Reference integral experiments databases and validation of nuclear data

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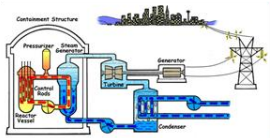
Outline

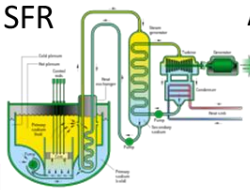
- *What is an integral experiment*
- *Integral experiments databases: ICSBEP and IRPHEP*
- *Visualization and databases search tools: DICE and IDAT*
- *NDaST tool*
- *Examples of validations*

❑ *The importance of Nuclear Data for energy and non-energy applications*

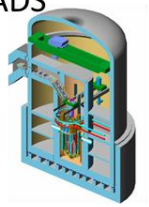
LWR



SFR



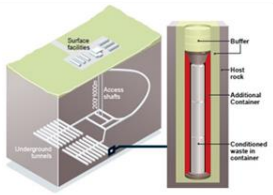
ADS



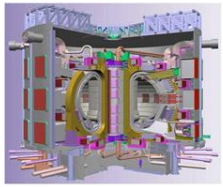
SMRs

Spent Fuel

DGR

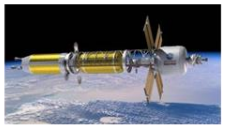


Fusion/ITER

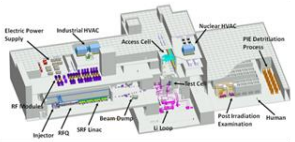


Nuclear Data for Applications (fission and fusion, radiation protection, nuclear medicine, nuclear security, object and materials analysis,…)
and Science (reactions and structure of nuclei, astrophysics, basic physics,…)

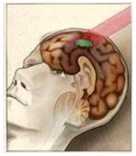
Neutrino's physics



Space technology



IFMIF/DONES



Medical applications

Astrophyscis

❑ Nuclear Data in the modelling

Boltzmann equation: Neutron transport, photon transport, charge particle transport, etc … → criticality, fission power distribution, reactivity coefficients, shielding, spent fuel storage, etc… safety analysis

$$\frac{1}{v}\frac{\partial f}{\partial t}+\mathbf{\Omega}\cdot\nabla f+\Sigma_T f = S+\int dE'd\mathbf{\Omega}'\, f(E',\mathbf{\Omega}')\Sigma_S(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})$$

$$S = S_{PF}+S_{dn}+S_{\alpha n}+S_{\text{ext}}$$

$$S_{PF} = \sum_i N_i \int dE'\, f(E')\overline{\nu}_i(E')\sigma_{F,i}(E')f_{P,i}(E',E)$$

$$\Sigma_{S(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')} = \sum_i N_i \frac{d^2\sigma_{s,i}}{dE'd\mathbf{\Omega}'}(E,E',\mathbf{\Omega}\cdot\mathbf{\Omega}')$$

$$\Sigma_T = \sum_i N_i\sigma_{T,i}$$

Doppler ignored

$$\Sigma_T = \Sigma_a+\Sigma_s$$

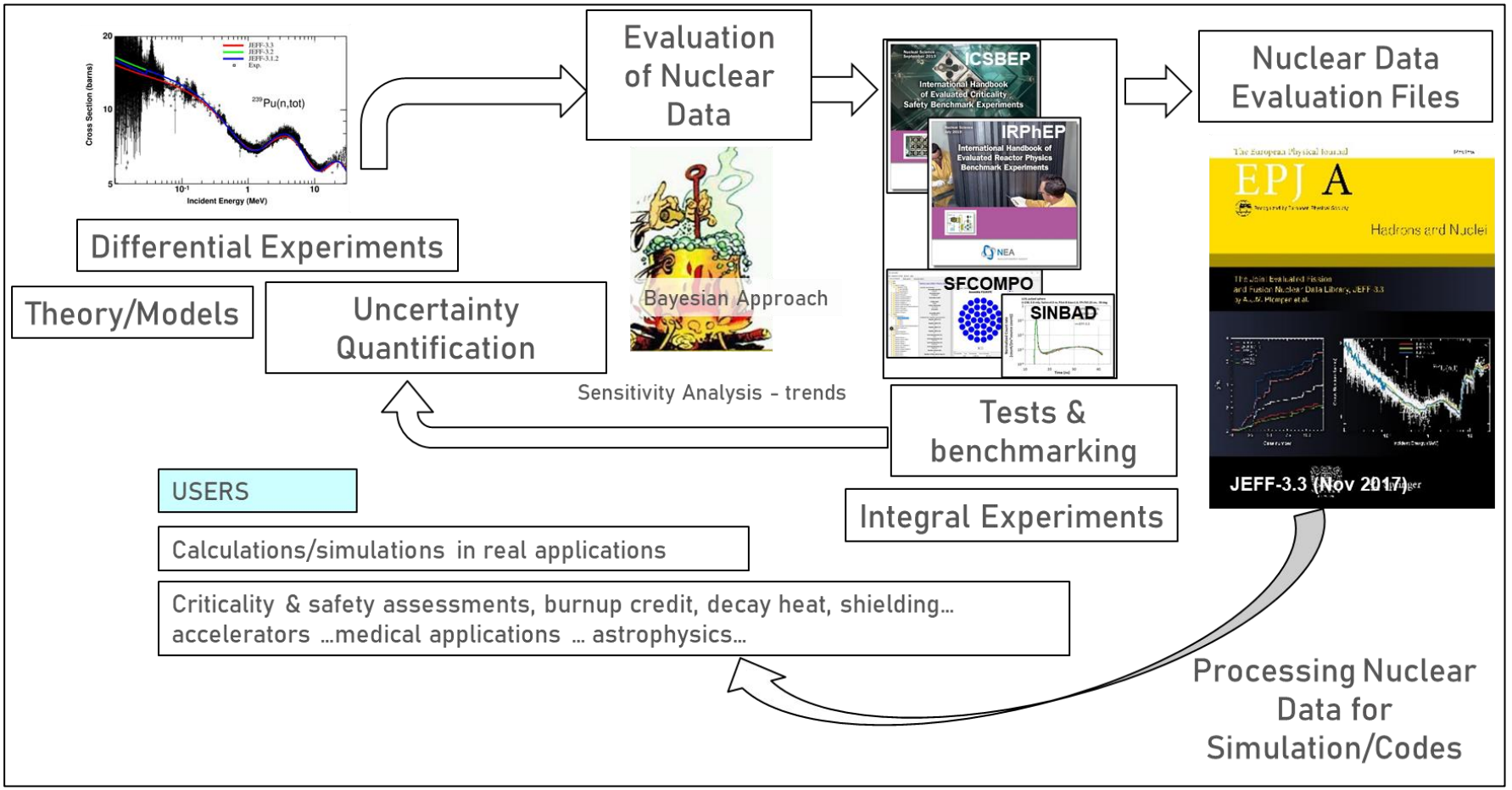
$$\Sigma_s = \int dE'd\mathbf{\Omega}'\,\Sigma_s(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')$$

Bateman equation: Inventory evolution -> radioactivity, decay heat, dose rates, waste management and environmental impact, etc …

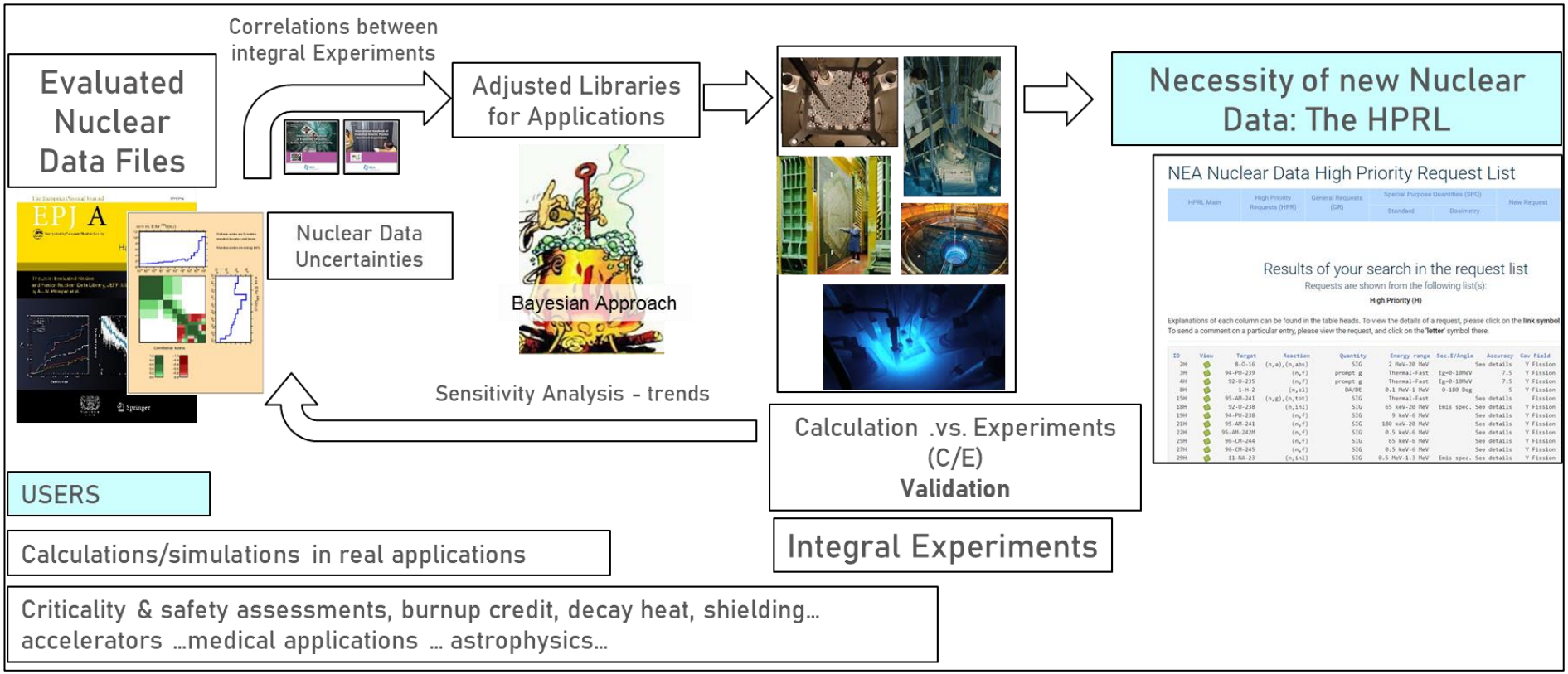
$$\frac{dN_i}{dt} = -\lambda_i N_i - r_i N_i + \sum_{j\neq i}\left\{\lambda_{j\to i}+r_{j\to i}\right\}N_j$$

Modelling for criticality, radiation damage, activation analysis, safegards, reactor emergency core cooling, shielding calculations, radioprotection, ….

- Nuclear Data are the bridge between the nuclear physics/the differential experiments and the simulations for applications



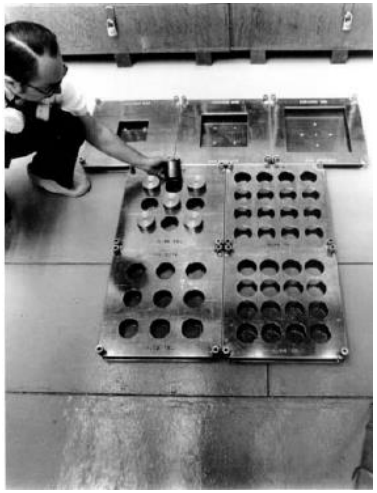
- The End-Users are the bridge between the applications and the necessity of new nuclear data

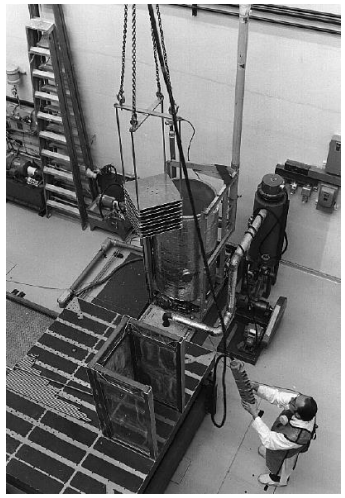


ICSBEP

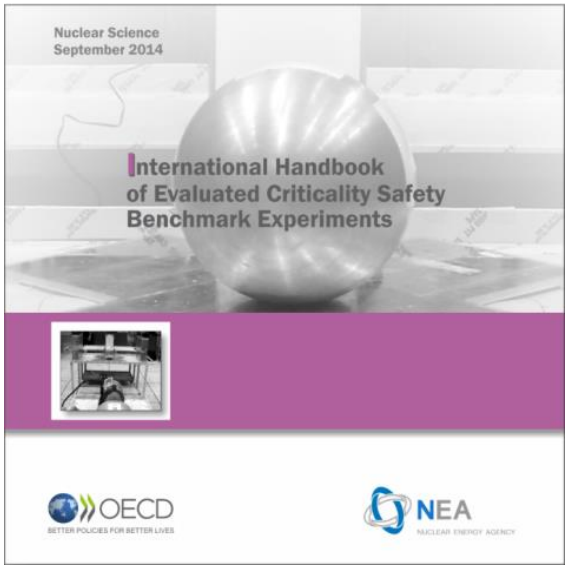
ICSBEP (**I**nternational Handbook of Evaluated **C**riticality **S**afety **B**enchmark **E**xperiments **P**roject) is a project whose objective is:

- To compile critical and subcritical benchmark experiment data into a standardised format that allows criticality safety analysis
- To easily use the data to validate calculation tools and cross-section libraries.
- Established 1992/1995, Handbook Released Yearly (DVD or Online)
- Over 5000 critical, subcritical and physics configurations





Rocky Flats Critical Mass Laboratory



https://www.oecd-nea.org/jcms/pl_24498/international-criticality-safety-benchmark-evaluation-project-icsbep

❑ "Benchmarks" are "Evaluated Experiments"

Content of an evaluation

1) Experimental data
2) Experiment and uncertainty evaluation … Experimental uncertainty: detectors,… Δk_{eff}^{exp}
3) Benchmark Model … Model versus the "Real" experiment
   - Dimension (e.g. radii,..), compositions, …. impact of these simplifications Δk_{eff}^{model} ?
     - correlation between experiments ?
   - Simplified Model – versus – detailed model…. differences in Sensitivity profiles? (e.g.PMI-2)
4) Sample calculations
5) Appendixes

$$k_{eff}^{EXP} \pm \Delta k_{eff}^{EXP} \rightarrow k_{eff}^{Model_1} \pm \Delta k_{eff}^{Model_1} \ldots \leftrightarrow k_{eff}^{CALC:Model_1:MCNP+JEFF-3.3} \pm \Delta k_{eff}^{CALC:Model_1:MCNP+JEFF-3.3}$$

$$\rightarrow k_{eff}^{Model_2} \pm \Delta k_{eff}^{Model_2} \ldots \leftrightarrow k_{eff}^{CALC:Model_2:MCNP+JEFF-3.3} \pm \Delta k_{eff}^{CALC:Model_2:MCNP+JEFF-3.3}$$

