot of neutron importance's for separate weight windows optimised for different foil locations through the ITER bulk shielding mock up



Preparation of CAD models

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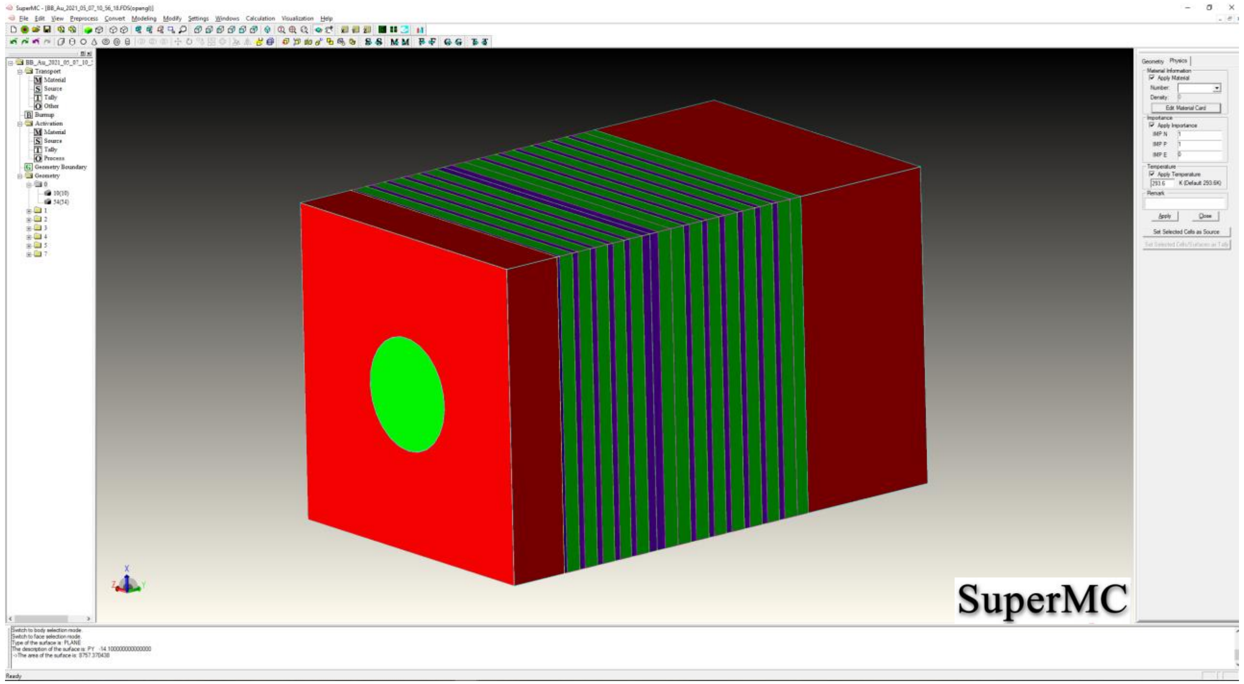
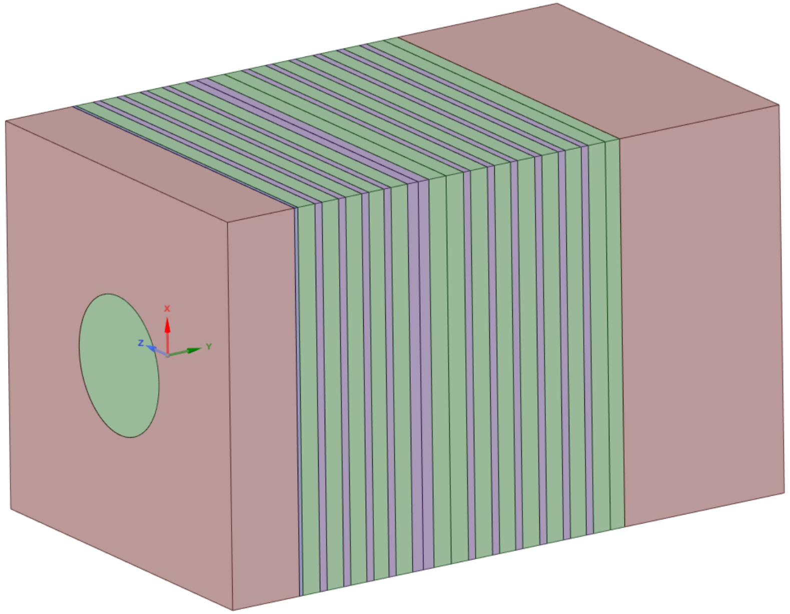
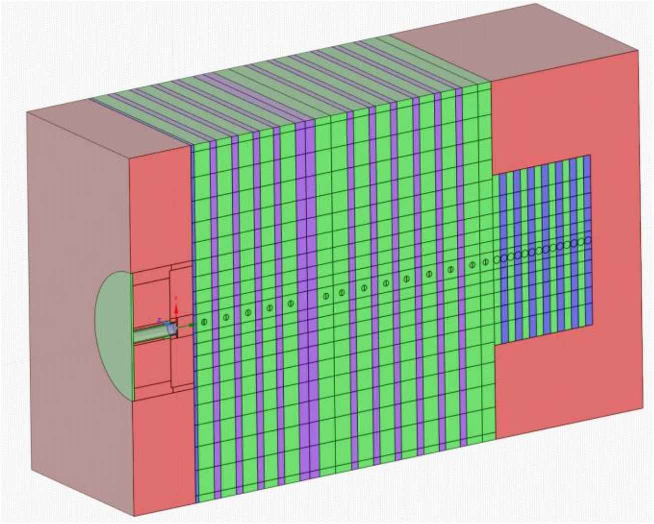
- The CAD model supplements the MCNP model while performing analysis.

