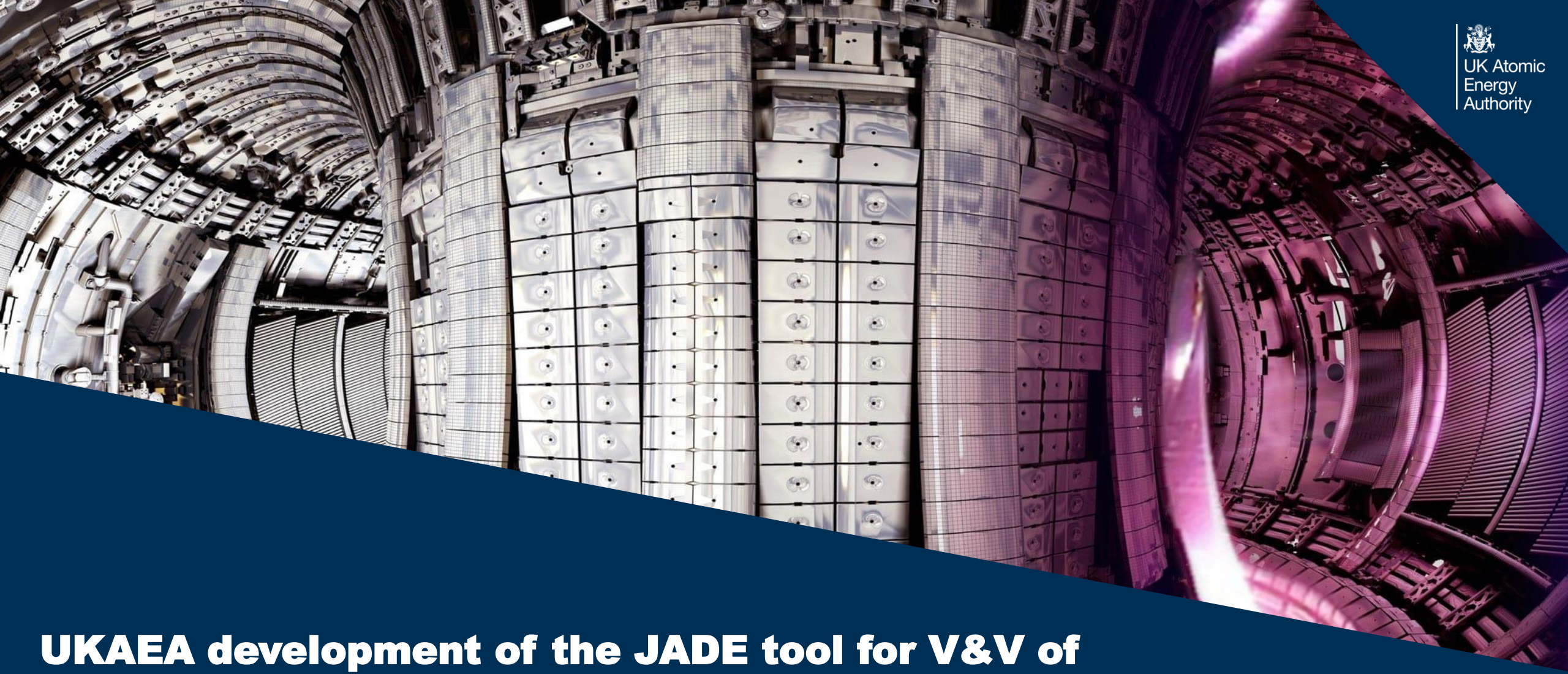


UK Atomic Energy Authority

# UKAEA development of the JADE tool for V&V of nuclear data and particle transport codes

Alex Valentine, Steven Bradnam, Dylan Wheeler + JADE development team

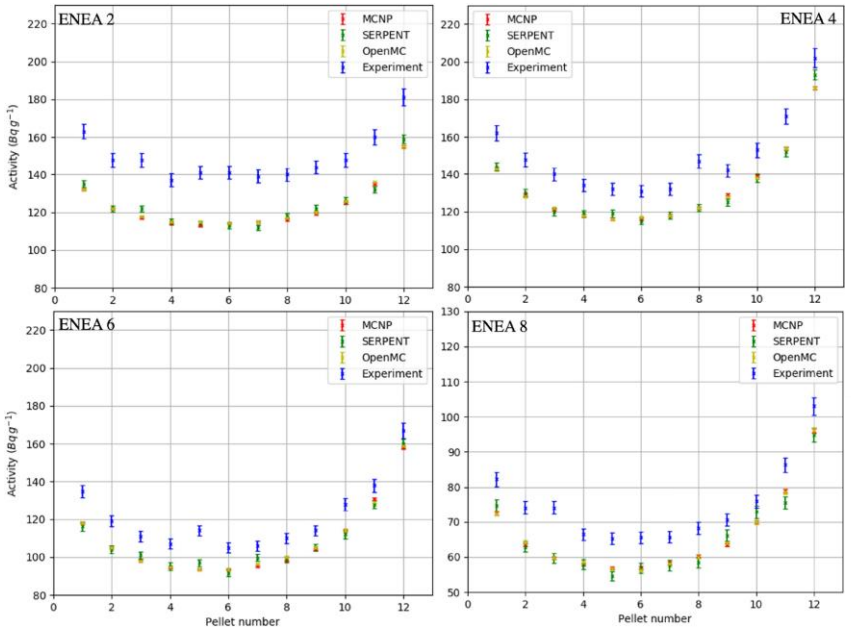
FENDL Consultants' Meeting, 01.11.23

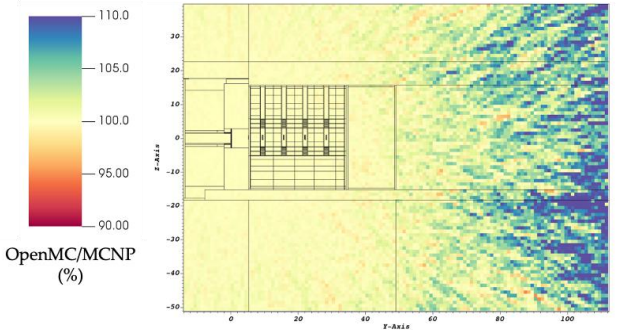
UK Atomic Energy Authority

# Changing landscape for particle transport codes

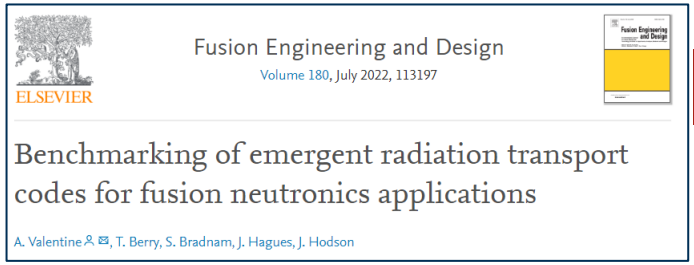
# Investigation of alternative codes

- MCNP is the reference transport code for fusion neutronics. It is heavily validated and well developed over the course of 40 years…
- Many patches for the code have been developed built on requirements for fusion neutronics and bugs that have been found. For most problems, it does what we want, and reasonably well.
- Alternatives to MCNP have emerged, particularly over the last ~10 years. UKAEA has actively investigated their potential application to fusion.

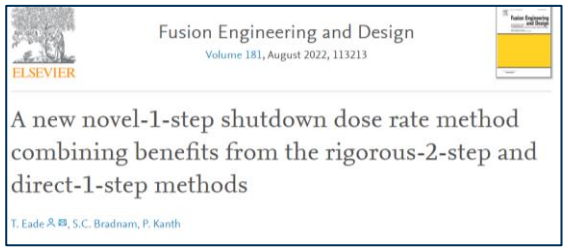









DAGMC
Direct Accelerated Geometry Monte Carlo Toolkit

Attila4MC

GEANT4
A SIMULATION TOOLKIT

MCNP6

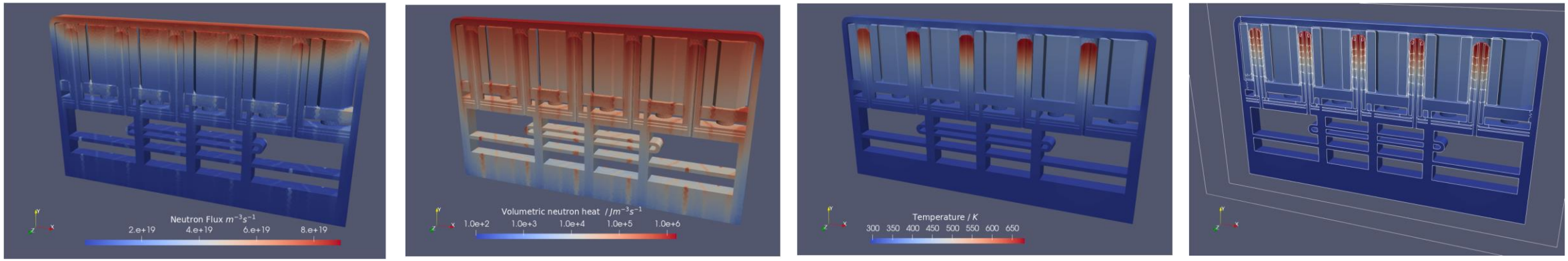
OpenMC

Serpent
a Continuous-energy Monte Carlo neutron and photon transport code

# Motivation – Integrated engineering

UK Atomic Energy Authority

- MCNP - single user, single site license is required, ~£1000 +. If running on computing network, system administrators are required to hold a license.
- In the design of fusion reactors, we need integrated multi-physics simulations capable of rapid exploration of a broad design space. Modern day advances in computing must also be harnessed.
- The **deployability** and **accessibility** of OpenMC has allowed development of such tools - UKAEA has developed AURORA code, coupling neutronics and thermal-mechanical FEA analysis (see https://github.com/aurora-multiphysics/aurora, H. Brookes et al.). Can be used for creating digital twins for test facilities – a key need for commercialization.