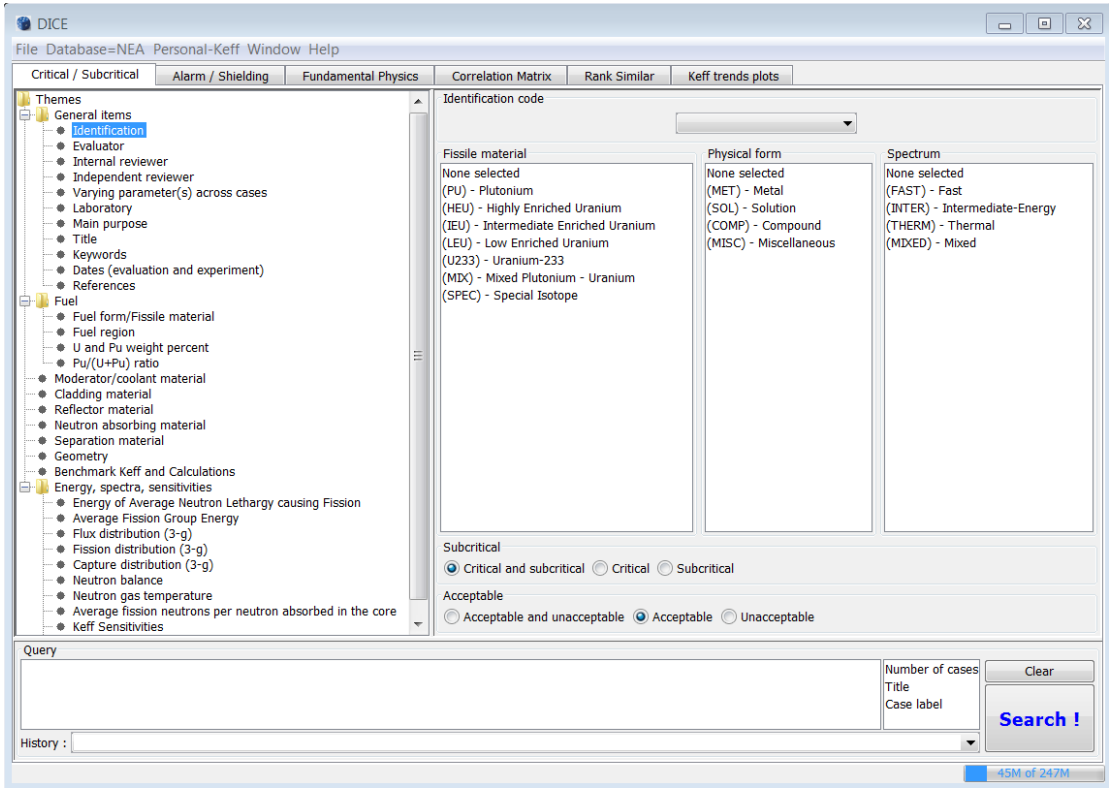
❑ ICSBEP was primarily devoted for "Criticality Safety Assessment" (CSA)

- Validation of computer-nuclear data
- Nuclear data validation or adjustment

❑ DICE

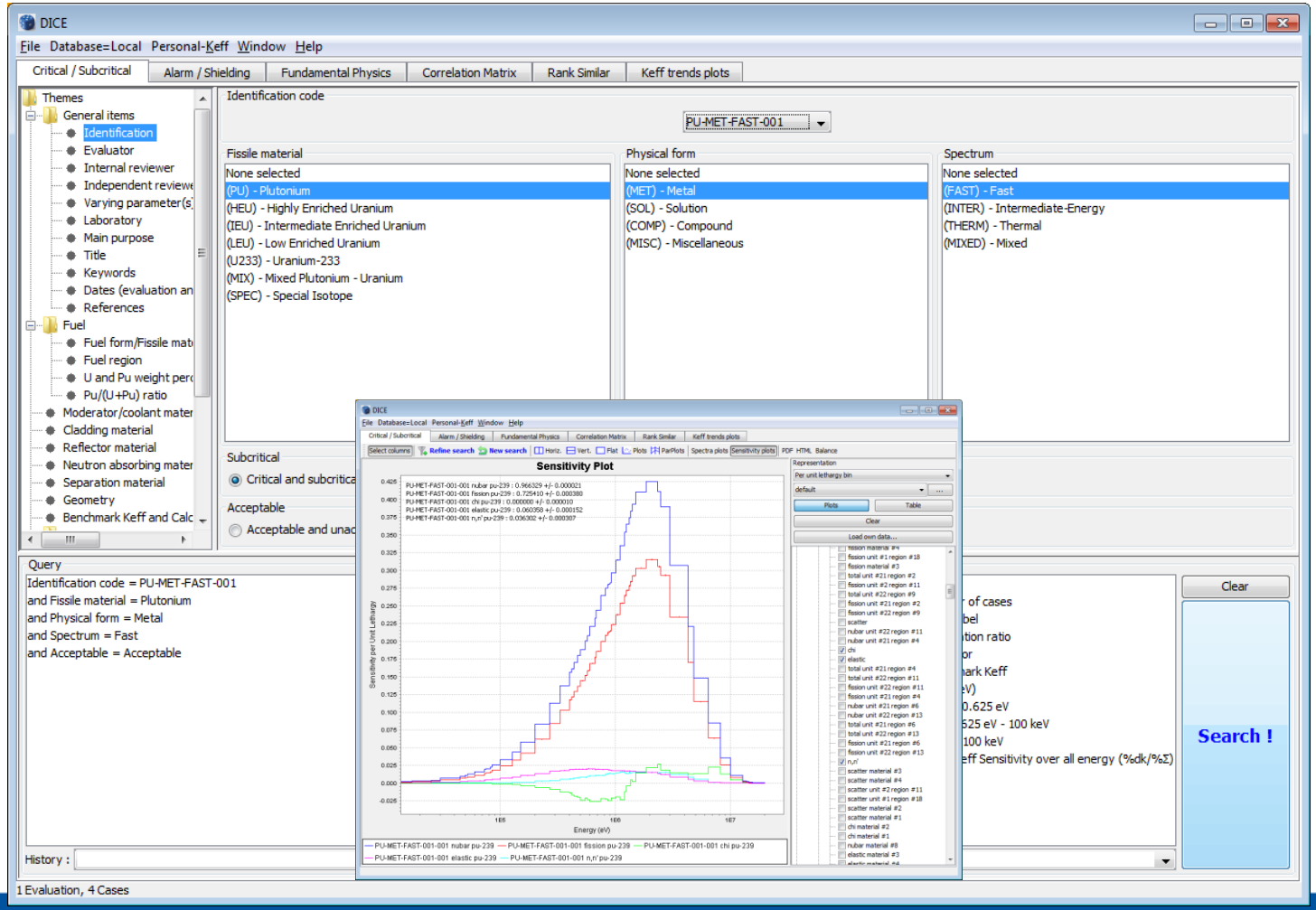
DICE is the Database for ICSBEP, provided with a searching tool in JAVA

- Distributed with Handbook since 2001
- Relational database
- User Friendly Way to Search
- DICE includes: Sensitivity data, tools using sensitivity data to identify useful benchmarks, load your own keff data, etc…

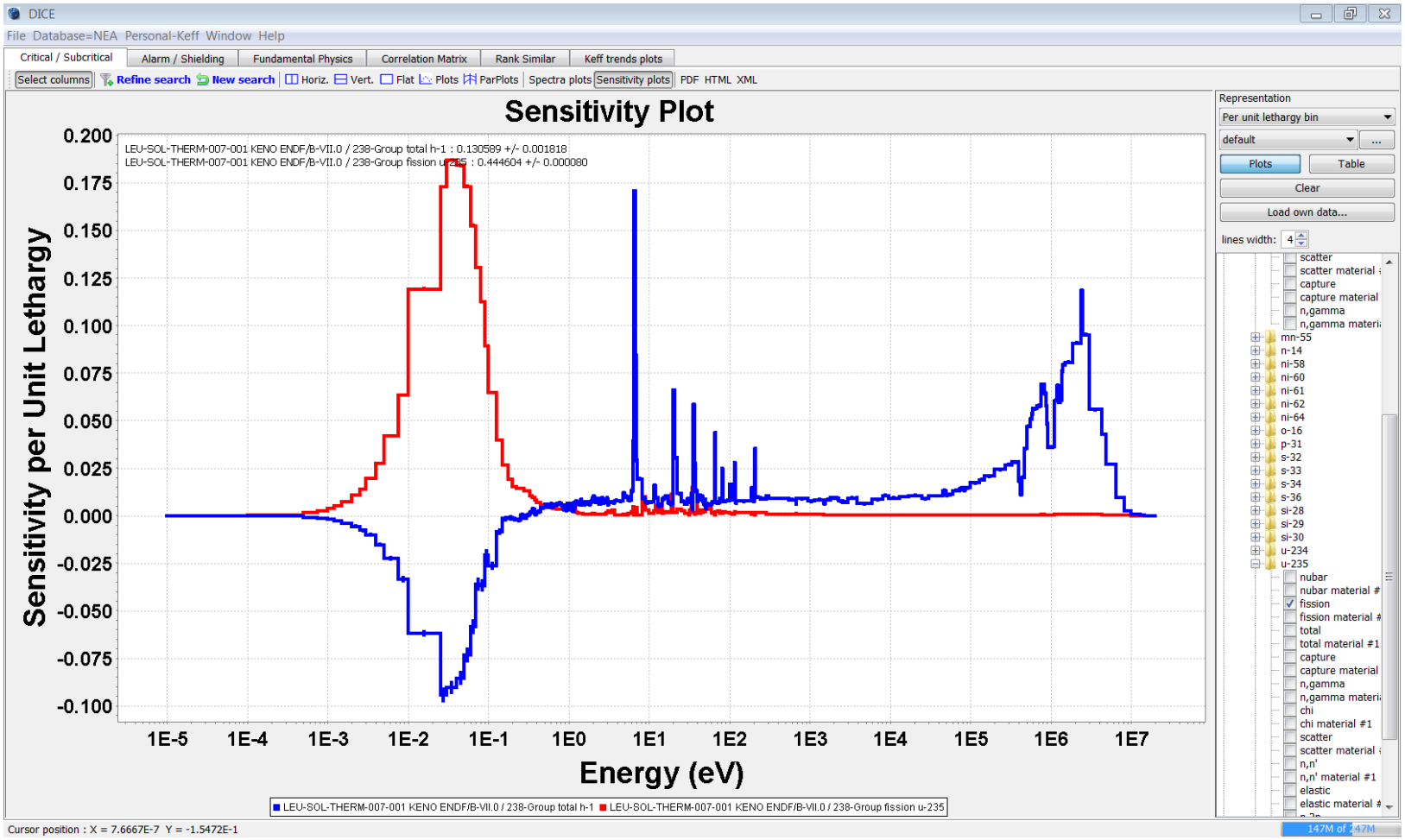


https://www.oecd-nea.org/science/wpncs/icsbep/dice.html

❑ Accessing benchmark information: PDFs for reading, inputs, …



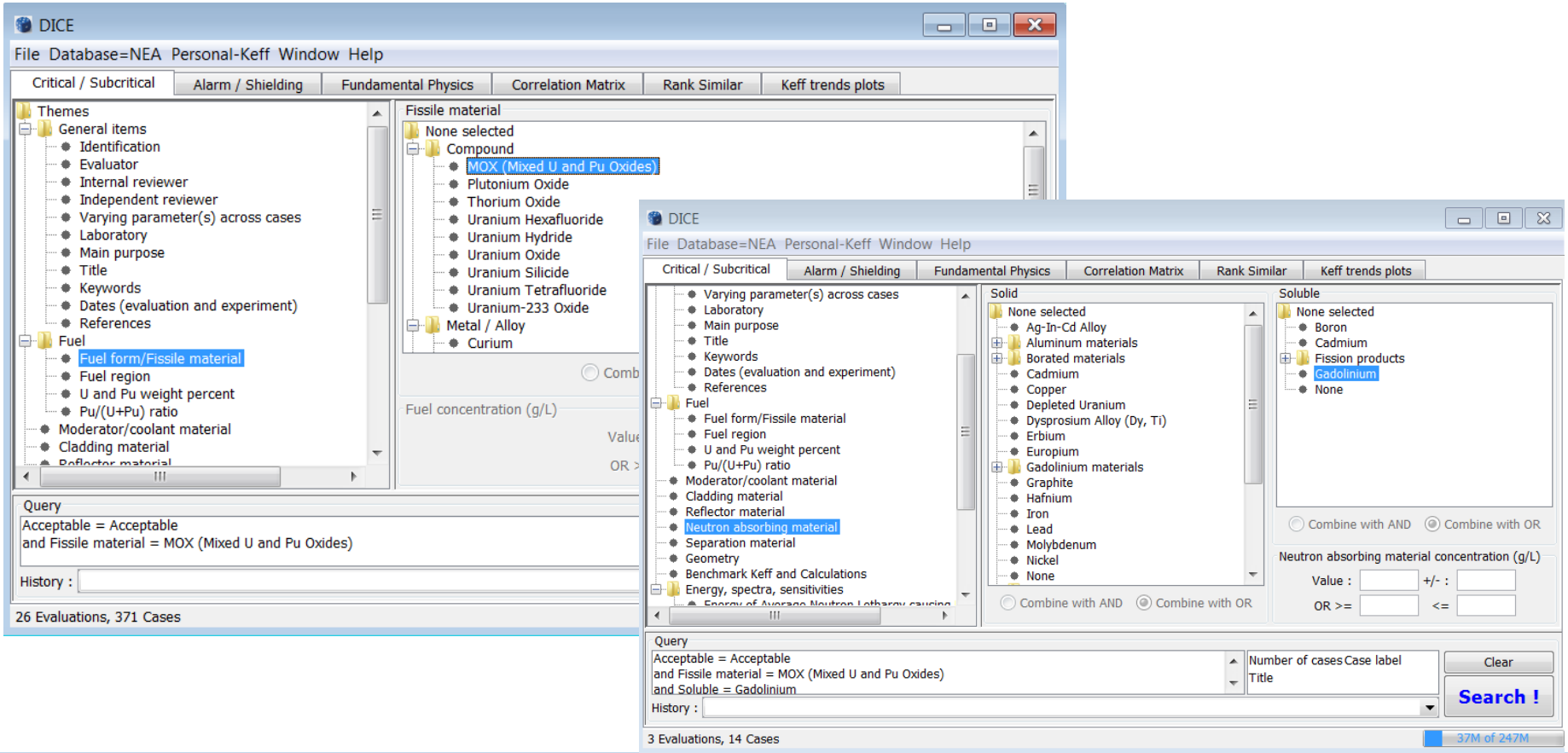
ND Sensitivity Viewer



❑ DICE: Searching tool

❑ Searching experimental benchmarks using different fields:

An example: MOX Experiments With Soluble Gd

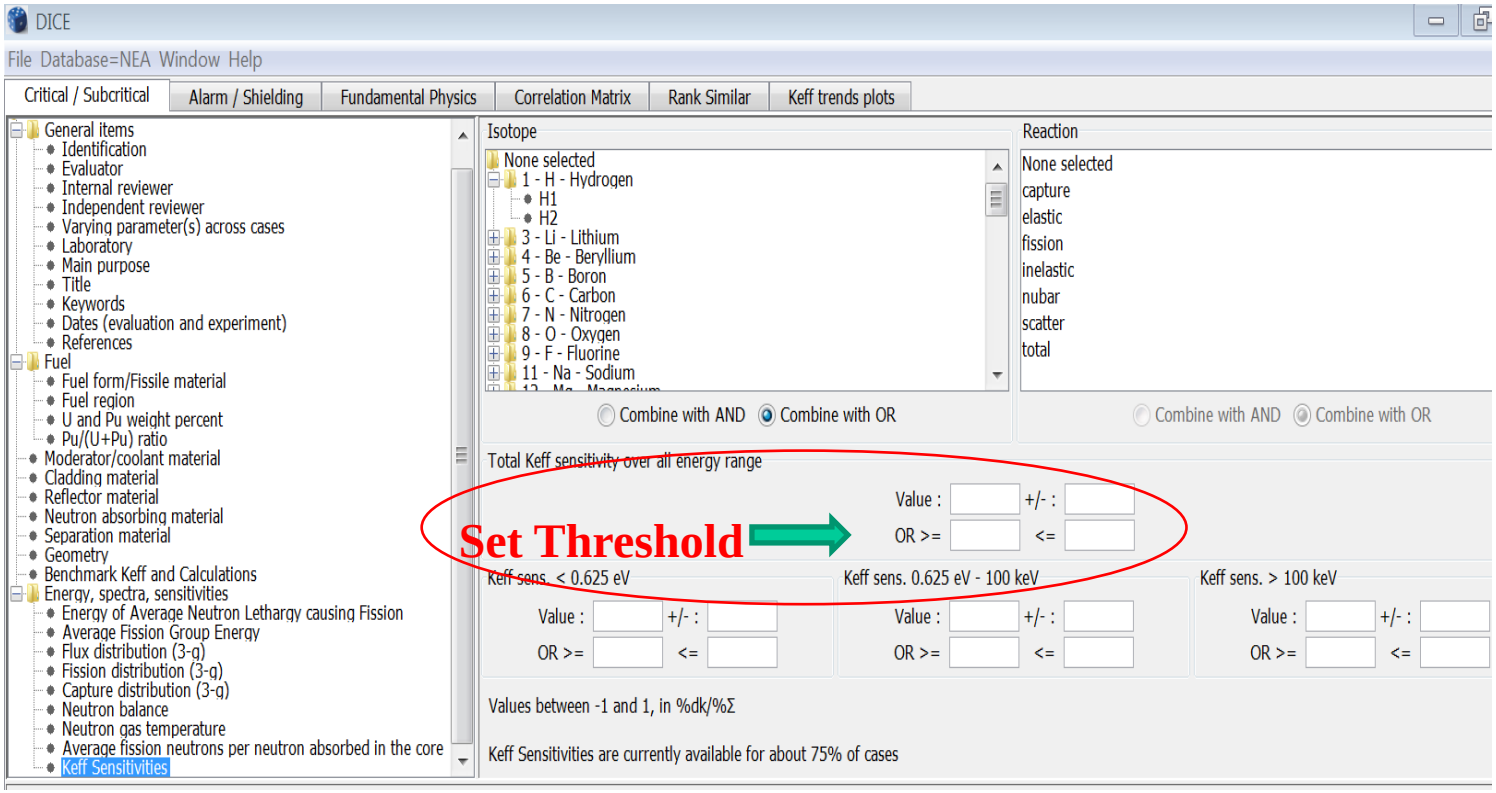


❑ DICE: Searching tool

❑ Searching experimental benchmarks using different fields:

e.g. Sensitivities

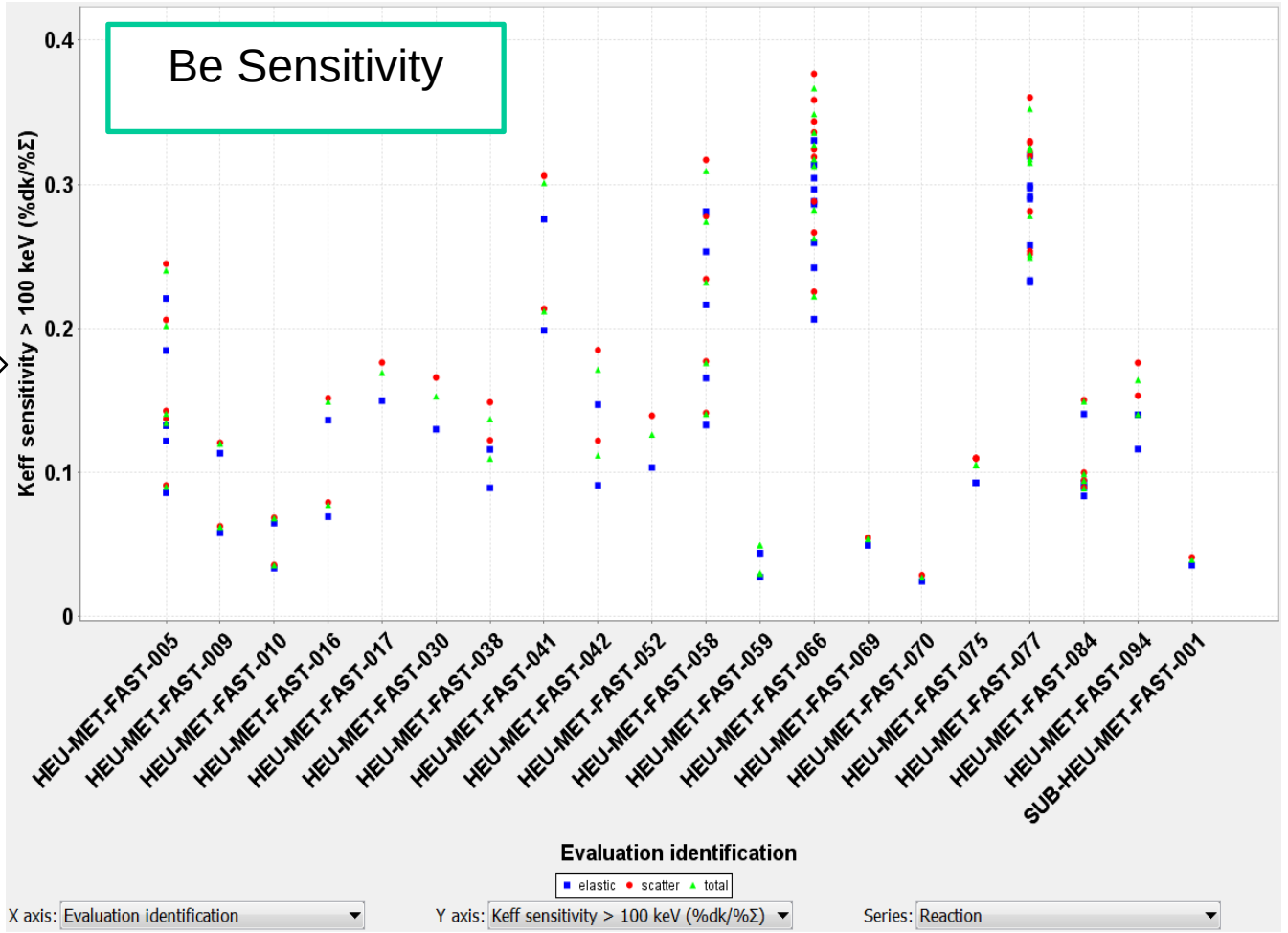
3-g search, full 238 Group SDF's are stored for plotting and computations



❑ DICE: Searching tool

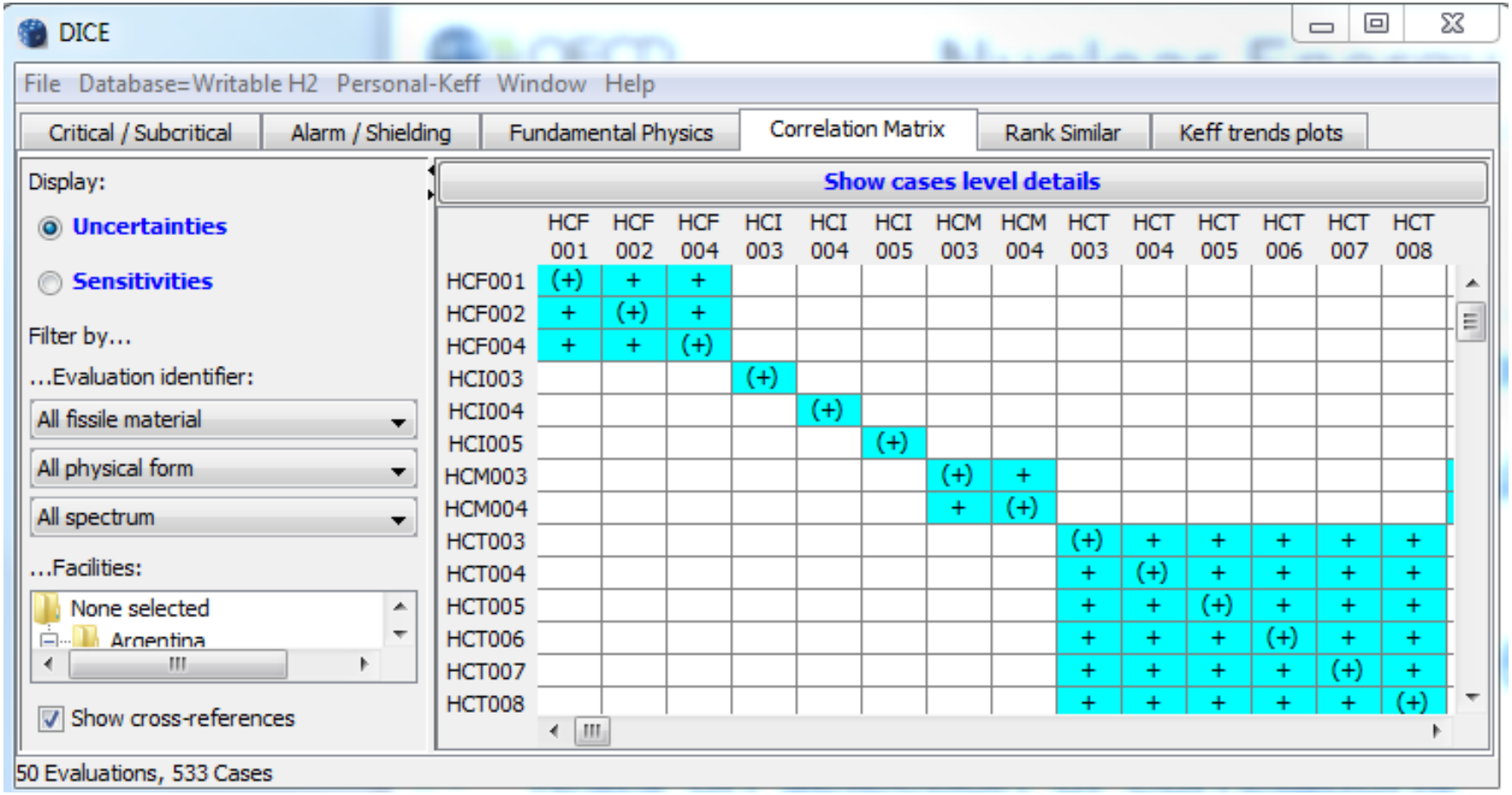
❑ Example: DICE Plotting of Be Sensitivity > 0.005 for HMF

Can also read as 1000 pcm/1% change in Σ



❑ DICE: Uncertainties/correlations

❑ Status of existing correlations “of benchmark model uncertainties”