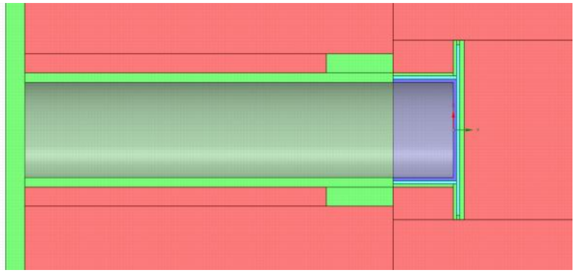
MCNP6 → SuperMC → SPACECLAIM CORPORATION

.sat files









ANSYS SpaceClaim

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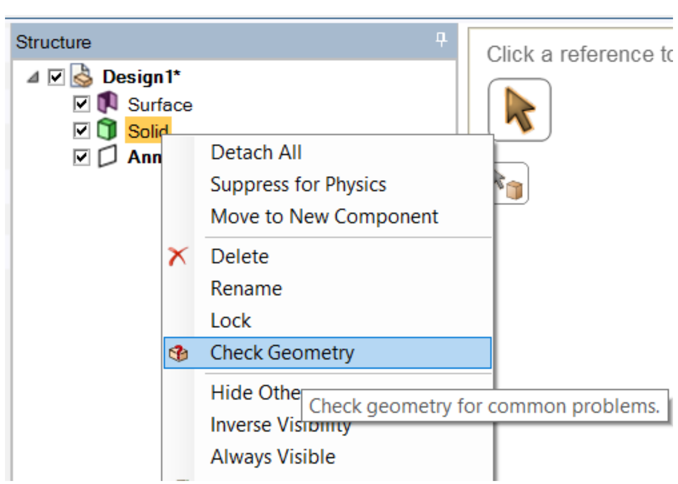
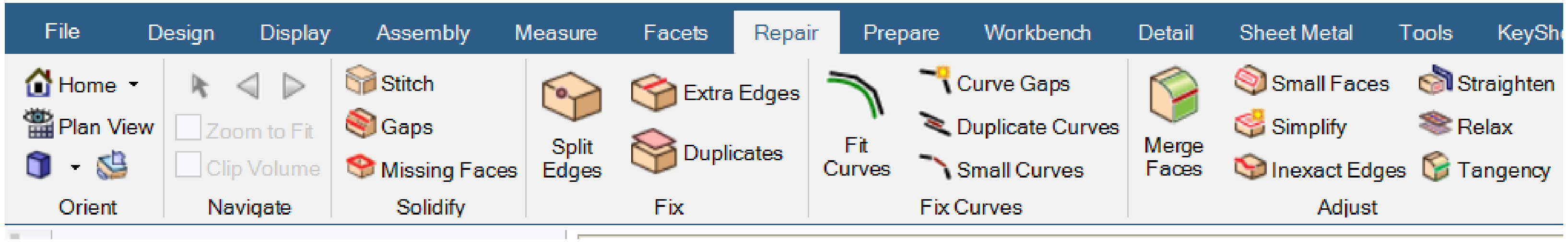
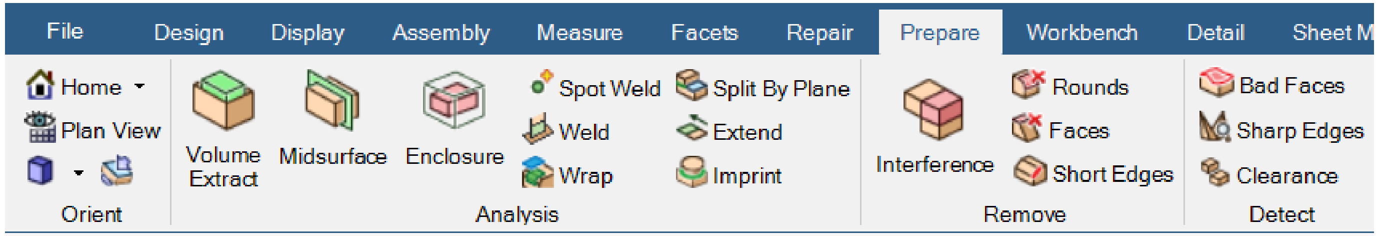
- Preferred CAD modelling software among neutronics community for last ~10 years.
- As well as being highly user friendly, there are some very useful in-built features that are tailored to our needs i.e. preparing a model for conversion to CSG or for import to meshing software.
- Any CAD used as a reference should pass all of these tests to be as clean as possible.

