UK Atomic Energy Authority

Benchmark experiment databases and sensitivity and uncertainty analysis tools for nuclear data V&V

I. Kodeli

ARIEL Meeting, March 16, 2023

Research Councils UK Energy For a Low Carbon Future
This work was funded by the RCUK Energy Programme
[Grant number EP/T012250/1]

CCFE CULHAM CENTRE FOR FUSION ENERGY

Neutron transport – Boltzmann equation

- *Rate of particle gain = Rate of particle loss*

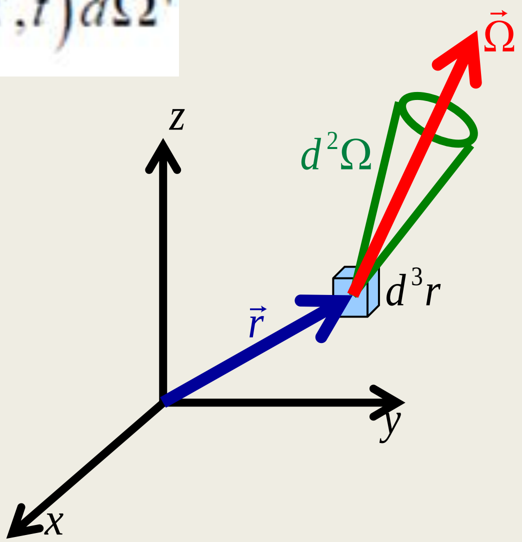
or:

- *Inscattering gain + Source production gain = Leakage loss + Outscattering loss*

$$\frac{1}{v}\frac{d\phi(\bar{r},E,\bar{\Omega},t)}{dt}+\bar{\nabla}\cdot\bar{\Omega}\phi(\bar{r},E,\bar{\Omega},t)+\Sigma_T(\bar{r},E)\phi$$
$$=S(\bar{r},E,\bar{\Omega},t)+\int dE'\int\Sigma_S(\bar{r},E'\rightarrow E,\bar{\Omega}'\rightarrow\bar{\Omega}')\phi(\bar{r},E',\bar{\Omega}',t)d\bar{\Omega}'$$

Statistical approach: n = average particle density in a particular region of phase space at a certain time t

$$\Phi(\vec{r},\vec{\Omega},E,t)=vn(\vec{r},\vec{\Omega},E,t)$$



Ludwig Boltzmann

Ludwig Boltzmann

Born	Ludwig Eduard Boltzmann February 20, 1844 Vienna, Austrian Empire (present-day Austria)
Died	September 5, 1906 (aged 62) Tybein near Trieste, Austria-Hungary (present-day Duino, Italy) Suicide
Residence	Austria, Germany
Nationality	Austrian
Fields	Physics
Institutions	University of Graz University of Vienna University of Munich University of Leipzig
Alma mater	University of Vienna
Doctoral advisor	Josef Stefan
Doctoral students	Paul Ehrenfest Philipp Frank Gustav Herglotz Franc Hočevar Ignacij Klemenčič
Other notable students	Lise Meitner
Known for	Boltzmann constant Boltzmann equation Boltzmann distribution H-theorem

BOLTZMANN transport equation: assumptions

$$\frac{1}{\mathrm{v}}\frac{\partial}{\partial \mathrm{t}}\Phi = B\Phi + Q = \left(P - L\right)\Phi + Q$$

- <u>**Diluted gas approximation:**</u> only collisions between 2 particles are considered, 3-body collisions are assumed to be very rare
- <u>**Molecular chaos approx.:**</u> no correlation between colliding particles, so that the movement is fully chaotic; (W_{12}=W_1 W_2)
- The <u>**collision time is much shorter**</u> than the time that elapses between collisions; time rate of change of W_1 and W_2 can be neglected.
- Over the range of the forces of interaction, the <u>**gradient of inhomogeneities in the transport medium may be ignored**</u>. This assumption effectively makes *W* a function of (r_1-r_2) only, and allows gradients of *W* to be neglected over a distance of the range of molecular forces.

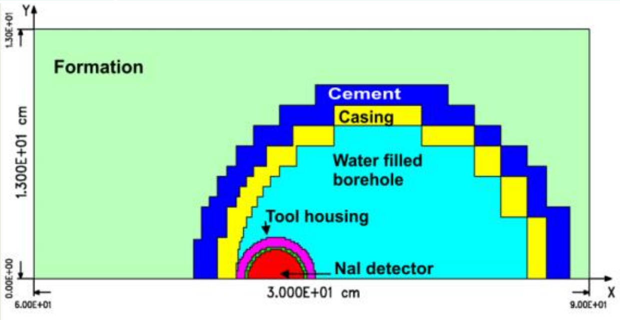
Boltzmann – Louville equations

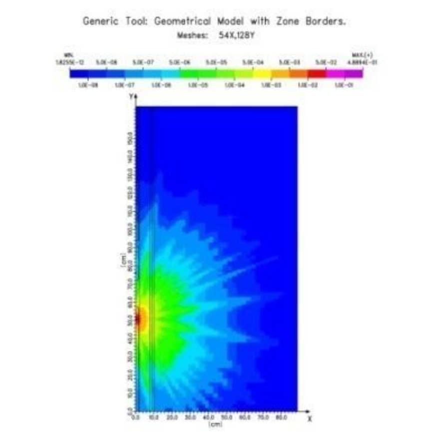
$$\frac{1}{\mathrm{v}}\frac{\partial}{\partial \mathrm{t}}\Phi = B\Phi + Q = (P - L)\Phi + Q$$

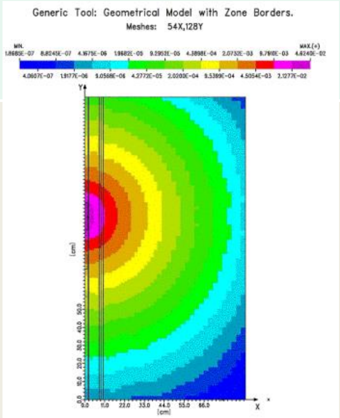
$f_1(r,v,t)$, as defined in Louville equation, is the probability (averaged over phase space) that particle number one is at position r with velocity v at time t. The Boltzmann equation, however, is a balance equation for $f(r,v,t)$, where $f(r,v,t)dr\, dv$ is the average number of particles in the volume element dr with velocity lying between v and $v+dv$ at time t.