❑ DICE: Uncertainties/correlations

❑ Cosine similarity of sensitivity profiles using the TSUNAMI-IP metric

DICE

File Database=Local Personal-Keff Window Help

Critical / Subcritical | Alarm / Shielding

Fundamental Physics | Correlation Matrix | Rank Similar | Keff trends plots

Display:
- Uncertainties
- Sensitivities

Filter by...
...Evaluation identifier:
HEU
MET
FAST
...Facilities:
LLNL

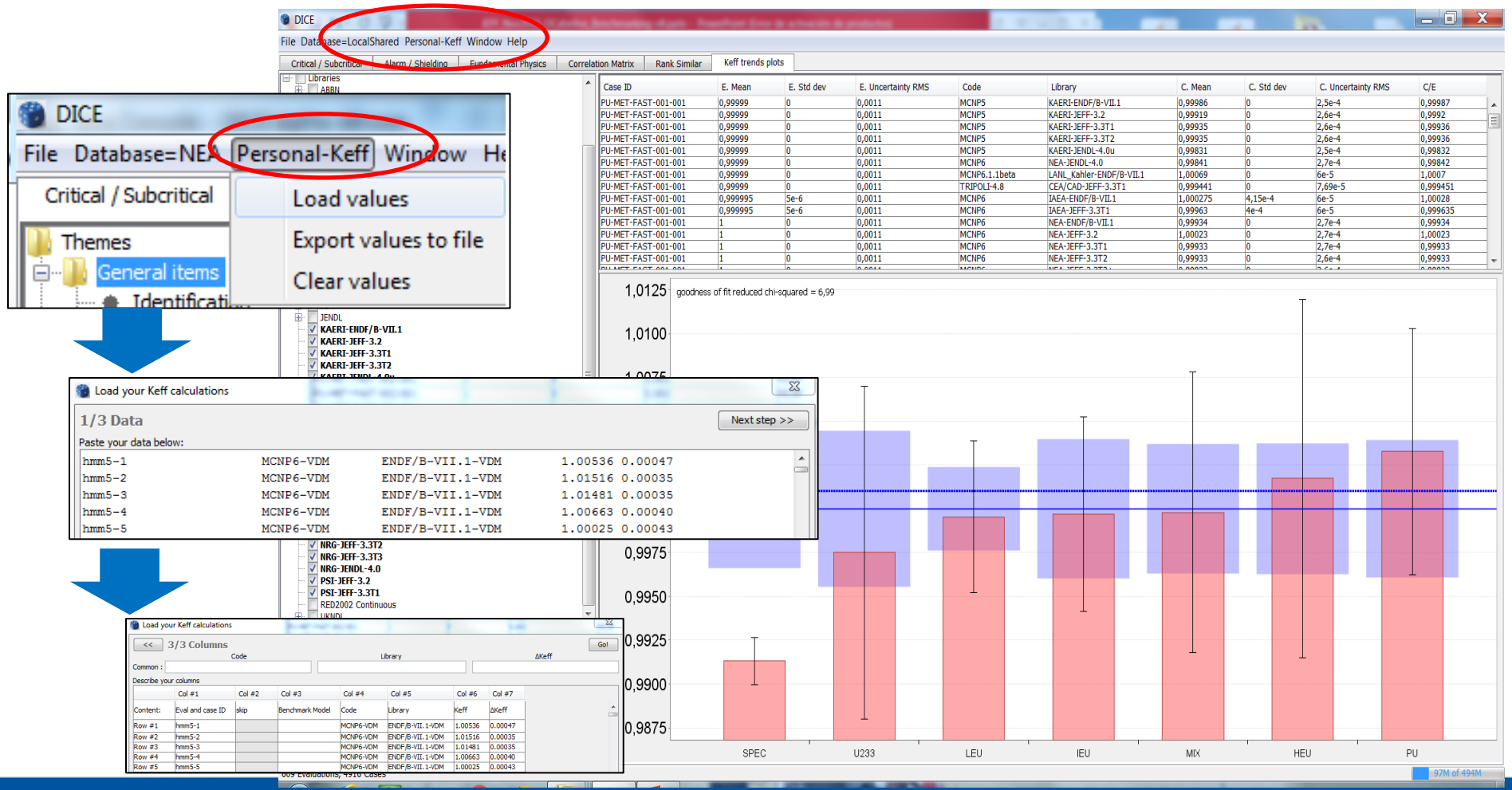
Return to evaluations level

	HMF057-001	HMF057-002	HMF057-003	HMF057-004	HMF057-005	HMF057-006	HMF058-001	HMF058-002	HMF058-003	HMF058-004	HMF058-005	HMF066-001	HMF066-002	HMF066-003	HMF066-004
HMF057-001	1000	998	998	998	999	999	883	923	947	965	973	895	931	948	831
HMF057-002	998	1000	997	999	997	999	888	929	952	971	979	900	936	953	836
HMF057-003	998	997	1000	997	999	999	881	921	945	962	970	894	929	945	830
HMF057-004	998	999	997	1000	996	998	889	930	954	972	980	901	937	954	836
HMF057-005	999	997	999	996	1000	999	881	921	945	962	970	894	929	946	831
HMF057-006	999	999	999	998	999	1000	885	925	948	966	974	897	932	949	833
HMF058-001	883	888	881	889	881	885	1000	991	978	959	946	994	984	975	990
HMF058-002	923	929	921	930	921	925	991	1000	996	985	976	996	998	994	975
HMF058-003	947	952	945	954	945	948	978	996	1000	996	991	986	998	999	953
HMF058-004	965	971	962	972	962	966	959	985	996	1000					
HMF058-005	973	979	970	980	970	974	946	976	991	998					
HMF066-001	895	900	894	901	894	897	994	996	986	969					
HMF066-002	931	936	929	937	929	932	984	998	998	990					
HMF066-003	948	953	945	954	946	949	975	994	999	996					
HMF066-004	831	836	830	836	831	833	990	975	953	925					

$$E \equiv \frac{\mathbf{S}_a^T \mathbf{S}_e}{\|\mathbf{S}_a\| \|\mathbf{S}_e\|}$$

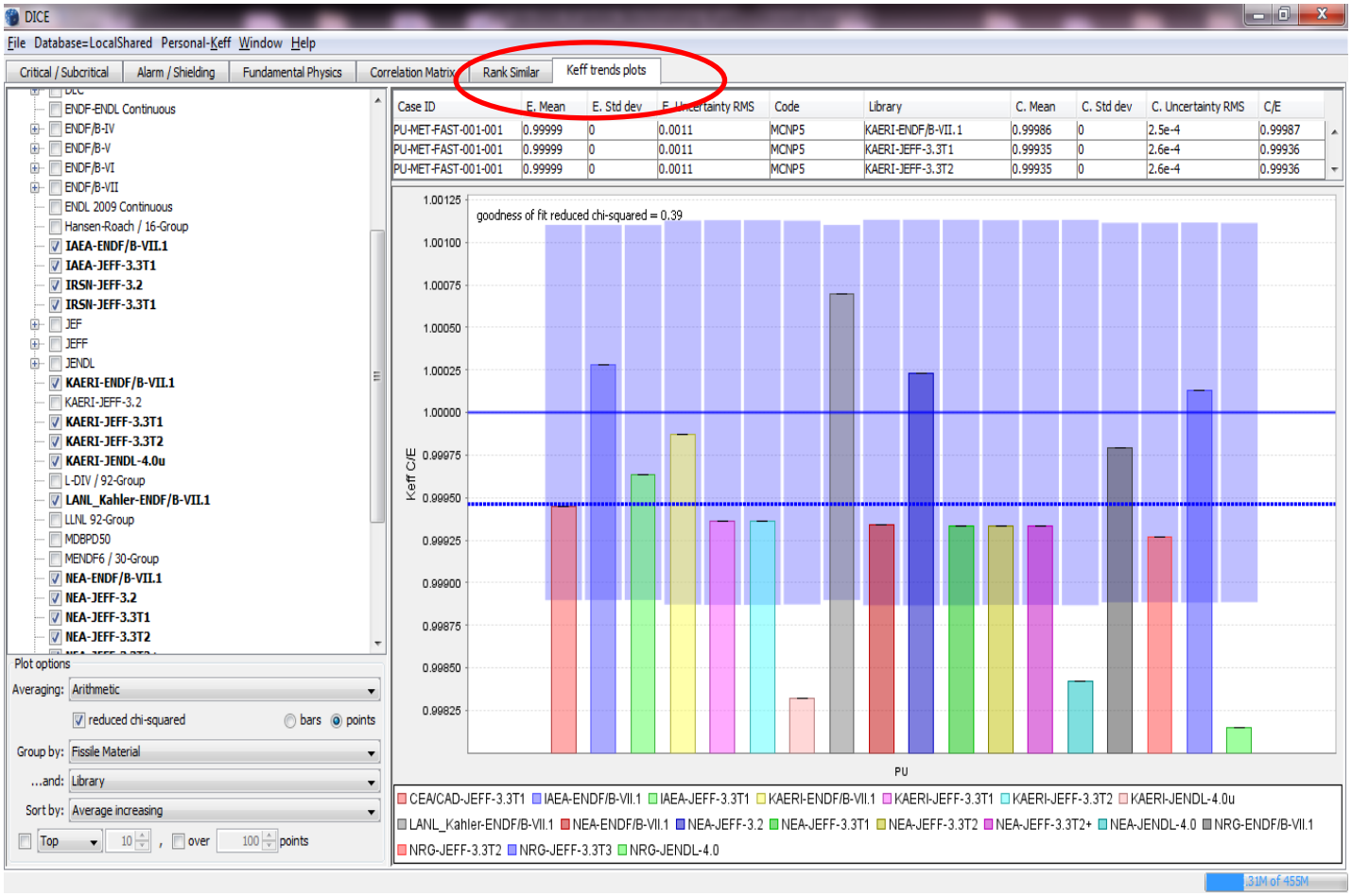
❑ DICE: Load personal-keff

❑ Providing own keff-calculated results of benchmarking



❑ DICE: Keff-trend plots

❑ keff trends plots… to see the performance of your own calculations



❑ DICE: Keff-trend plots

❑ The use of Figure of Merit (FoM) to assess the performance of ND in keff

These metrics can give reliable indications of the nuclear data performance

- ❑ **Average C/E**
- ❑ **Average difference, r.m.s. Delta-k**
  - magnitude of the average difference between C and E
  - smaller values better fit to benchamrk

$$\langle|\Delta|\rangle = \Sigma\frac{|k_{calc} - k_{exp}|}{n}$$

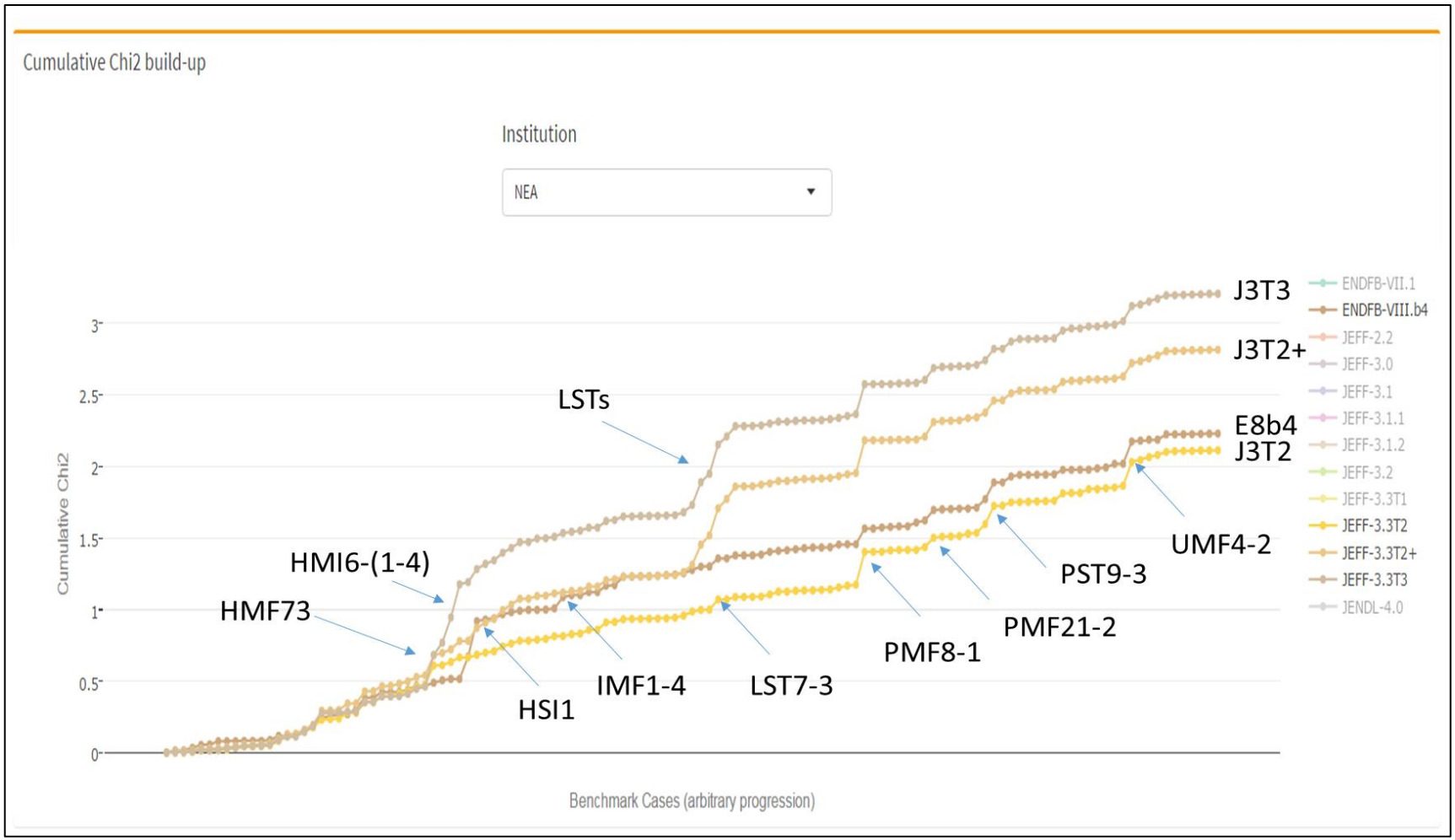
- ❑ **Residuals:** $(k_{calc}\text{-}k_{exp})/\Delta k_{exp}$
- ❑ **Chi-squared, X^2/DoF**
  - accounts for the uncertainty in the experimental value
  - sensitive to cases with unrealistically small uncertainties
  - If x<1 then , on average calculations math benchmarks to within one exp. std.

$$\text{“}\chi^2\text{“} = \Sigma\frac{((k_{calc} - k_{exp})/\delta k_{exp})^2}{n}$$

- ❑ **PDFs, CDFs, … % of results within experimental std. dev**

❑ ICSBEP
Keff-trend plots

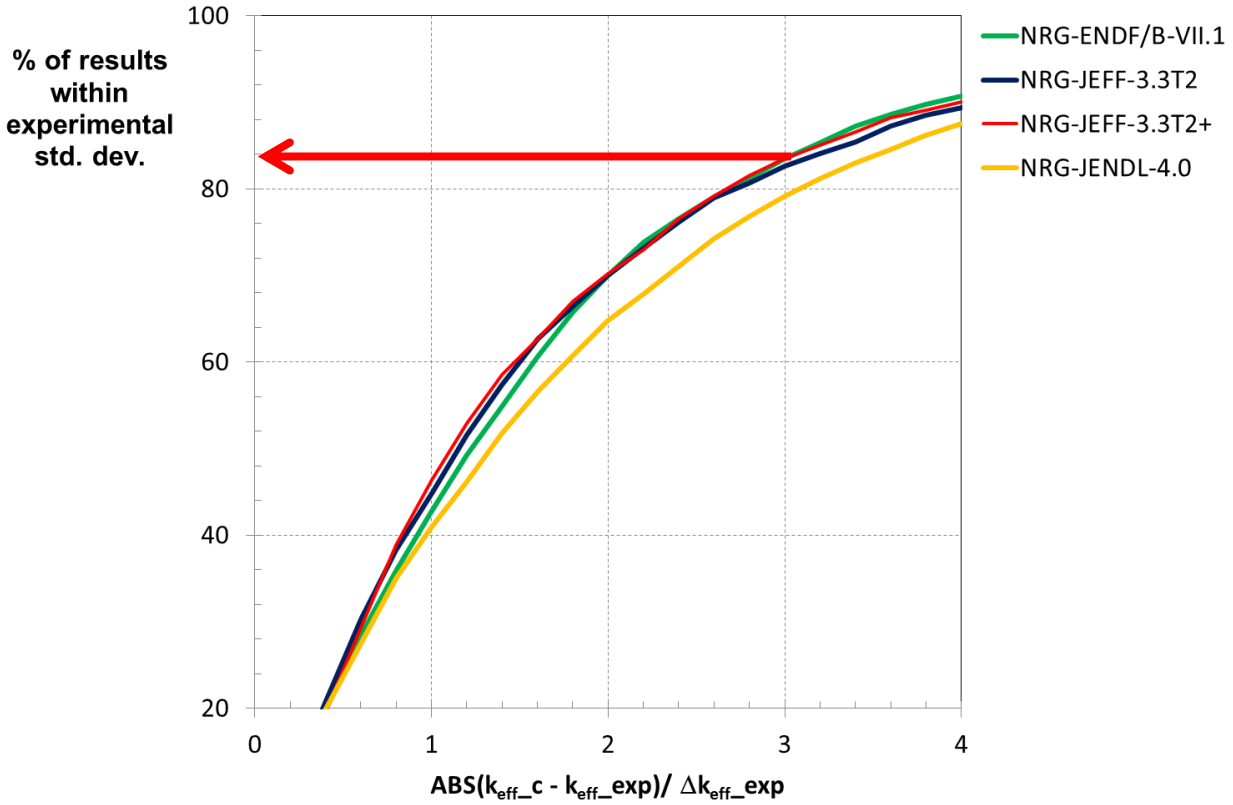
❑ Results of criticality benchmarking using ICSBEP