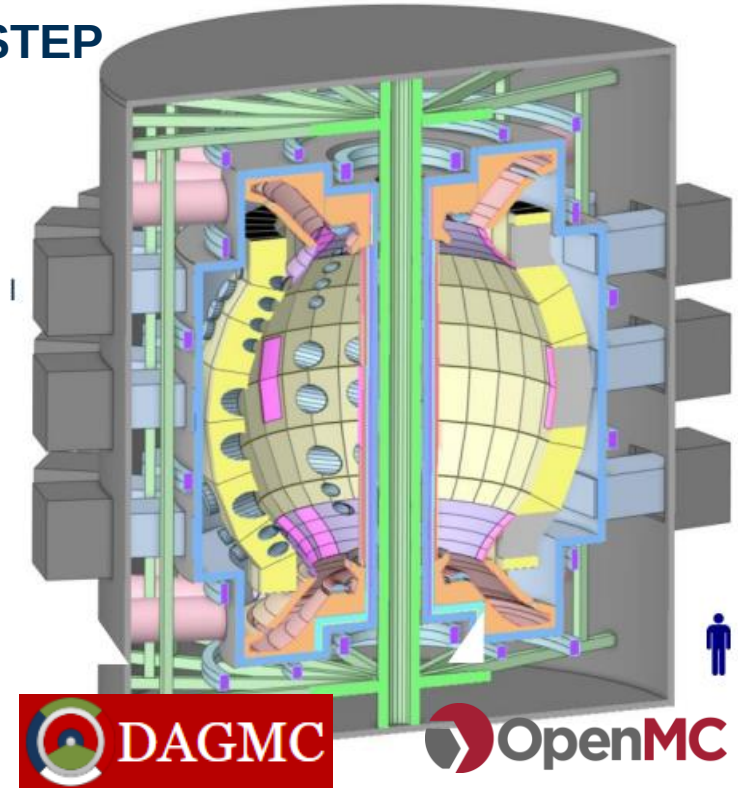


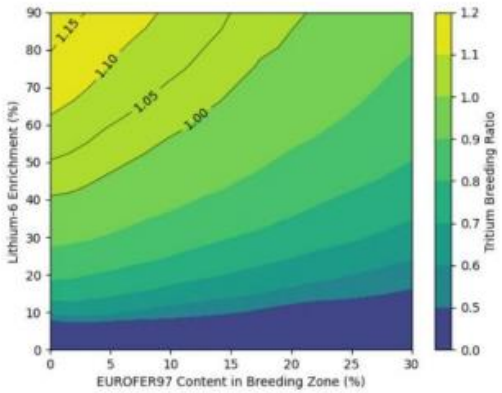

AURORA: **A** **U**nified **R**esource for **O**penMC (fusion) **R**eactor **A**pplications
Simulation of HCPB blanket concept