Deterministic vs. Monte Carlo Methods

	Deterministic (DOORS, PARTISN, ATTILA, DENOVO, THOR)	Monte Carlo (MCNP, SERPENT, TRIPOLI, OpenMC, MCBEND)
+	• Low CPU time • Detailed flux distributions • Suitable for sensitivity and uncertainty analyses	• Exact geometry description • Pointwise cross section treatment
-	• Discretisation ➔approximate representation in space, energy, angle • Case dependent multigroup cross sections (self-shielding, weighting spectra) • Memory needs	• Long CPU time • Statistical uncertainties, difficulty in using variance reduction • “Limited” information (integral quantities)







Evaluated Cross Section Files Data and Formats

General purpose lib.

- **BROND-3.1**
- **CENDL-3.1**
- **ENDF/B-VIII**
- **JEFF-3.3**
- **JENDL-5.0**
- **RUSFOND-2010**
- **TENDL-2021**

E ~ 10^{-5} eV – 150 MeV

- **MF=1**: description text
- **MF=2**: resonances parameters
- **MF=3**: energy cross-sections
- **MF=4**: angular Distributions
- **MF=5**: energy Distributions
- **MF=6**: energy-angle distributions
- **MF=7**: thermal scattering data
- **MF=8**: radioactive data
- **MF=9-10**: nuclide production data
- **MF=12-15**: photon production data
- **MF=30-40**: covariance data

Main uncertainties in Neutronics Calculations

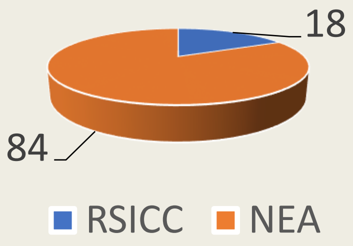
- Mathematical methods and simplifications: e.g. M/C statistics, S_N space/energy/angular discretization, anisotropic scattering order, convergence criteria
- **Nuclear data uncertainties**: nuclear cross-sections, fission spectra (U, Pu), standards, response functions (kerma, dpa)
- Radiation source description (space/energy distribution)
- Geometry modelling, material compositions, conditions (1D/2D/3D, temperature, exact locations…)
- "Human factor"
- **Validation & Verification**
  - **Benchmark experiments**
  - **Sensitivity and uncertainty analysis**

- Benchmark experiments
- ND Sensitivity/uncertainty analysis & SUSD3D/XSUN-2023

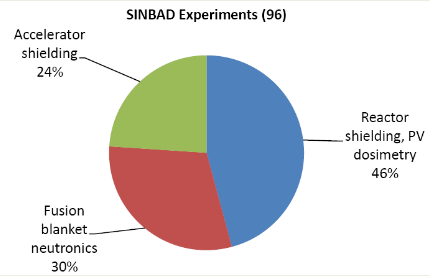
Benchmark experiments

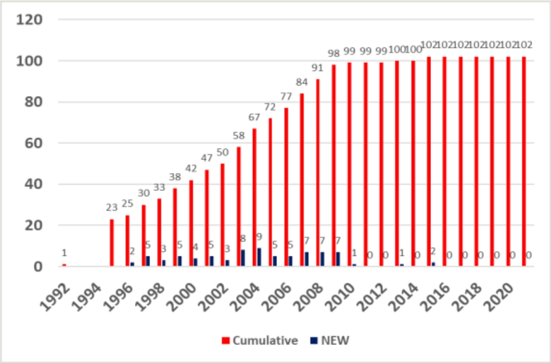
- **Preserve results from expensive experiments in an user-friendly format**
- **Evaluate the quality, consistency and completeness of experimental information**
- **Validation of** radiation transport codes, nuclear data performance, reactor design concepts / components
- Developing an approach of global method and data validation, using integral experiments
- **Education & training**
- OECD/NEA NSC sponsored projects on integral experiments:
  - **SINBAD** - Radiation **Shielding** Experiments
  - **ICSBEP** - International Handbook of Evaluated **Criticality Safety** Benchmark Experiments
  - **IRPhEP** - **Reactor Physics** Experiments

SINBAD - Radiation Shielding Experiments



- Objective: Compilation of high-quality experiments for validation and benchmarking of computer codes and nuclear data used for radiation transport and shielding problems encompassing:
  - reactor shielding, PV dosimetry **(48)**
  - fusion blanket neutronics **(31)**
  - accelerator shielding **(23)**





- **Quality review – 51 benchmarks**

Simplicity of use; easy & low-cost maintenance

- **OECD/NEA Working Party on Scientific Issues of Reactor Systems (WPRS) Expert Group on Physics of Reactor Systems (EGPRS): monitor, steer and support the continued development of SINBAD (Chair R. Grove, ORNL)**
- **Working Party on Evaluation Cooperation (WPEC) - SG47 "Use of SINBAD for Nuclear Data Validation" 2019 – 2022 (I. Kodeli)**
- **NEA Task Force on SINBAD development (>2022) (T. Miller, ORNL, O. Buss, NEA)**