❑ ICSBEP: Keff-trend plots

❑ Results of criticality benchmarking using ICSBEP

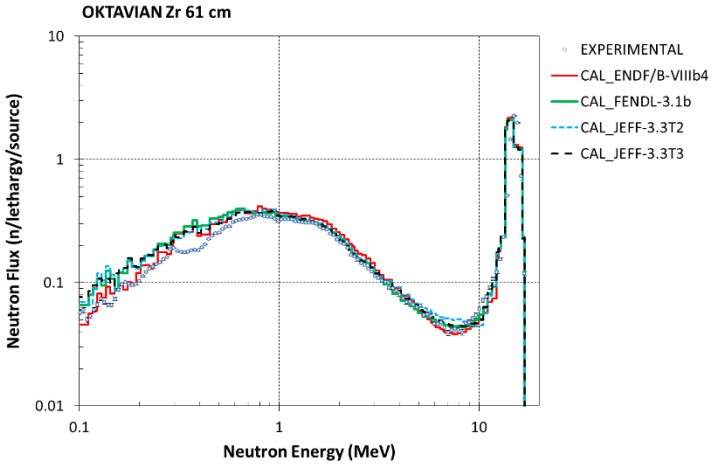
Figure. % of results within experimental std. dev.



❑ Other Benchmarking

❑ Shielding and fusion application: **SINBAD Database**

- Reactor shielding (46)
- Fusion neutronics shielding (31)
- Accelerator shielding (23)



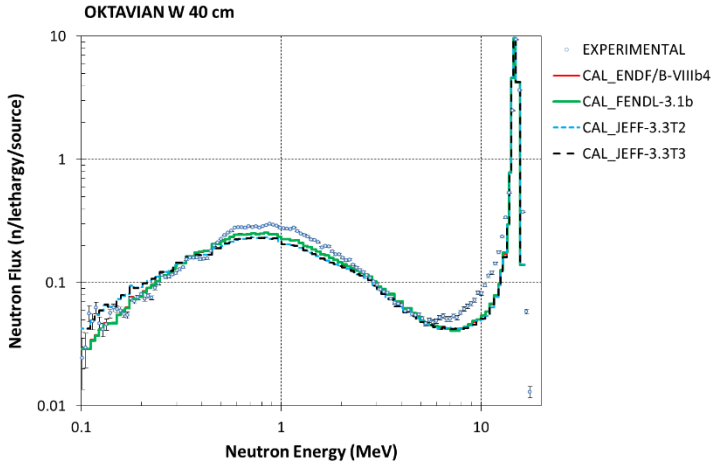
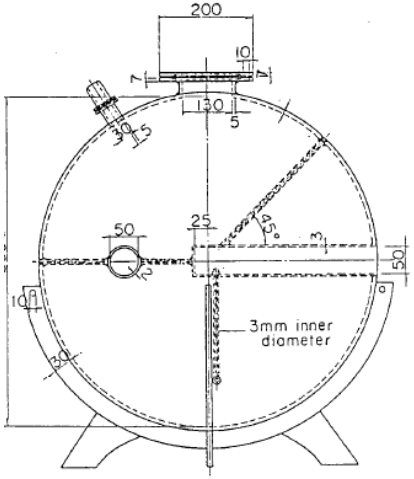


Figure. An example: Neutron leakage from OKTAVIAN pulsed sphere 61 cm sphere - Type I

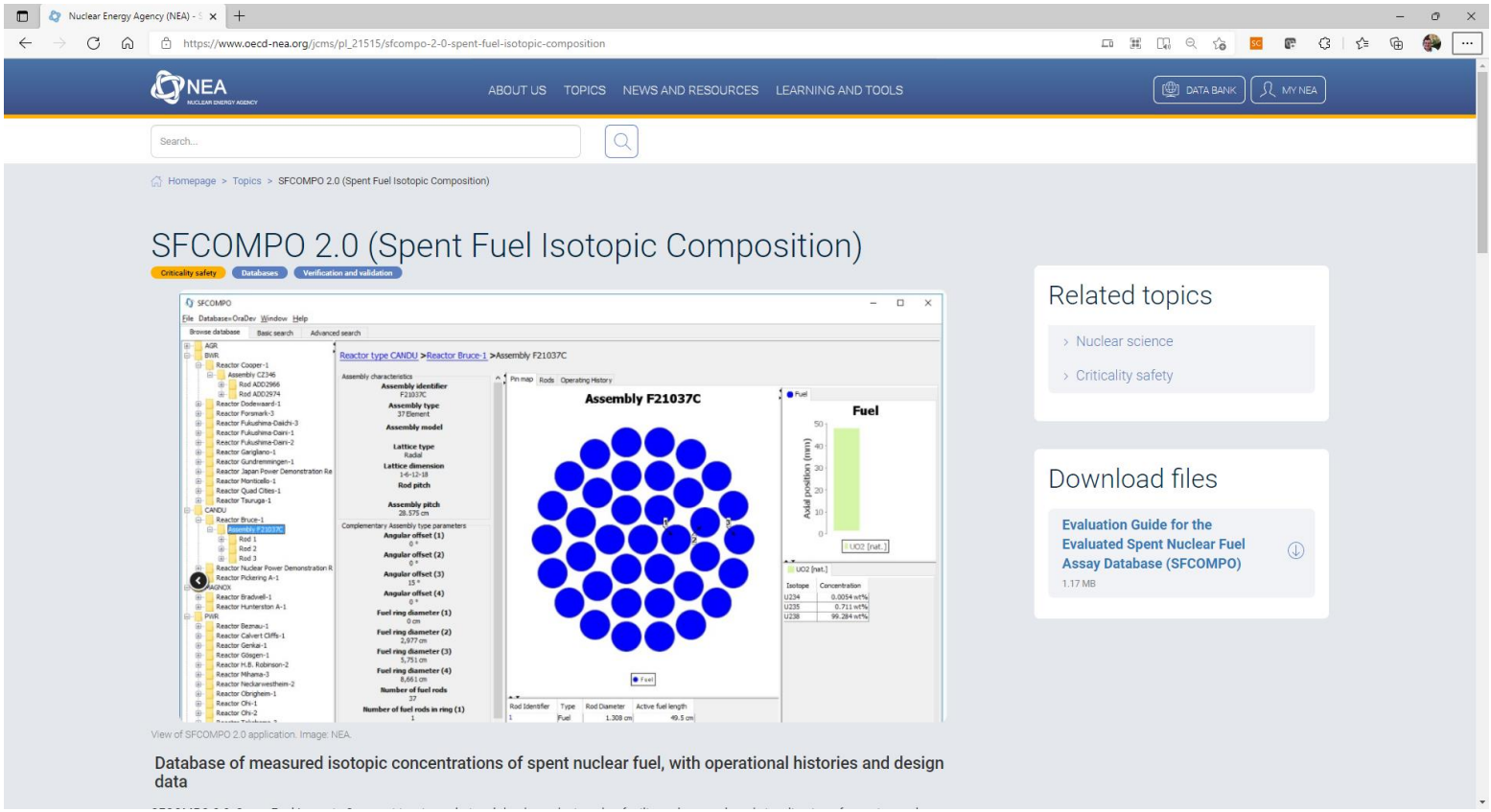


https://www.oecd-nea.org/jcms/pl_32139/shielding-integral-benchmark-archive-and-database-sinbad

❑ Other Benchmarking

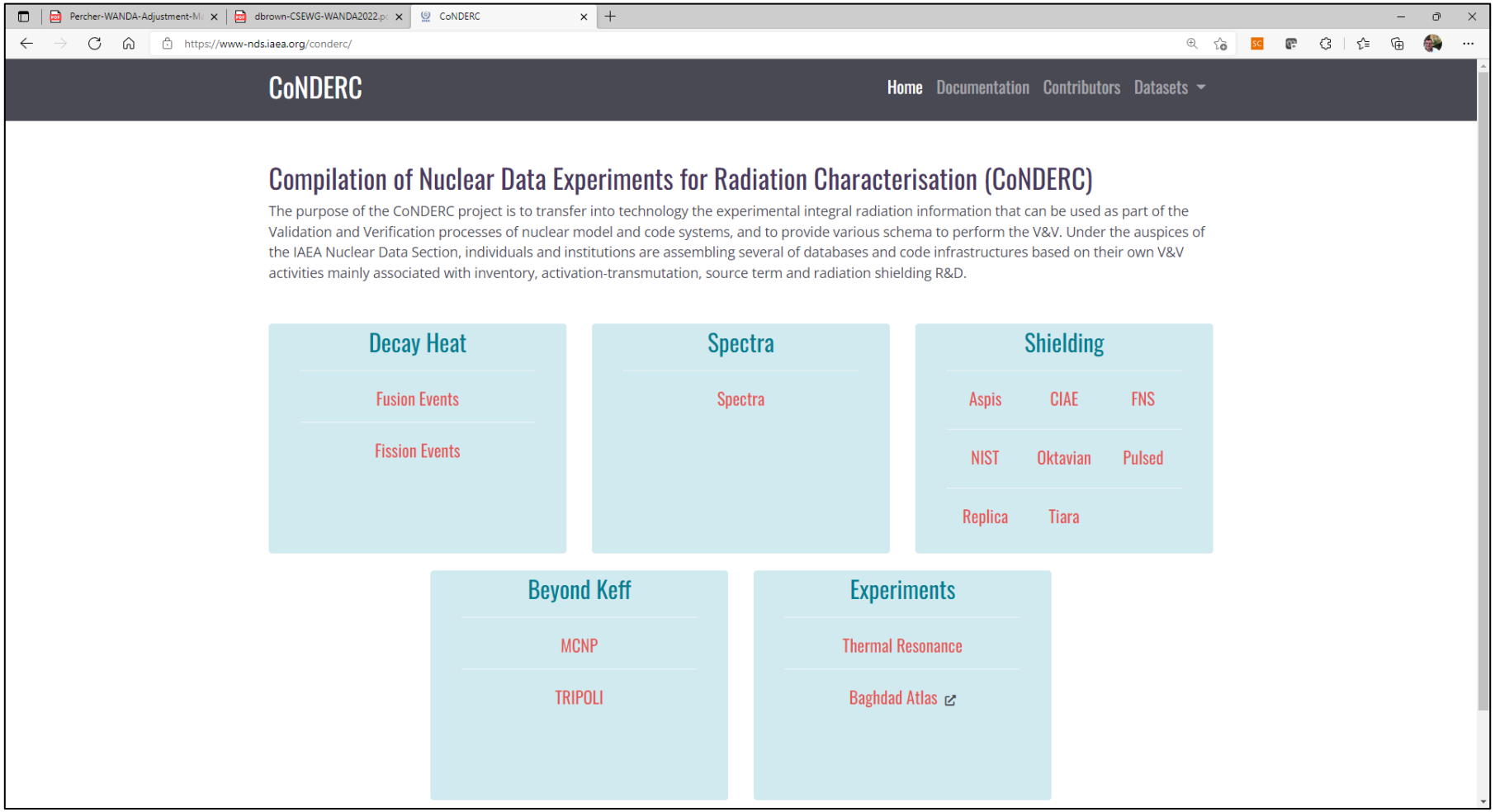
❑ SFCOMPO: Post Irradiation Experimental Measurements

- 700 samples



https://www.oecd-nea.org/jcms/pl_21515/sfcompo-2-0-spent-fuel-isotopic-composition

❑ Other Benchmarking

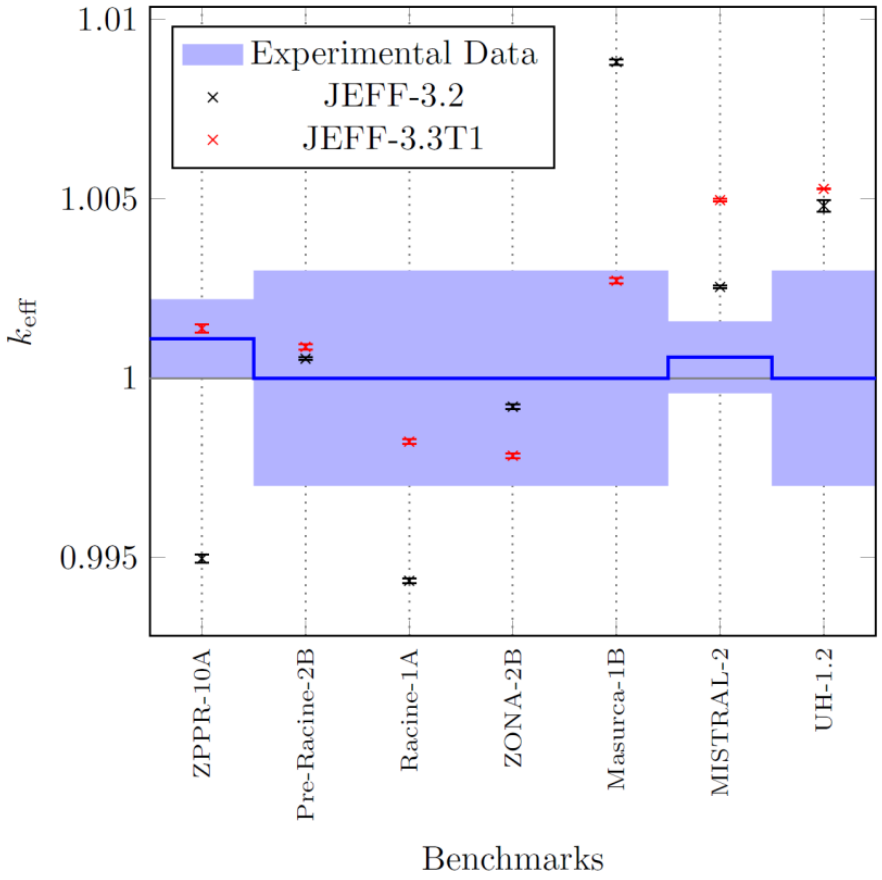


https://www-nds.iaea.org/conderc/

❑ Other Benchmarking

❑ Experimental reactors

Ref. P. Tamagno, JEF/DOC-1752 (2016)

