Status of the Nuclear Data Sensitivity Tool (NDaST)

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WPEC SG46
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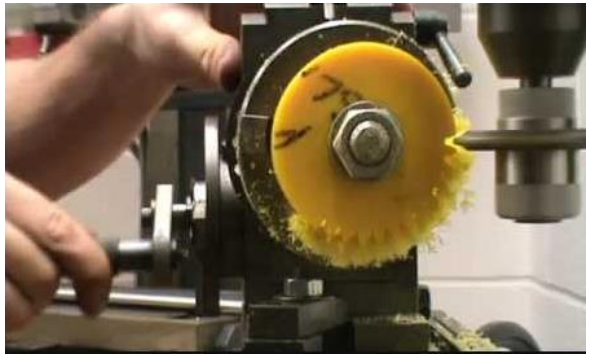
What Is NDaST?

- Some java code resulting in a GUI that connects nuclear data (JANIS) to integral experiments (DICE, IDAT, SINBAD, NEA Benchmarks).

https://www.oecd-nea.org/ndast



Industrial engineering: is a branch of engineering which deals with the optimization of complex processes, systems, or organizations. **Industrial engineers** work to eliminate waste of time, money, materials, person-hours, machine time, energy and other resources that do not generate value. According to the Institute of Industrial and Systems Engineers, they create engineering processes and systems that improve quality and productivity.[1]

Nuclear Data Sensitivity Tool (NDaST) Flowchart

Benchmarks (Sensitivities) → Nuclear Data (% Change or Covariance) → Integral Results

XML and GUI

Select / load benchmarks

Sensitivities (S) & C/E data

DICE

IDAT

Personal

Numerical Benchmarks

Database of over 4000 Sensitivity Data Files

User Input Perturbation (P)

isotope/reaction/energy cross section

AND /OR

Covariance data via JANIS (C)

Built in processed data for major libraries

Load personal (coverx)

M energy groups (fixed)

S*P

Δk_{eff} for selected cases

C/E output plot grouped by criteria

S*C*S^T

$U_{C(XS)}$ for selected cases

Additional uncertainty on output plot grouped by criteria

Matrix plot showing individual contribution to $U_{C(XS)}$ by isotope-reaction

JANIS MF33: ENDF/B-VII.1 = 2138 files, JEFF-3.2 = 5688 files JENDL-4.0 = 2155 files TENDL-2013 = 77811 files, SCALE6.2

Sensitivity Profiles Available [DICE + IDAT]