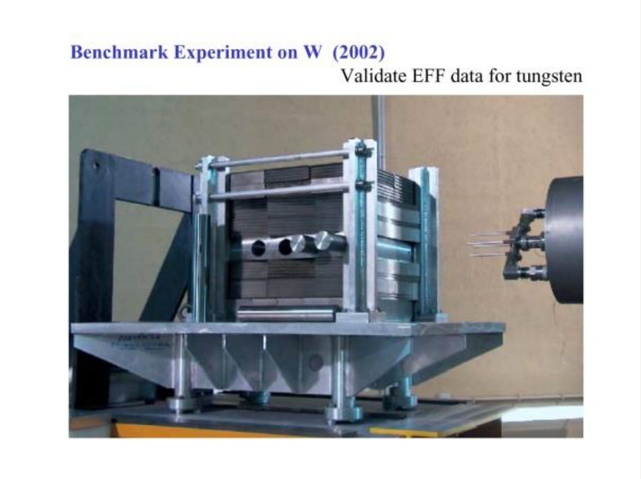
Distribution on CD-ROM by the NEA DB and the RSICC.

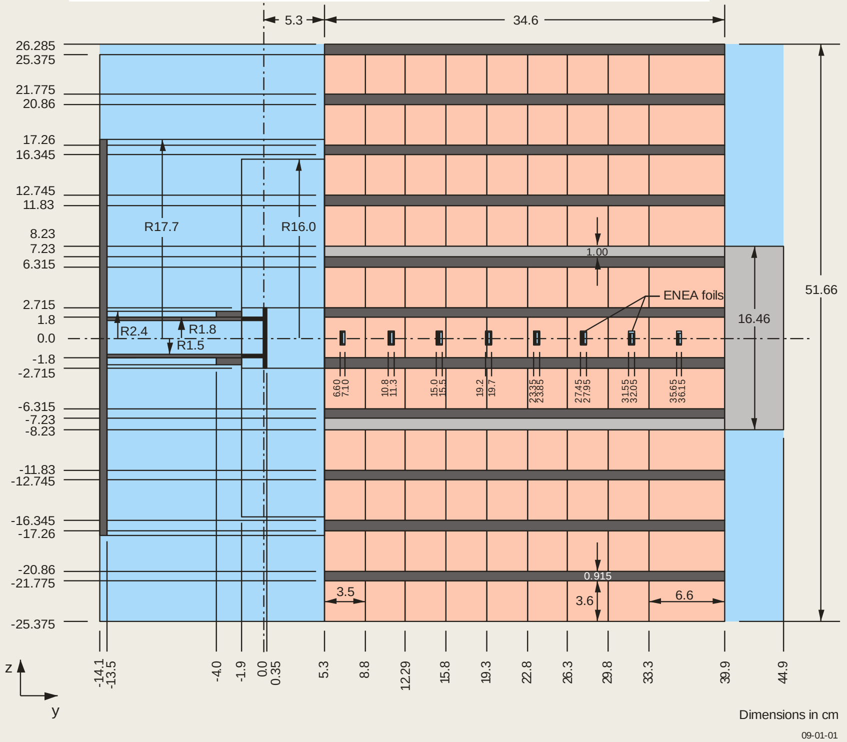
- https://www.oecd-nea.org/science/wprs/shielding/sinbad/
- http://www-rsicc.ornl.gov/BENCHMARKS.aspx

SINBAD (Radiation Shielding Experiments Data Base)

Shielding Materials

- Fe/SS (27 benchmarks)
- H_2O (11)
- Air (9)
- Na (6)
- Concrete (5)
- Pb, W, Si/SiC (4)
- Graphite, Al (3)
- O, V, Cu (2)
- Li, Mn, Ni, N, Nb, Be, Th, Bi, $(CH_2)_{2n}$ (1)
- Multiple materials (18)

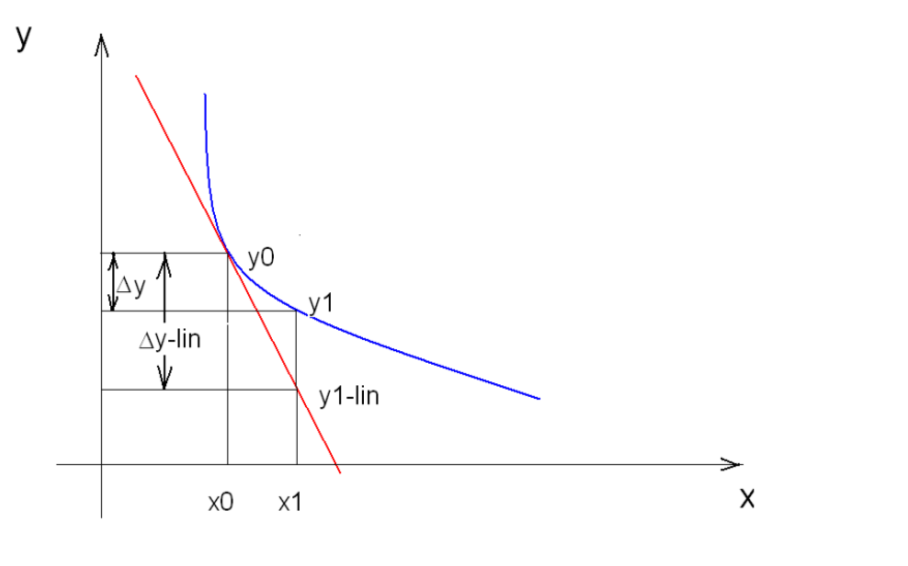




- Benchmark experiments
- ND Sensitivity/uncertainty analysis & SUSD3D/XSUN-2023

Propagation of uncertainty – "sandwich" formula

Often a quantity (y) is not measured directly, but is obtained from other quantities (x). In first order approximation:



$$y_j = y_j(x_i)$$

$$\vec{y} = (y_i^t), \vec{x} = (x_i^t)$$

$$y = ax$$

$$\delta y = a\,\delta x + x\,\delta a + \delta a\,\delta x$$

$$\frac{\delta y_j}{y_j} = \sum_i \left.\frac{x_i \partial y_j}{y_j \partial x_i}\right|_{x=\langle x\rangle} \frac{\delta x_i}{x_i} + \ldots$$

$$V(\vec{y}) = S^t \cdot V(\vec{x}) \cdot S$$

$$V_{ij} = \frac{<\delta x_i \delta x_j>}{<x_i><x_j>} = \text{relative covariance matrix}$$

$$S_{ij} = \frac{x_j}{y_i}\frac{\partial y_i}{\partial x_j} = \frac{\partial \ln y_i}{\partial \ln x_j} = \text{relative sensitivity matrix}$$

Derivatives are evaluated at 1st order, i.e. assumed constant for the variations around <x> within the interval described by the corresponding uncertainties (δx) ⇒ ***valid for linear relations between quantities within few σ (or small uncertainties).***

Methods for Cross-section Sensitivity Analysis

- Analytical method
- **Several independent calculations (brute force)** – time consuming but possible with todays computers (**total M/C-** TENDL, XSUSA)
- **Perturbation methods: sensitivity of a small number of responses to a very large number of uncertain inputs;**
  - forward and adjoint (deterministic, Monte Carlo) flux calculations; 1^{st} order perturbations;
  - Monte Carlo differential operator perturbation method, correlated sampling;
- Examples of available computer codes:

  ERANOS, TSUNAMI, SUSD3D, SERPENT, MCSEN, MCNP-6, XSUSA, TENDL based code systems

Eugène P. WIGNER « Effect of Small Perturbations on Pile Period » classified document of Manhattan Project (CP 3048, 13 june 1945).

L. N. USACHEV: Equations for the Importance of neutrons, reactor kinetics and the theory of perturbations, Int. Conf. Peaceful Uses of Atomic Energy 5, 503-510, UN, N.Y. (1955).

L.N. USACHEV, « *Perturbations theory for the breeding ratio and for other number ratios pertaining to various reactor processes* », J. Nucl. Energy, 18 p.571 (1964)

A.GANDINI, « *A generalized perturbation method for bilinear fuctionals of the real and adjoint fluxes* » J. Nucl. Energy, 21, 735-745, 1967.

M. L. Williams, Perturbation Theory for Nuclear Reactor Analysis, CRC Press, 1986

- **Multiplication factor**
- **BOC peak to average power**
- **Control rod worth**
- **Breeding ratio**
- **Moderator void coefficient**
- **Absorbed radiation dose**
- **Material damage**
- **Detector reading, ex core**
- **Peak transient power**
- **EOC fuel inventory**
- **EOC reactivity and EOC neutron flux**

Direct and adjoint transport equation – importance fonction

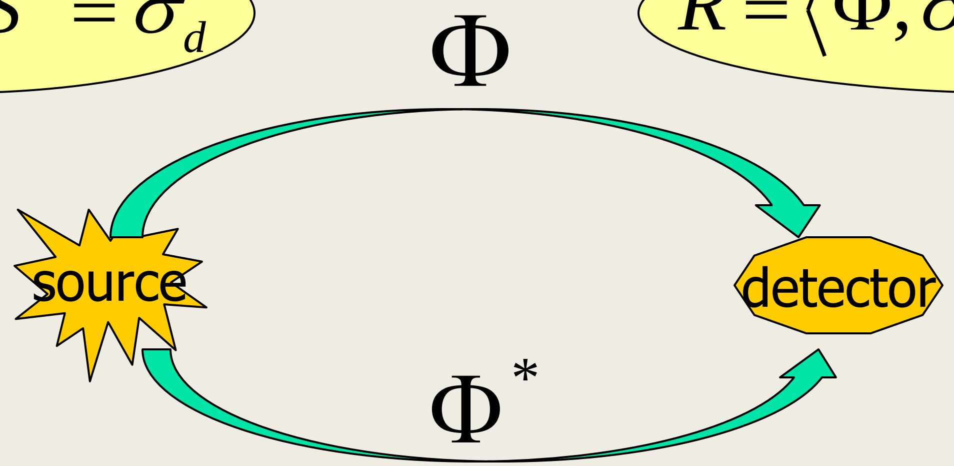
Calculation of the reaction rates:

$$R = \langle \sigma_d \cdot \Phi \rangle = \int_V \int_0^{E_{\max}} \int_{4\pi} \Phi(\vec{r}, \vec{\Omega}, E) \sigma_d (\vec{r}, \vec{\Omega}, E) \, d\vec{r} dE d\vec{\Omega}$$