# Advanced modelling

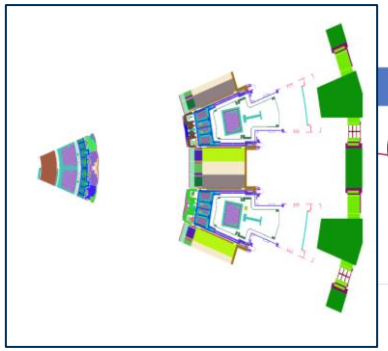
UK Atomic Energy Authority

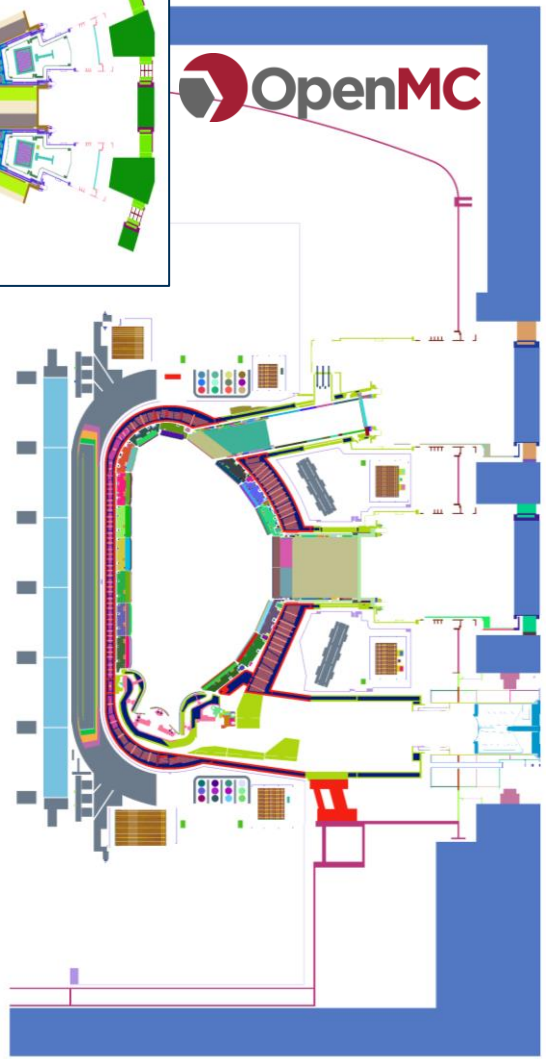
**STEP**



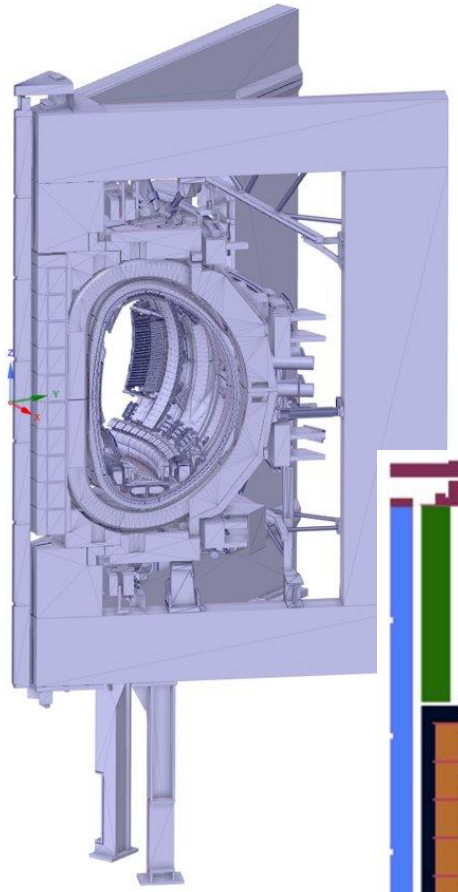




*TBR for different BZ structural content*

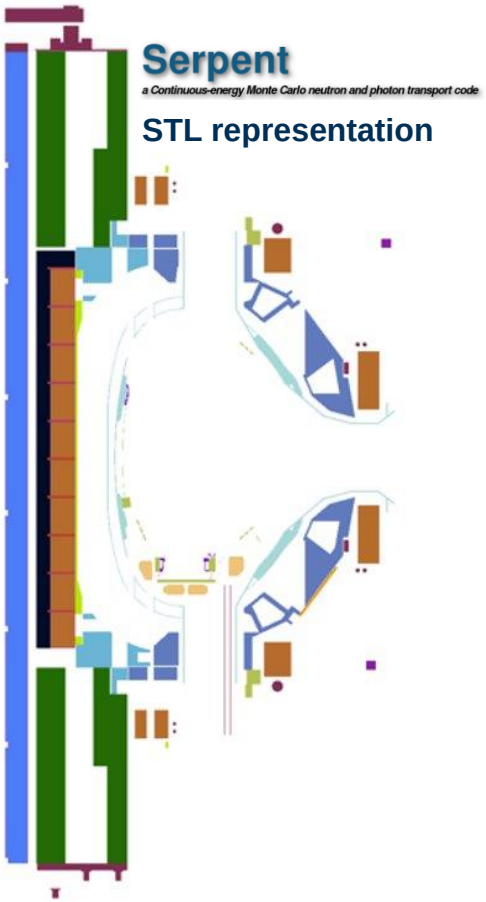





**ITER** *C-Model R181031*



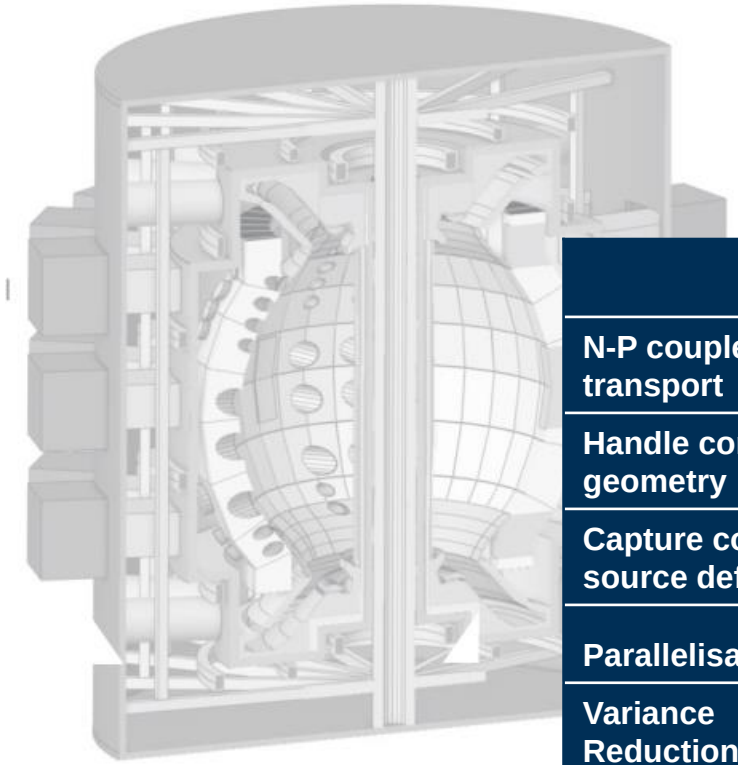
**JET**
*heterogenous waste analysis model*

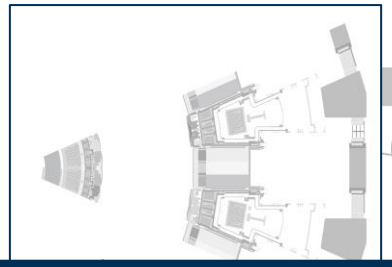



**STL representation**

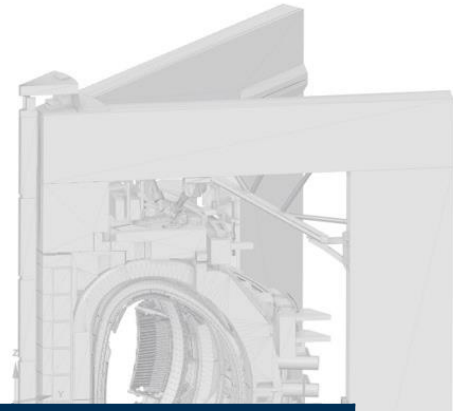
# Advanced modelling

UK Atomic Energy Authority



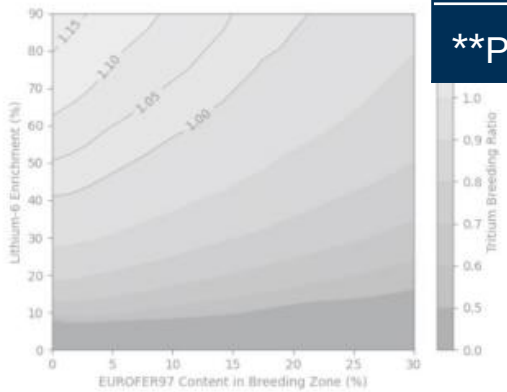


OpenMC

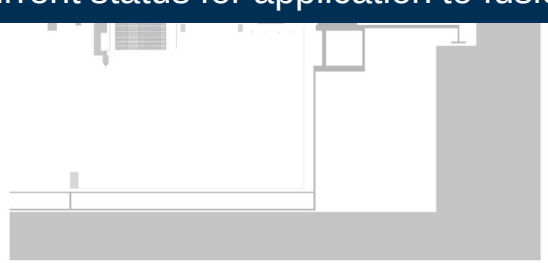


| | MCNP | OpenMC | Serpent |
|---|---|---|---|
| N-P coupled transport | | | |
| Handle complex geometry | | | |
| Capture complex source definitions | | | |
| Parallelisation | | | |
| Variance Reduction | | | |

**Personal view only of current status for application to fusion problems.




*TBR for different BZ structural content*



**ITER** *C-Model R181031*

*heterogeneous waste analysis model*


**STL representation**

UK Atomic Energy Authority

# JADE V-V tool

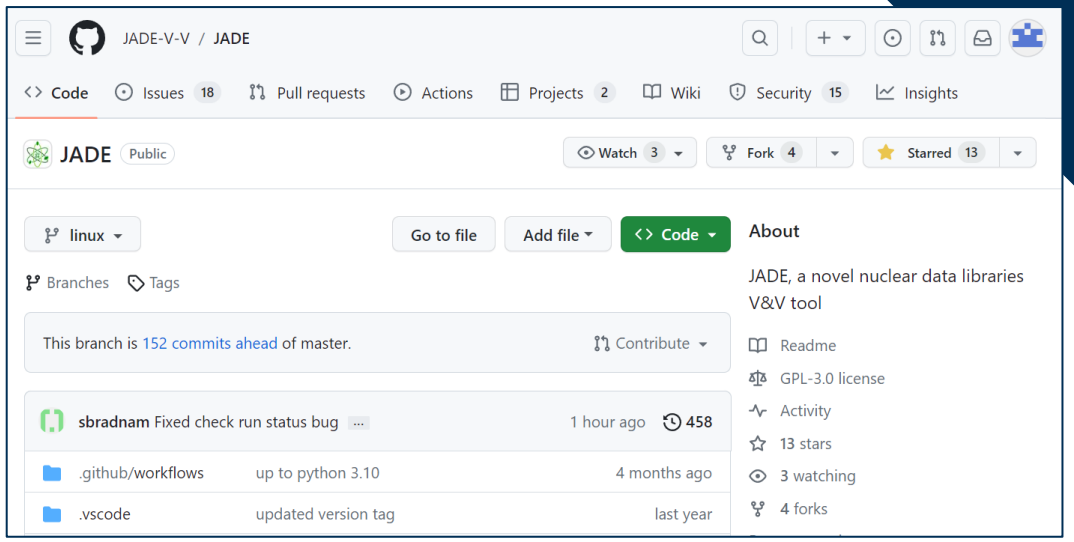
Extending the capability of the tool

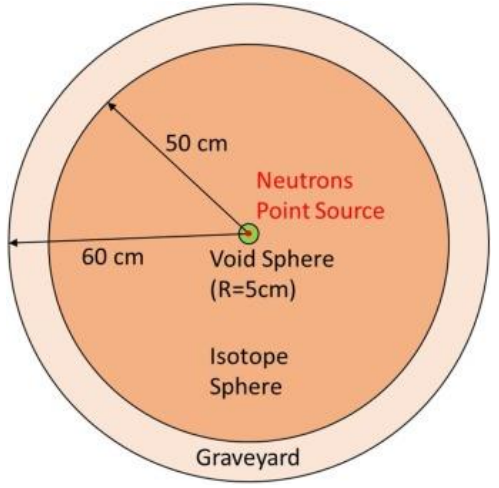
# The JADE tool for V&V

- JADE[1] is an **open source** python based tool for the validation and verification of nuclear data libraries (**see talk by D.Laghi**).
- The windows application provides a set of computational and experimental benchmarks that are performed using MCNP for given nuclear data libraries, with extensive output for analysis and examination of results.
- Recent application demonstration for JEFF-4T2 and FENDL-3.2.

- UKAEA have been contributing to the development of the tool with the following primary objectives:
  - **Develop a Linux compatible version**
  - **Restructure JADE to include additional transport codes**
  - **Develop workflow for submission in parallel**

- For the initial proof of principle, we have been using the 'sphere leakage' computational benchmark included in the JADE.

