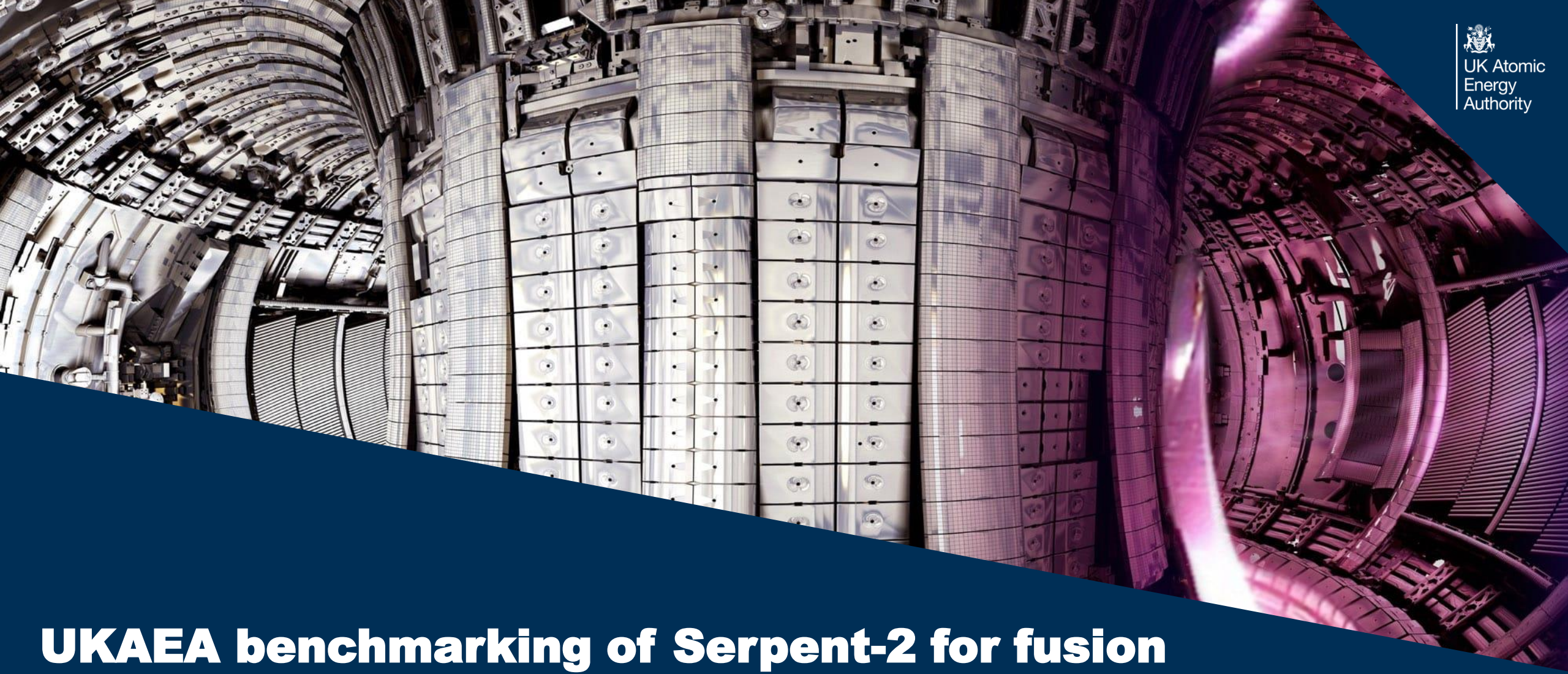


UK Atomic Energy Authority

UKAEA benchmarking of Serpent-2 for fusion neutronics applications

Serpent User Group Meeting 2020, held virtually.

Alex Valentine

Contents

1. UKAEA organisation overview
2. Summary of Serpent benchmarking at UKAEA
3. Variance reduction in fusion neutronics
4. Variance reduction in Serpent 2
5. FNG Bulk Shielding Benchmark – Application of VR and results
6. DEMO HCPB benchmark – Application of VR and results
7. Summary and outlook for future work

UK Atomic Energy Authority

RACE

CCFE CULHAM CENTRE FOR FUSION ENERGY

MATERIALS RESEARCH FACILITY

AS

UK Atomic Energy Authority

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

Applied Radiation Technology group (Neutronics)

UK Atomic Energy Authority

FISPACT-II

SPACECLAIM CORPORATION

MCNP6

SuperMC

visit

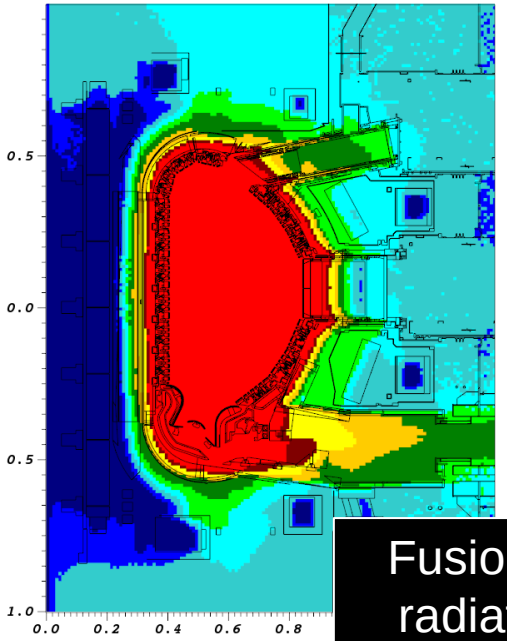
OpenMC

DAGMC

McCad

Serpent

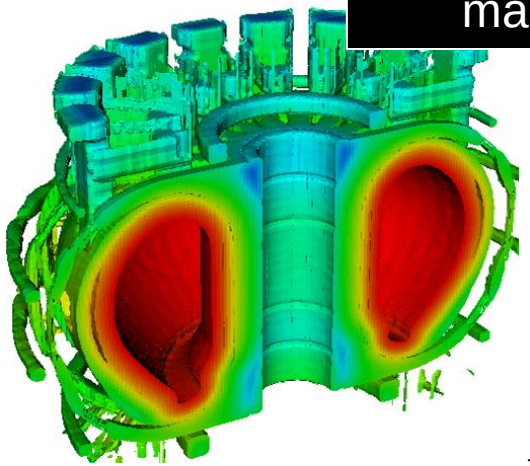
OAK RIDGE National Laboratory



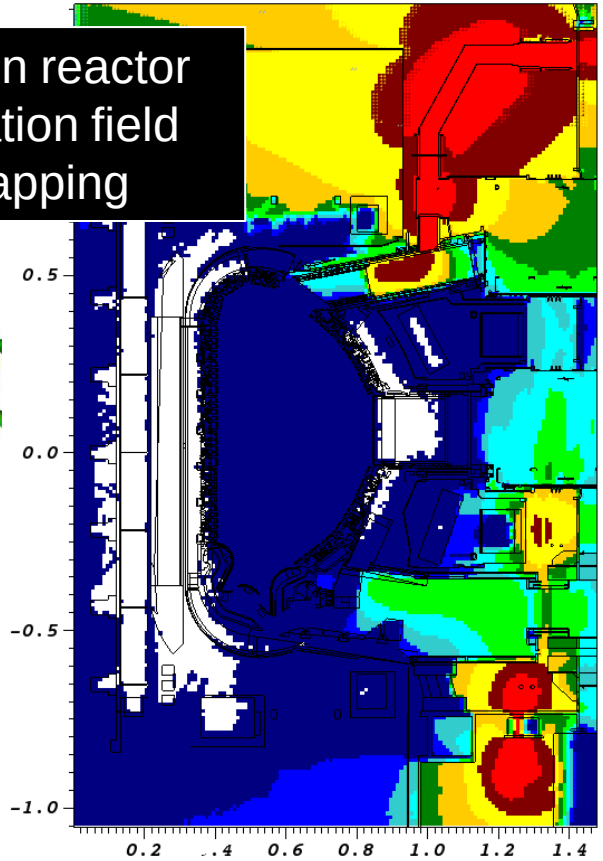
Plasma Source

ITER

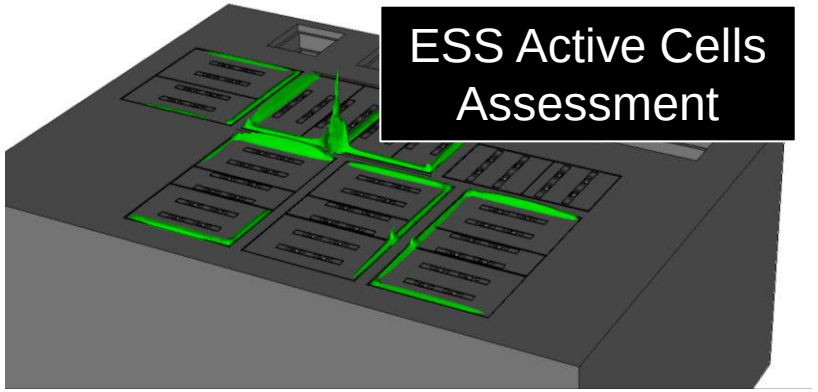
Fusion reactor radiation field mapping



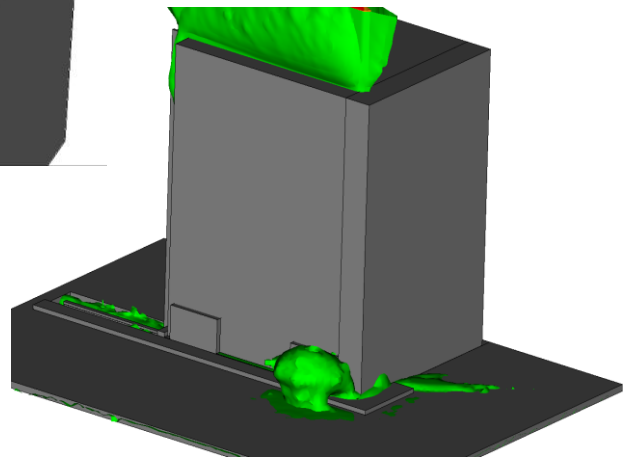
EU DEMO



Cooling Water System Source



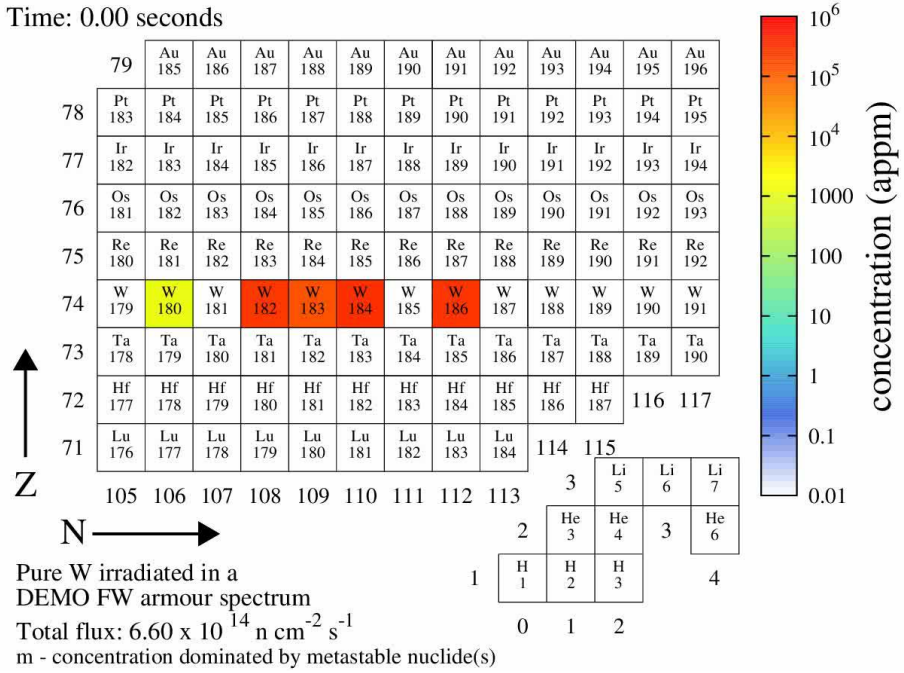
ESS Active Cells Assessment

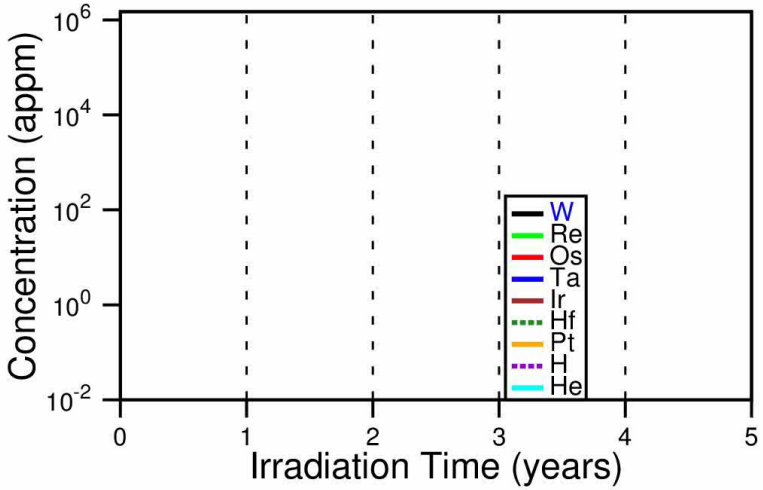


Hot Cell commissioning

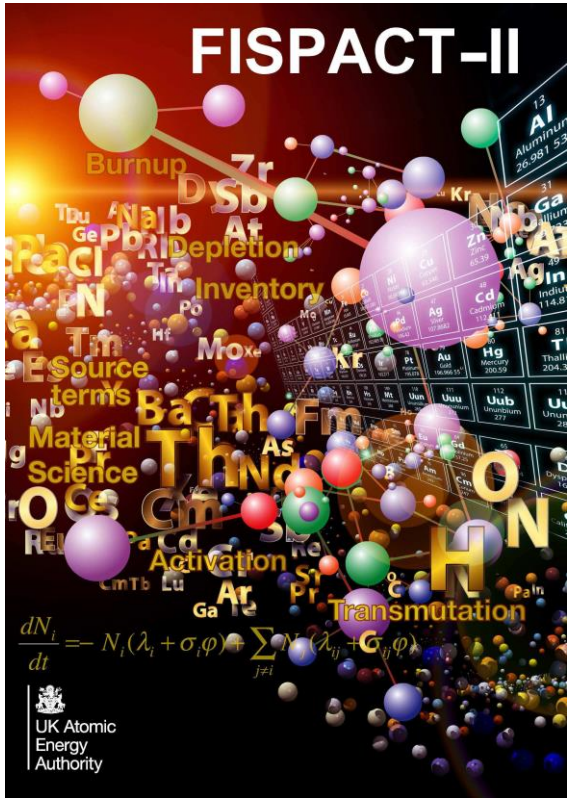
Nuclear Inventory Simulation

- 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



Neutronics workflow

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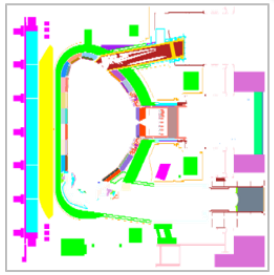
Neutronics model