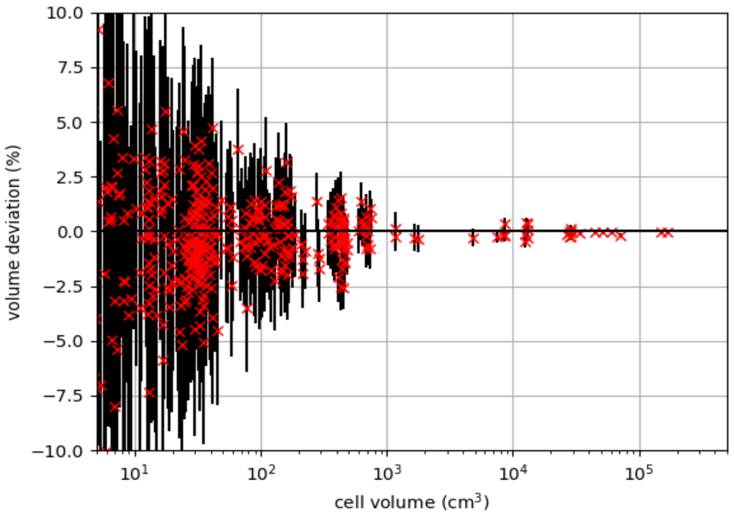




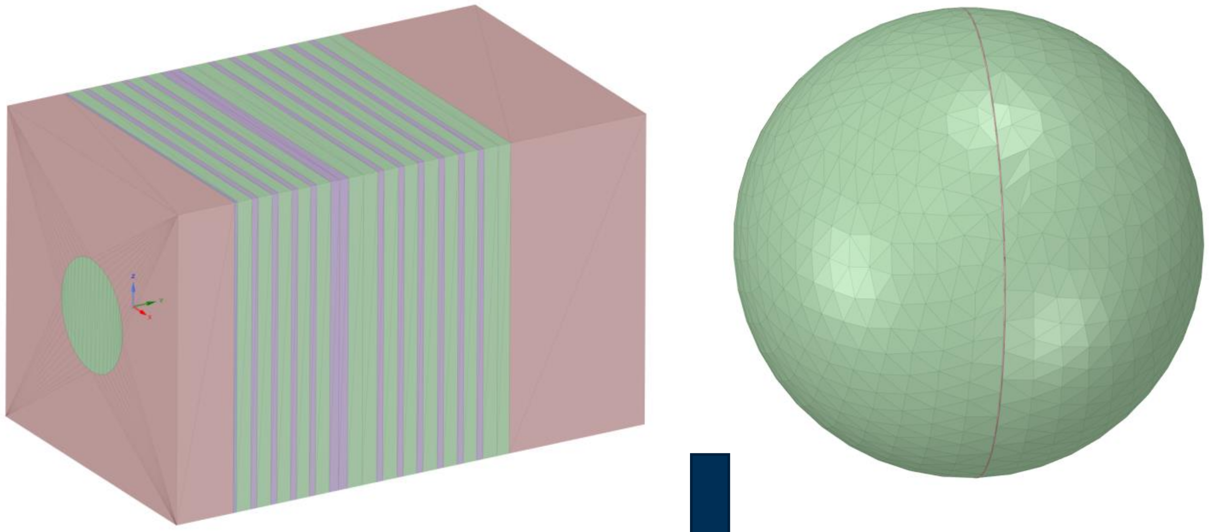


Validation of model and conversion to STL

- From the CAD model, as well as providing a more readable format for the experiment, CAD based particle transport models can be produced. The first step is accurate production of the CAD in suitable file format (.sat, .step etc).
- One example is production of STL files that can be read into Serpent.



All CAD models should include a validation of this form – MC stochastic volume against CAD



Neutron photon transport on STL with weight window in Serpent 2