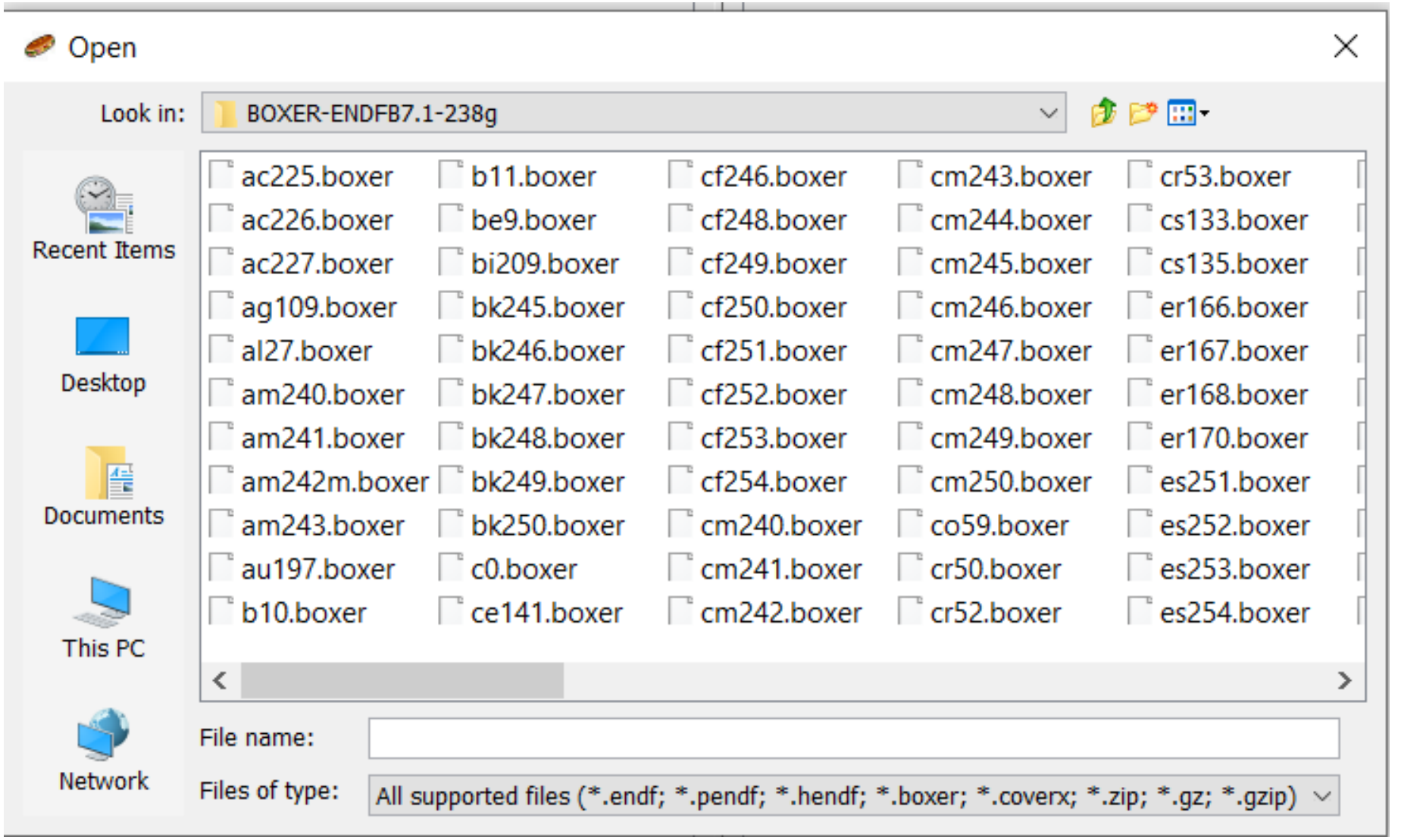
Handbook Edition	Number of Unique Cases	Sources
2012	727	TSUNAMI1D+TSUNAMI3D [VALID]+MMK-KENO
2013	3575	Previous +Non VALID cases SCALE6.0 from Balance Inputs
2014	4011	Previous + MCNP6 + SCALE6.2BClutch
2015	4065	Previous + New Cases
2016	~4200	Previous + New Cases + P1 Sensitivities [~400 cases]
2017	~4200	Previous+P1 Sensitivities [~700 cases]
2017	~600	IDAT Sensitivities [Waiting input +Code GPT]

- Sensitivity dot product to characterise similarity.

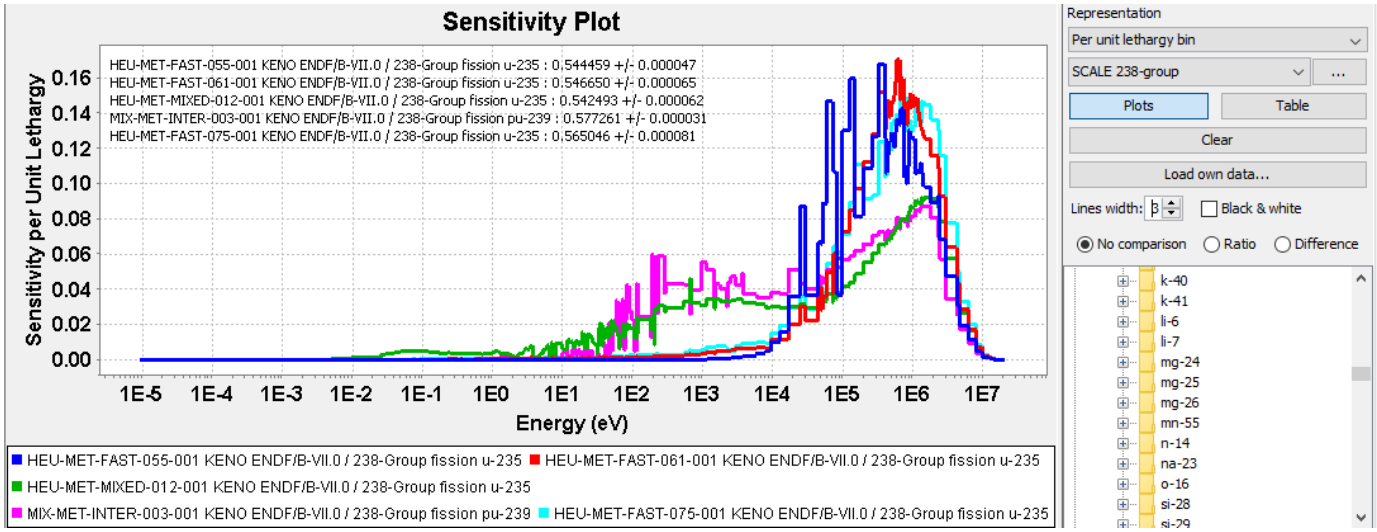
Covariance Data Available [JANIS]