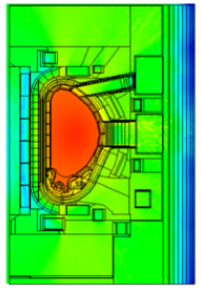


CAD conversion

ANSYS SpaceClaim

FDS SuperMC

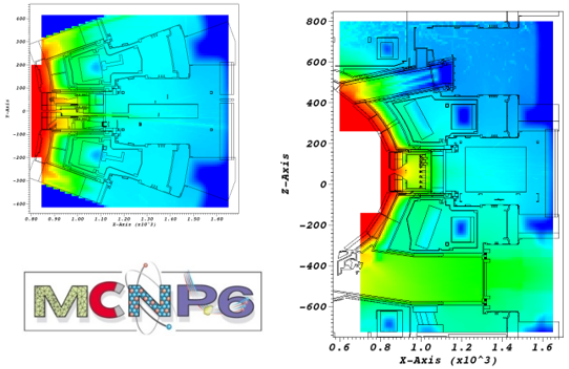
Global variance reduction (GVR)



WWITER

ADVANTG

Oak Ridge National Laboratory



MCNP6

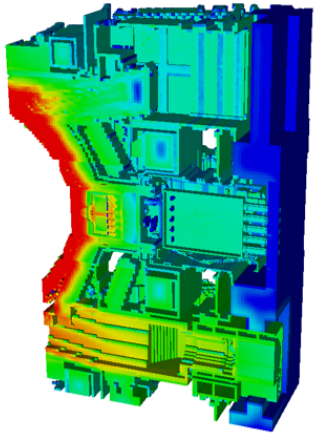
Coupled neutron-photon transport with GVR

Secondary responses:

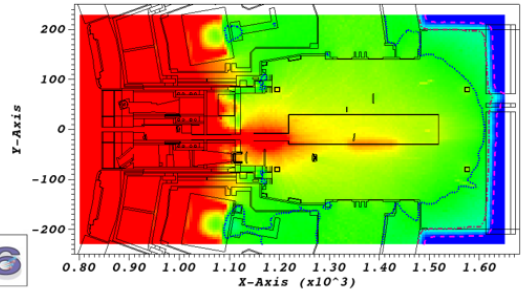
- Nuclide inventory
- Radioactive waste
- Shutdown dose rates

MCR2S

Decay gamma source from MCR2S



Photon Transport (SDDR)

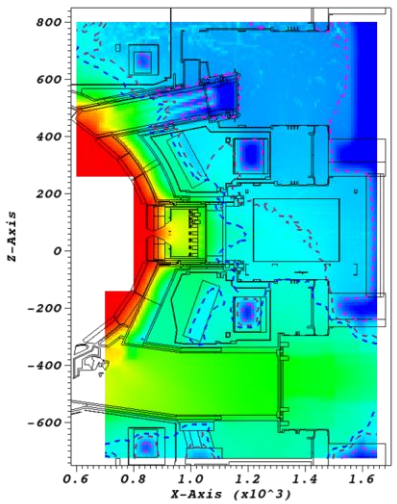


MCNP6

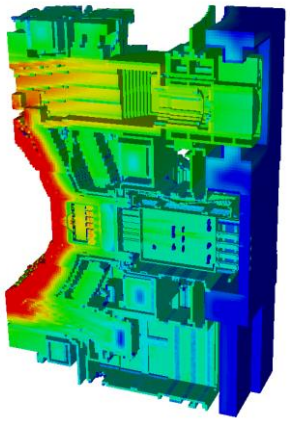
Primary responses:

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

Integration of Serpent with MCR2S

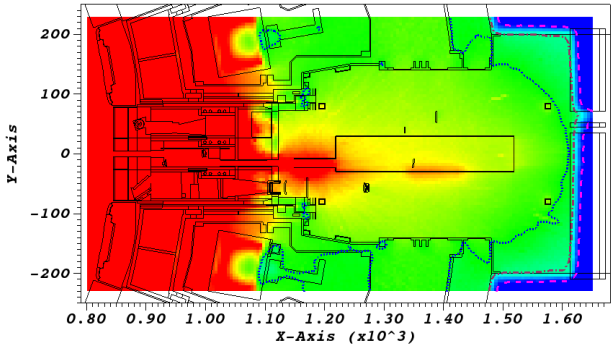


Neutron Flux

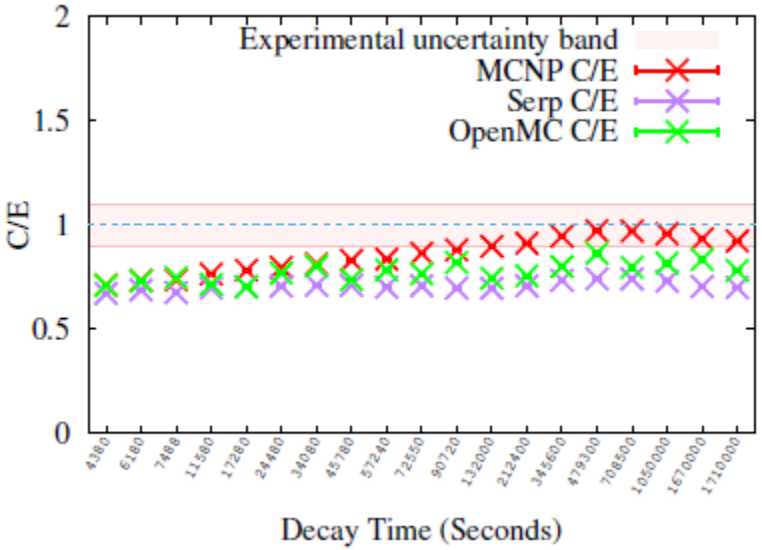


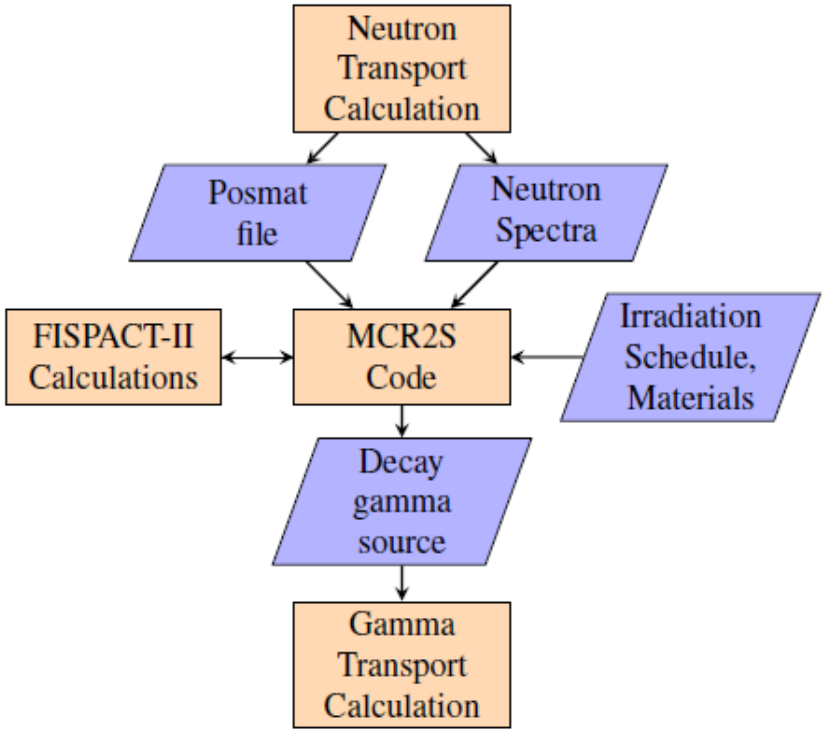
Gamma Source

Shutdown Dose



- Inventory analysis (FISPACT-II)
- MCR2S couples shutdown inventory with space and time
- Full 3D activation and shutdown dose analysis tool
- Serpent 2 now fully integrated in to MCR2S for





T. Eade et al 2020 Nucl. Fusion 60 056024
https://iopscience.iop.org/article/10.1088/1741-4326/ab8181/meta

Fusion neutronics: Requirements

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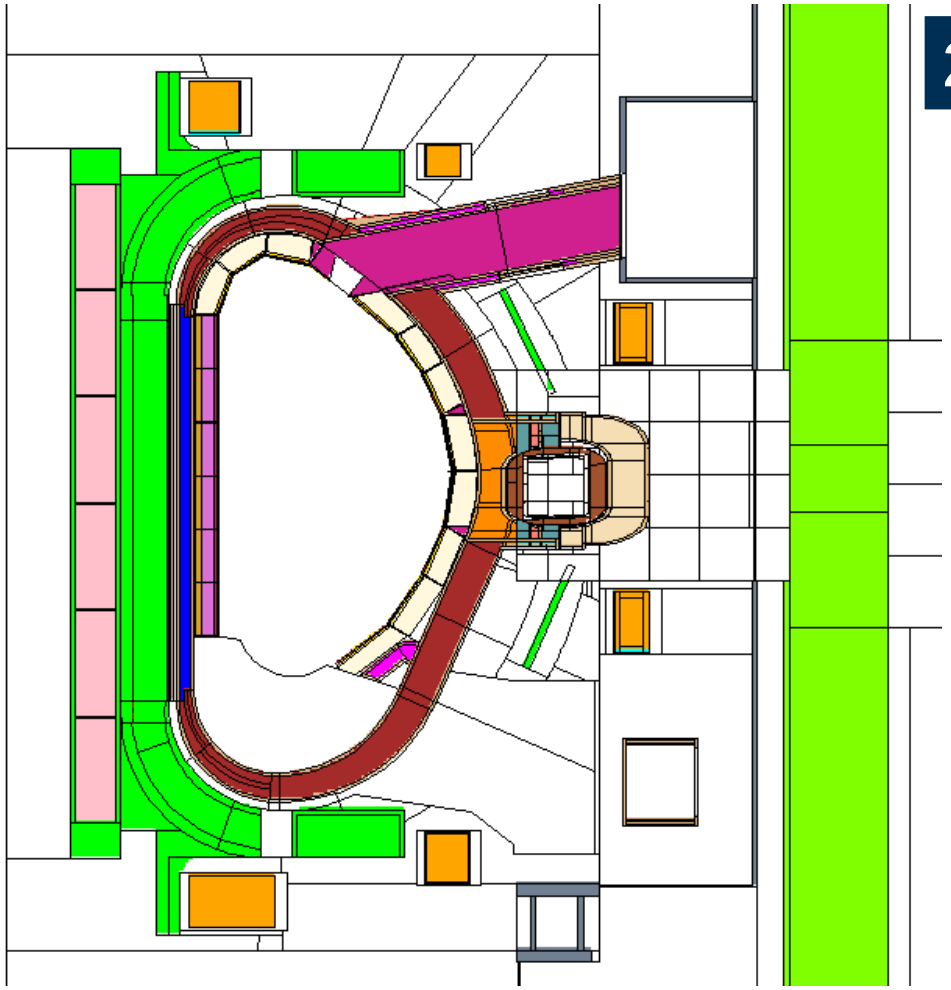
- There are several requirements for a new code to be used for this application and be adopted by the wider neutronics community
  - Capable of performing both neutron and photon transport coupled transport using point wise cross section libraries.
    - ✓ Photon mode in 2015 and coupled transport ~2017 in E range 1 keV to 100 MeV
  - Geometric representation of the model in all its complexity
    - ✓ CSG geometry and STL capability ~2014
  - Parallelisation capability of deployment on HPC architectures
    - ✓ Support for MPI and OpenMP as well as hybrid approach
  - Accommodate plasma neutron source definitions
    - ✓ User defined sources easily defined and called
  - Capable of employing acceleration techniques
    - ✓ Variance reduction
  - Validated for this application!

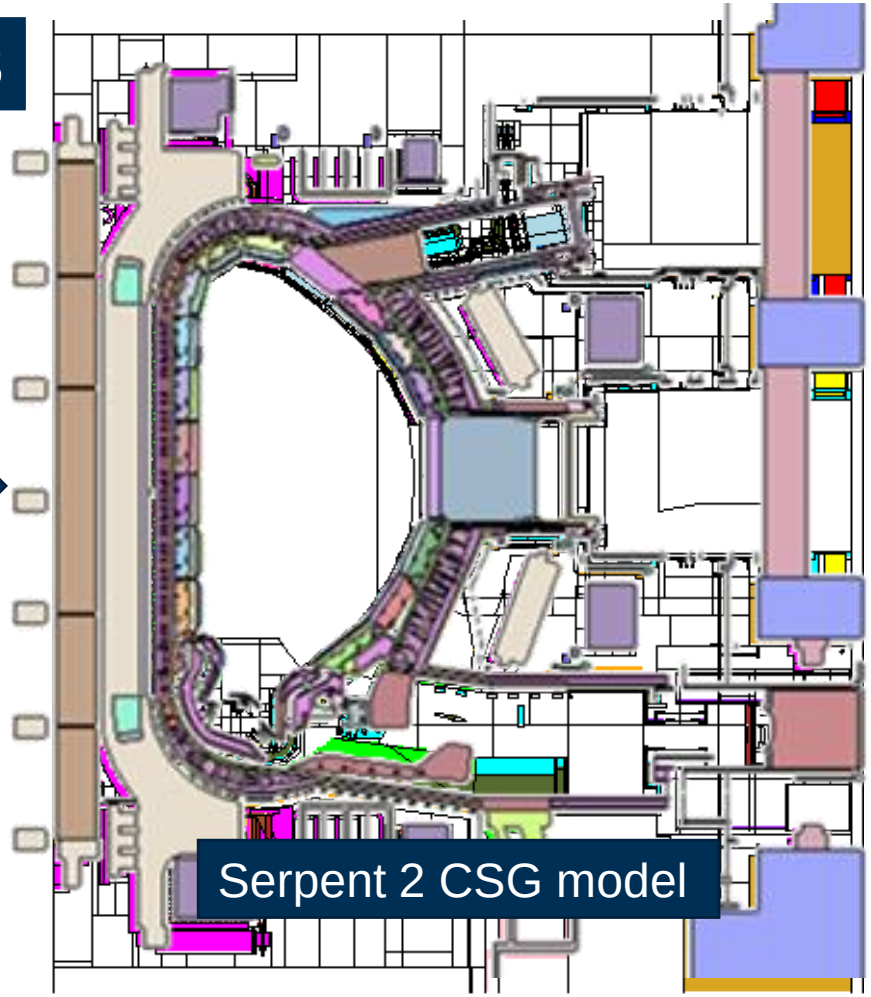
Fusion neutronics: Stretching the geometrical capabilities of MCNP