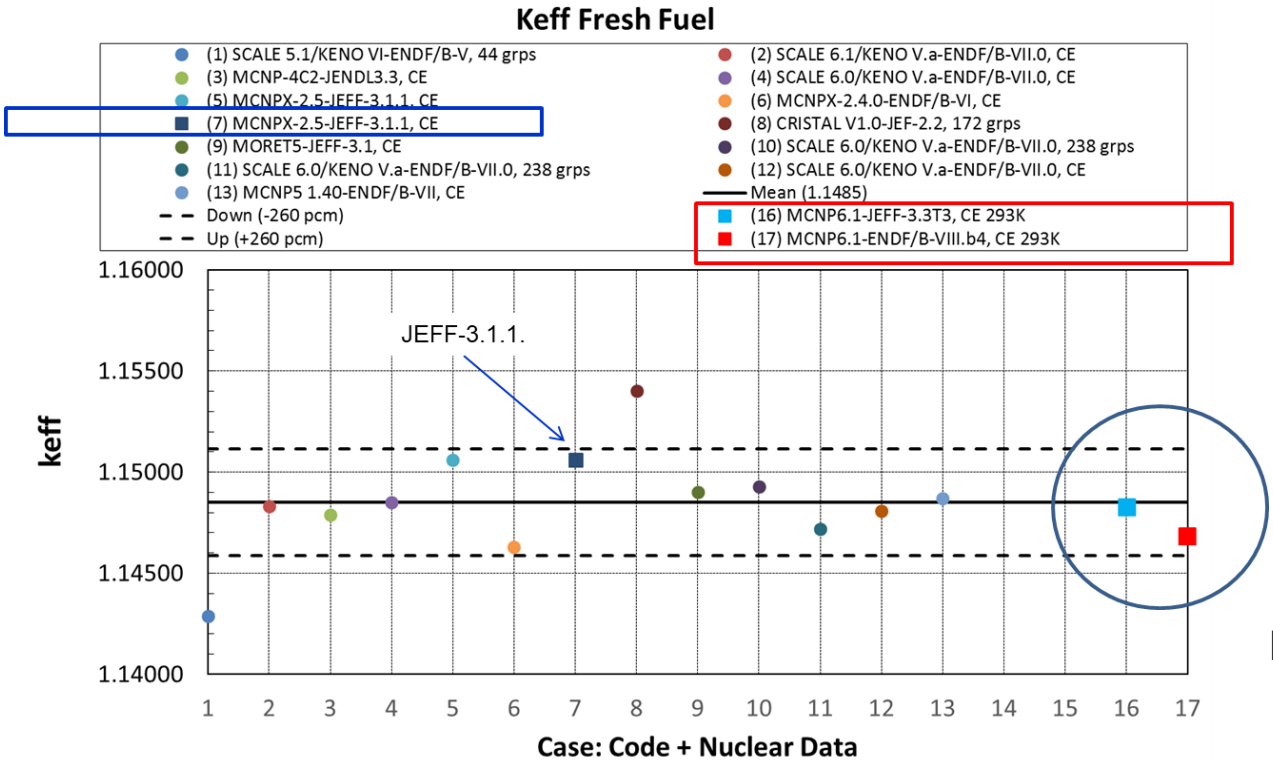


Experiment	Δρ(JEFF33T1-JEFF32) [pcm]
ZPPR-10A	+644
Pre-Racine-2B	+33
Racine-1A	+391
ZONA-2B	-137
Masurca-1B	-603
Mistral-2	+240
UH1.2	+51

❑ Other Benchmarking

❑ Computational Benchmarking

Reference: *John C. Wagner and Georgeta Radulescu, Specification for Phase VII Benchmark UO2 Fuel: Study of spent fuel compositions for long-term disposal, NEA Expert Group on Burn-up Credit, November, 2008*



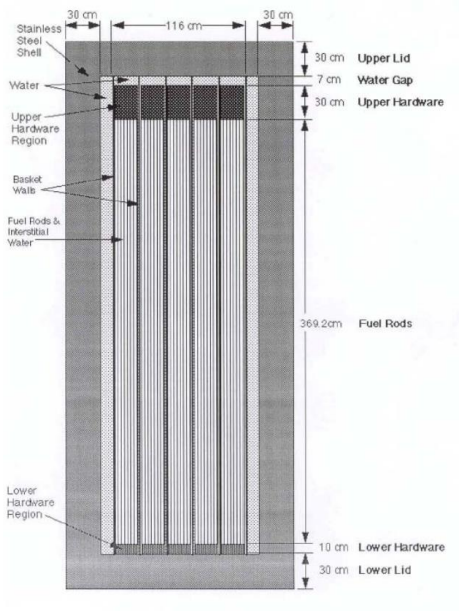
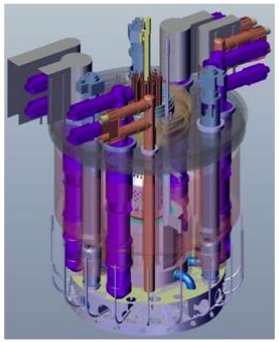


Figure. Cask model (side view)

❑ Other Benchmarking

❑ Computational Benchmarking: new reactor designs

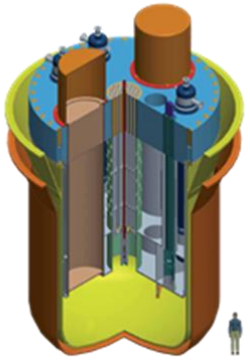
ASTRID prototype
(600 MWe)
Interm. Na circuit
Driver core ~ MOX



MOX	JEFF-3.2	JEFF-3.3T1	Diff.
k_{eff}	0.99829	1.0018	+351 pcm
Total fission probability	0.340	0.344	+1.0%
Total capture probability	0.658	0.654	-0.6%

P. Romojaro, JEFF/DOC-1756(2016)

MYRRHA concept
(50-100 MWe)
Cooled by lead-bismuth I
Driver core ~ MOX
Start-up core ~ UO_2 fuel



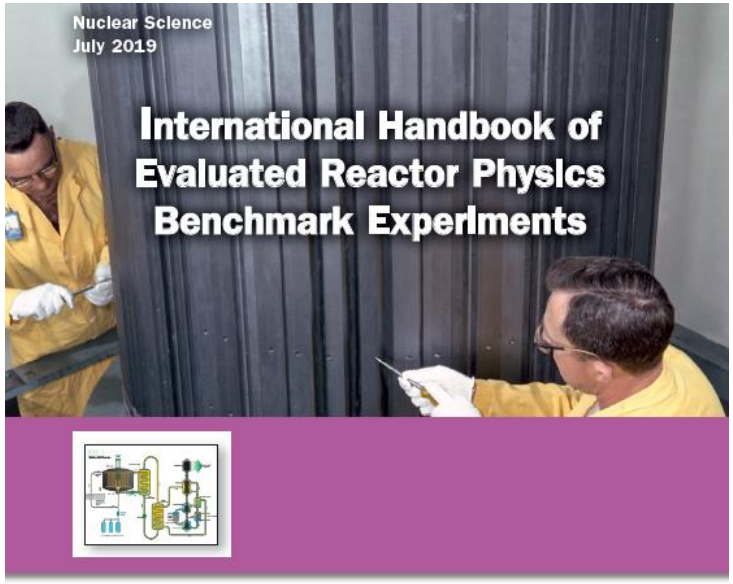
MOX	JEFF-3.2	JEFF-3.3T1	Diff.
k_{eff}	1.00479	1.00737	+258 pcm
Total fission probability	0.343	0.346	+1.0%
Total capture probability	0.664	0.660	-0.5%
UO2	**JEFF-3.2**	**JEFF-3.3T1**	**Diff.**
k_{eff}	1.01003	1.00001	-1002 pcm
Total fission probability	0.408	0.404	-1.0%
Total capture probability	0.596	0.600	+0.7%

International Reactor Physics Benchmark Experiment Evaluation Project

- Established in 2000
- 10+ types of measurements. (Only k-eff in ICSBEP … with exceptions see FUND)

  Reaction Rate Distribution, Spectral Characteristics, Power Distributions, Reactivity Effects, Isotopic Composition, Reactivity Coefficients,…

  - 200 reactor benchmarks
  - 200 spectra benchmarks
- Organised by reactor type
- Similar format to ICSBEP, with subsections for each measurement type

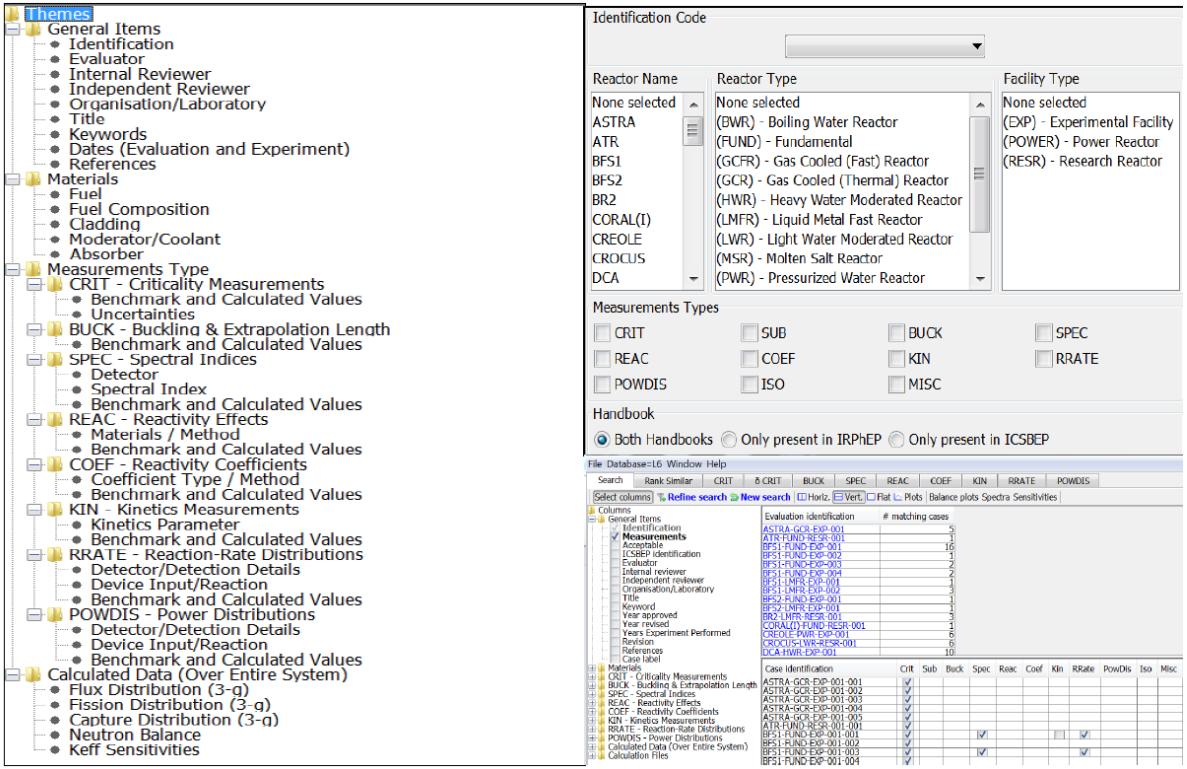


NEA
NUCLEAR ENERGY AGENCY

https://www.oecd-nea.org/jcms/pl_20279/international-handbook-of-evaluated-reactor-physics-benchmark-experiments-irphe

❑ IDAT

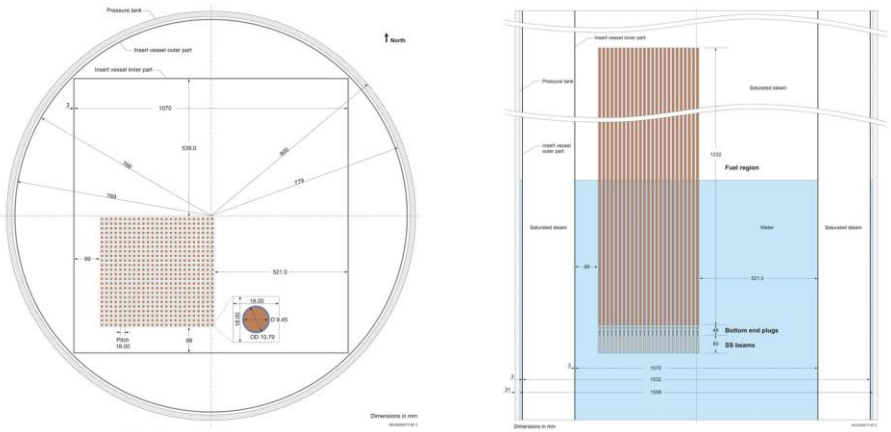
- The IRPhEP Database and Analysis Tool (IDAT) was first released in 2013 and is included on the IRPhE Handbook DVD. This database and corresponding user interface allows easy access to handbook information.