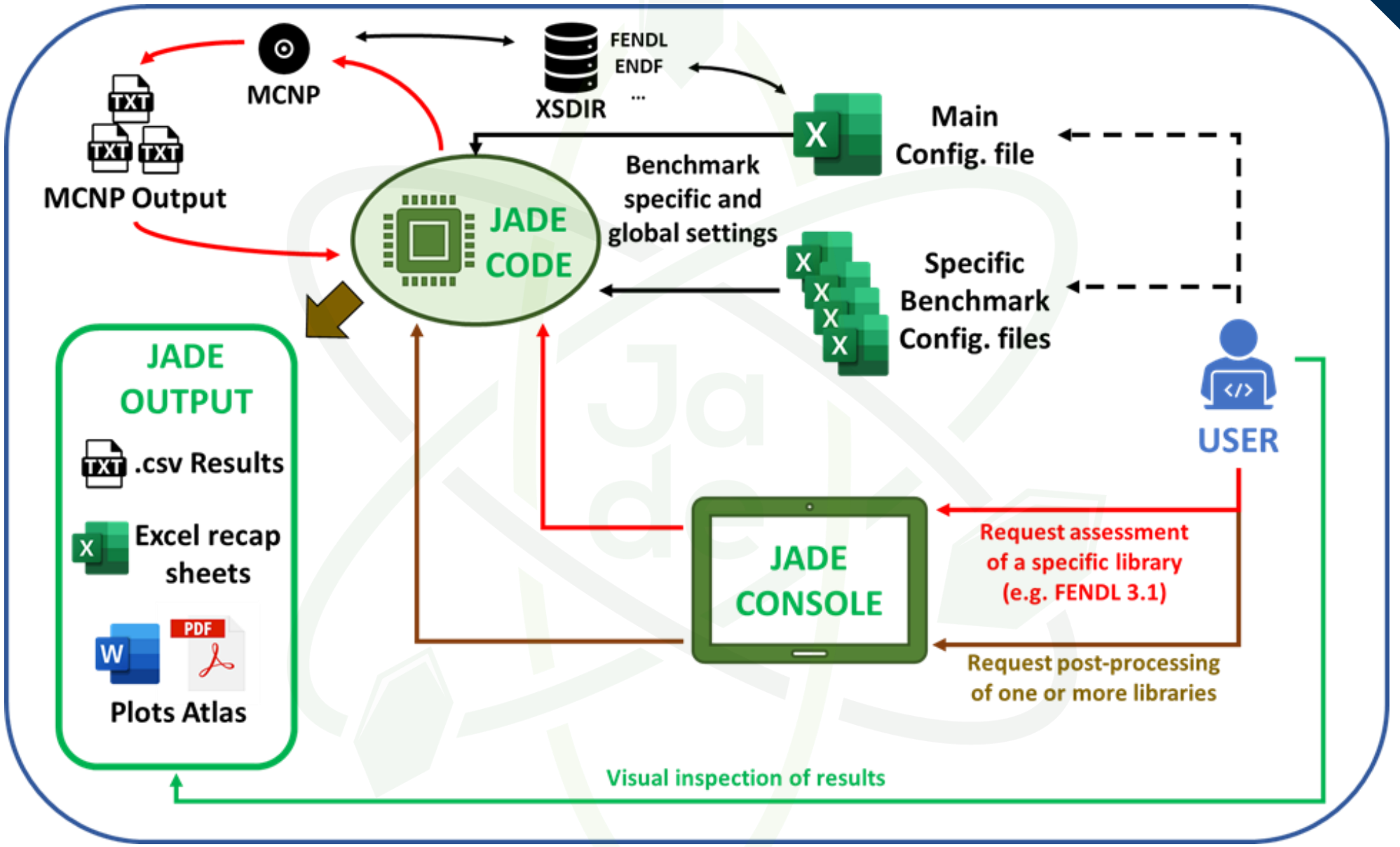


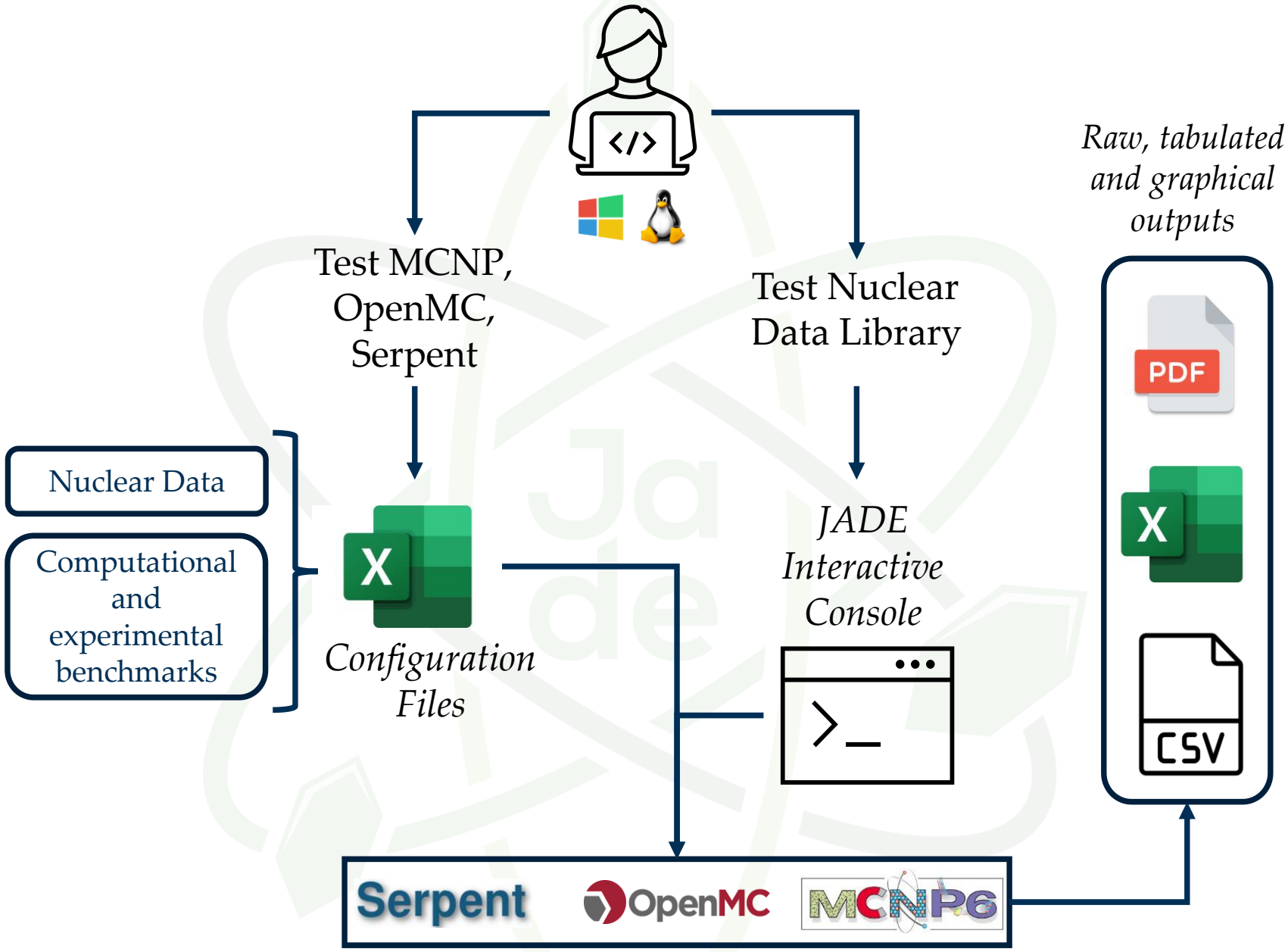

*JADE: Sphere Leakage computational benchmark.*



*[1] Davide Laghi, Marco Fabbri, Lorenzo Isolan, Raul Pampin, Marco Sumini, Alfredo Portone, Andrej Trkov, JADE, a new software tool for nuclear fusion data libraries verification & validation, Fusion Engineering and Design, Volume 161, 2020, https://doi.org/10.1016/j.fusengdes.2020.112075.*