2011



A-lite Neutral Beam sector

2018



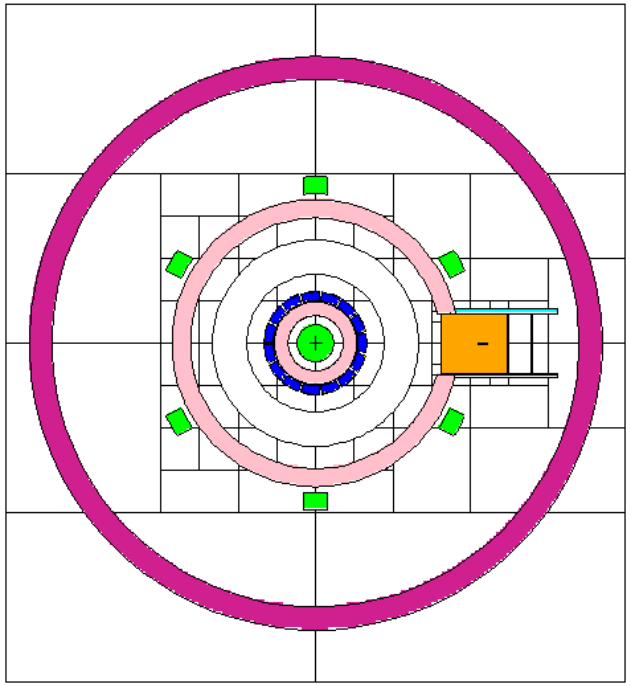
C-model R181031

- *Cells= 114,285*

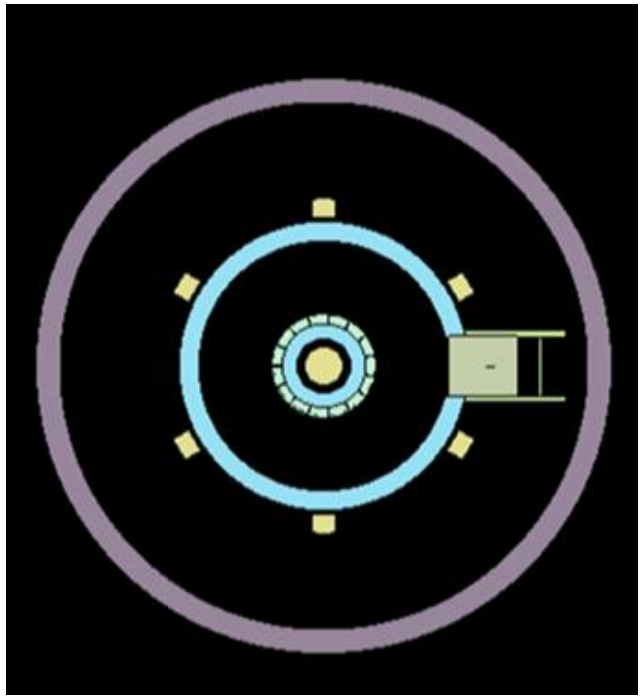
Serpent 2 tool development

- Python neutronics toolkit
  - Serpent 2 output reader (tally post-processing and plotting) and converter to VTK format
  - MCNP to Serpent 2 conversion tool
- ‘csg2csg’ (https://github.com/makeclean/csg2csg). All models presented e
  - Python scripts, supporting conversion of MCNP files to Serpent, OpenMC, Fluka and PHITS

MCNP



Serpent



Serpent 2 Benchmarking: Summary

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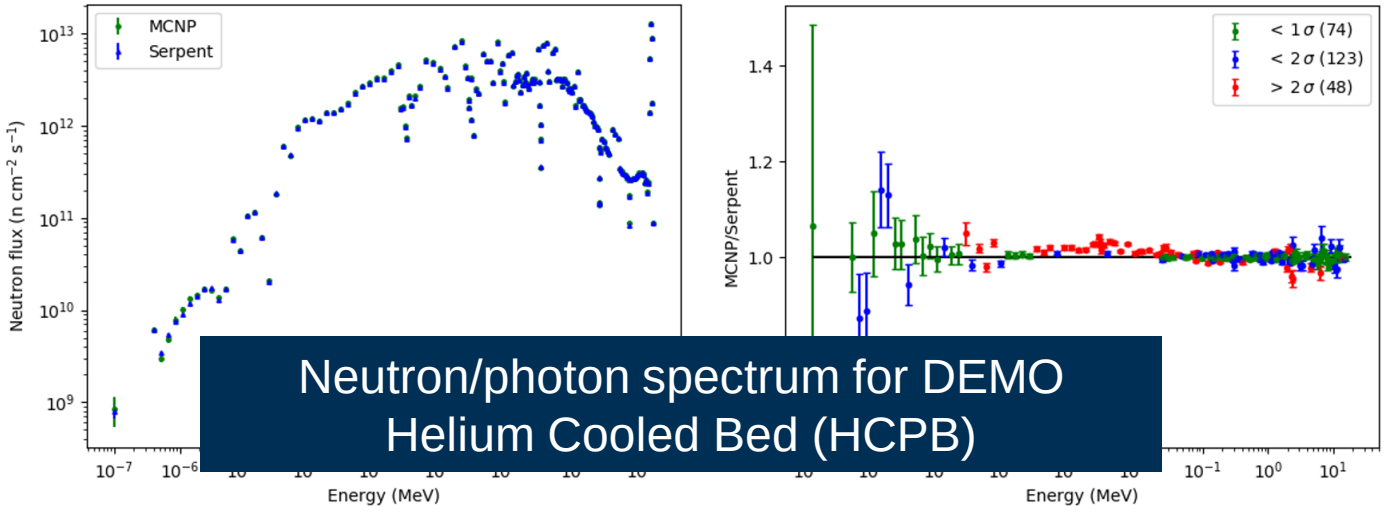
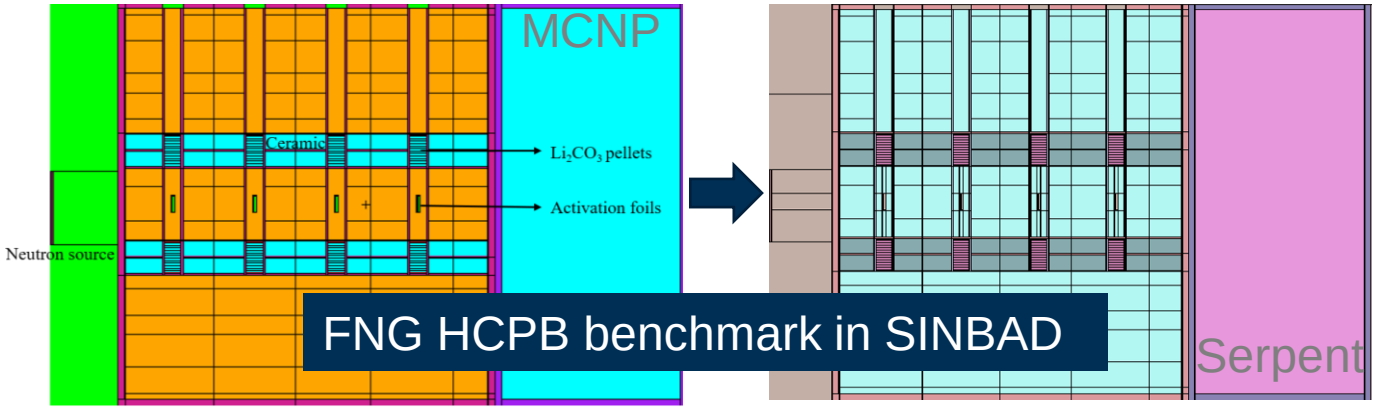
- UKAEA started looking into Serpent for fusion applications ~5 years ago.
- In this time, 3 EUROfusion reports have been produced documenting the various benchmarking activities.
- Other Serpent related activities: Serpent benchmarking has been reported at the past two WPEC meetings hosted by the NEA. This is the fourth SUGM attended by UKAEA. In Oct.2019, A Valentine and R.Worrall visited VTT for one week. Serpent was also presented at the ITER neutronics meeting in 2017.
- The tasks have focussed on:
  - Benchmarks available in SINBAD relevant to fusion neutronics
  - Geometry definitions: Translation of MCNP models to Serpent using available tools
  - Producing relevant source terms: 14 MeV neutron generators or plasma sources.
  - Performing calculation and comparing results against MCNP calculations. For SINBAD benchmarks comparison is possible against experimental data. For Tokamak reactor models, benchmarking has focussed on typical nuclear responses including **neutron/photon flux, tritium production rate** (TPR), **displacements per atom** (dpa) and the neutron/ photon **nuclear heating**
- A paper was published in the proceedings of PHYSOR 2020 : Valentine, A., et al. Benchmarking of the Serpent 2 Monte-Carlo code for fusion neutronics applications.

Serpent task 2020

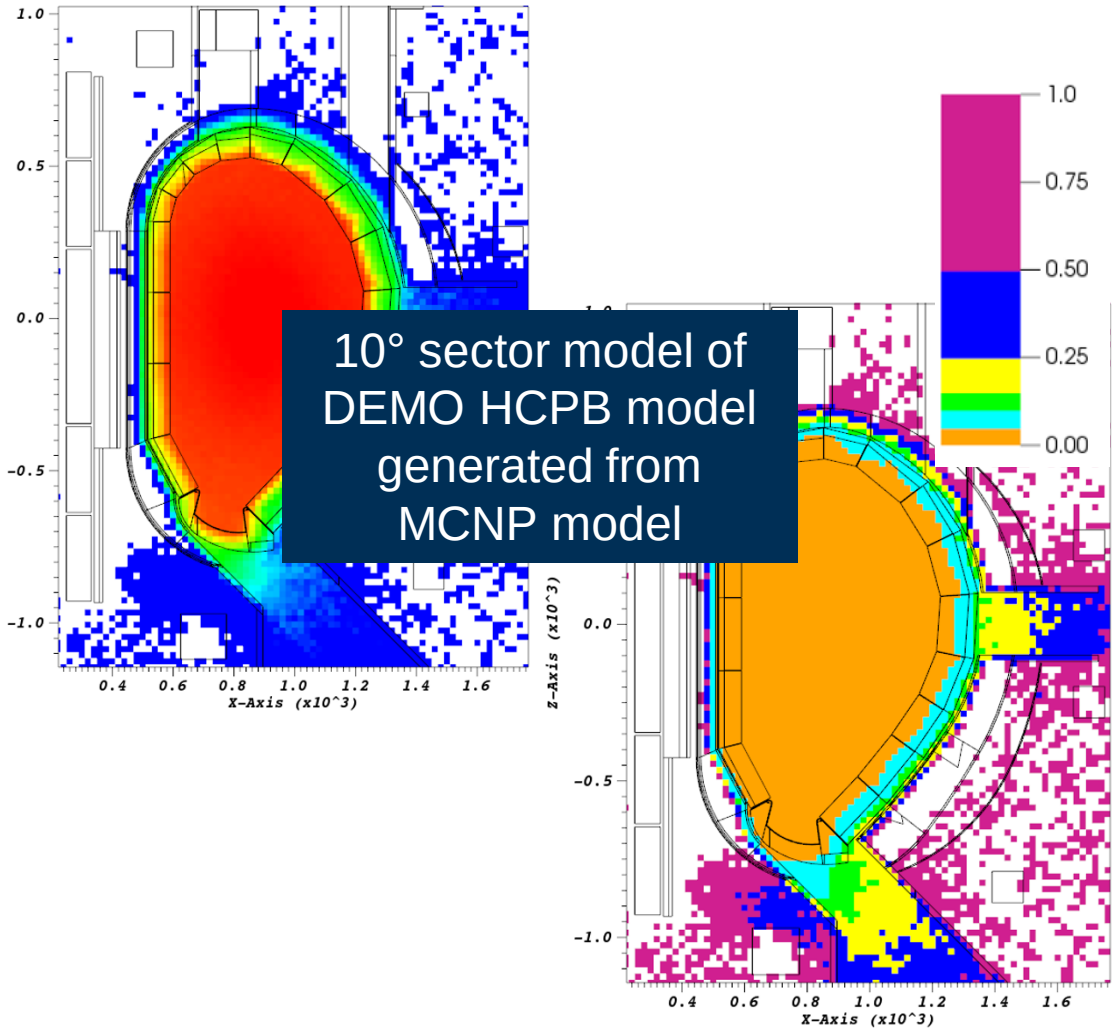
- The work undertaken this year is funded through EUROfusion (PMI_3.3_T042_D002). This follows on naturally from last years task (D001).



Neutron/photon spectrum for DEMO Helium Cooled Bed (HCPB)