- All major libraries have BOXER files with MF32/MF33 processed. (~30 libraries with covariances, ~40 libraries)
- Users can add MF31. In the future these will be available
- No MF34. Will come in the future.
- Supports user entered BOXER / COVERX files
- Supports some versions of the SCALE covariance library

Load Own Covariance

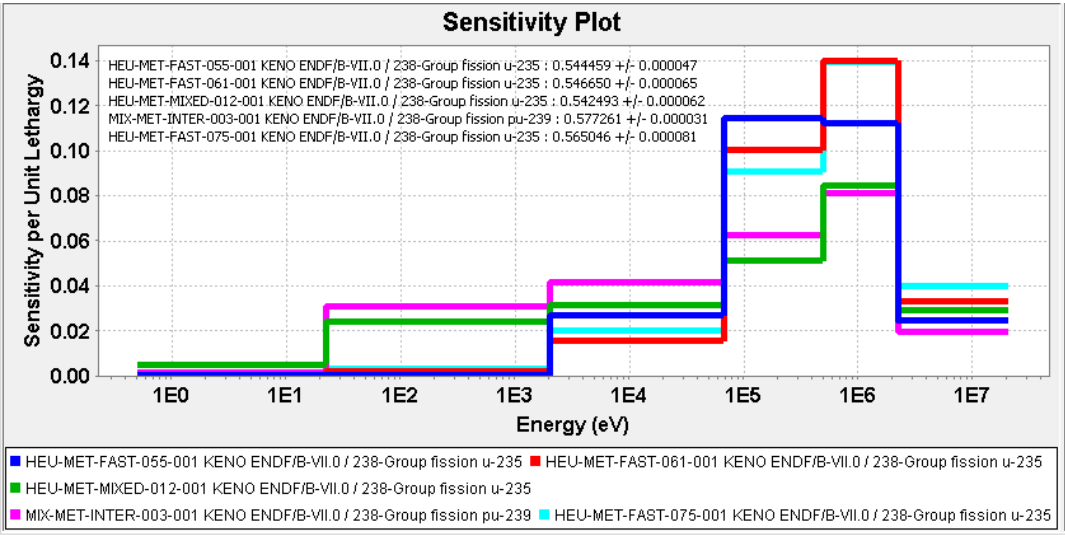


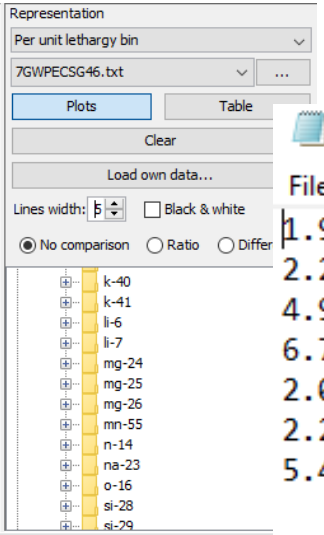
DICE+IDAT With Proposed 7 Group Structure