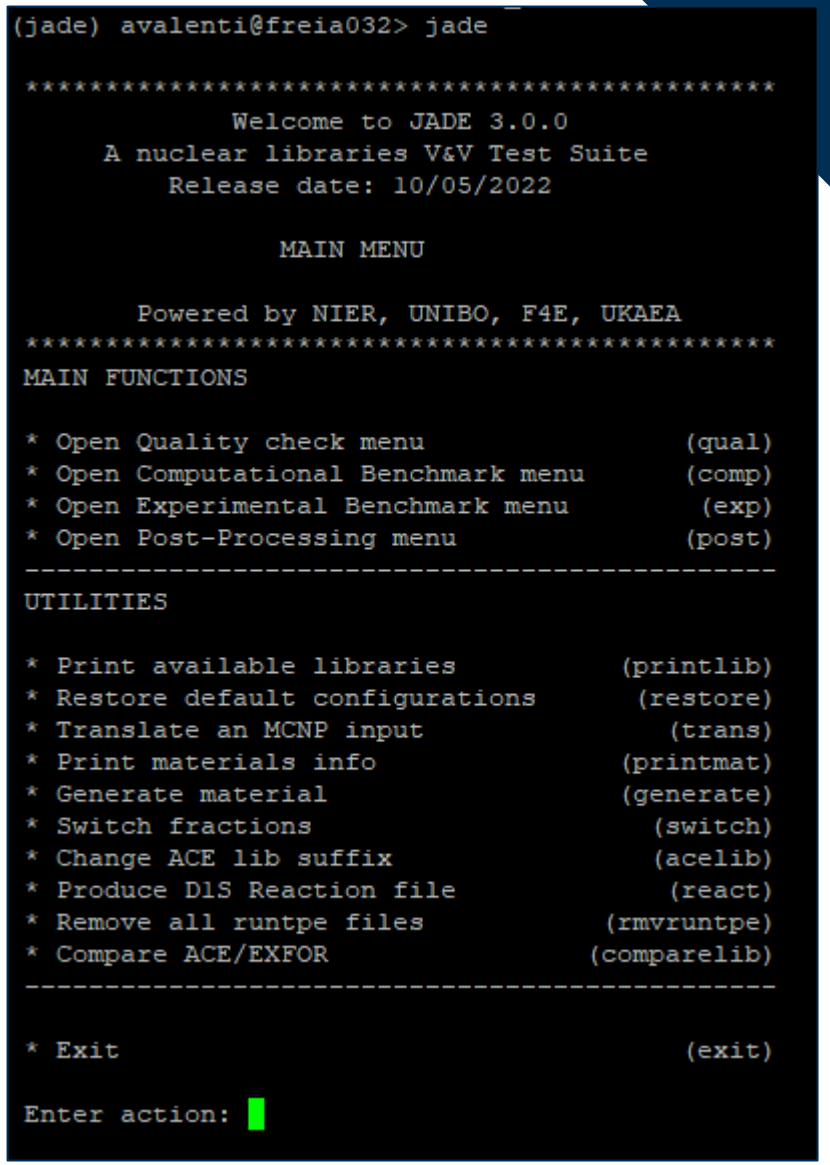

*JADE: Overview of framework*


Test MCNP, OpenMC, Serpent
Test Nuclear Data Library
Raw, tabulated and graphical outputs
Nuclear Data
Computational and experimental benchmarks
Configuration Files
JADE Interactive Console
PDF
CSV
Serpent
OpenMC
MCNP6
Execute Simulations in Parallel

# Linux compatible version of JADE

UK Atomic Energy Authority

- Dependency handling is now managed by *pip* rather than *conda*:
  - Re-configured as a command line tool that can be called with single command line argument, *'jade'.*
  - Removed the dependency on *conda*, allowing any python3 installation to be used.
- Windows-only packages have been removed.
  - Alternative multiplatform packages were implemented where needed.
  - As much as possible, retain original JADE functionality. **Tool must be able to run on both platforms**



# Modifications to configuration files

UK Atomic Energy Authority

- Configuration file extended to OpenMC and Serpent.

## Computational benchmark additional options

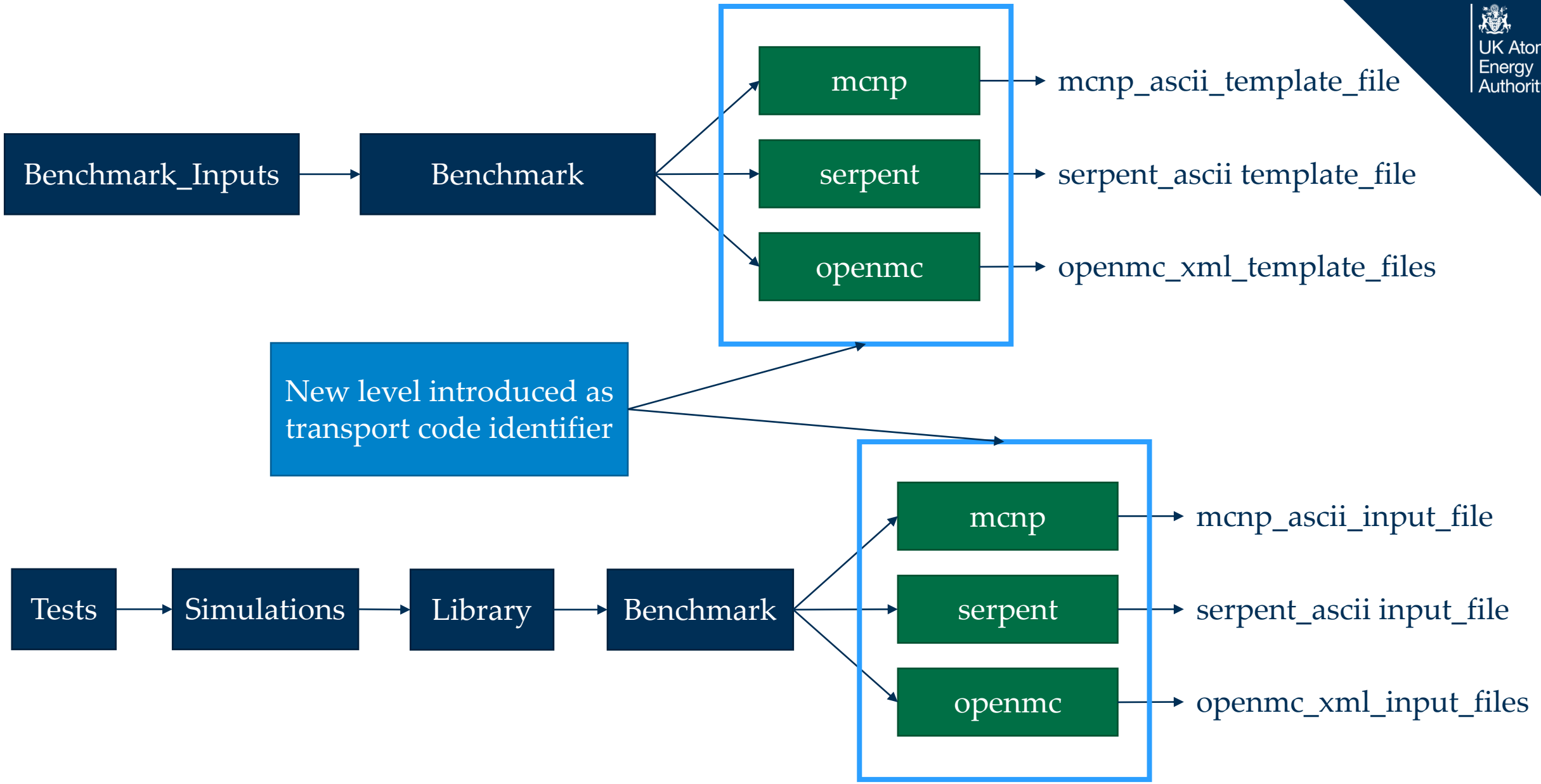
### Default Benchmarks

| Description | Folder Name | OnlyInput | MCNP | Serpent | OpenMC | d1S | Post-Processing | NPS cut-off | Custom Input |
|---|---|---|---|---|---|---|---|---|---|
| Sphere Leakage Test | Sphere | true | true | true | true | false | true | 1.00E+06 | 10 |
| ITER 1D (by M. Sawan) | ITER_1D | false | false | false | false | false | true | 5.00E+07 | |
| Helium Cooled Pebbled Bed Test Blanket Module (1D) | HCPB_TBM_1D | false | false | false | false | false | true | 1.00E+07 | |
| Water Cooled Lithium Lead Test Blanket Module (1D) | WCLL_TBM_1D | false | false | false | false | false | true | 1.00E+07 | |
| C-Model R181031 rev190715 | C_Model | false | false | false | false | false | false | 1.00E+08 | |
| ITER Cylindrical benchmark for SDDR | ITER_Cyl_SDDR | false | false | false | false | false | false | 5.00E+08 | |
| Sphere SDDR | SphereSDDR | false | false | false | false | false | false | 1.00E+08 | |

## Experimental benchmark additional options

### Default Benchmarks

| Description | Folder Name | OnlyInput | MCNP | Serpent | OpenMC | d1S | Post-Processing | NPS cut-off | Custom Input |
|---|---|---|---|---|---|---|---|---|---|
| Oktavian Experiment | Oktavian | false | false | false | false | false | true | 1.00E+07 | |
| Frascati Neutron Generator SDDR experiment | FNG | false | false | false | false | false | false | 5.00E+08 | |


Benchmark_Inputs
Benchmark
mcnp
serpent
openmc
mcnp_ascii_template_file
serpent_ascii template_file
openmc_xml_template_files
New level introduced as transport code identifier
Tests
Simulations
Library
Benchmark
mcnp
serpent
openmc
mcnp_ascii_input_file
serpent_ascii input_file
openmc_xml_input_files

# Running JADE in parallel

UK Atomic Energy Authority

- To perform validation and verification optimally for a large number of benchmarks and for complex geometries, HPC systems should be utilised for parallel submission of Monte-Carlo simulations.
- JADE can now be run either on the command line or submitted as a job. Demonstration on *LoadLeveler* submission system on the UKAEA '*freia*' HPC cluster and other UKAEA workload managers (i.e. *SLURM*).
- In principle, any workload manager can be supported by creating a template job submission file – deployment on Marconi or CSD3 (UK HPC centre) for example.

```
1   #!/bin/sh
2
3   #SBATCH --job-name="JADE"
4   #SBATCH --workdir=INITIAL_DIR
5   #SBATCH --output=OUT_FILE
6   #SBATCH --error=ERROR_FILE
7   #SBATCH --mem-per-cpu=8000
8   #SBATCH --time=16-48:00
9   #SBATCH --ntasks=MPI_TASKS
10
11  CONFIG_SCRIPT
12
13  ENV_VARIABLES
14
15  COMMAND
```

| MAIN CONFIGURATION VARIABLES | |
|---|---|
| **MCNP executable** | /home/mcnp/mcnpexecs/drake/mcnp6v2_ifort2018_n1s |
| **MCNP config** | mcnp_config.sh |
| **Serpent executable** | /home/avalenti/software/freia/Serpent2_src/v2.1.32_ccfe/sss2 |
| **Serpent config** | serpent_config.sh |
| **OpenMC executable** | /home/avalenti/software/openmc_0.13.3/build/bin/openmc |
| **OpenMC config** | openmc_config.sh |
| **d1S executable** | |
| **d1S config** | |
| **OpenMP threads** | 1 |
| **MPI tasks** | 8 |
| **Batch system** | sbatch |
| **Batch file** | Job_Script_Templates/Slurmtemplate.sh |