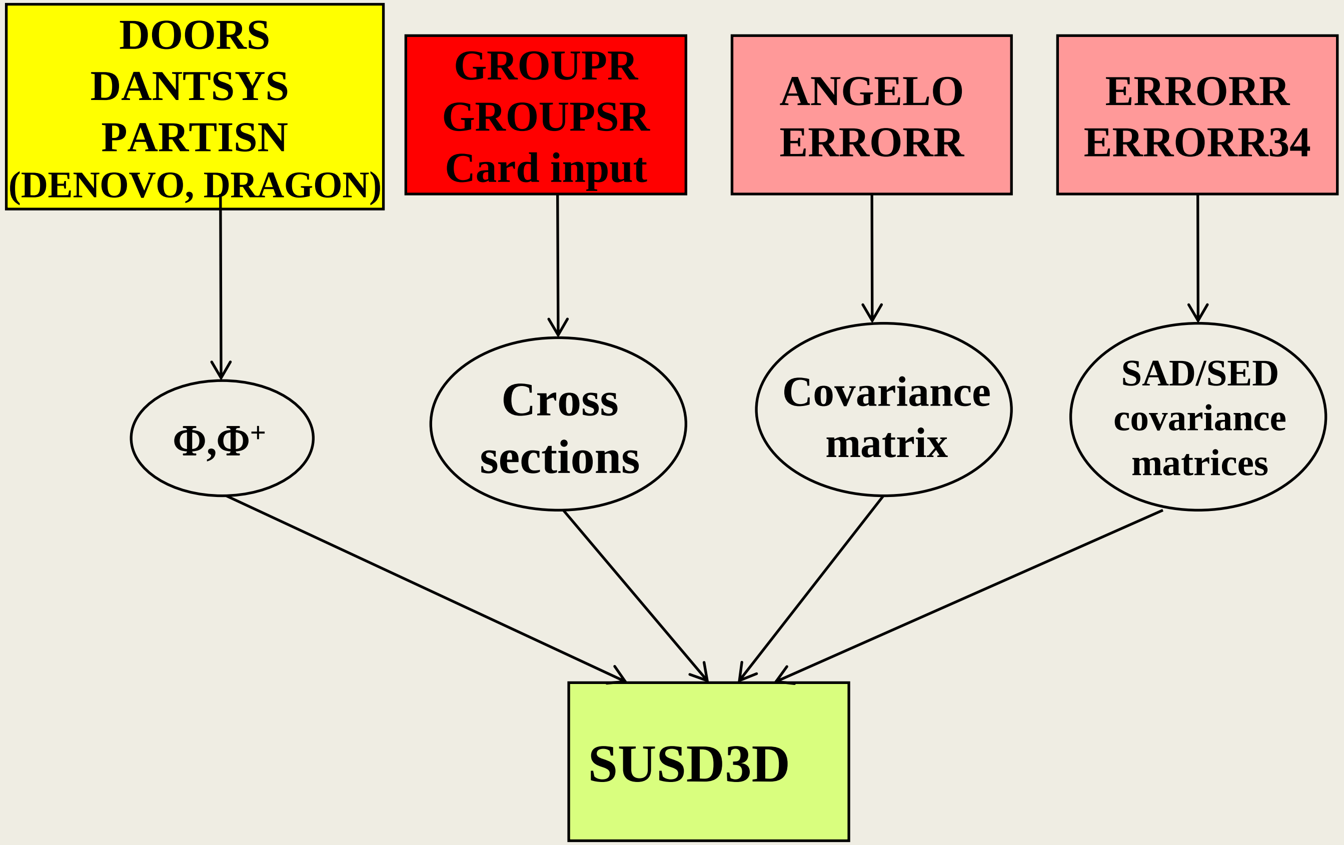
- Corresponding adjoint operator can be defined as:

$$B^* \cdot \Phi^* = S^* = \sigma_d$$

$$R = \langle \Phi, \sigma_d \rangle = \langle \Phi^*, Q \rangle$$



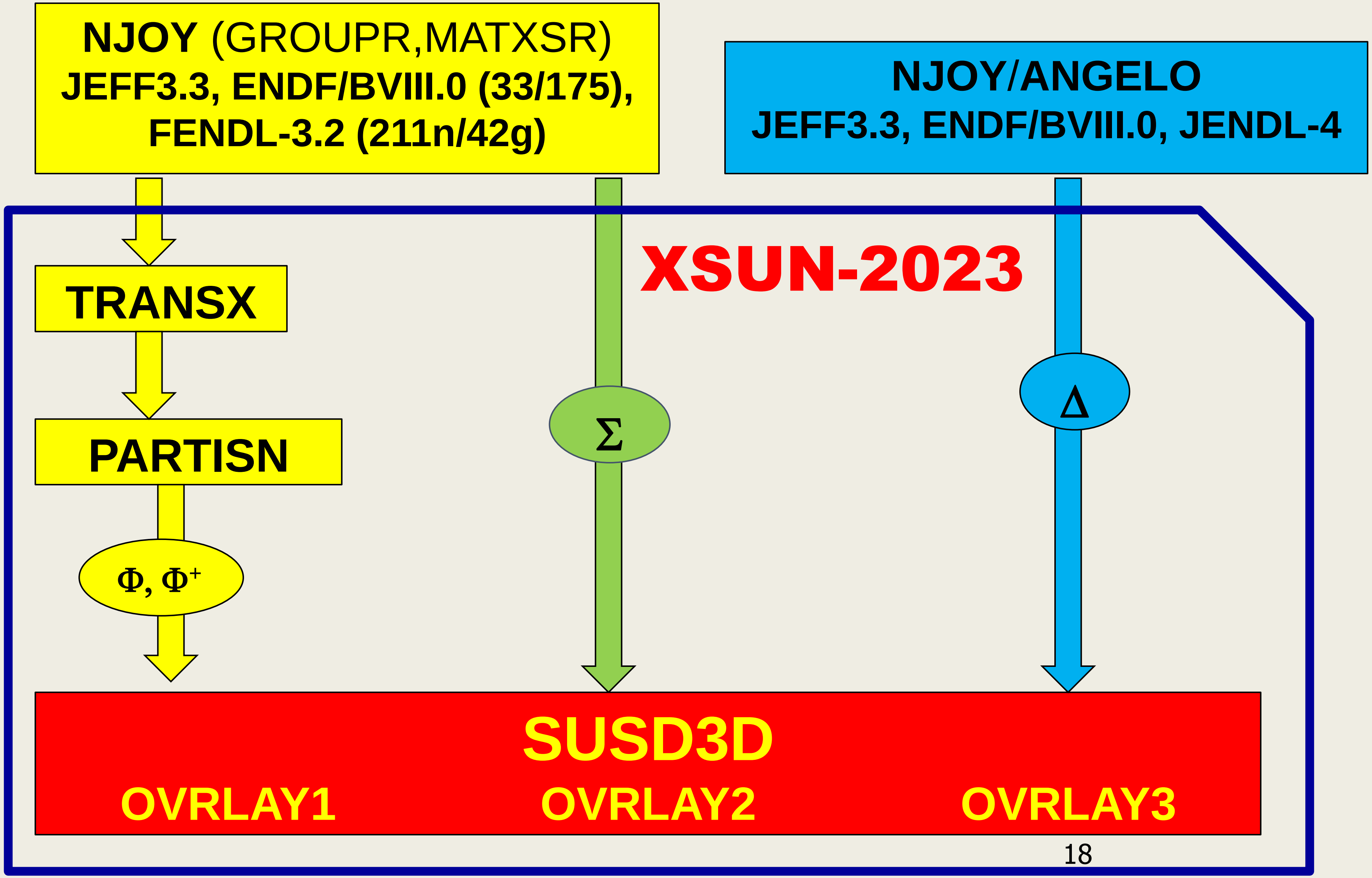
SUSD3D: Nuclear data sensitivity & uncertainty based on generalized perturbation theory