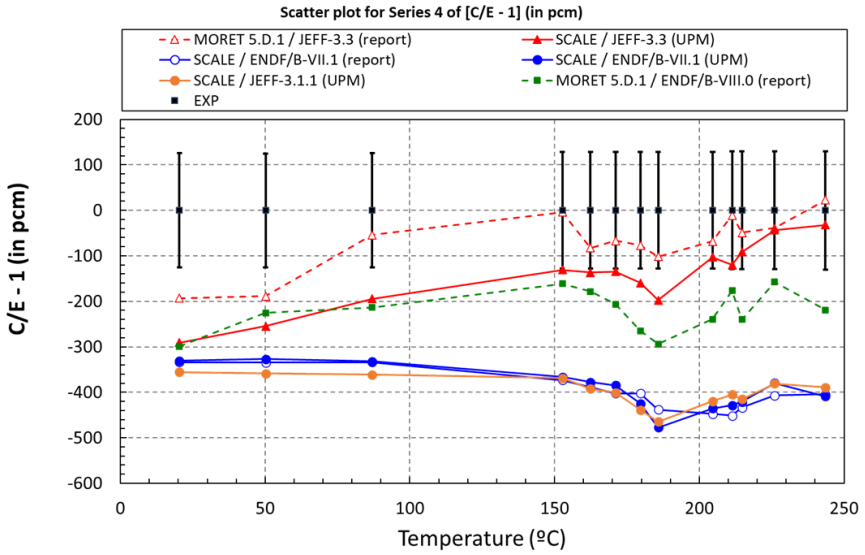


https://www.oecd-nea.org/jcms/pl_20296/international-reactor-physics-handbook-database-and-analysis-tool-idat

❑ **An example IRPHEP Benchmark:** Light-water reactor lattices at KRITZ reactor in Studsvik (Sweden) for criticality at room and elevated temperatures

Figure 1. Schematic top and side views of the core are presented





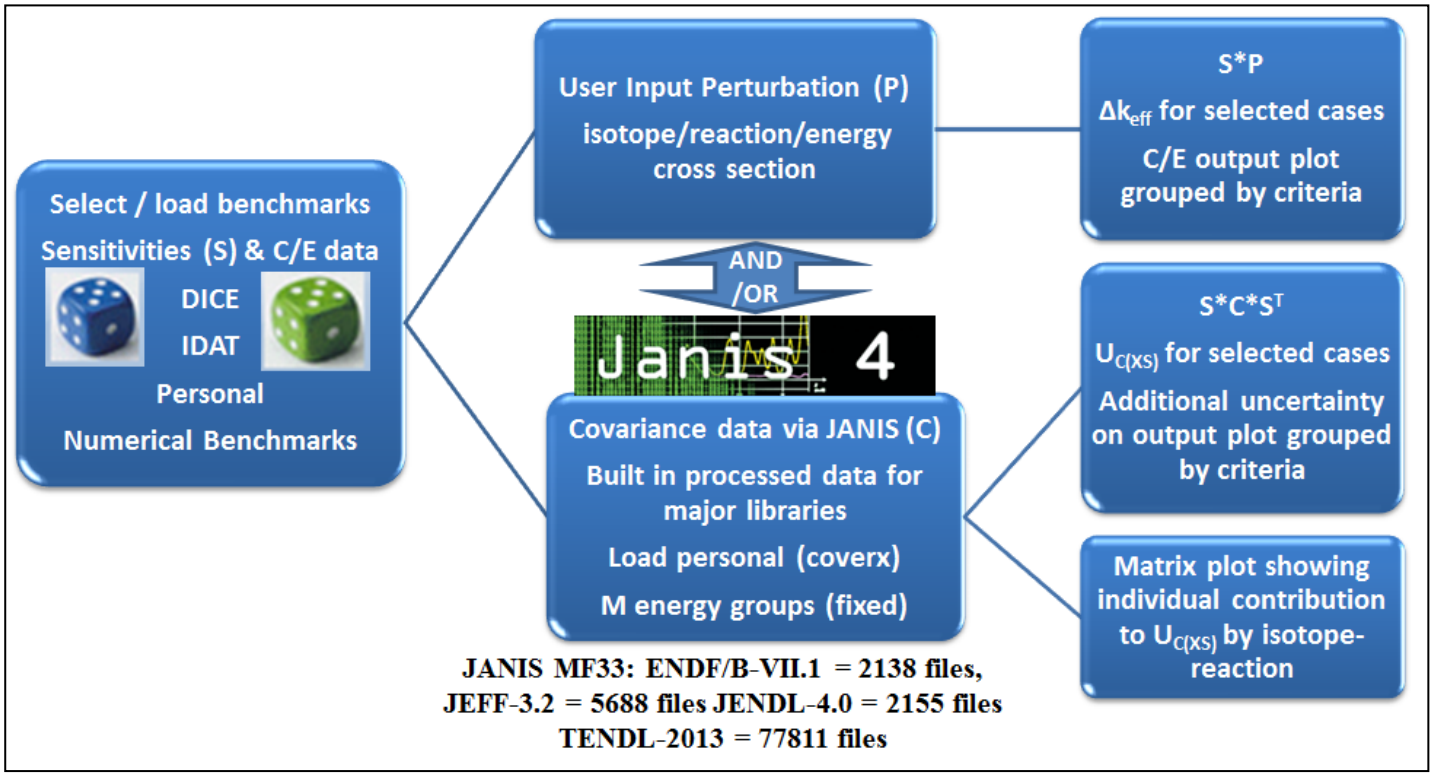
- IRPHEP **"KRITZ-LWR-RESR-004 Evaluation Report. 2019 Rev.0"**
- 37 criticality measurements at room and elevated temperatures (critical water heights of active fuel covered by water)
- UO2 fuels 1.35wt% in ^{235}U

❑ In JEFF-3.3, the trend with temperature becomes stronger

❑ NDAST

NDaST (**N**uclear **Da**ta **S**ensitivity **T**ool) brings together the existing capabilities of both DICE and JANIS, whose main objective is:

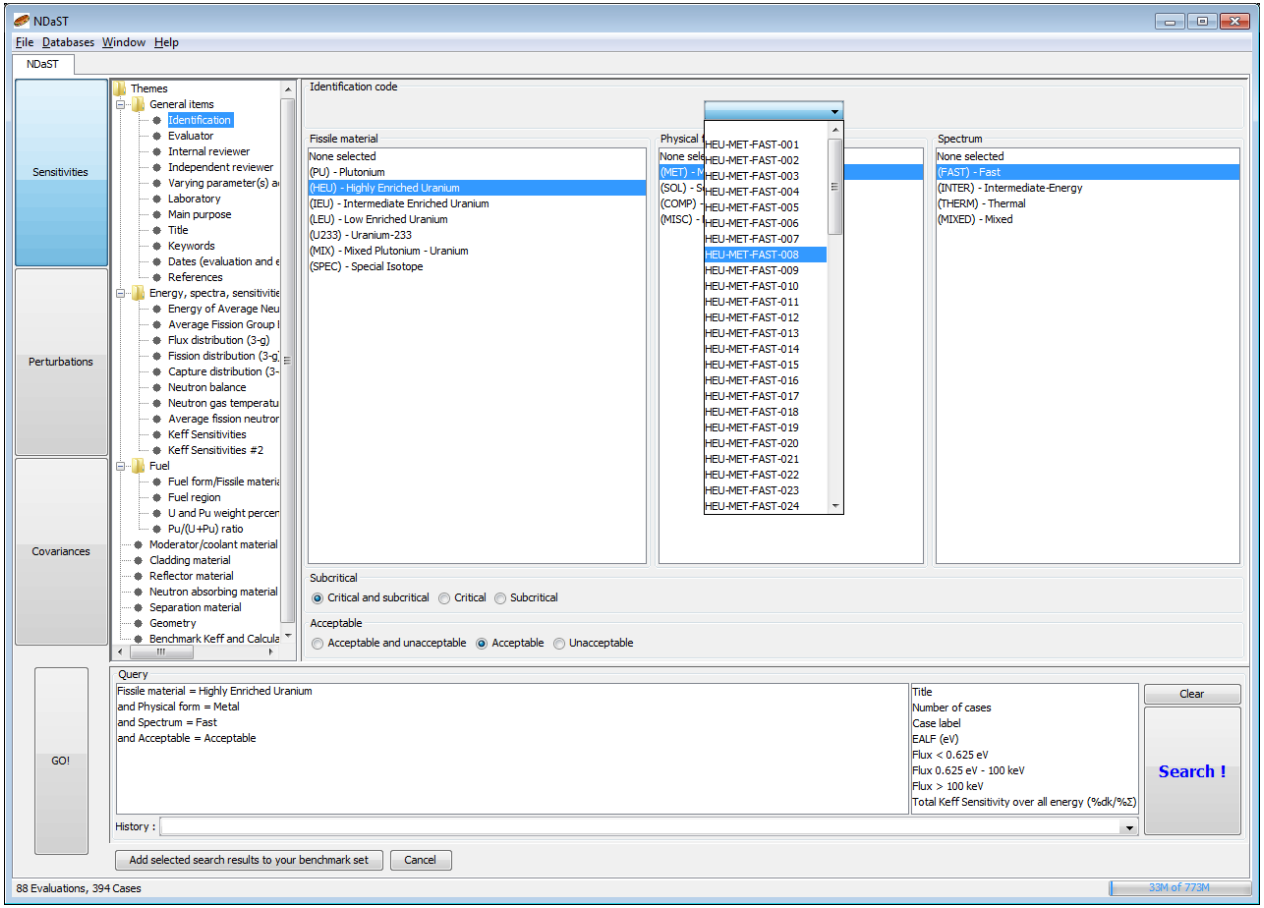
- to quickly propagate the impact of changes in nuclear data cross sections and nuclear data covariances to benchmarks



https://www.oecd-nea.org/jcms/pl_32450/nuclear-data-sensitivity-tool-ndast

❑ NDAST: Sensitivities

Sensitivities Panel: Data needs to be added in order to provide the cases for which the subsequent calculations will be carried out



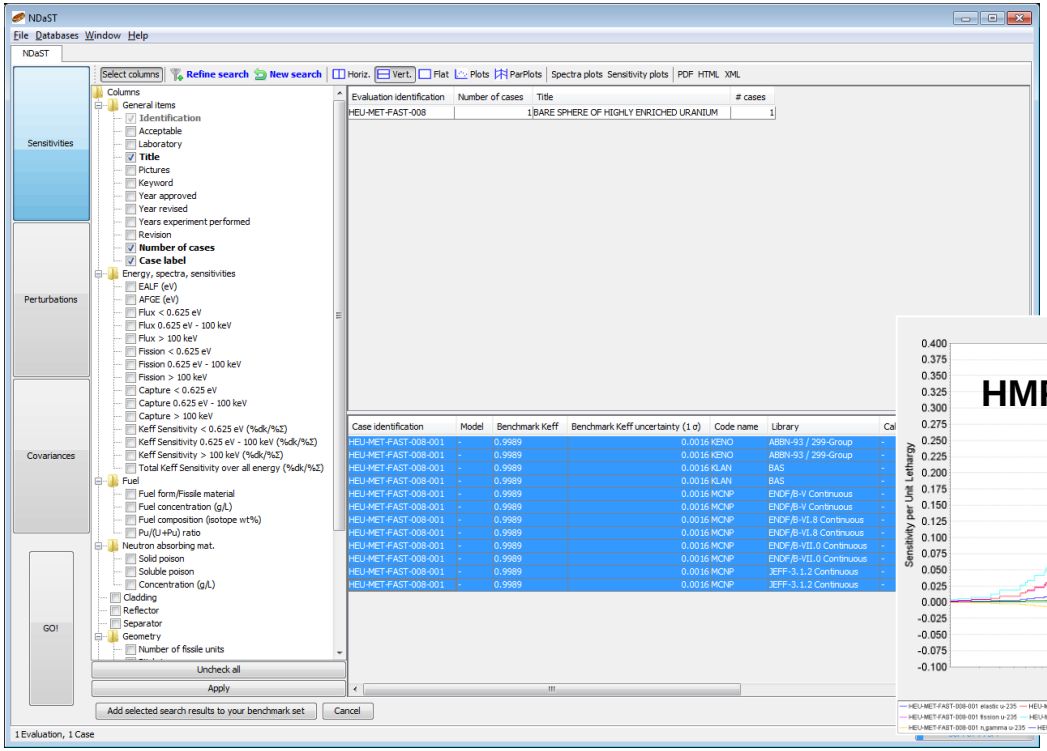
❑ NDAST: Sensitivities

Current Databases:

- Experimental benchmarks in DICE and IDAT (useful only when benchmarks have sensitivity profiles)
- Nuclear data covariance in JANIS database

Formats

- Sensitivity data: SCALE, ABBN formats
- Covariance data: ENDF-6, BOXER and COVERX (SCALE6.1)

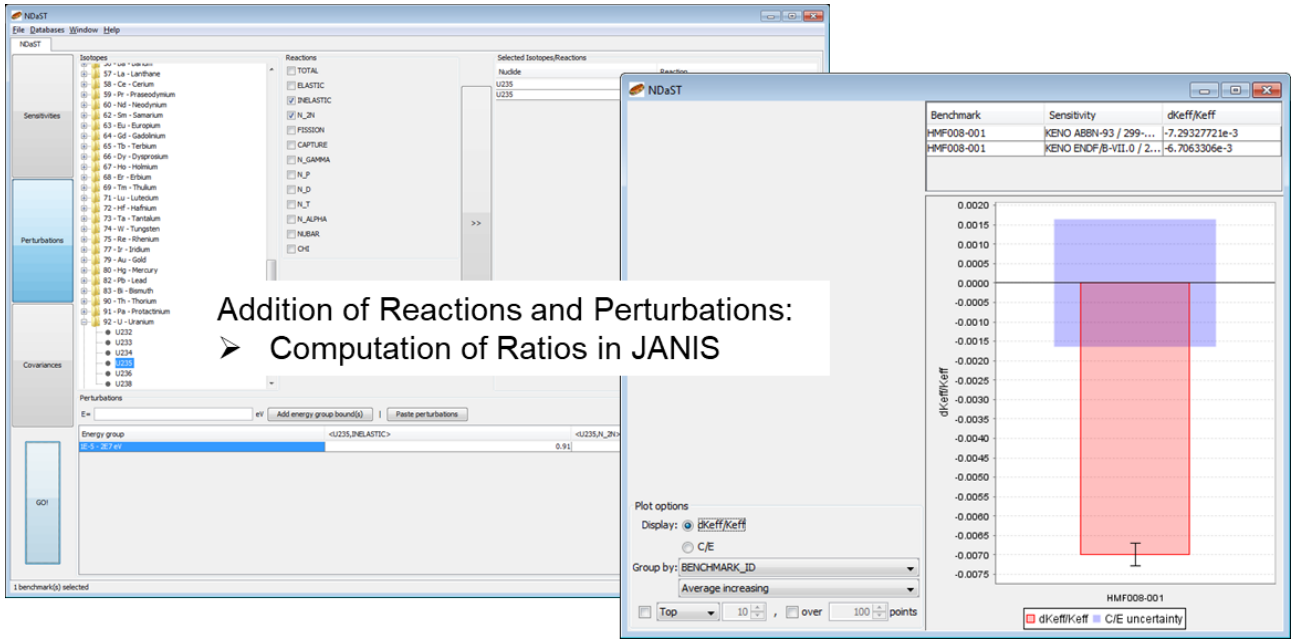


"*Add selected search results to your benchmark set*" at bottom left of the panel