# Handling multiple transport codes

UK Atomic Energy Authority

- For all transport codes, we need an accurate representation of the **geometry, source term and physics.**

- ***csg2csg***[1] and are ***openmc_mcnp_adaptor*** used for conversion of geometry and materials for all current JADE benchmarks.
- Simple source terms manually replicated. For FNG, we have developed a wrapper to the MCNP source routine in OpenMC and Serpent. Material definitions for each code handled using *XsdirTable* object and developed material card writers for Serpent and OpenMC.
- Nuclear data: OpenMC uses HDF5 format nuclear data [see https://openmc.org/official-data-libraries/ ]. Distributed by FENDL? Serpent and MCNP equivalent ACE files.
- Different implementations for tallies:
  - OpenMC does not support surface flux tallies.
  - F4 + tally multiplier only applicable to MCNP.
  - Serpent only supports single isotope entry for reaction rates.
  - Different normalisations/units for each code – post processing must handle.
- Unique implementations for variance reduction.
- For the sphere benchmark, the inherent differences between the codes mean a direct translation of the full MCNP benchmark model cannot be achieved.



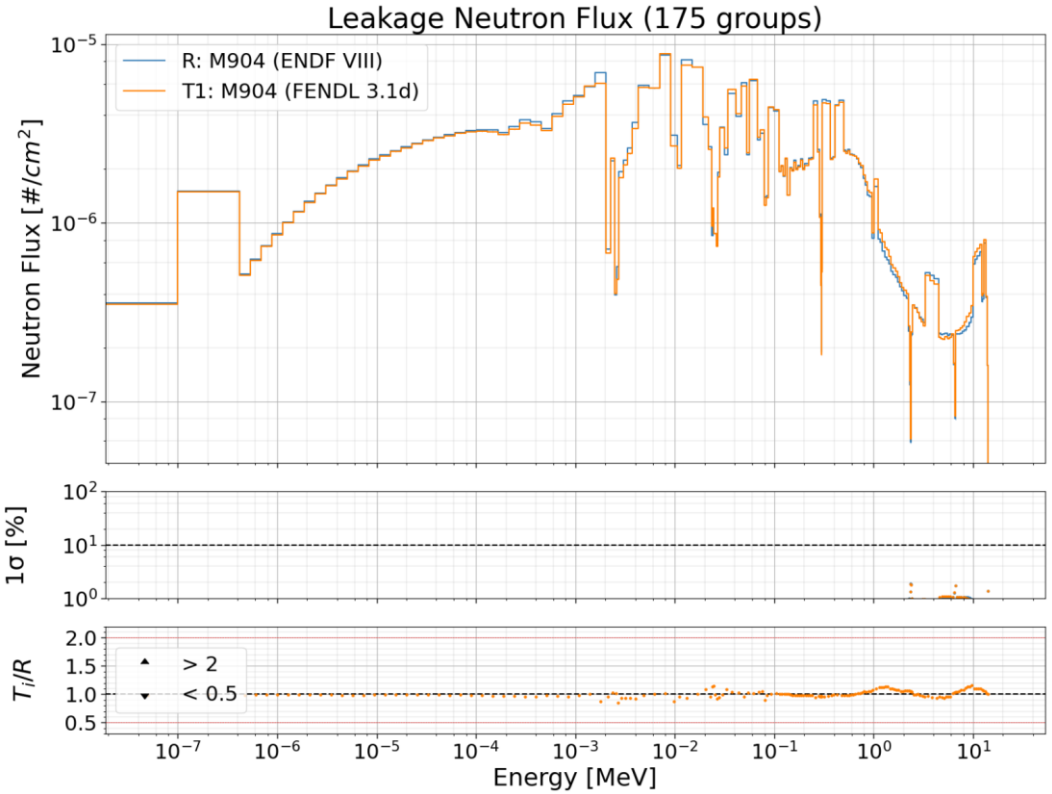
*[1] Davis, Andrew & Lilley, Steven & Shimwell, Jonathan. (2021). csg2csg: A TOOL TO ASSIST VALIDATION & VERIFICATION. EPJ Web of Conferences. 247. 04012. 10.1051/epjconf/202124704012.*

# Post-processing development

| | Output Reader | Single Library | Cross-Library | Cross Code |
|---|---|---|---|---|
| *MCNP* | ✓ | ✓ | ✓ | ◌ |
| *OpenMC* | ✓ | ✓ | ✓ | ◌ |
| *Serpent* | ◌ | ◌ | ◌ | ◌ |

*Current development status*

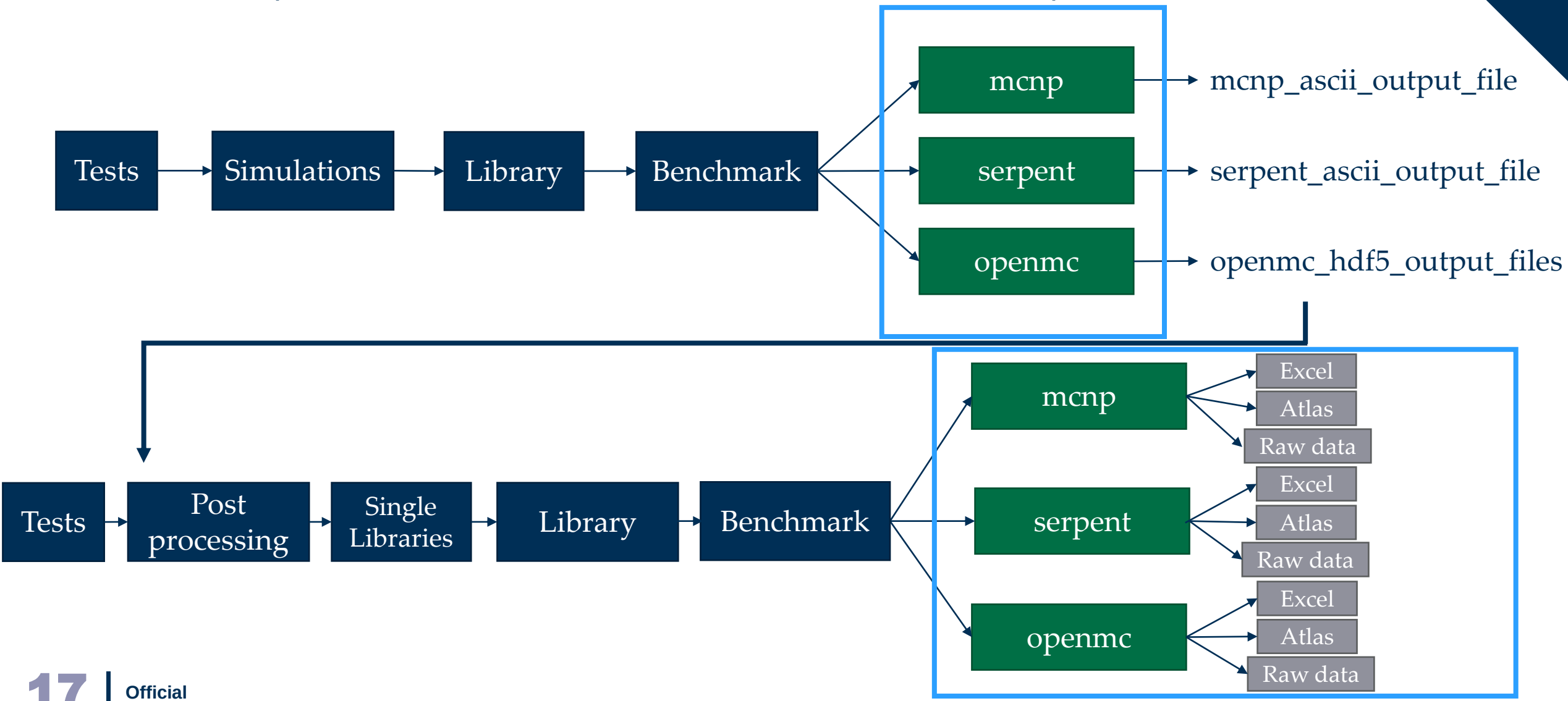
- New output parsers have been developed for OpenMC and Serpent, minimizing dependencies.