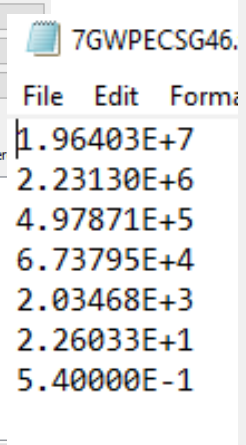


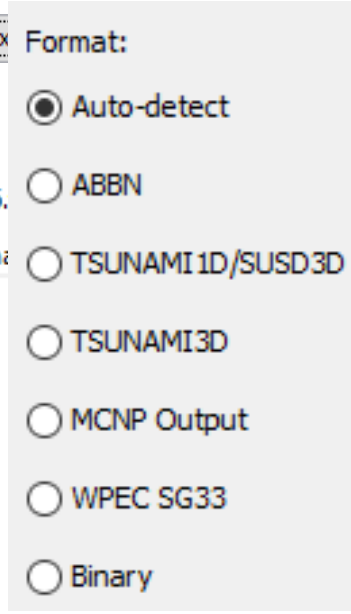
Some ZPPR Fission Sensitivity Profiles

Support added for MCNP6.2 created TSUNAMI3D format following JEFF 2021 winter meeting

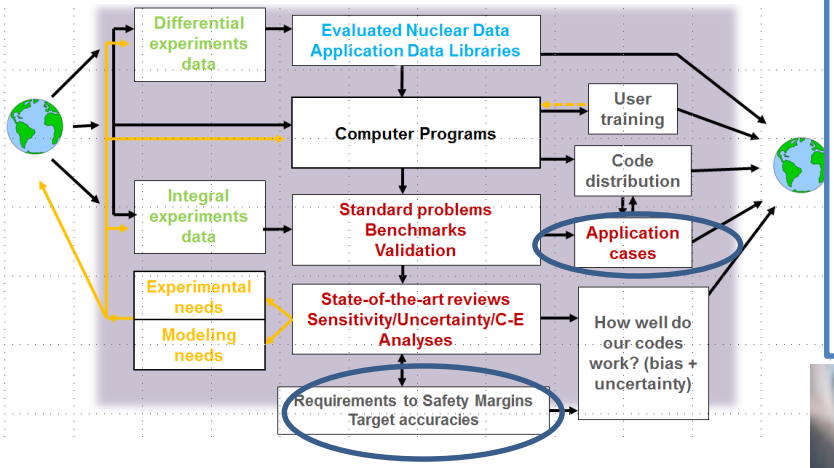




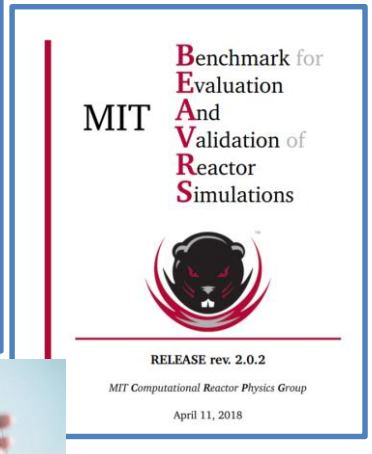


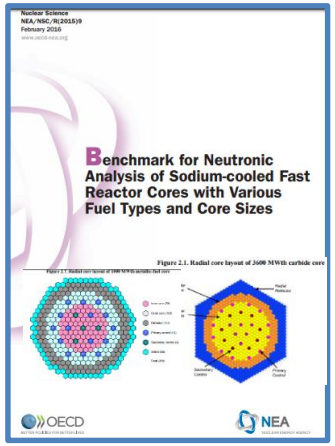


Linking to representative benchmarks from various application



Collect benchmarks and automate the impact of new data on these activities

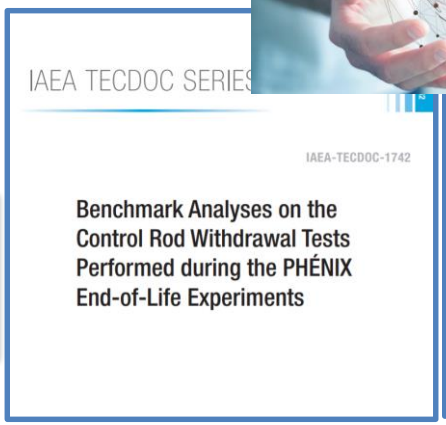


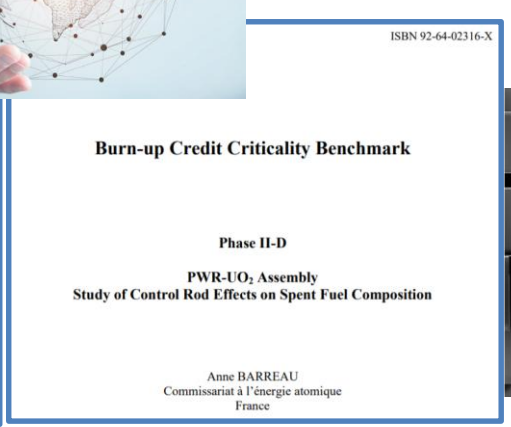


Candidate Reactors for Target Accuracy Requirements

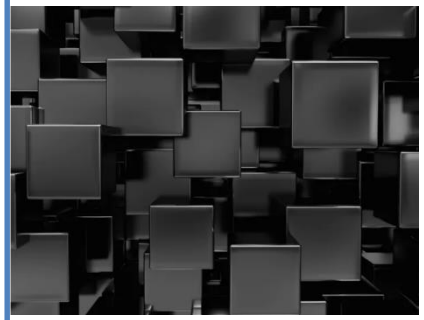
- From SG26:
  - ABTR, SFR, EFR, GFR, LFR, ADMAB, VHTR, PWR
- From SG33:
  - ABR (metal), ABR (oxide), FBR
- New ones with available data:
  - MYRRHA (critical, subcritical)
  - JSFR
  - Westinghouse LFR
  - MOSART (Fast MSR)
  - Fast MSR with chloride salt
  - Low sodium void SFR
  - SPX1
  - INL HTGR
  - Not easy to get (proprietary) but possible: VHTR, INL microreactor, TWR from TerraPower
- Would be nice to have also: MSR (Flibe ?), SMR (Thermal, fast), ASTRID, microreactors (earth, space)

WPEC SG46: **Efficient** and **Effective** Use of Integral Experiments for Nuclear Data Validation





Industry surrogate models/response functions



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https://www
REGULAR ARTICLE
OPEN

A comparison of uncertainty propagation techniques using NDaST: full, half or zero Monte Carlo?

James Dyrda, Ian Hill, Luca Fiorito, Oscar Cabellos, and Nicolas Soppera*
OECD Nuclear Energy Agency, Boulogne-Billancourt, France