UKAEA Perspective: Future Benchmarks

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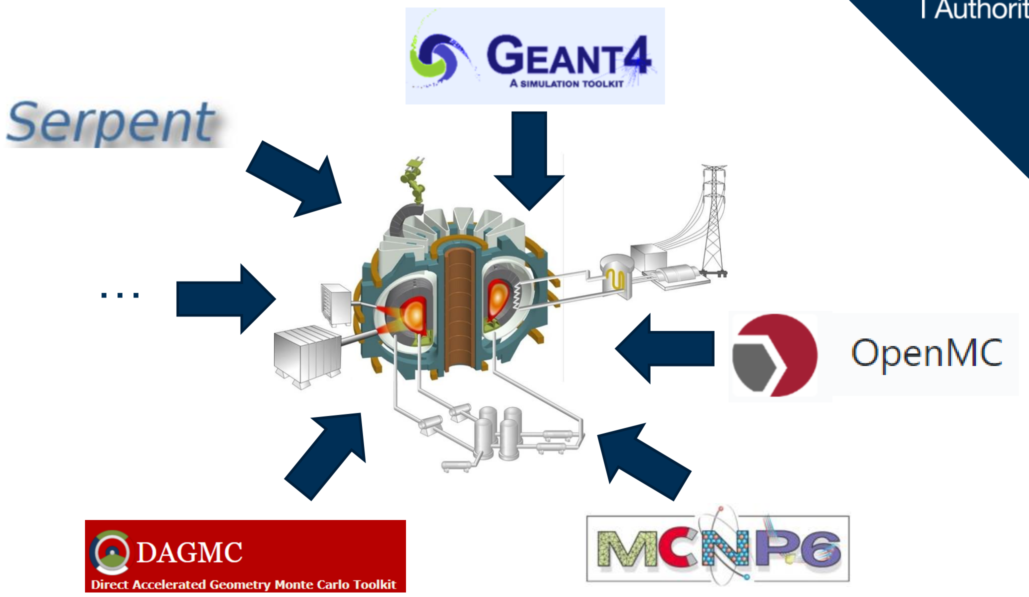
- Government announced £220 million of funding for UKAEA to create a concept design of a spherical tokamak for energy production (STEP).
- This highly ambitious research program draws on the experience of industry and academia in the UK and aims to identify a pathway to supply net energy by the 2040s.
- STEP is first of a kind = Inevitably requires significant R&D, specifically further 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:

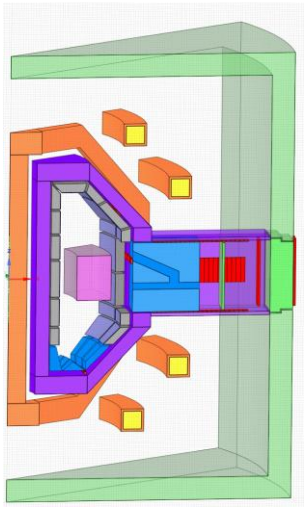
W, Mo, Cr, Y, Ti, C, Zr, Li, Pb, Be, Si, Nb, La, Cu, Fe, Vn

SINBAD for validation of emergent radiation transport codes

- UKAEA neutronics group will be exploring emergent radiation transport codes under core research grant. Licence restrictions, engineering and design requirements has motivated exploration of alternative/complementary codes.
- Interest in SINBAD? Two or three of the benchmarks will be adopted but we also aim to automate a lot of the testing. The automation is heavily reliant on the quality of the available benchmarks.



Computational



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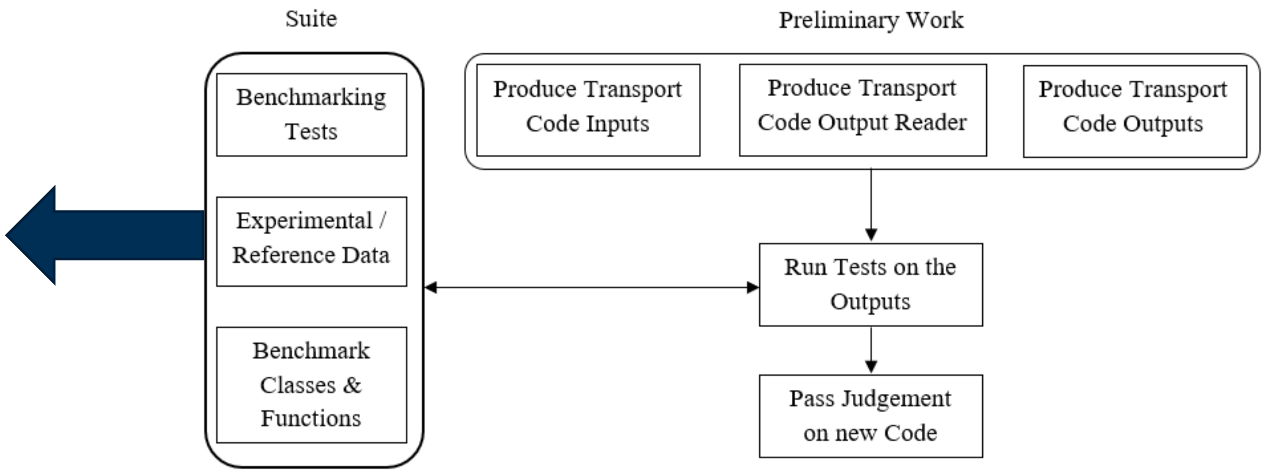
SINBAD

Several quality reviewed experiments depending on application



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

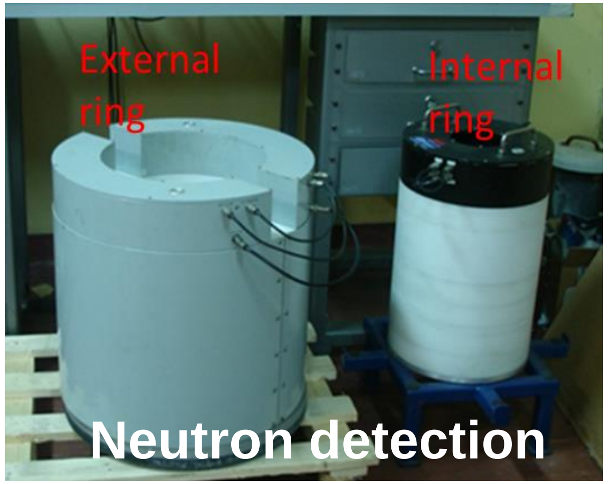
- The collaboration measured ^{16}N and ^{17}N production in water activated by DT neutrons and compared with calculations validate the methodology for water activation assessment.
- The main sources of uncertainty currently being due to modelling and nuclear data, and hence safety factors between 8.2 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), γ (3.7% @ 0.87 MeV).