*Example of a cross library comparison of neutron flux for MCNP in the sphere leakage benchmark.*

# Post Processing

- As with the input – JADE has been restructured for additional transport codes



# Post processing

- The Excel outputs provide a powerful visualization for analysis and interpretation. This has been preserved on Linux. No changes to A*tlas* files.
- Previous, *xlwings* dependency removed. Rather than using template files, now create and write Excel file containing the post processed data using pandas and *XLSXwriter.*

| LIBRARY | 00c_Vs_31c | Target library Vs Reference library (Reference-Target)/Reference |
|---|---|---|

**SPHERE LEAKAGE % COMPARISON RECAP**

ZAID — TALLY

LEGEND
- >|20|%
- |20|%≤|10|%
- |10|%≤|5|%
- <|5|%

| Zaid | Zaid Name | 1e-07 [MeV] [t4] | 4.14e-07 [MeV] [t4] | 5.316e-07 [MeV] [t4] | 6.826e-07 [MeV] [t4] | 8.764e-07 [MeV] [t4] | 1.125e-06 [MeV] [t4] | 1.445e-06 [MeV] [t4] | 1.855e-06 [MeV] [t4] | 2.382e-06 [MeV] [t4] | 3.059e-06 [MeV] [t4] | 3.928e-06 [MeV] [t4] | 5.043e-06 [MeV] [t4] | 6.476e-06 [MeV] [t4] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1001 | H-1 | -0.001924221 | -0.00135666 | 0.000394808 | 0.001129611 | 9.9442E-05 | 0.000690478 | 0.000637707 | 0.00021077 | 0.000112808 | 0.000186848 | 0.000394182 | -0.000375637 | 0.000540307 |
| 1002 | H-2 | 0.03547722 | 0.039111703 | 0.032864011 | 0.018601666 | 0.048988675 | 0.037060221 | 0.025207034 | 0.030567043 | 0.03551103 | 0.029176764 | 0.037970908 | 0.030991795 | 0.033814517 |
| 1003 | H-3 | 2.09434E-05 | -1.7701E-05 | 9.39538E-05 | -3.2355E-05 | 5.68867E-05 | 1.00677E-05 | 1.94231E-05 | -7.04671E-06 | 1.82404E-05 | Identical | 3.21384E-06 | Identical | 2.98309E-06 |
| 2003 | He-3 | Not Available | Not Available | Not Available | Not Available | Not Available | 0.001968784 | 0.001801894 | Not Available | 0.001718885 | Not Available | 0.001426892 | 0.001533082 | 0.001669799 |
| 3006 | Li-6 | Not Available | Not Available | Not Available | Not Available | Not Available | 0.000327636 | 0.000328343 | Not Available | 0.000342789 | Not Available | 0.000387335 | 0.000402149 | 0.000792378 |
| 3007 | Li-7 | -7.68626E-06 | 6.33718E-05 | 9.45776E-06 | 5.38757E-06 | -0.000793521 | -9.3308E-06 | 1.42525E-05 | Identical | 7.74006E-05 | Identical | 4.56249E-05 | 0.011444462 | -0.008515467 |
| 4009 | Be-9 | 0.000806998 | 0.00124002 | 0.00133502 | 0.003734853 | 0.003200038 | -1.76838E-05 | 0.003381877 | 0.000919165 | 0.002858739 | 0.000731212 | 0.003330858 | 0.002081058 | 0.003550204 |
| 5010 | B-10 | Not Available | Not Available | Not Available | Not Available | Not Available | -0.000847666 | -0.000830007 | Not Available | -0.000768667 | Not Available | -0.000601044 | -0.000530192 | -8.14298E-05 |
| 5011 | B-11 | -0.000292379 | -0.000225422 | 0.000463253 | -3.37136E-05 | 9.18493E-06 | -0.000114033 | -0.000559416 | 0.000319015 | -0.00022825 | -7.3977E-05 | 0.000237037 | -0.000222869 | 1.91647E-05 |
| 6012 | C-12 | 0.008433724 | 0.007313056 | 0.005699427 | 0.004464129 | 0.004663368 | 0.004061473 | 0.004614031 | 0.005106228 | 0.003896254 | 0.003417881 | 0.003663339 | 0.003775828 | 0.004081135 |
| 6013 | C-13 | 0.421709453 | 0.251551921 | -0.185447727 | -0.191863271 | -0.199437094 | -0.20002315 | -0.209865084 | -0.21431554 | -0.218446501 | -0.225635386 | -0.231314783 | -0.236897382 | -0.245957765 |
| 7014 | N-14 | Not Available | Not Available | Not Available | Not Available | Not Available | Identical | Identical | Not Available | Identical | Not Available | Identical | Identical | Identical |
| 7015 | N-15 | Not Available | Not Available | Not Available | Not Available | Not Available | Identical | Identical | Not Available | Identical | Not Available | Identical | Identical | Identical |
| 8016 | O-16 | Not Available | Not Available | Not Available | Not Available | Not Available | Identical | Identical | Not Available | Identical | Not Available | Identical | Identical | Identical |
| M101 | SS316L(N)-IG | -0.066043839 | -0.041555803 | -0.069184258 | -0.080374098 | -0.073125 | -0.068473237 | -0.067394981 | -0.066466462 | -0.063236719 | -0.06361713 | -0.061197676 | -0.055023823 | -0.054477566 |
| M901 | olyethylene (non-borate | -0.000906151 | -0.000181224 | 0.001025546 | 0.001275421 | 0.002701598 | 0.000237836 | 0.000468305 | 0.00321608 | 0.002155598 | 2.52773E-05 | 0.000752448 | 0.001911431 | 0.002199026 |
| M904 | Resistive_magnet | 0.019907667 | 0.010214111 | 0.01865274 | 0.01109531 | 0.011834153 | 0.012453345 | 0.007935881 | 0.006267674 | 0.010346922 | 0.0098175 | 0.011911765 | 0.018720645 | 0.013267567 |
| M905 | mat_Thermal_Shield | -0.142739711 | -0.062302974 | -0.042658563 | -0.042135648 | -0.045576739 | -0.04737036 | -0.059829669 | -0.062137262 | -0.064061195 | -0.066513444 | -0.062924859 | -0.057211791 | -0.053017991 |
| M903 | mat_PF_coil_casing | -0.142739711 | -0.062302974 | -0.042658563 | -0.042135648 | -0.045576739 | -0.04737036 | -0.059829669 | -0.062137262 | -0.064061195 | -0.066513444 | -0.062924859 | -0.057211791 | -0.053017991 |
| M902 | at_TF_Coil_inb inb_tf_ta | -0.000983393 | 0.000800827 | 0.002239686 | 0.001016973 | 0.00190137 | 0.001635419 | 0.007243558 | 0.010295114 | 0.003639734 | 0.011136934 | 0.01050927 | -0.003070894 | 0.012257824 |
| M909 | mat_Shield_inboard_3 | 0.040038937 | 0.010281627 | 0.012732987 | 0.019451192 | 0.031280321 | 0.019863738 | 0.008671636 | 0.01350653 | 0.010000884 | -0.005481736 | 0.020354941 | 0.009537481 | 0.009136451 |
| M200 | Ordinary Concrete | 0.043804384 | 0.011108788 | -0.00240026 | -0.00368184 | -0.003050864 | 9.24682E-05 | -0.002325551 | -0.006602414 | -0.00474687 | -0.003688773 | -0.0029268 | -0.007727929 | -0.003920163 |
| M906 | mat_VV vv_steel | -0.004192636 | -0.004309583 | -0.004364616 | -0.001362998 | 0.000608059 | -0.004393215 | -0.000757066 | 0.001250784 | -0.004010782 | 0.003605748 | -0.003318341 | -0.001769325 | 0.006155134 |
| M907 | mat_Shield_inboard_1 | 0.022866286 | 0.013741349 | 0.019084322 | -3.12301E-05 | 0.011506928 | 0.010972879 | 0.021710655 | 0.013581293 | -0.003875144 | -0.005446633 | 0.018346051 | 0.020964006 | 0.003320579 |
| M911 | IFW_W80_E7_h2o13 | -0.02433174 | -0.00416192 | 0.039804976 | -0.002722465 | 0.031367763 | -0.037938785 | 0.013510725 | -9.18437E-05 | -0.003433815 | 0.015313588 | 0.052303217 | 0.012111482 | 0.018988091 |
| M400 | Water | -0.004170168 | -0.003834117 | -0.002714601 | -0.000935588 | -0.003528757 | -0.001375134 | -0.002129894 | -0.001028843 | -0.003044598 | -0.002458647 | -0.001252296 | -0.003223166 | -0.001818585 |
| M203 | Boron Carbide | -0.1376399 | -0.311432409 | Reference = 0 | -0.001016922 | -0.790099471 | -5.73547E-06 | -0.003601414 | -0.023401764 | -0.006967725 | -0.137489275 | 0.2686655 | 0.137024516 | -0.00715216 |
| M900 | Natural Silicon | Not Available | Identical | 3.18947E-06 | 3.3842E-06 | 7.91039E-06 | 6.5392E-06 | 4.23409E-06 | 4.20495E-06 | 6.99291E-06 | 6.41626E-06 | 3.93767E-06 | 3.04532E-06 | -4.8453E-05 |
| M908 | mat_Shield_inboard_2 | -0.010139347 | -0.007005009 | -0.002201916 | 0.001576067 | -0.002092215 | -0.001998208 | 0.001099141 | 0.000526179 | -0.009058682 | -0.001796027 | -0.003506908 | -0.007635543 | -0.001403528 |