SUSD3D
- **Complex geometries 1D, 2D, 3D**
- **Sensitivity-uncertainty to distributions in (E,Θ) of emitted neutrons**
- **Shielding, criticality (fusion, fission)**
- PC DOS, LINUX
- written **Fortran 95**

- First use for the PV surveillance (REP 900), 3D version developed in the scope of the EFF project in the early 1990-ies., Used for the FNG benchmark pre- and post-analyses.
- Available from NEA Data Bank and RSICC since 2000.
- XSUN-2013 & 2017 released at NEADB, **XSUN-2023 in preparation**

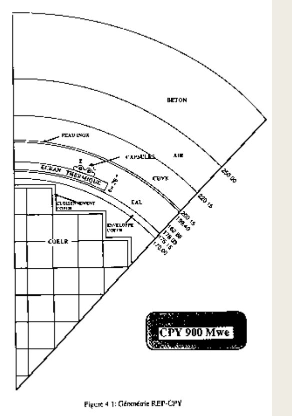
Computational scheme



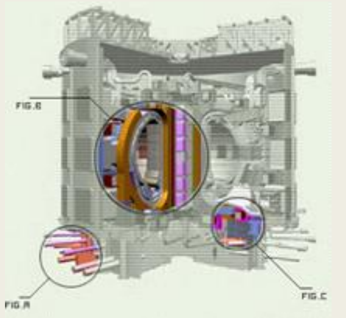
SUSD3D, A FEW MAIN / NOVEL FEATURES

- Sensitivity to different cross-section types: **MF=3** (gain term), **MF=6** (loss term), **MF=2** (direct term-response function), **MF=4** (SAD uncertainty), **MF=5** (SED uncertainty).
- Covariance terms **MF=33, 34, 35** can be used to propagate these uncertainties using the « sandwich » equation;
- Nuclear data for up to up to 440 nuclides from JEFF-3.3 and ENDF/B-VIII.0 in 175- and 33-groups, FENDL-3.2 (211n/42g)
- Sensitivity calculations make use of **angular moments** rather than angular fluxes (considerable computer space savings – **3D**).
- SAD/SED distributions: Re-normalisation of **prompt/delayed fission spectra** covariance matrices can be applied using the **constrained sensitivity method**. This option is useful in case if the fission spectra covariances used do not comply with the ENDF-6 Format Manual rules.
- Sensitivity of the effective delayed neutron fraction (β_{eff})
- **Sensitivity to gamma-ray** quantities (gamma flux, heating, …)
- Available from NEA-DB and RSICC since 2000: Present packages available in SUSD3D (NEA 1628/01-/03) and XSUN (NEA-1882)

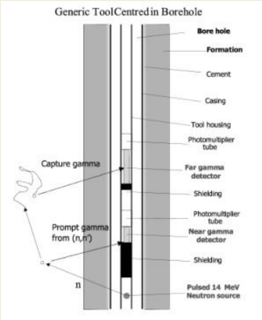
Examples of SUSD3D Analysis



- ***Reactor pressure vessel surveillance dosimetry:*** uncertainty in predicted dosimeter reaction rates and PV exposition, determination of safety margins → **reactor lifetime predictions,**
- ***Critical & shielding benchmarks (fission):***
  - thermal (KRITZ-2, VENUS-2) and fast (SNEAK-7A/7B, ….);
  - PV surveillance: ASPIS-Fe, -FE88 (2D), VENUS-3 (3D)



- ***Shielding experiments for fusion reactors for ITER:***
  - Preparation and analysis of 9 benchmarks at **FNG, Frascati**: validation of cross sections and of design of some components; XS of Fe, SiC, W, Be, Pb, Cu and **tritium production** in HCPB, HCLL & WCLL modules;
- ***Validation of M/C sensitivity method (MCSEN, SERPENT) against Discrete Ordinates***
- ***Beta-eff SU analysis (several fast benchmarks, MYRRHA ADS reactor)***: reactor safety, XS data adjustment.