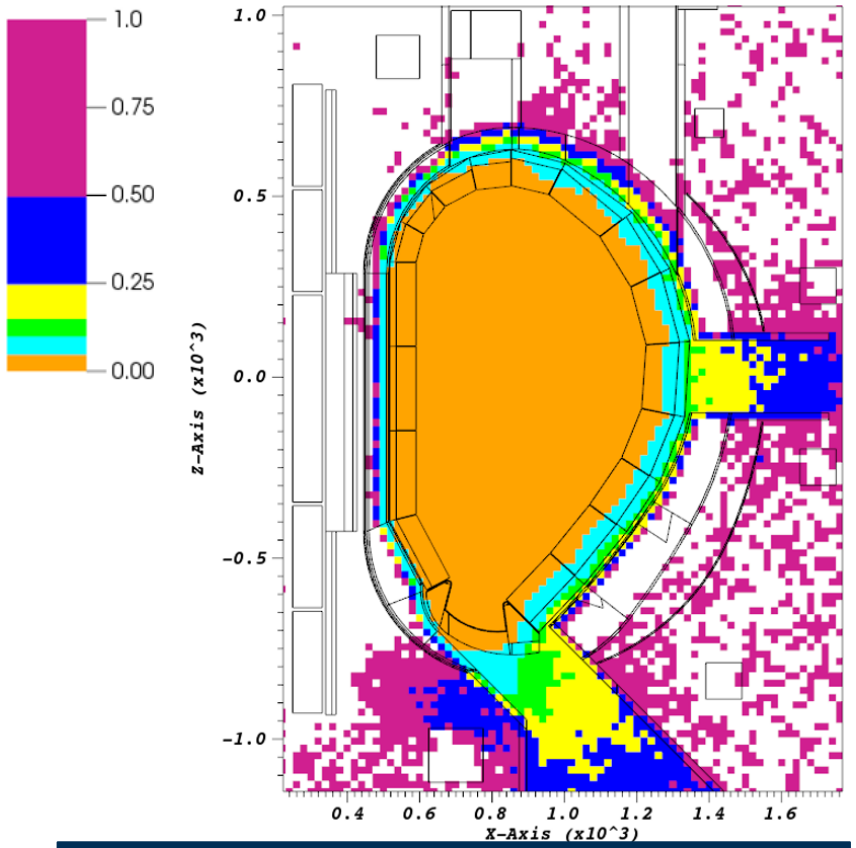


FNG HCPB benchmark in SINBAD



10° sector model of DEMO HCPB model generated from MCNP model

Serpent task 2020

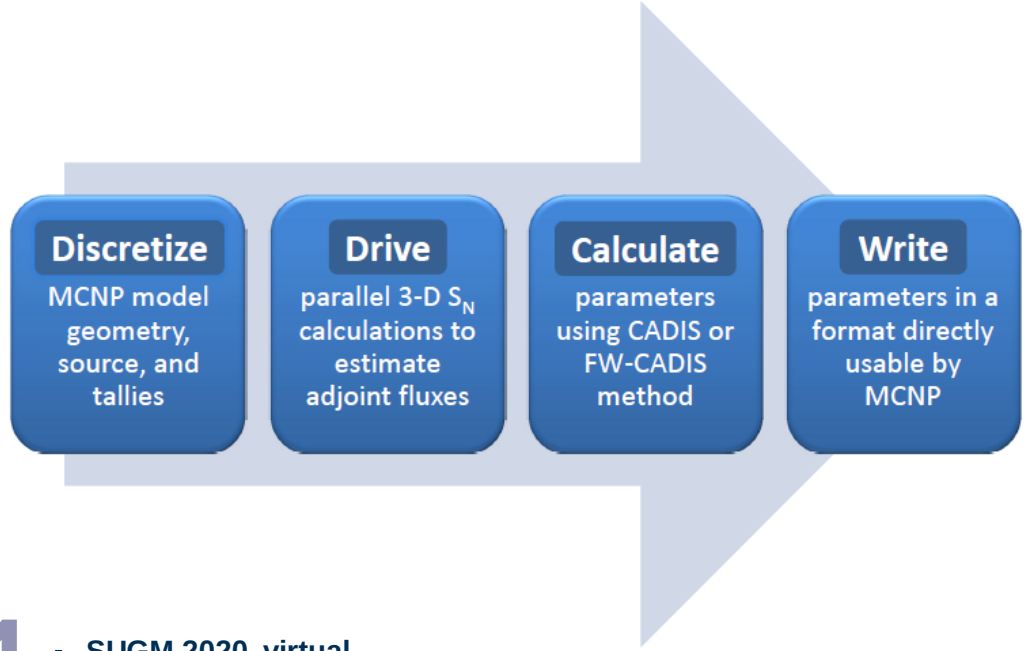


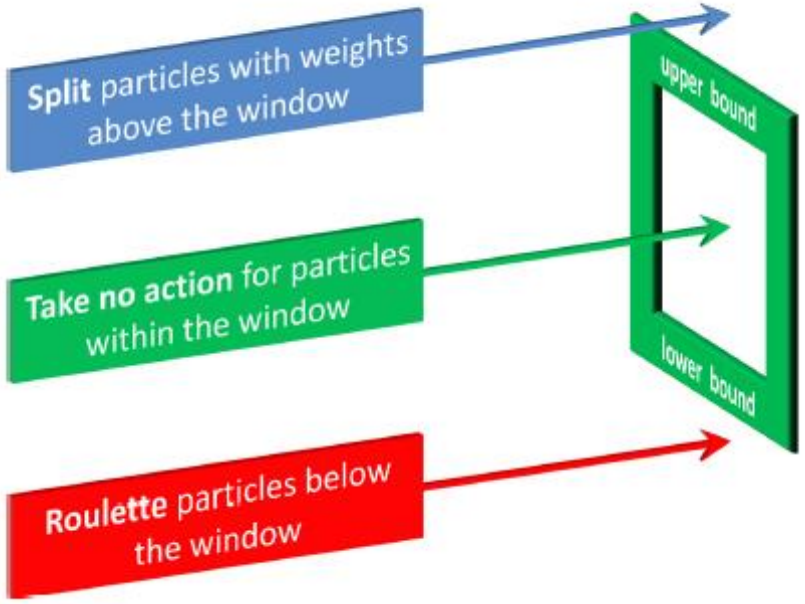
Statistical error map for Serpent 2 calculation – Only in the blanket modules, the error <10%

- So far, all studies have been limited to looking at in-vessel responses e.g. tritium production/ nuclear heating/ DPA in the blanket (first plasma facing layer)
- Often, analysis is interested in responses in the ex-vessel region and even beyond this in to surrounding buildings. We would like for example to calculate the neutron flux in the ports that can be used in activation analyses to determine our strategy for remote maintenance
- For this we require variance reduction techniques.
- Investigation into the new variance reduction capabilities in Serpent is the focus of the work conducted this year.

Variance Reduction

- The idea is that we control the populations of particles and encourage them to regions of higher **importance** using two techniques, **rouletting** and **splitting**. The calculation is not biased by ensuring that the **statistical weight** is preserved.
- The fusion community have since ~2016 focussed on using **ADVANTG (https://info.ornl.gov/sites/publications/files/Pub56840.pdf)** . The time for weight window generation was reduced from the order of days to hours relative to previous workflows.
- ADVANTG is a very powerful tool for completely automating the variance reduction parameters through use of a **deterministic transport solver**. Capability to target individual responses (CADIS) or achieve uniform statistical precision across multiple tallies or regions of phase space (FW-CADIS)





Variance Reduction in Serpent 2

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- The importance map which is used to derive the weight mesh is found as a solution to the adjoint transport problem. This can be found using **deterministic transport codes** as in ADVANTG or by using the Monte Carlo method to run the transport simulation backwards or back-track stored events.
- Serpent includes a **response-matrix based solver** which uses a series of coupling coefficients calculated via the Monte Carlo method.
- Serpent also has the capability to read in the weight window mesh generated by ADVANTG and therefore use the same WW as MCNP (WWINP format)
- This is also capable of targeting multiple responses as well as a single response. **Global variance reduction** is achieved through gradually populated different regions of the phase space to achieve better statistics. The calculation proceeds iteratively and in this respect is automated.

J. Leppänen. "Response Matrix Method Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code." Nucl. Technol. DOI: 10.1080/00295450.2019.1603710

How to we know the suitability of the WW?

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- When performing variance reduction, it is very important that we ensure that the more precise result is also accurate. In MCNP, we rely on a number of in built tests provided in tally fluctuation charts which provide information as in the examples below. There are in total 10 statistical tests.
- Is there such detailed statistics we can look at in Serpent beyond the FOM and Relative Error?

Mean	1. Nonmonotonic behavior for the last half of the problem
Relative Error	2. An acceptable magnitude (< 0.05 for point detector; < 0.10 otherwise) 3. Monotonically decreasing for the last half of the problem 4. A $1/\sqrt{N}$ decrease rate for the last half of the problem
VOV	5. Magnitude less than 0.10 6. Monotonically decreasing for the last half of the problem 7. A $1/N$ decrease rate for the last half of the problem
FOM	8. Statistically constant value for the last half of the problem 9. Nonmonotonic behavior for the last half of the problem

tally 14

nps	mean	error	vov	slope	fom
64000	1.8133E-11	0.1375	0.0407	0.0	243
128000	1.8744E-11	0.1031	0.0428	0.0	218
192000	2.0642E-11	0.0863	0.0274	0.0	206
256000	2.2710E-11	0.1030	0.3157	0.0	108
320000	2.1464E-11	0.0904	0.2733	0.0	112
384000	2.1538E-11	0.0795	0.2187	0.0	121
448000	2.0859E-11	0.0735	0.1843	2.5	122
512000	2.0658E-11	0.0678	0.1558	2.8	125
576000	2.0425E-11	0.0629	0.1374	3.1	129
640000	2.0105E-11	0.0590	0.1245	3.0	132
704000	2.1964E-11	0.0993	0.5536	2.3	42
768000	2.3479E-11	0.1116	0.3533	2.0	31
832000	2.3702E-11	0.1029	0.3421	2.0	33
896000	2.4088E-11	0.0987	0.2883	2.0	34
960000	2.3655E-11	0.0942	0.2838	2.0	35
1000000	2.3394E-11	0.0917	0.2814	2.1	35

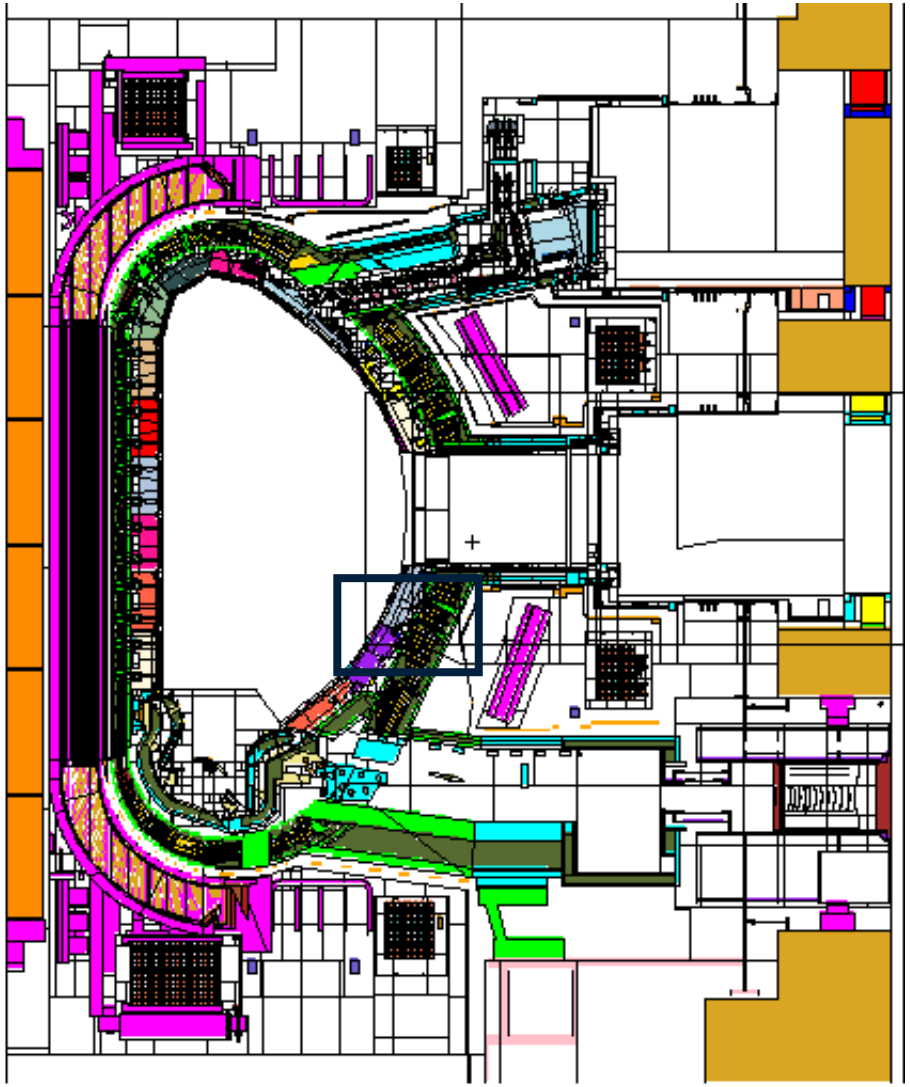
Probably significant

tally 115

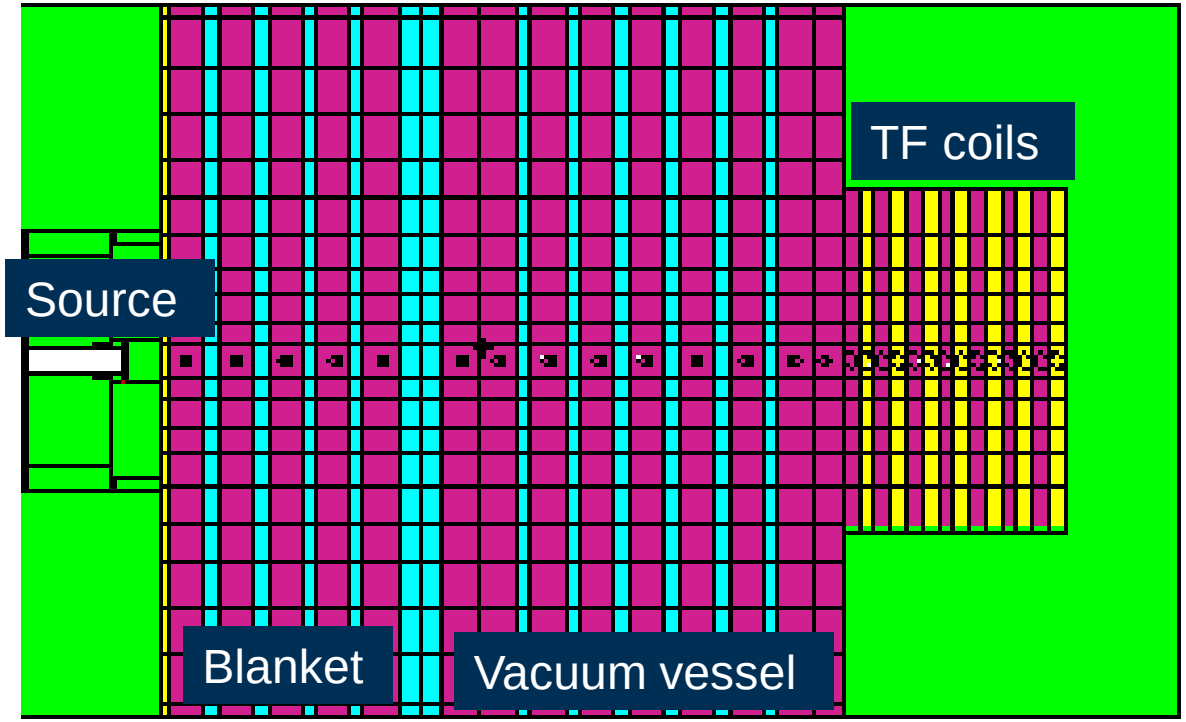
nps	mean	error	vov	slope	fom
512000	5.7432E-09	0.0155	0.0036	4.3	40
1024000	5.6874E-09	0.0110	0.0017	4.2	40
1536000	5.7057E-09	0.0092	0.0018	2.8	38
2048000	5.7247E-09	0.0080	0.0015	2.8	38
2560000	5.7226E-09	0.0071	0.0011	3.5	38
3072000	5.7210E-09	0.0065	0.0008	8.0	38
3584000	5.7220E-09	0.0060	0.0007	10.0	39
4096000	5.7253E-09	0.0056	0.0006	10.0	39
4608000	5.7305E-09	0.0053	0.0005	10.0	39
5120000	5.7354E-09	0.0050	0.0006	10.0	39
5632000	5.7442E-09	0.0048	0.0005	10.0	38
6144000	5.7348E-09	0.0046	0.0005	10.0	39
6656000	5.7269E-09	0.0044	0.0004	10.0	39
7168000	5.7283E-09	0.0043	0.0005	8.3	38
7680000	5.7240E-09	0.0041	0.0005	10.0	38
8192000	5.7201E-09	0.0040	0.0004	8.9	38
8704000	5.7311E-09	0.0039	0.0004	6.5	38
9216000	5.7357E-09	0.0038	0.0007	4.3	37
9728000	5.7462E-09	0.0037	0.0006	4.2	37
10000000	5.7410E-09	0.0037	0.0006	4.2	37