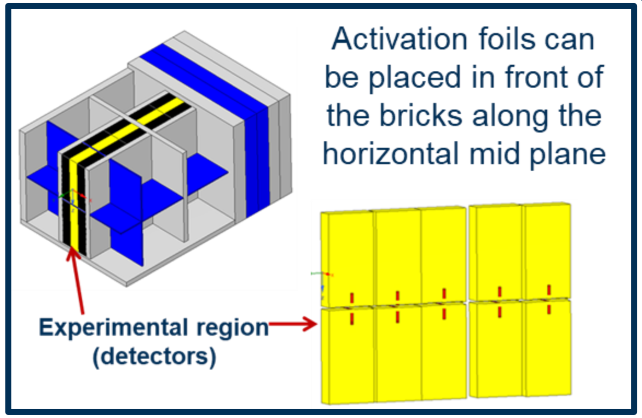
- The results provided good C/E agreement for ^{16}N, and highlighted inconsistencies in the nuclear data for ^{17}N - with a factor of 5 difference for some libraries.
- Fluid activation modelling codes both Actiflow and Gammaflow developed at UKAEA. This continues to identify the requirements of a common fluid activation code for use by the EUROfusion community in ITER and DEMO projects.

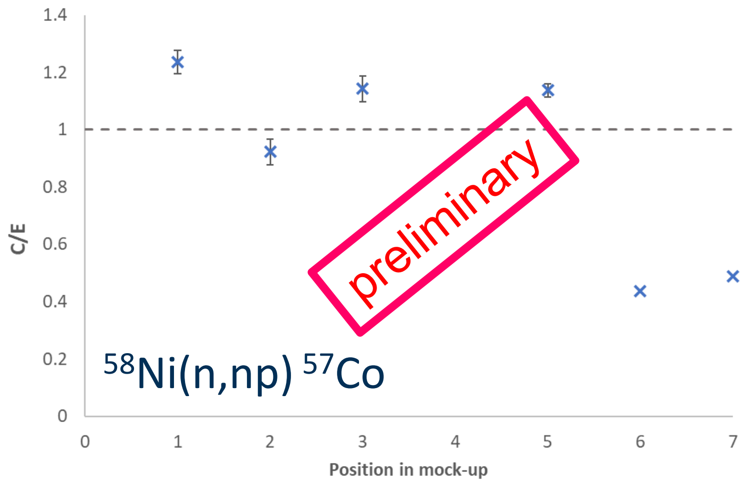
C.R.Nobs, et al., Computational evaluation of N-16 measurements for a 14 MeV neutron irradiation of an ITER first wall component with water circuit, preprint submitted to ISFNT, 2019.

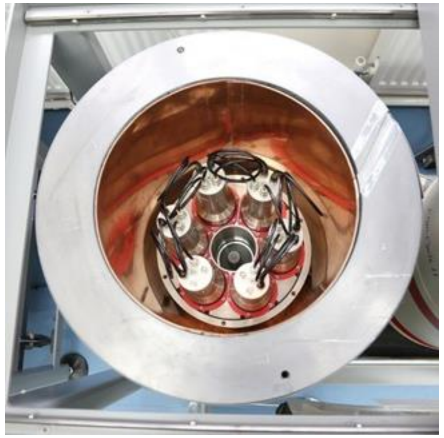


Fusion experiments: Water Cooled Lithium Lead (WCLL) neutronics mock-up experiment

- The nuclear design and performance of breeder blankets fully rely on the results provided by neutronics calculations. This experiment aimed 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.
- The first experimental campaign at ENEA FNG was performed in September 2020 to irradiate activation foils (Ta, Fe, Ni, Y and Sc) embedded at 6 positions throughout the mock-up to monitor the local flux.
- Following irradiation at ENEA FNG, spectroscopy measurements were performed at ADRIANA – UKAEA Gamma Spectroscopy laboratory.
  - Ongoing work this year to understand discrepancies at back positions (6 & 7)
- This experiment will be folded into SINBAD. Uncertainty/sensitivity analysis performed by I.Kodeli







ADRIANA BEGe detector used to measure activation foils

Results expected to be published 2021

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

SINBAD: General comments on status

UK Atomic Energy Authority

Quality

- Recognised that quality review is still required for several benchmarks. For example, several MCNP input decks are not valid and cannot be ran without modification to input file. Transition to GitLab should aid in quality review through pull requests.
- 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. More emphasis needed on calculation side of database.
- HTML format is OK, however may benefit with additional report on the calculational model distributed with each benchmark, particularly if we start to make CAD models available.