Received: 23 October 2017 / Received in final form: 18 January 2018 / Accepted: 4 May 2018

Have I see it before?

April 2015-2017

JEF/DOC-1840	JEFF-3.3T13 Processed Covariances: Uncertainty Propagation Analysis and Comparison	J. Dyrda, O. Cabellos
JEF/DOC-1789	CIELO Pu-239 data testing with NDAST tool, Ian HILL, NEA	
JEF/DOC-1772	JEFF-3.3T1 processed covariances : uncertainty propagation analysis and comparison, J. Dyrda	
JEF/DOC-1759	JEFF-3.3-T1 processed covariances: uncertainty propagation, analysis and comparison, J. Dyrda	
JEF/DOC-1727	Use of the NDaST tool for Benchmarking and Validation, J. Dyrda	
JEF/DOC-1639	Development of a new Nuclear Data Sensitivity tool at NEA, J. Dyrda	

- Used for CIELO
- Presented at NCSP2017 Annual Meeting
- Presented at WONDER2018
- Presented at ND2018
- Presented at ANS2018

And as parts of other presentations, example:

EPJ Web of Conferences **146**, 02001 (2017)
ND2016

with a feedback loop leading to the optimization of the reaction model parameters and ultimately of the evaluated data files. Nuclear reaction theory and modeling codes for coupled channels, statistical reactions and fission, and R-matrix, continue to be refined. The community is also starting to understand the benefits, and use of, sensitivity tools such as the NEA's NDaST codes to help focus research efforts. Also, various insights from the NEA/WPEC Subgroup 39 adjustment project have been useful.

jefdoc-1991	Feedbacks on JEFF-3.3 Evaluation	Oscar Cabellos	UPM	Spain	April 2020

NDaST fast, and keeps getting faster

JEFF3.3 test set (146 cases for 54 covariance files) runs in under 1 minute. Previously 20-30 minutes.