Probably not significant

FNG ITER bulk shielding benchmark

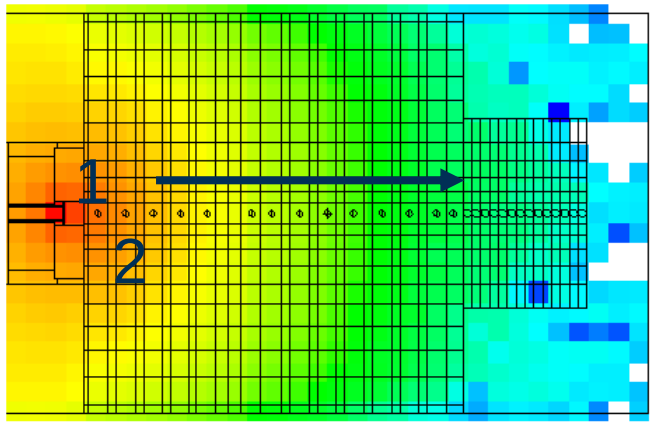


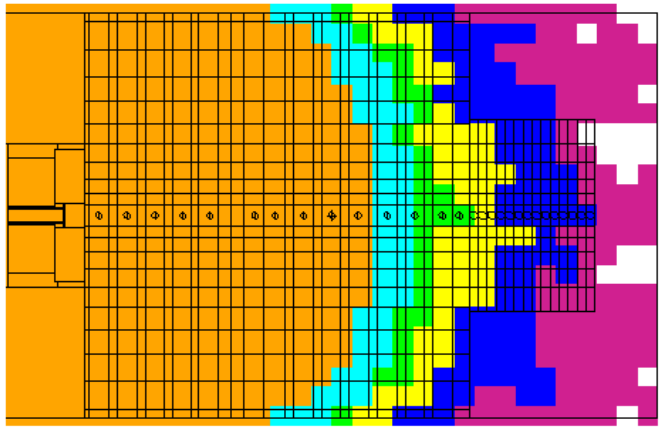
- Mock up designed in 1995 for validation of ITER in-board shielding. Includes a description of the first wall, blanket, vacuum vessel and the toroidal field coils. Consists of a copper, stainless steel/perpex sandwich, with a smaller block at the rear of the mock-up comprising alternating layers of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



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 197Au(n,g).
- Frascati Neutron Generator (14 MeV neutron source) rewritten in C.



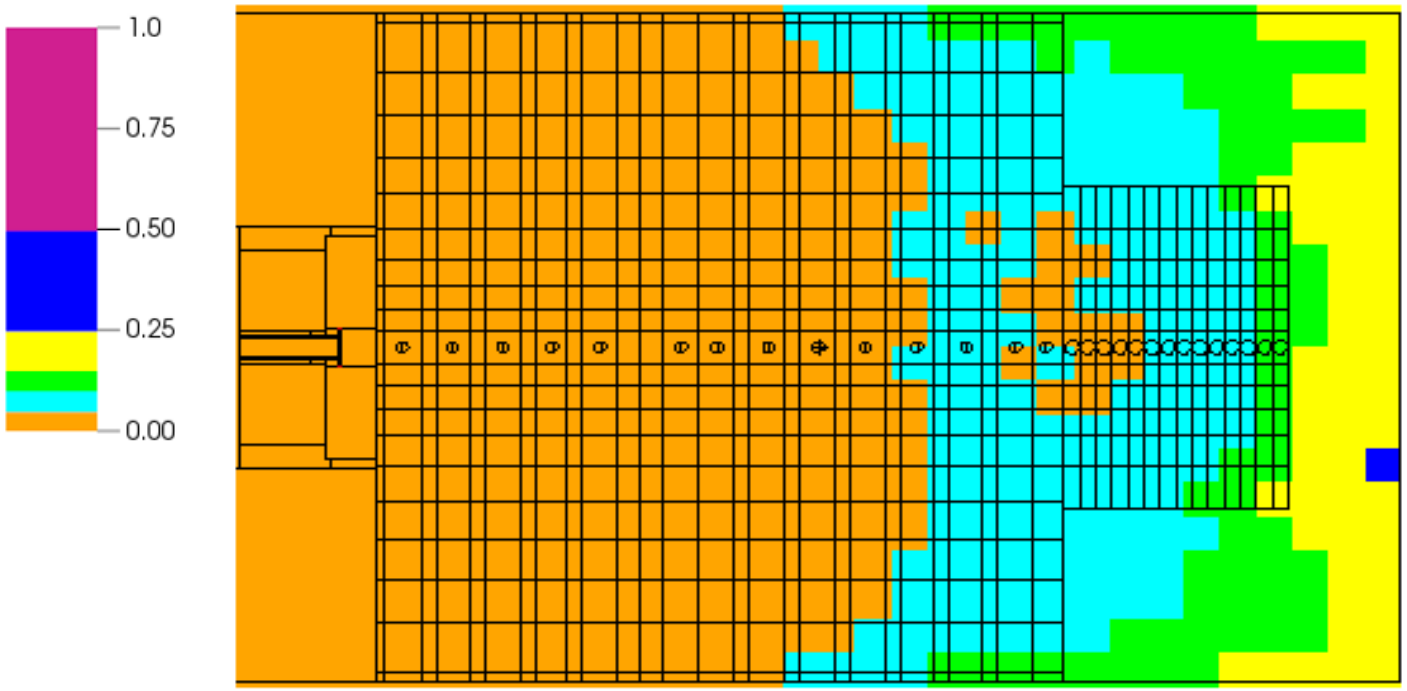


Det	Depth (cm)	Experiment	RR	Error	C/E
1	3.43	6.37E-03	5.97E-03	6.70E-02	9.38E-01
2	10.32	9.72E-03	9.47E-03	5.22E-02	9.74E-01
3	17.15	5.50E-03	5.41E-03	6.66E-02	9.83E-01
4	23.95	2.44E-03	2.62E-03	9.66E-02	1.07E+00
5	30.8	9.47E-04	7.55E-04	1.68E-01	7.97E-01
6	41.85	1.65E-04	1.60E-04	3.17E-01	9.73E-01
7	46.85	6.64E-05	6.60E-05	6.81E-01	9.93E-01
8	53.8	3.76E-05	5.57E-05	5.70E-01	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	-

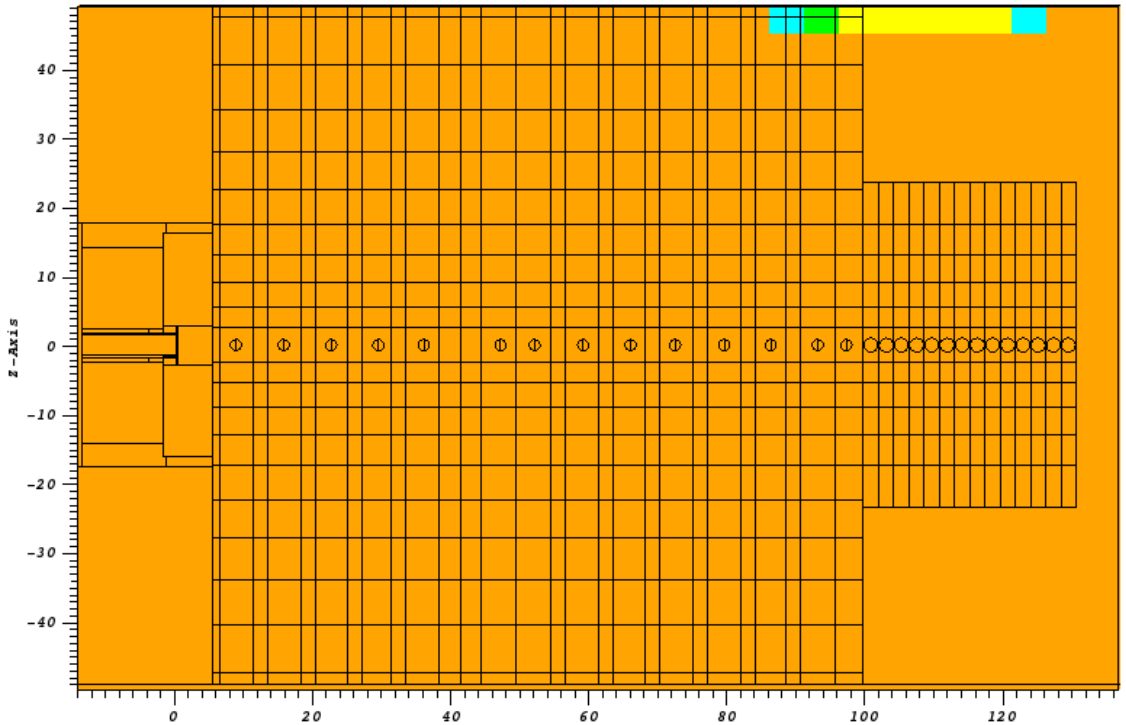
Analog calculation: 1E8 histories. Only to the 4th detector is the relative error reasonably small and the results comparable to experiment

Variance Reduction

- In this case, the built in WW generator in MCNP was used as well as ADVANTG. The former can take many hours to optimise the mesh. ADVANTG with FW-CADIS ran in minutes.
- For Serpent, the GVR scheme was first used with 3 iterations. Time taken to generate the WW was of the order of seconds



ADVANTG with GVR using FW-CADIS



Serpent with GVR for 3 iterations

Serpent global and targeted response

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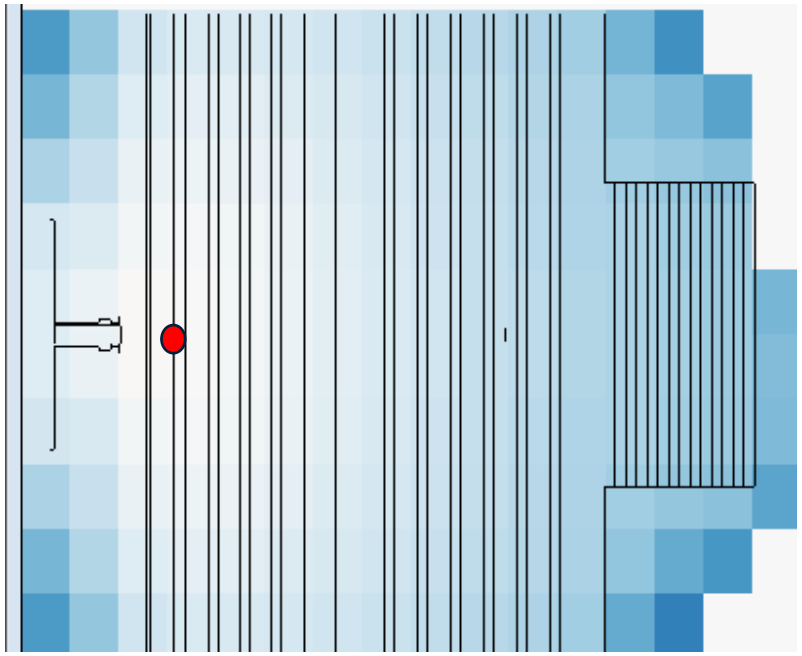
- Different number of iterations were trialled and 3 found to be most optimal. No gain after this.
- Also trialled targeting specific detectors in which case only this response should be considered valid
- Optimal case for deep shielding (TF coil region) was GVR and subsequent targeted response….

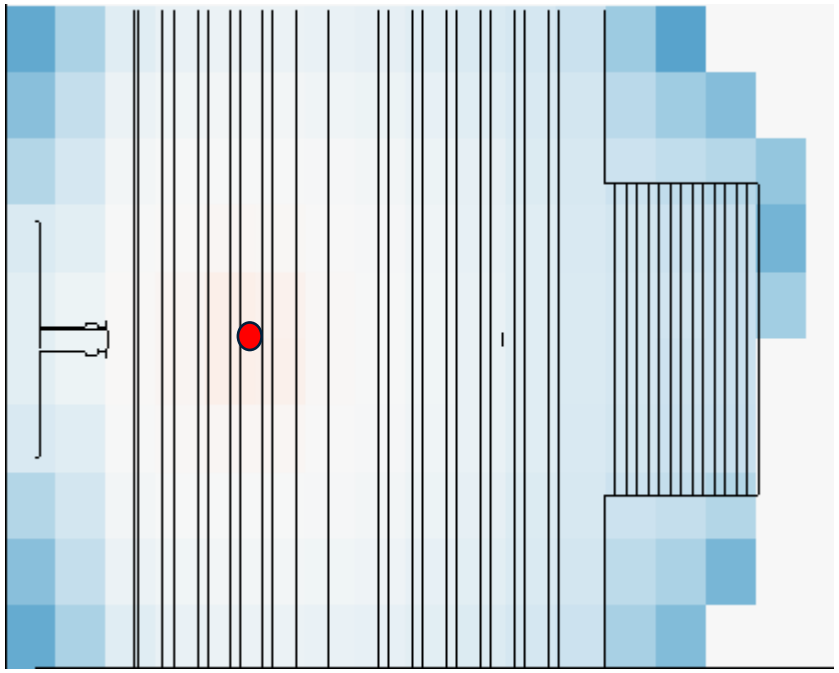
			GVR 3 iterations			Det 1 target			Det 5 target			Det 7 target		
Det	Depth (cm)	Experiment	RR	Error	C/E	RR	Error	C/E	RR	Error	C/E	RR	Error	C/E
1	3.43	6.37E-03	6.11E-03	4.63%	9.59E-01	6.33E-03	4.77%	9.94E-01	6.06E-03	3.19%	9.94E-01	6.51E-03	3.35%	1.02E+00
2	10.32	9.72E-03	9.41E-03	3.56%	9.68E-01	9.71E-03	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	0.00E+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	0.00E+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	0.00E+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	0.00E+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	0.00E+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	0.00E+00	0.00E+00	0.00E+00	0.00%	0.00E+00

Targeted Response plots of neutron importance

- Serpent allows for plotting of the importance, providing some information on whether the WW is working as intended. User specified logarithmic scale and bounds for importance.
- Plots below are for targeted detector responses through the mock up