Availability

- Benchmarks available through NEA data bank and RSICC. Clear limitations from not being open however tra

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. Same applies to produced CAD models (accompanying pdf files, clear illustrations at multiple slices etc)

Completeness

- There is a lack of solely photon and photonuclear benchmarks
- Neutron and photon heating benchmarks are also of high relevance in fusion and should be a priority
- Many of the older benchmarks are not distributed with MCNP models
- Other Monte Carlo inputs to be included as well as CAD model?

Conclusions

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- The SINBAD database provides valuable experimental data used in validation of nuclear data and benchmarking of radiation transport codes.
- UKAEA have used several of the benchmarks as part of investigations into Serpent 2 Monte Carlo code for fusion applications. This years' activities have demonstrated a robust new workflow with its in built variance reduction scheme.
- 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 may be part of dedicated shielding mock ups which will be critical to current design phase fusion reactors such as STEP.
- Ongoing efforts in benchmarking emergent radiation transport codes will seek to automate much of the available data. This relies on quality and clarity in the database.

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Thank you for listening

Alex.Valentine@ukaea.uk

Back Slides

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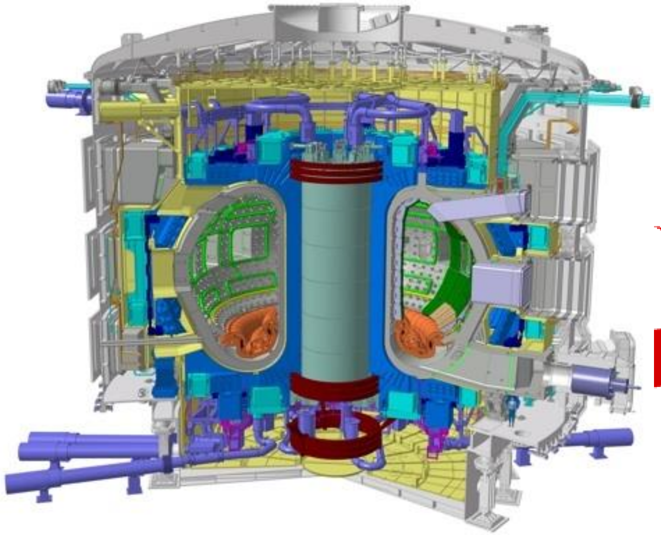
Goals on the path to delivering fusion power

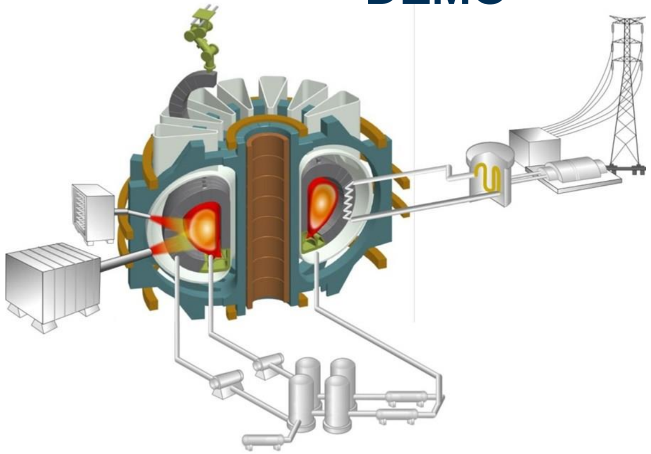
UK Atomic Energy Authority

ITER



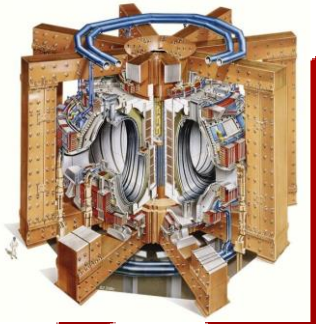
Enable the delivery of sustainable fusion power plants