❑ NDAST: Perturbation

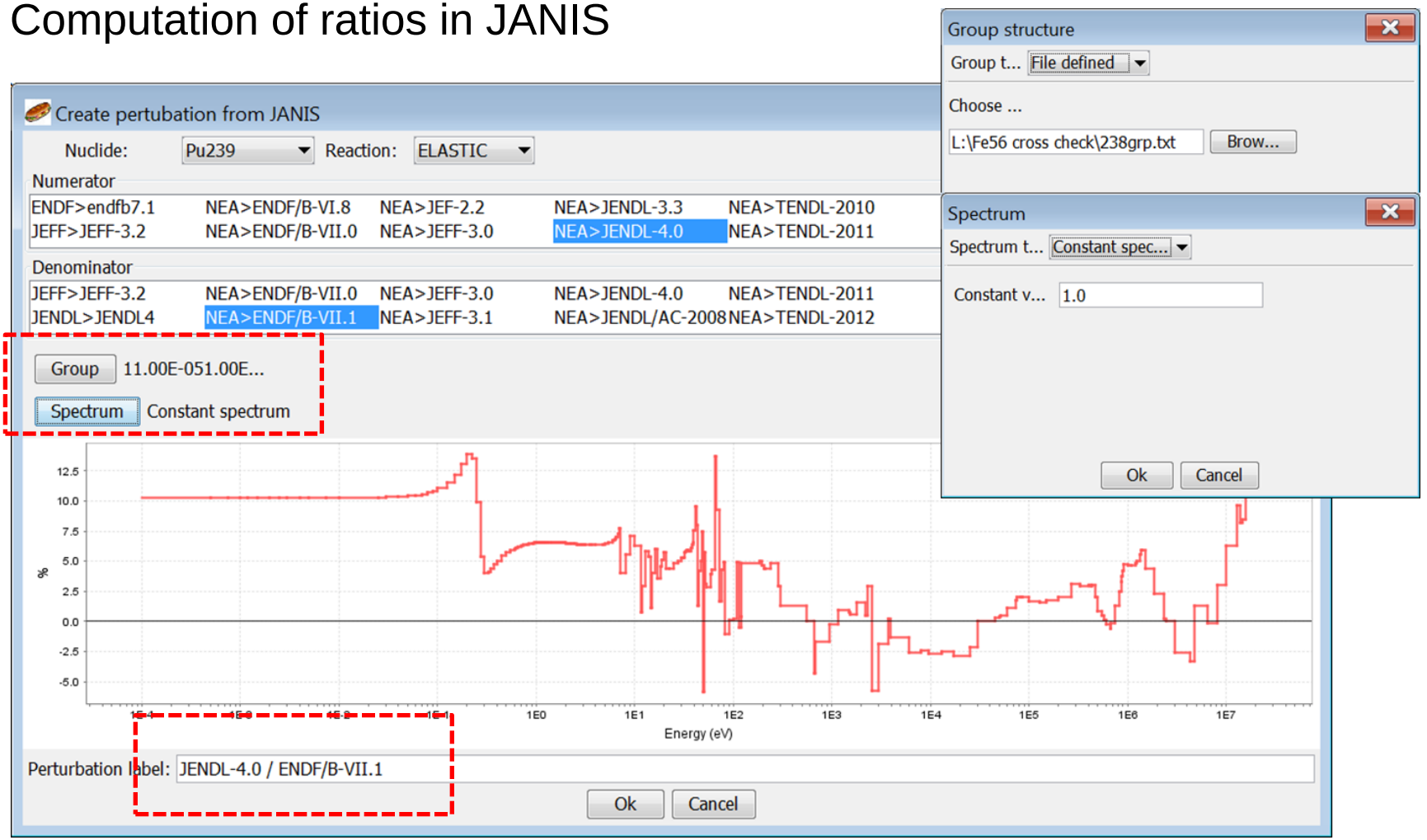
- **NDasT performs matrix multiplication** for calculating keff perturbations and keff uncertainties
- **Plotting capability:**
  - experimental keff + uncertainty
  - calculated keff + perturbation (including breakdown) + uncertainty
- **Save status** (benchm./perturb./covariance selections) in XML format file

Perturbation Panel



❑ NDAST: Perturbation

❑ Computation of ratios in JANIS

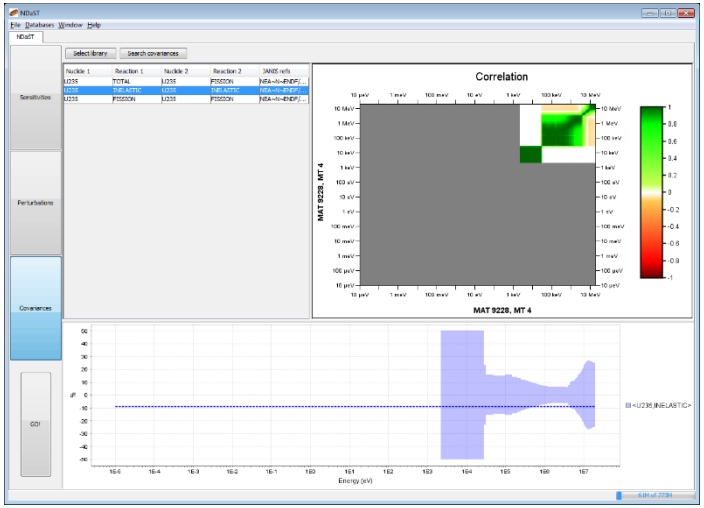


❑ NDAST: Covariances

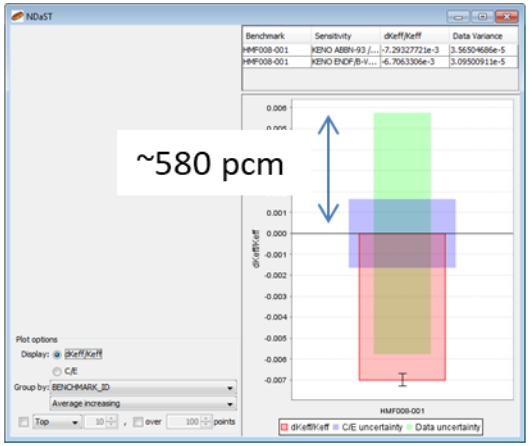
Covariances Panel

Search covariances and press ‘ok’:

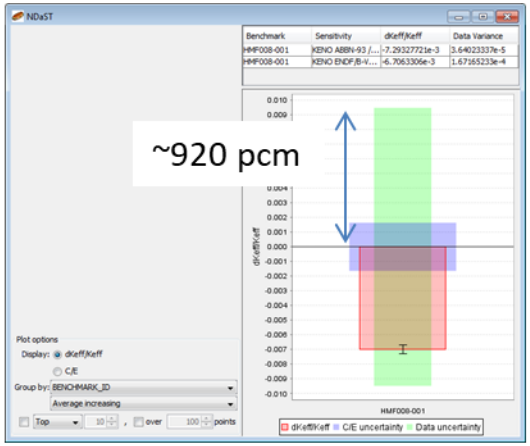
- JANIS Database
- Format: ENDF, BOXER



Go! and Output Results Panel



Only inelastic ENDF/B-VII.1



All ENDF/B-VII.1 covariances

- Δk/k perturbation (**red**)
- Δk/k benchmark uncertainty (**blue**)
- Δk/k based on the ENDF7.1 covariance file (**green**)

Conclusion

- *What is an integral experiment*
- *Integral experiments databases: ICSBEP and IRPHEP*
- *Visualization and databases search tools: DICE and IDAT*
- *NDaST tool*
- *Examples of validations*

Back-up slides

❑ Create a new database in JANIS

… to be used with NDAST

Import WIZARD tool

- Use the “Database > Import Wizard” to create a permanent database

Following steps:

1) **New folder** shall be created with three sub-folders, one per type of file (i.e. hendf, boxer and inter). Then, the files generated shall be copied to their corresponding sub-folders. **IMPORTANT**! Delete those empty files
2) Open JANIS, and at the toolbar click on “**database -> import wizard**“
3) Add HENDF/PENDF files. For that use either “**Add directory**" or “**add files**" options. Click on “next“
4) “**Automatic detection**” should work fine. Click on “next"
5) Choose a **library name,** e.g. JEFF-4.0T1, (less than 20 characters). Click on “next“
6) Select “**a new base**“ when importing HENDF, that means for the first import. For BOXER and INTER files, “an existing base" shall be selected, and then, selecting the created database for HENDF files
7) Choose “**path to the folder”** where the database will be created. Click on “next"

Back-up slides

❑ Create a new database in JANIS

Following steps:

7) ….

8) The "base root" shall point to the folder created with the three sub-folders (one for each kind of file type). Click on "next"

9) Type a "**database" name**, e.g. "NUDATA", for showing later in JANIS. Click on "next"

10) A summary of the task to do, plus input parameters, is presented before importing data from files. Click on "Finish"

11) Once imported HENDF files, for BOXER and INTER files **repeat these instructions** until step (5), where to change to "existing base" option

12) Errors might arise if empty files are read, so remove them from the importing list

13) Check that once the BOXER files have been imported into the database, a "Others" tag does not appear in the "Nuclide / Compound tree". If this tag exists, then, there is an issue in regard to cross-correlation covariance data, likely to be missing data for one of the two isotopes present in the cross-correlation matrix

14) At the end of this process, a "**db.h2.db**" le is created, plus the importing logs

Back-up slides

- Two distinct methods of **nuclear data adjustment methodologies**:
  - **Deterministic**
    - Generalized Linear Least Squares (GLLS)

$$[E - C'(\sigma')]^T V_E^{-1} [E - C'(\sigma')] + [\sigma' - \sigma_0]^T V_\sigma^{-1} [\sigma' - \sigma_0] = \chi^2_{min}$$

Assumptions:
- Experimental and nuclear data are normally distributed
- Linear approximations between all observables
- Model and experimental data are uncorrelated

  - **Stochastic/Monte Carlo methods**
    - Bayesian MC techniques -> direct application of Bayes' Theorem

$$(\sigma|E) \propto p_0(\sigma|\sigma_C, V_C) \times L(y_E, V_E|\sigma)$$

    - To avoid the need to linearize non-linear models
    - To handle model which are not necessarily normally distributed

Back-up slides

❑ Generalized Linear Least Squares (GLLS)

- First-order Taylor series approximation

$$C(\sigma) \approx C(\sigma_0) + S(\sigma - \sigma_0)$$
$$V_C \approx S V_{\sigma_0} S^T$$

- "A posteriori" mean and variance-covariance matrix

$$\sigma' = \sigma_0 + V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E \right]^{-1} [E - C(\sigma_0)]$$

$$V_{\sigma'} = V_{\sigma_0} - V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E \right]^{-1} S V_{\sigma_0}$$

$$C'(\sigma') \approx C(\sigma_0) + S(\sigma' - \sigma_0) = C(\sigma_0) + S V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E \right]^{-1} [E - C(\sigma_0)]$$

$$V_C' \approx S V_\sigma' S^T = S V_{\sigma_0} S^T - S V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E \right]^{-1} S V_{\sigma_0} S^T$$

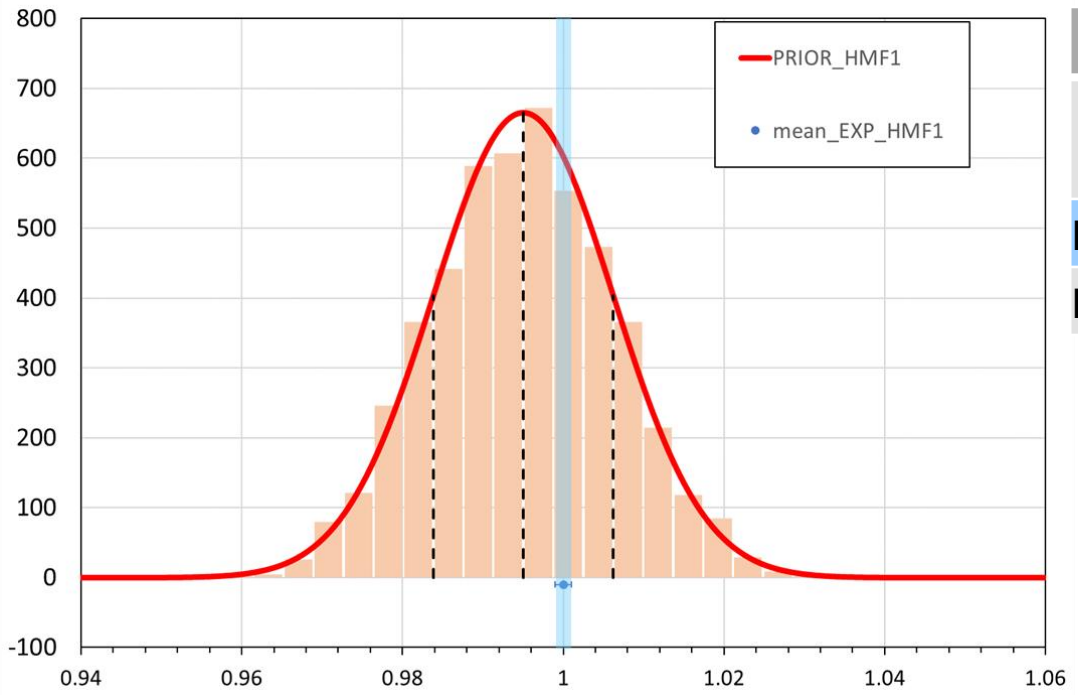
$$V_E' = V_E - V_E \left[S V_{\sigma_0} S^T + V_E \right]^{-1} V_E$$

$$V_{E-\sigma}' = V_E \left[S V_{\sigma_0} S^T + V_E \right]^{-1} S V_{\sigma_0}$$

GLLS: "*This approach is a Bayesian approach in the sense that experimental data are used to adjust prior values. Although probability density functions are not considered explicitly.*"

Back-up slides

❑ HMF1 – Godiva Benchmark

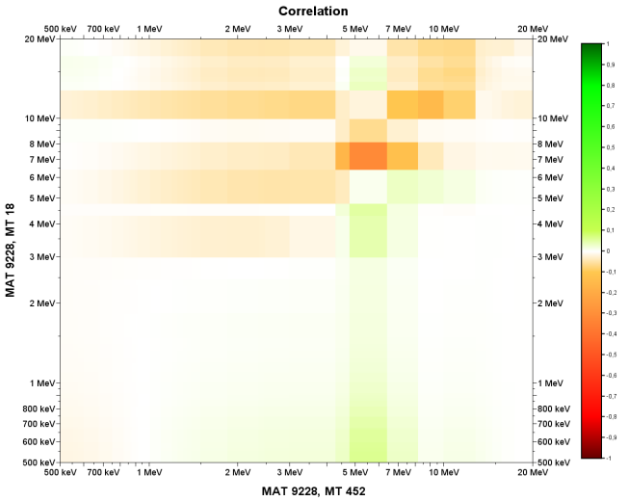


	HMF1	
	keff (MEAN)	Dkeff (STD)
PRIOR....	0.99504	0.01119
POST....	0.99992	0.00100

- **Exercise:** BMC adjustment with criticality
  5000 random files 235U/TENDL2014
  Calculations with MCNP6.1.1

Correlation: MT18 –MT452

PRIOR



POSTERIOR with HMF1