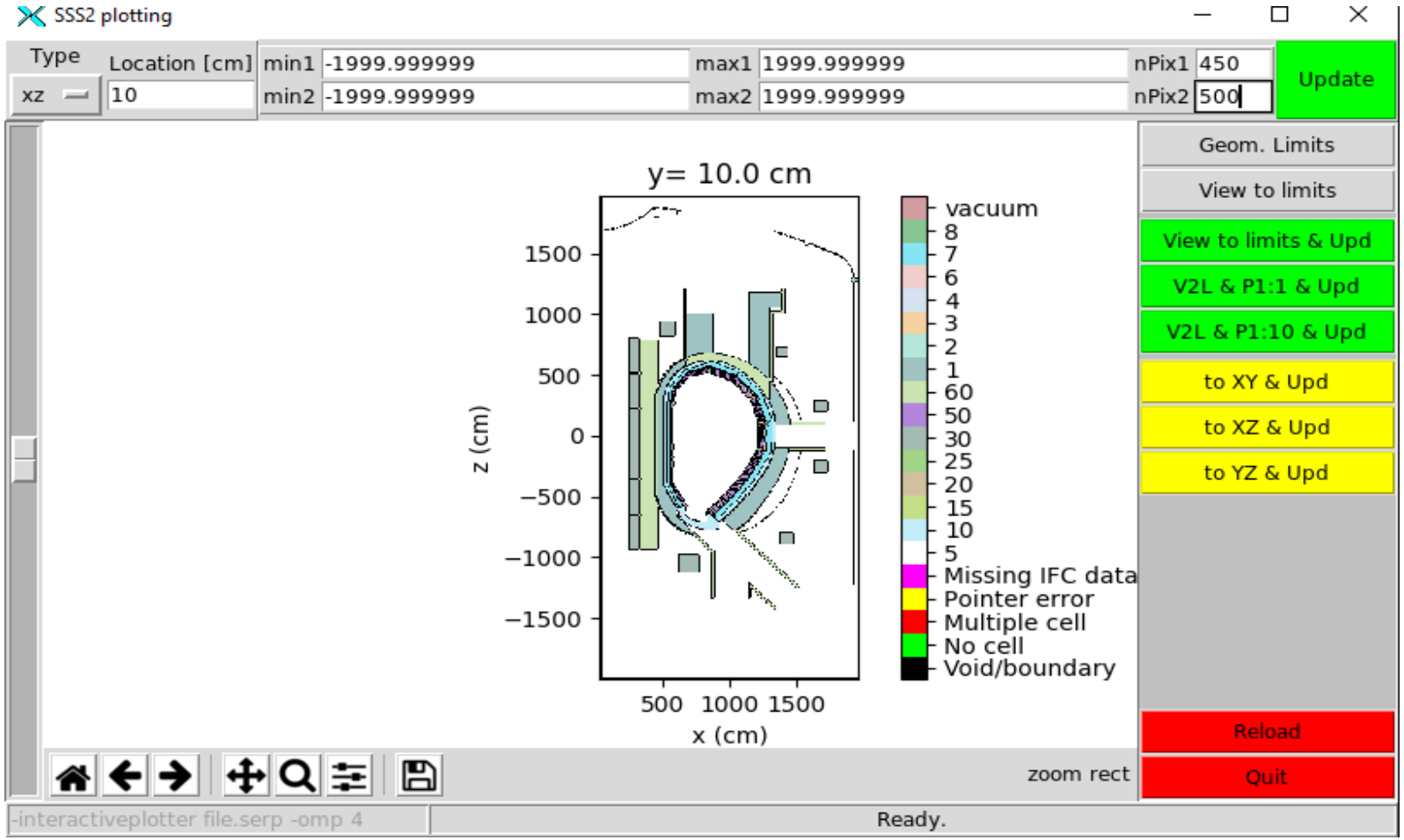
DET 1 target= 3 cm from source



DET 5 target= 31 cm from source

DEMO HCPB - Visualisation in Interactive plotter

- Interactive plotter provides a very powerful tool for plotting geometries. Particularly useful for increasing complexity to identify errors and overlaps



Python plotter: https://pypi.org/project/pysss2/

Global variance reduction with DEMO HCPB model

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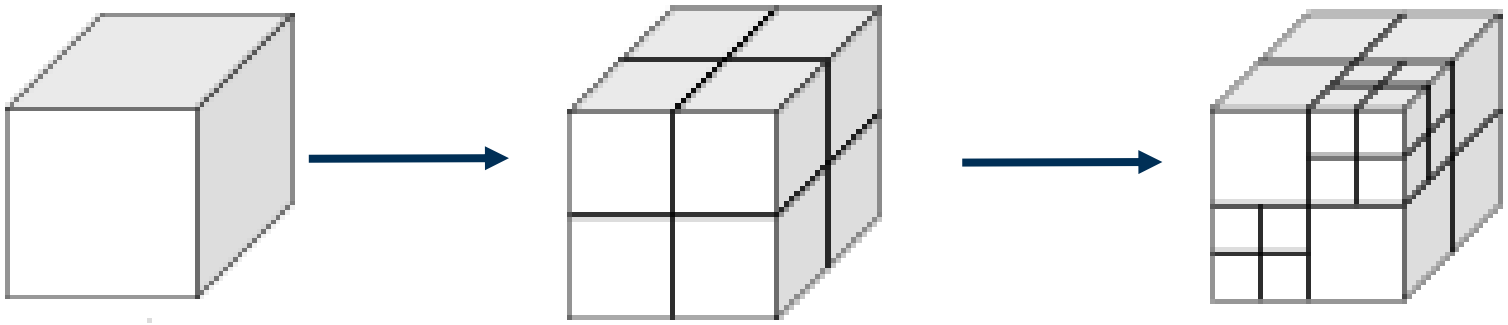
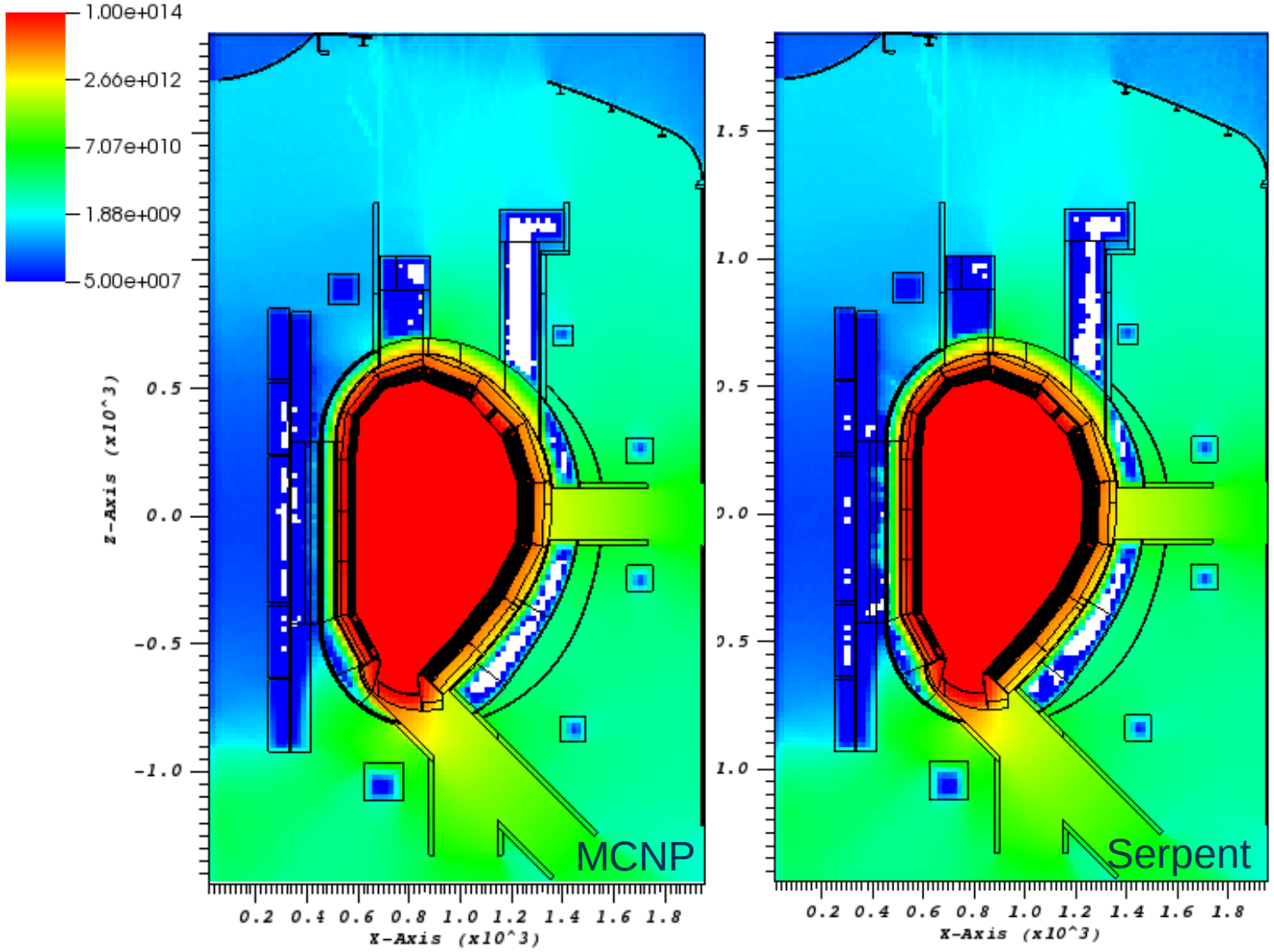
- For the DEMO geometry with deep shielding, global variance reduction is required for ex-vessel responses.
- Results are compared to ADVANTG using FW CADIS in the GVR scheme
- In Serpent, it was found that 4 iterations was optimal, after which little improvement was seen
  - The **adaptive mesh option** was used in which the cartesian mesh is recursively split based on a user define density criterion and minimum mesh voxel dimensions
  - This gives much higher resolution in areas where there is a steep gradient in the importance

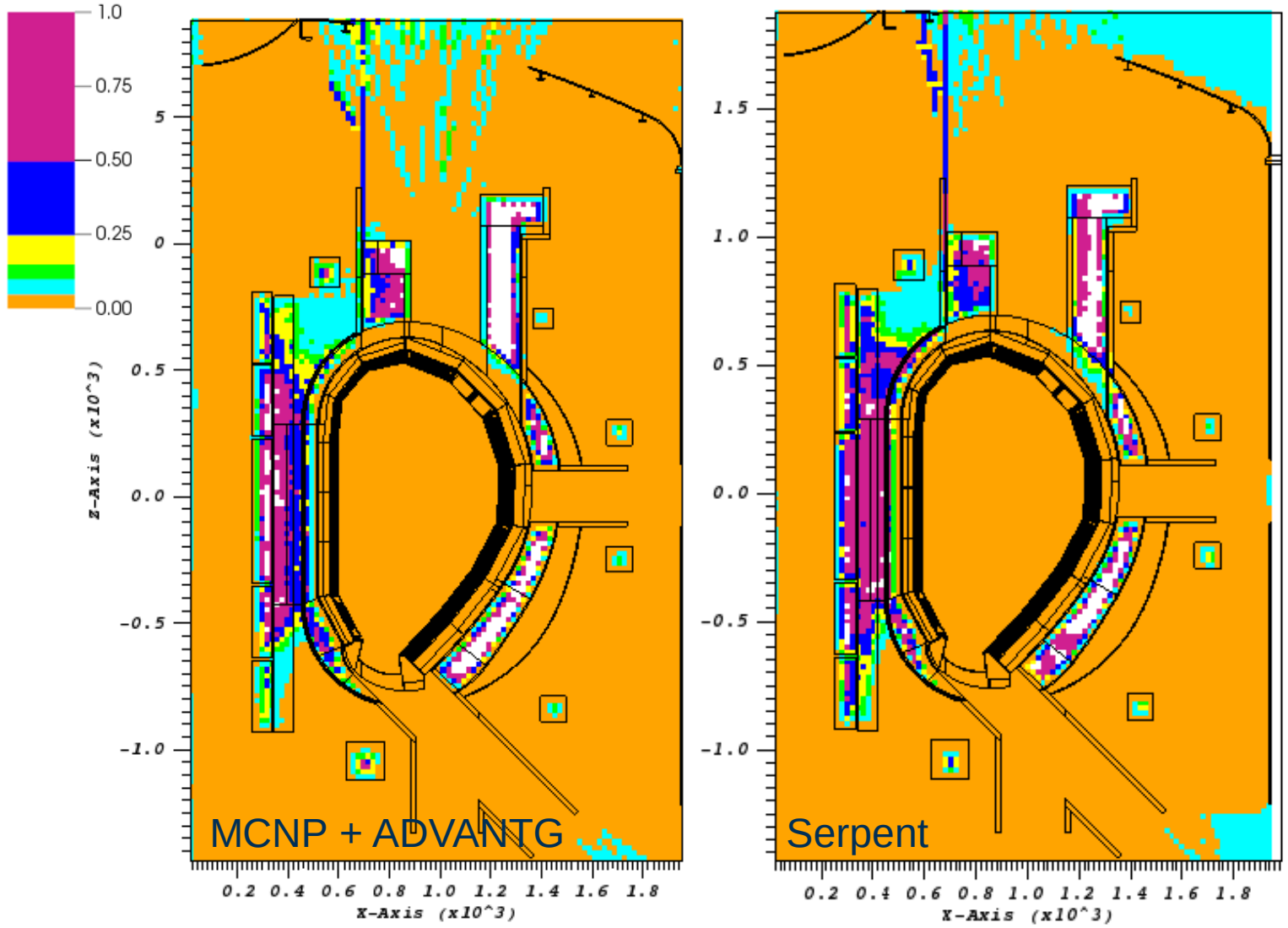


Neutron flux (neutrons s^{-1} cm^{-2})



- All Serpent calculations are performed with hybrid OpenMP+MPI using 8 MPI tasks and 8 OMP threads
- All MCNP calculations MPI using 64 CPUs.
- Calculations ran to **1E8** histories.
- **JEFF 3.3** nuclear data used for both Serpent and MCNP
- FORTRAN parametric plasma source has been rewritten in C for use in Serpent
- Assumes DEMO operational power of 1998 MW giving 7.094E20 neutrons s^{-1}.

DEMO HCPB: Relative Error



- ADVANTG WW generated in 1.6 hours using FW CADIS method.
  - Target mesh: 10 cm
- Serpent iterations completed in 2.1 hours
- Calculations took several hours in both cases however ADVANTG required detuning in order to achieve comparable time scales.
- **Both considerably better than other VR techniques for unform statistical precision across ex-vessel region**

Neutron Flux comparison

- Neutron flux (neutrons cm^{-2} s^{-1}) calculated for the 6 poloidal field coils (PFC) which are located poloidally around tokamak ex-vessel region.