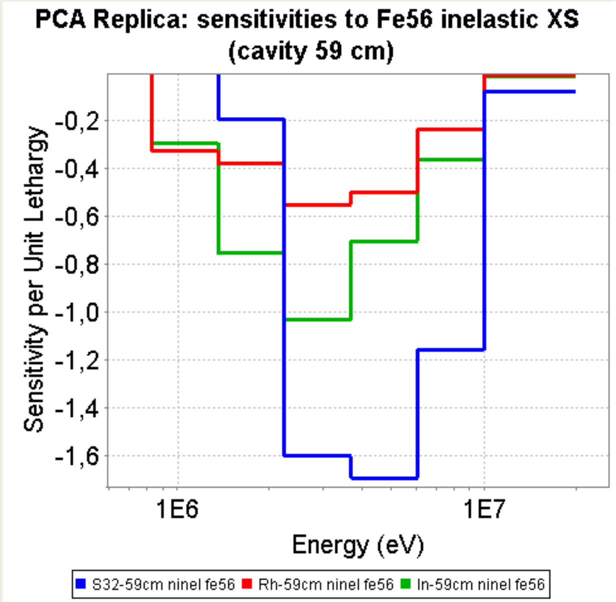


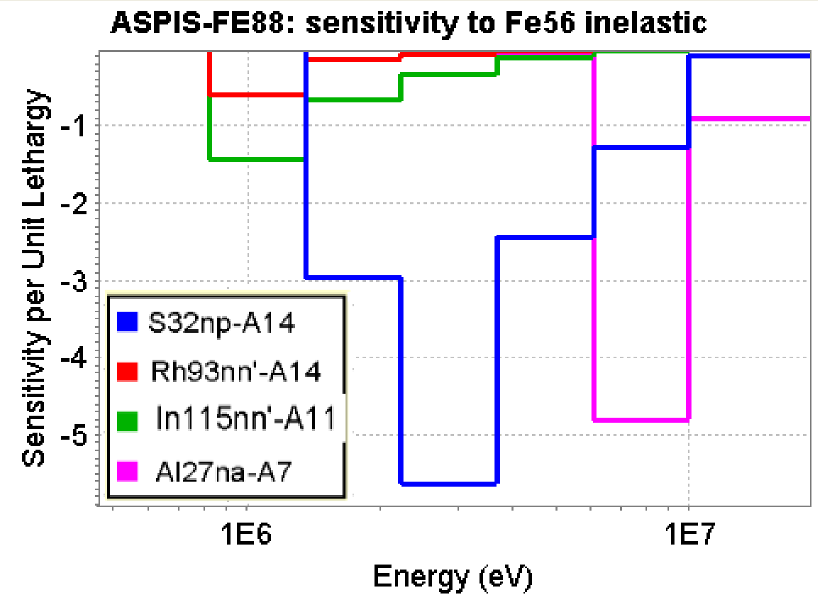
- ***Activation analysis:*** FISPACT II
- ***Gamma-ray S/U analysys:*** gamma spectra benchmark studies, oil well logging C/O logging (S/U of C/O gamma ratio)

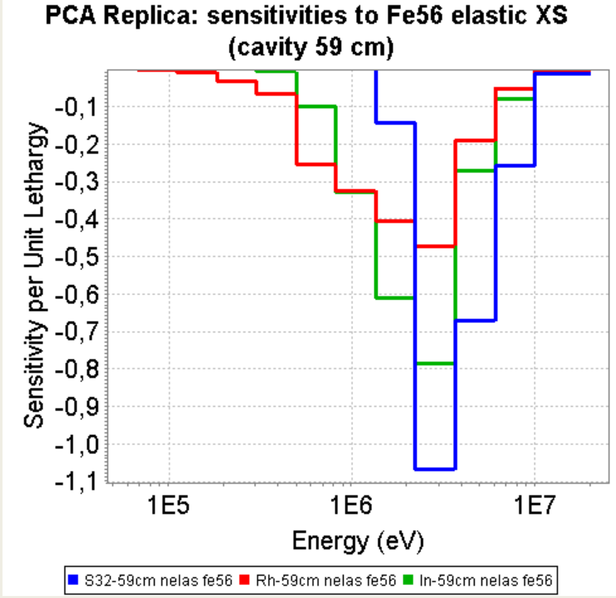
i=1

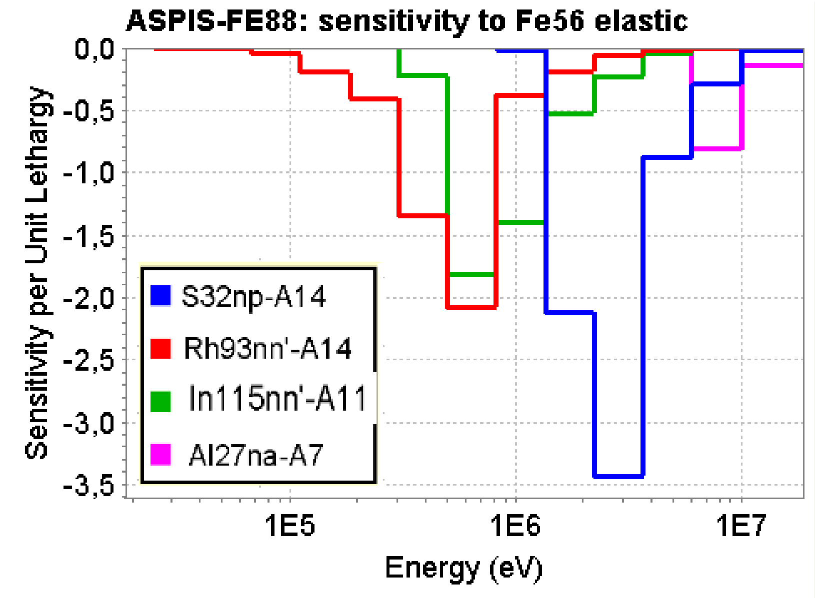
$$\Delta t = \frac{ln\left(1 + \frac{\Delta R}{R}\right)}{\lambda}$$