**GLOBAL QUICK RESULT: % of cells per range of comparison differences**

| Range | 1e-07 [MeV] [t4] | 4.14e-07 [MeV] [t4] | 5.316e-07 [MeV] [t4] | 6.826e-07 [MeV] [t4] | 8.764e-07 [MeV] [t4] | 1.125e-06 [MeV] [t4] | 1.445e-06 [MeV] [t4] | 1.855e-06 [MeV] [t4] | 2.382e-06 [MeV] [t4] | 3.059e-06 [MeV] [t4] | 3.928e-06 [MeV] [t4] | 5.043e-06 [MeV] [t4] | 6.476e-06 [MeV] [t4] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 < % of cells < 5.0 | 0.772727273 | 0.826086957 | 0.869565217 | 0.913043478 | 0.869565217 | 0.931034483 | 0.862068966 | 0.826086957 | 0.862068966 | 0.782608696 | 0.793103448 | 0.827586207 | 0.862068966 |
| 5.0 < % of cells < 10.0 | 0.045454545 | 0.086956522 | 0.043478261 | 0.043478261 | 0.043478261 | 0.034482759 | 0.103448276 | 0.130434783 | 0.103448276 | 0.130434783 | 0.137931034 | 0.103448276 | 0.103448276 |
| 10.0 < % of cells < 20.0 | 0.136363636 | 0 | 0.043478261 | 0.043478261 | 0.043478261 | 0 | 0 | 0 | 0 | 0.043478261 | 0 | 0.034482759 | 0 |
| % of cells > 20.0 | 0.045454545 | 0.086956522 | 0.043478261 | 0 | 0.043478261 | 0.034482759 | 0.034482759 | 0.043478261 | 0.034482759 | 0.043478261 | 0.068965517 | 0.034482759 | 0.034482759 |

UK Atomic Energy Authority

# UKAEA Future Effort

FENDL validation and importance for future applications

# Additional benchmarks in JADE

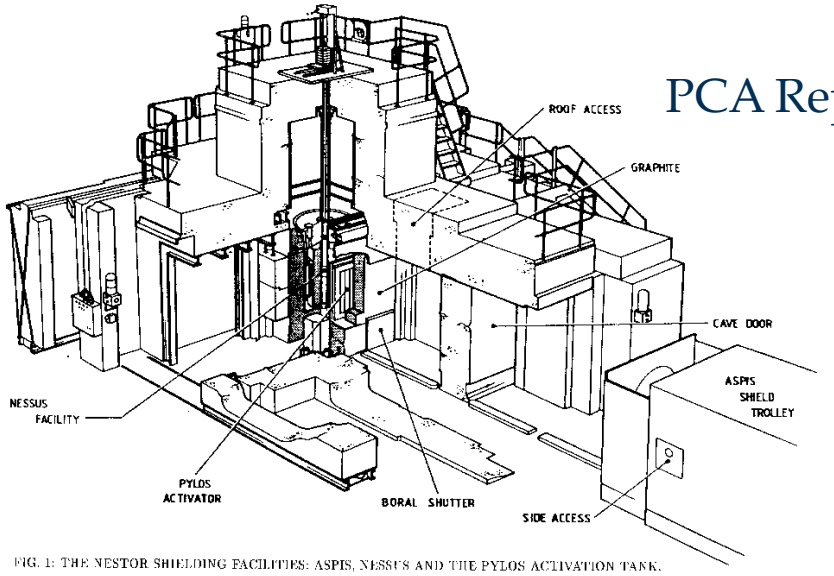
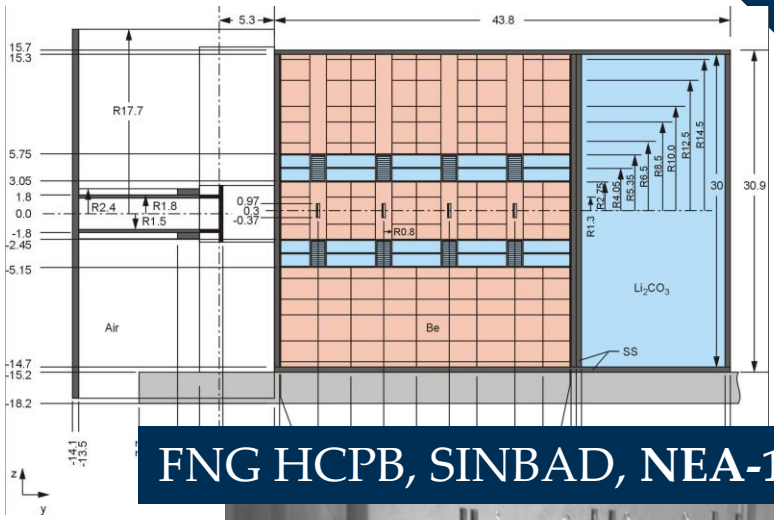
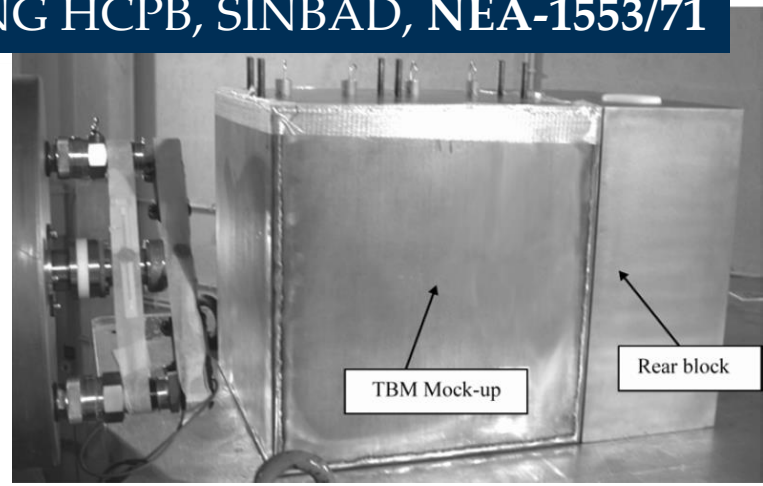


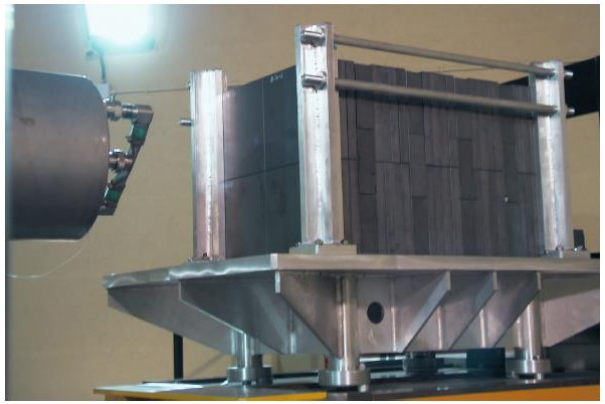
FIG. 1: THE NESTOR SHIELDING FACILITIES: ASPIS, NESSUS AND THE PYLOS ACTIVATION TANK.

PCA Replica, **NEA-1517/75**

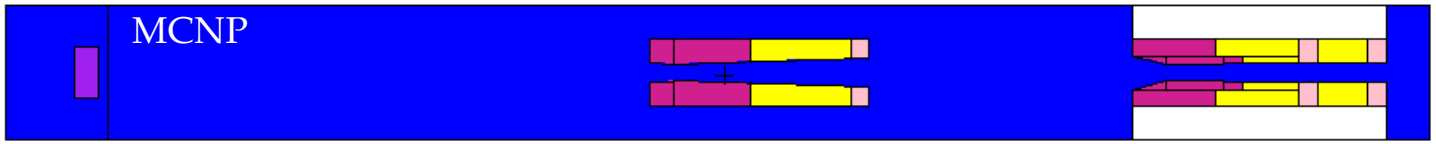



FNG HCPB, SINBAD, **NEA-1553/71**



FNG SiC, SINBAD, **NEA-1553/56**




CIAE Fe, **CoNDERC, IAEA**

**Openly available, interoperable benchmark data is fundamental to these efforts**

# Future work

UK Atomic Energy Authority

- Currently working towards a release **v3.0.0** of the code in Q1 2024. Complete JADE portability to Linux without feature loss from current version.

- ❑ Complete functionality for OpenMC and Serpent across all benchmarks.
- ❑ Further addition of 1D benchmarks – consider parametric builds. Important for STEP and UKAEA Fusion Futures programme.
- ❑ Addition of FNG Cu.
- ❑ Variance reduction techniques developed where required.
- ❑ JADE GUI
- ❑ Work with OpenMC and Serpent developers on addressing needs for JADE.

UK Atomic Energy Authority

# Thank you for listening

Alex.Valentine@ukaea.uk


https://github.com/JADE-V-V