PFC	Serpent				MCNP + ADVANTG				GVR: (MCNP-Serp)/Serp
	Analog	Error	GVR	Error	Analog	Error	GVR	Error	
1	4.27E+14	25%	3.65E+14	2.10%	3.53E+14	67%	3.69E+14	1.40%	1.05%
2	4.09E+15	7%	4.57E+15	0.40%	4.59E+15	15%	4.69E+15	0.30%	2.68%
3	2.49E+16	4%	2.40E+16	0.30%	2.41E+16	17%	2.46E+16	0.20%	2.40%
4	2.58E+16	3%	2.60E+16	0.30%	2.75E+16	15%	2.68E+16	0.20%	2.98%
5	1.59E+16	4%	1.55E+16	0.30%	1.67E+16	15%	1.59E+16	0.20%	2.76%
6	6.09E+16	2%	6.34E+16	0.10%	6.45E+16	12%	6.54E+16	0.20%	3.10%

Targeting specific responses

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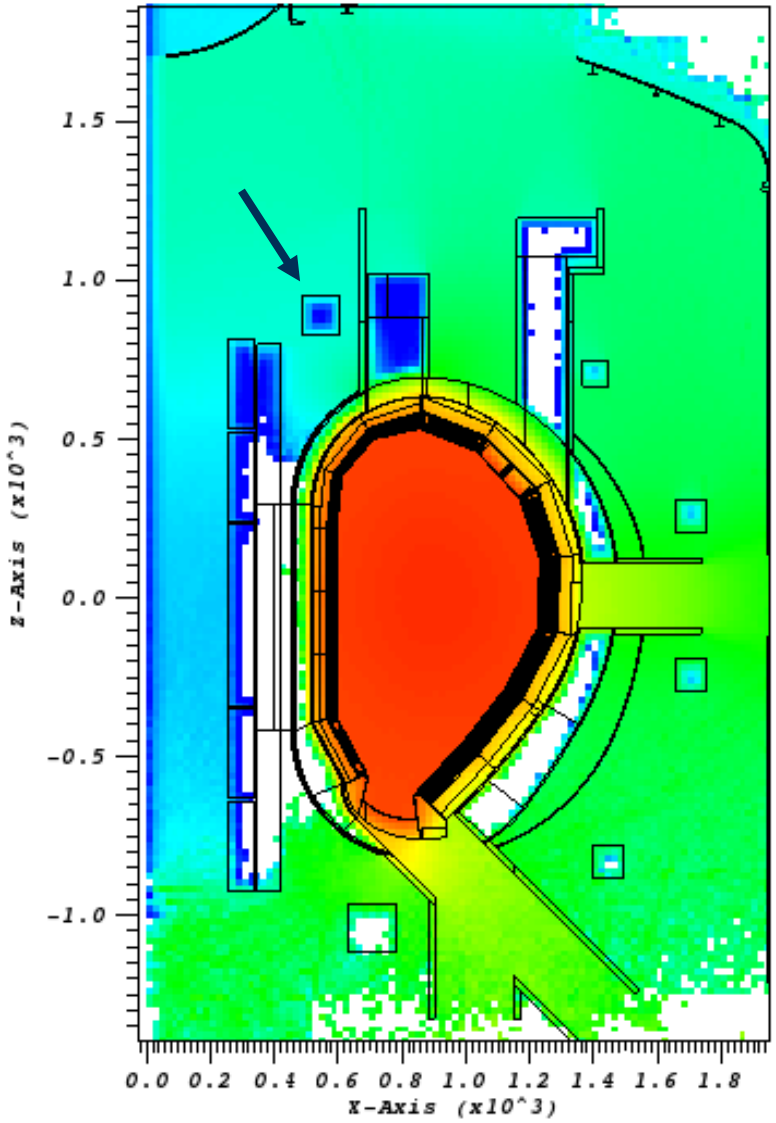
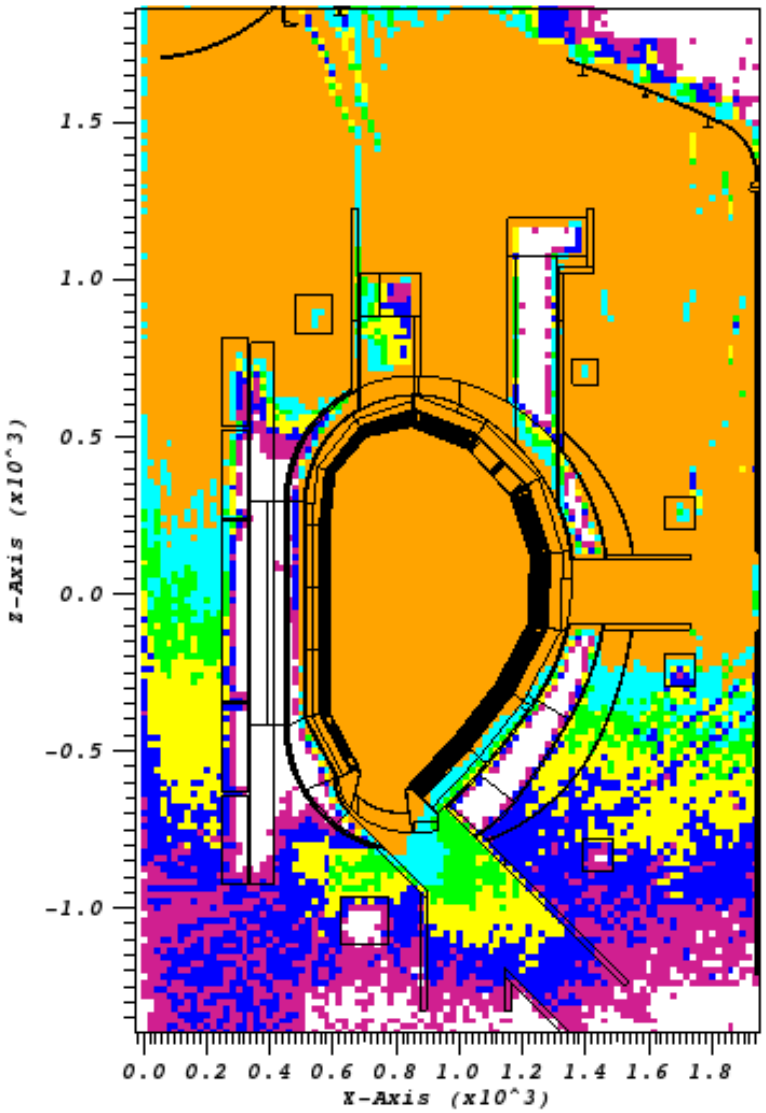
- Targeting individual responses is difficult because of poor statistics -Monte Carlo simulation fails to provide the coupling coefficients for the response matrix method-based importance solver.
- In this case, the most effective method was found to be using GVR scheme and then performing a subsequent simulation which targets the response of interest.
- Therefore, using the previously generated GVR map, specific poloidal filed coils were targeted.
- The calculation is now a three step process:

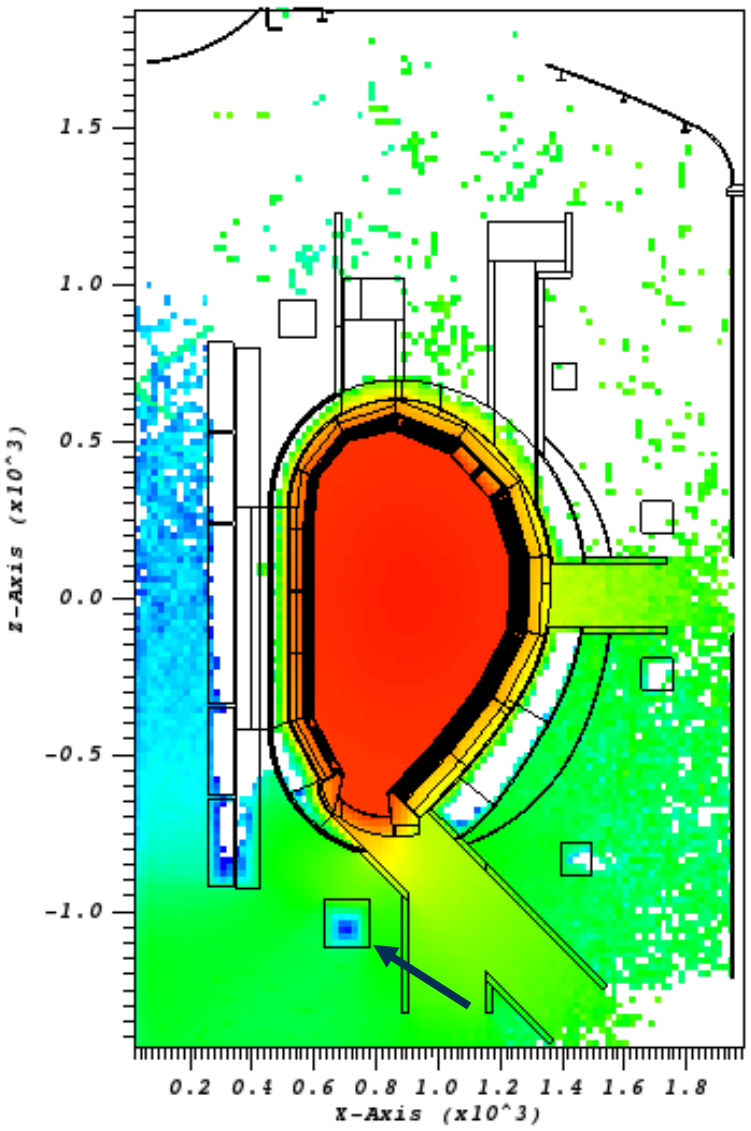
Run GVR iterations → Optimise mesh for specific detector → Run with optimised mesh