Sensitivity profiles

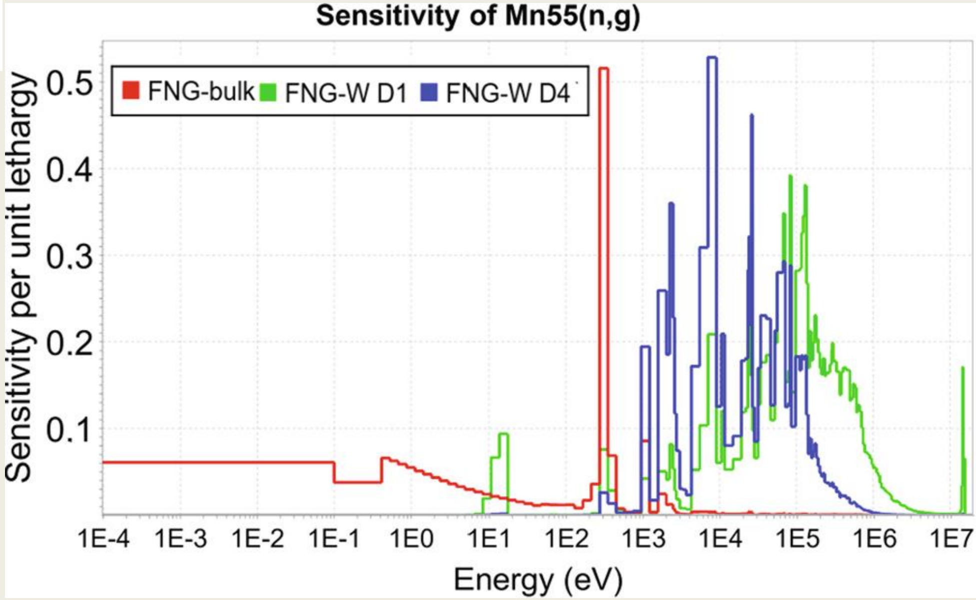








- **S/U provide uncertainty in the result**
- **Ranking key parameters** (most sensitive, contributing the most to the uncertainty)
- **Gives confidence in the simulation results**
- **sensitivity profiles available for: ASPIS Fe88, PCA Replica, FNG (Cu, W, HCPB, HCLL, …), VENUS-3, LLNL.**



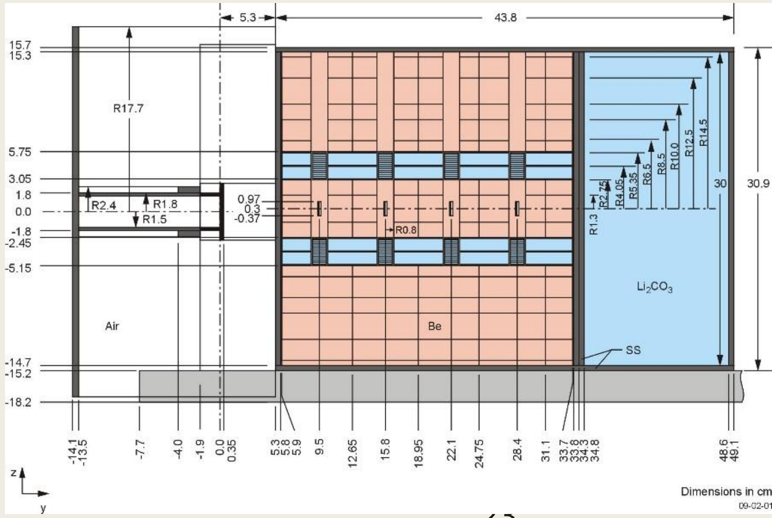
Format: SensitivitiesViewer (N.Soppera) https://www.oecd-nea.org/sensitivities-viewer/webstart/SensitivitiesViewer.jnlp

Conclusions

- Reactor design and safety parameters are biased due to uncertainties in nuclear data. Improved safety and better cost efficiency can be achieved by the reduction of uncertainties in design parameters.
- Monte Carlo and deterministic codes and nuclear data used for n/g transport need to be validated
- Uncertainties of calculated results can be estimated by sensitivity & uncertainty analysis and by comparison with experiments.
- Sensitivity and uncertainty analysis can also identify areas of weakness in data files and guide further evaluations.
- Powerful computational tools and databases needed for such analysis are available.

Benchmarking activities at UKAEA

- Focus on nuclear fusion: analyses typically involve large and complex geometries, neutron & gamma source terms, higher energy neutrons than fission.
- Involved in fusion reactor projects such as **JET, ITER, STEP, MAST-U, DEMO**;
- **Licencing needs: V&V, understand and eventually reduce uncertainties**
- **Fusion research** needs (W, Cu, Fe, V, Mo, Cr, Y, Ti, C, Zr, Li, Pb, Be, Si,...)
- Predominantly MCNP M/C calculations using acceleration methods, but use of alternative codes is actively studied: **Serpent2, OpenMC, GEANT4, TRIPOLI**,
- SINBAD database serves for validation of transport codes and nuclear data,
- **CAD based computational workflows**
- Project on automation of benchmark analysis.
- Nuclear data **sensitivity and uncertainty** analysis
- Activation & nuclear waste studies (**Fispact II**)
- Open to international collaboration: with NEA (SINBAD Task Force), IAEA (Conderc, FENDL), F4E (JADE)



FNG –HCPB

THANK YOU FOR YOUR ATTENTION