DEMO

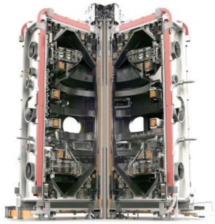


Be a world leader in fusion research and development

JET



MAST-U



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

STEP

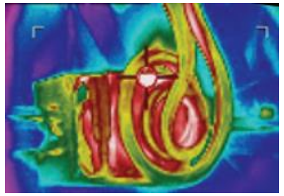
Create places that accelerate innovation and develop skilled people for industry to thrive

OAS

RACE

MRF

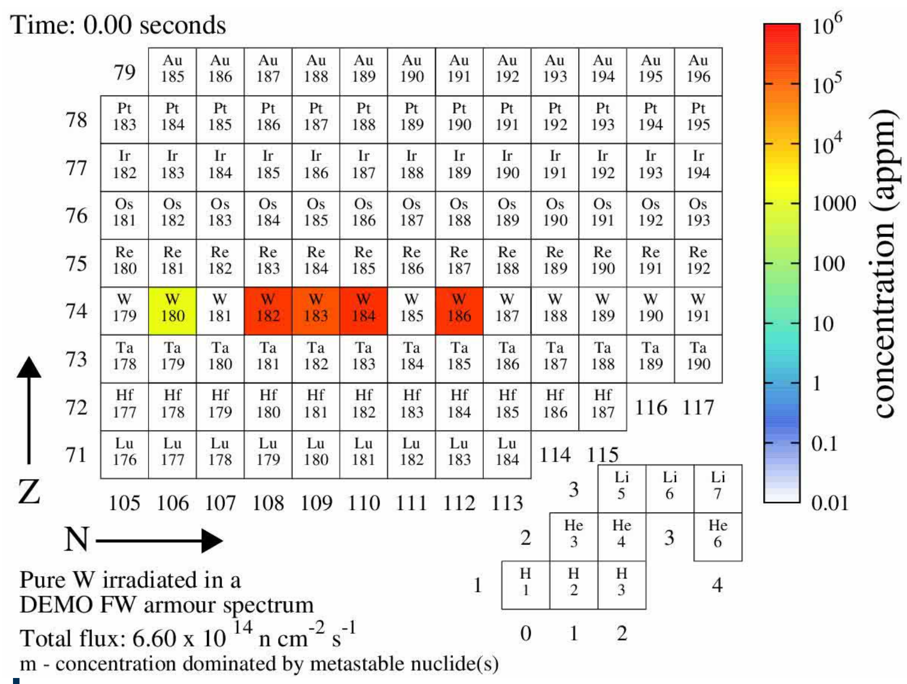
H3AT

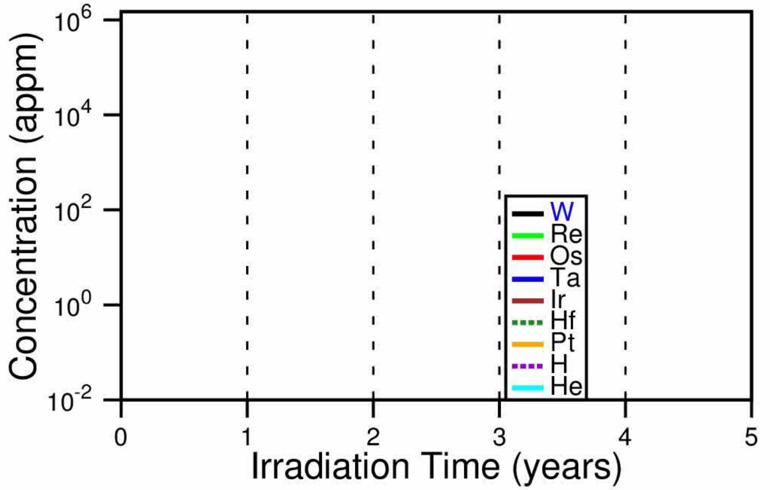


FTF

Nuclear 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