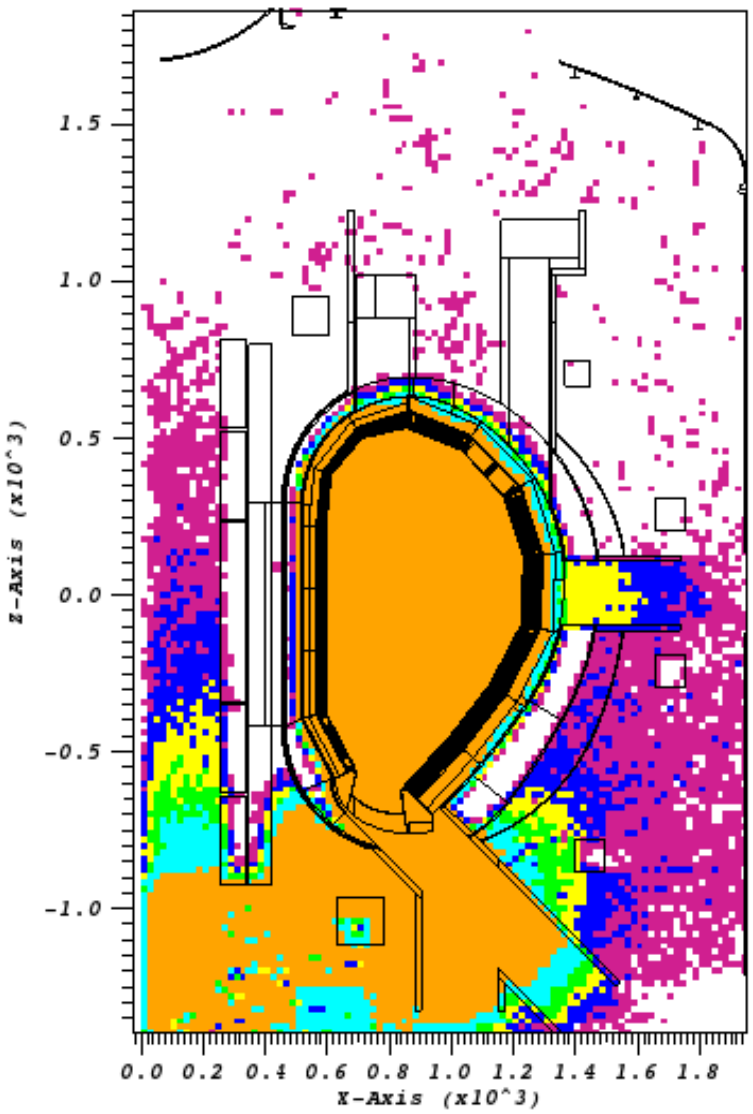
Targeted Response: PFC 1



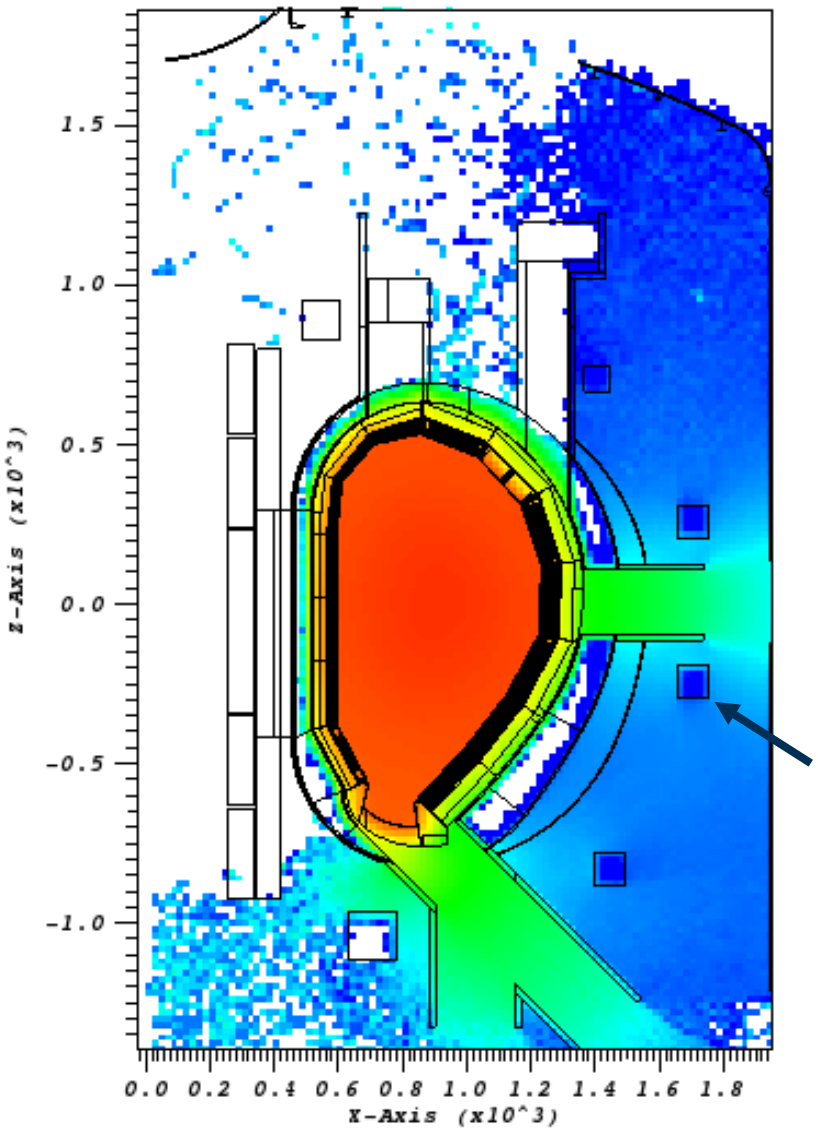


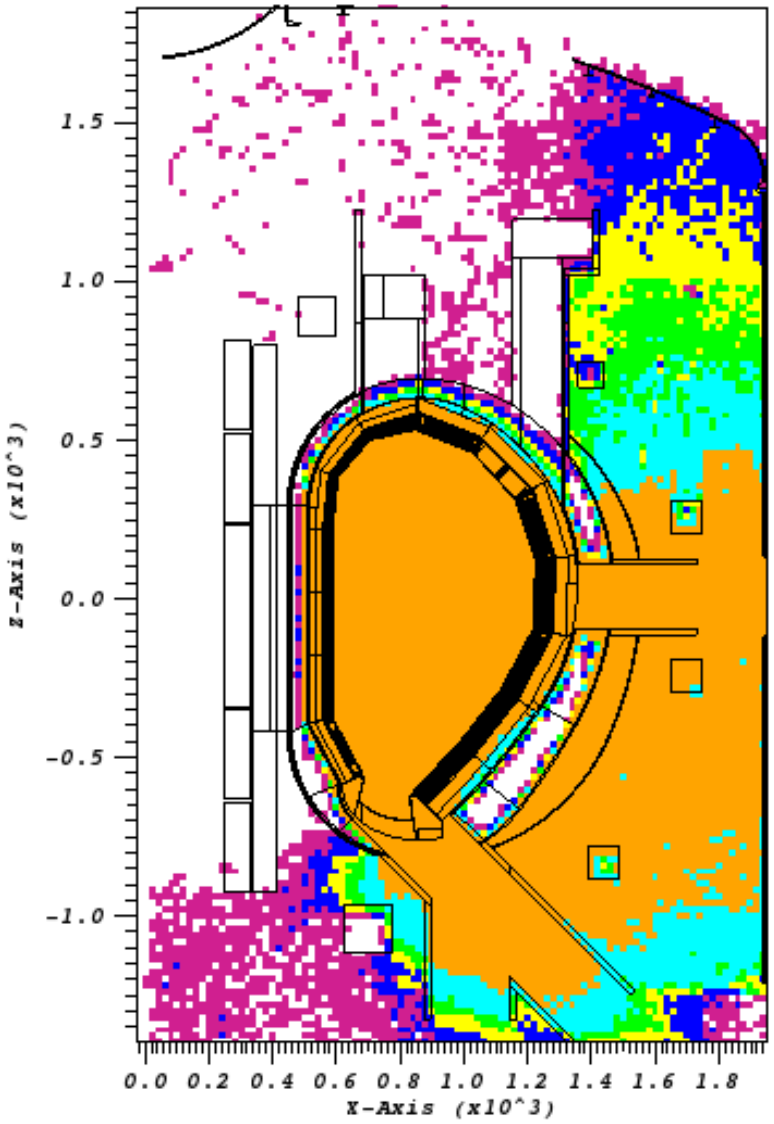
Targeted Response: PFC 6

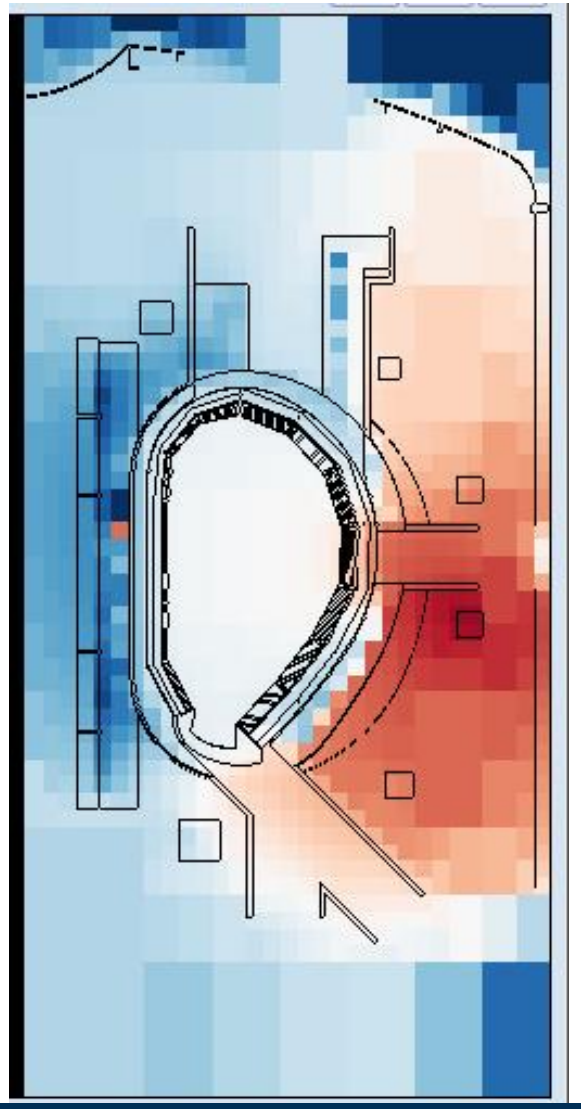




Targeted Response: PFC 4



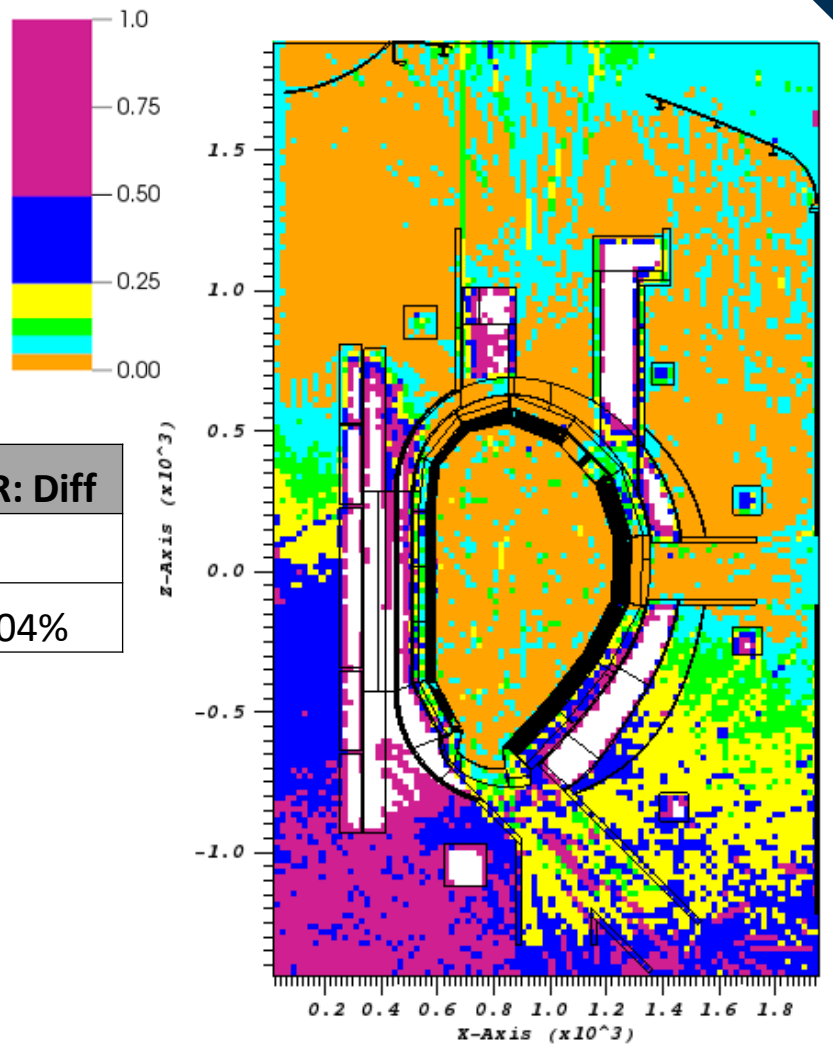




Importance plot from 1E-5 to 1E5. Log scale.

Comparison with MCNP + ADVANTG

- For single detector response in ADVANTG, a single F4 tally (PFC 1) is used as the target
- More ‘noisy’ than Serpent however this is done using a single ‘iteration’ – requires some tuning of quadrature set and the deterministic spatial mesh
- In this case, the FOM improvement from the analog calculation was ½ that of Serpent



PFC	Serpent				MCNP				GVR: Diff
	Analog	Error	GVR + Target	Error	Analog	Error	Target	Error	
1	4.27E+14	25%	3.55E+14	0.07%	3.53E+14	67%	3.69E+14	1.50%	4.04%

Summary

- Many of the features needed in the fusion domain are now implemented in the code
- Variance reduction justifiably regarded as a delicate art rather than an exact science. Many methods exist from simple importance profiling to more esoteric methods
- For such an art, it is better if as much as possible can be automated, and the response matrix method in Serpent provides a powerful way to do this as demonstrated for the SINBAD benchmark ITER mock up and DEMO reactor model.
- Some user iterations is need as well as a fair level of intuition but this is expected and will be improved (novel development in Serpent). For ADVANTG we often the refine the deterministic spatial mesh, quadrature set, or other computational options to obtain high-quality variance reduction parameters
- The methodology shows great promise for application to more complex geometries- JET/ITER

Open questions

- Are there more statistical tests we can use for assessing VR accuracy?
- Are long histories seen as a potential issue?
- Is there a possibility to introduce a rendezvous to allow for run restart/continue?
- Will the interactive plotter be extended to plot mesh results and maps of importance?

What's next?

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- If funding should be available next year, the focus could be on the use of unstructured meshes which is the clear future for fusion neutronics workflows.
- With the current workflow, most of the changes are made downstream (in MCNP) which gives a very rigid, opaque way of working.
- The ideal is to move to a CAD-centric workflow. The CAD model is then the reference making revisions much more traceable.
- **DAG-MC (https://svalinn.github.io/DAGMC/index.html)** is one such example that performs particle transport directly on the CAD model. The use of STL geometry in Serpent also provides a powerful route for doing this.
- Using a hybrid CSG STL approach would be useful on studies of existing reference models where the CAD model does not exist (ITER).

Serpent User guide (Fusion)

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October 15, 2019

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October 15, 2019

Serpent User Guide for Fusion Applications

October 15, 2019

Serpent User Guide for Fusion Applications

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October 15, 2019

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UKAEA Page 3 of 21

CONTENTS refno
October 15, 2019 Serpent User Guide

Contents

1 Introduction **5**

2 Default data cards **5**
2.1 Set options 5
2.2 Volume Calculation 6
2.3 Plotting 7
2.4 Nuclear Data 7

3 MCNP to Serpent conversion **7**
3.1 CSG2CSG 7
3.2 MCNP2SERPENT 8

4 Definition of Sources **8**
4.1 Parametric Plasma Source . 9
4.2 FNG source 9

5 Detectors **10**
5.1 General 10
5.2 Nuclear Heating 10
5.3 DPA 11
5.4 Tritium Production 11
5.5 Mesh tallies 11
5.6 Post-processing 11

6 Parallelisation and HPC submission **12**
6.1 Serpent on Erik 12
6.2 Serpent on Cumulus 12

7 Modelling of sectors with reflecting boundaries **12**

8 Errors **13**

9 Correspondence with Jaakko Leppänen **13**
9.1 Email Correspondence . . . 13
9.2 From Serpent forum 18

10 Literature **20**

References **21**

Thank you for listening

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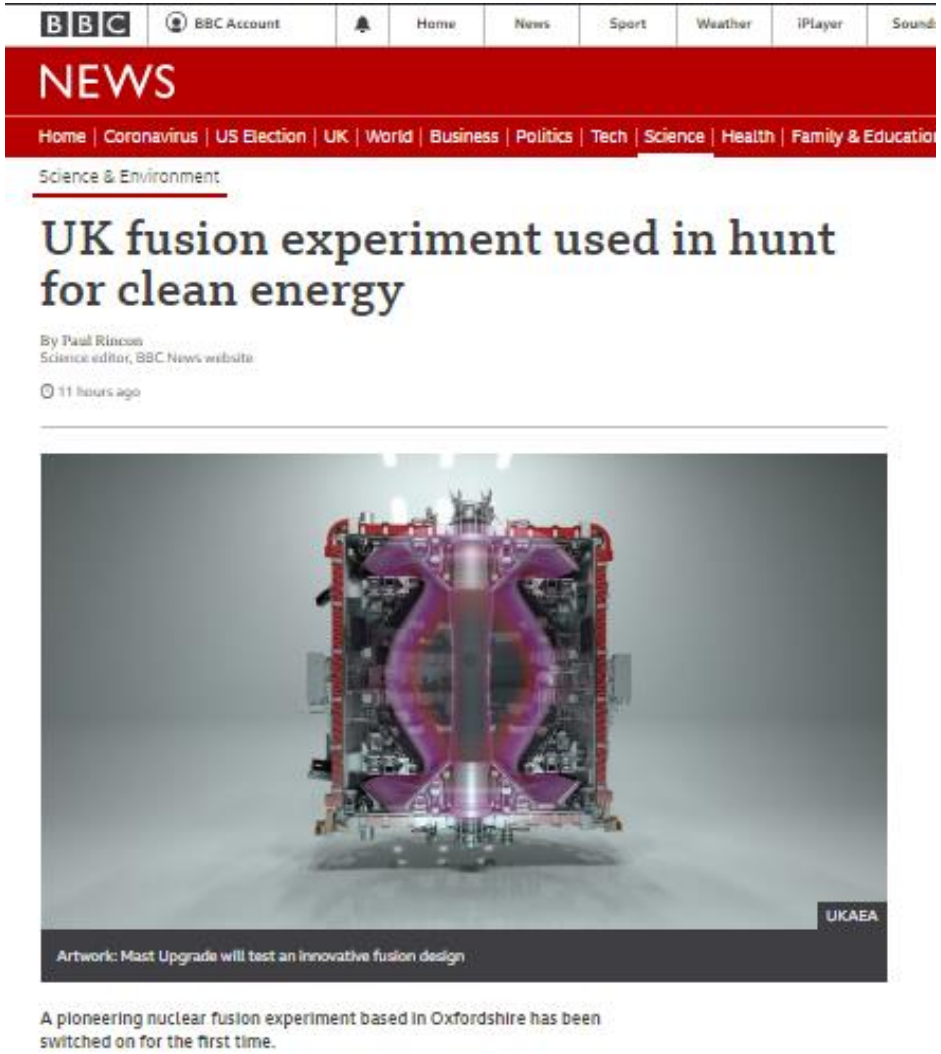

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By Paul Rincon
Science editor, BBC News website

11 hours ago

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Artwork: Mast Upgrade will test an innovative fusion design

A pioneering nuclear fusion experiment based in Oxfordshire has been switched on for the first time.