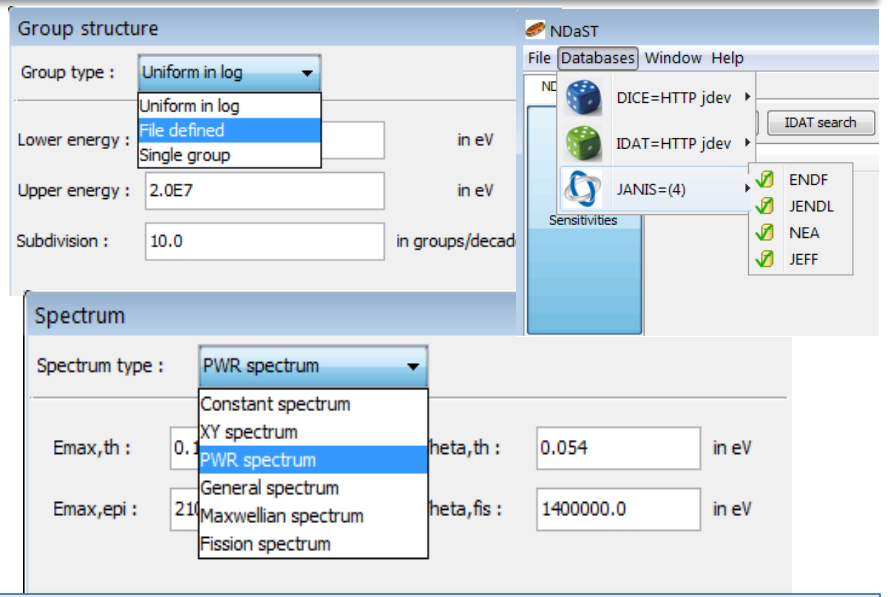
Some changes included:

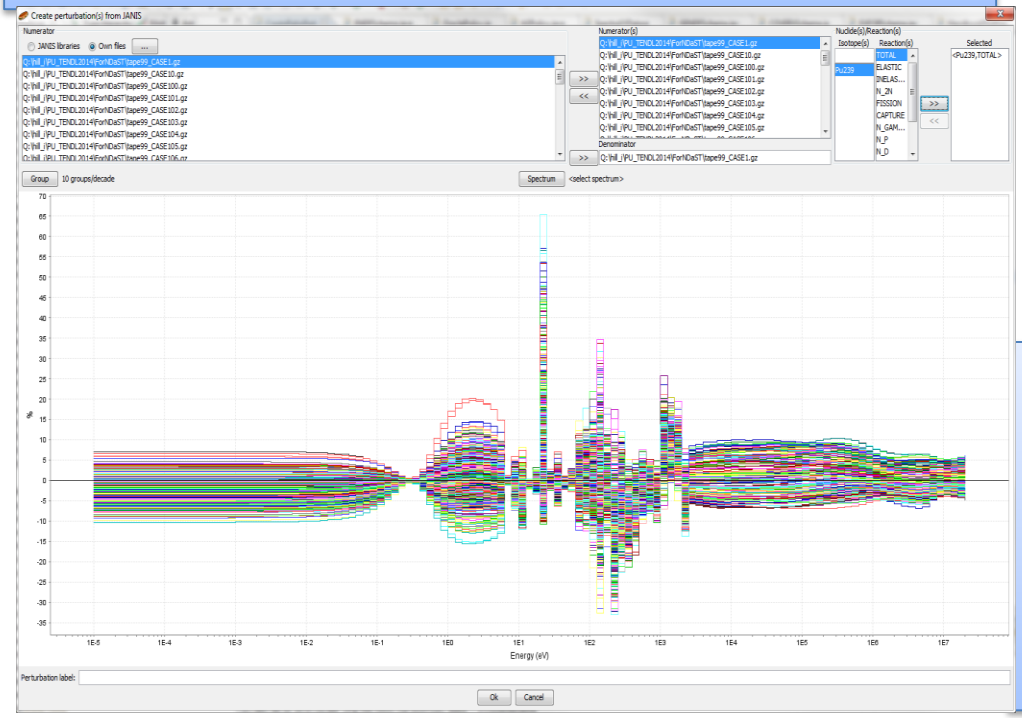
- Discarding zones in sensitivity profiles
- Discarding sensitivity nuclide reactions with 0's.
- Using a custom binary format to optimise compression and transfer

NDaST: Automated JANIS Computations

- An automated link has been introduced to the JANIS nuclear data software to generate the perturbation ratios between two evaluations.

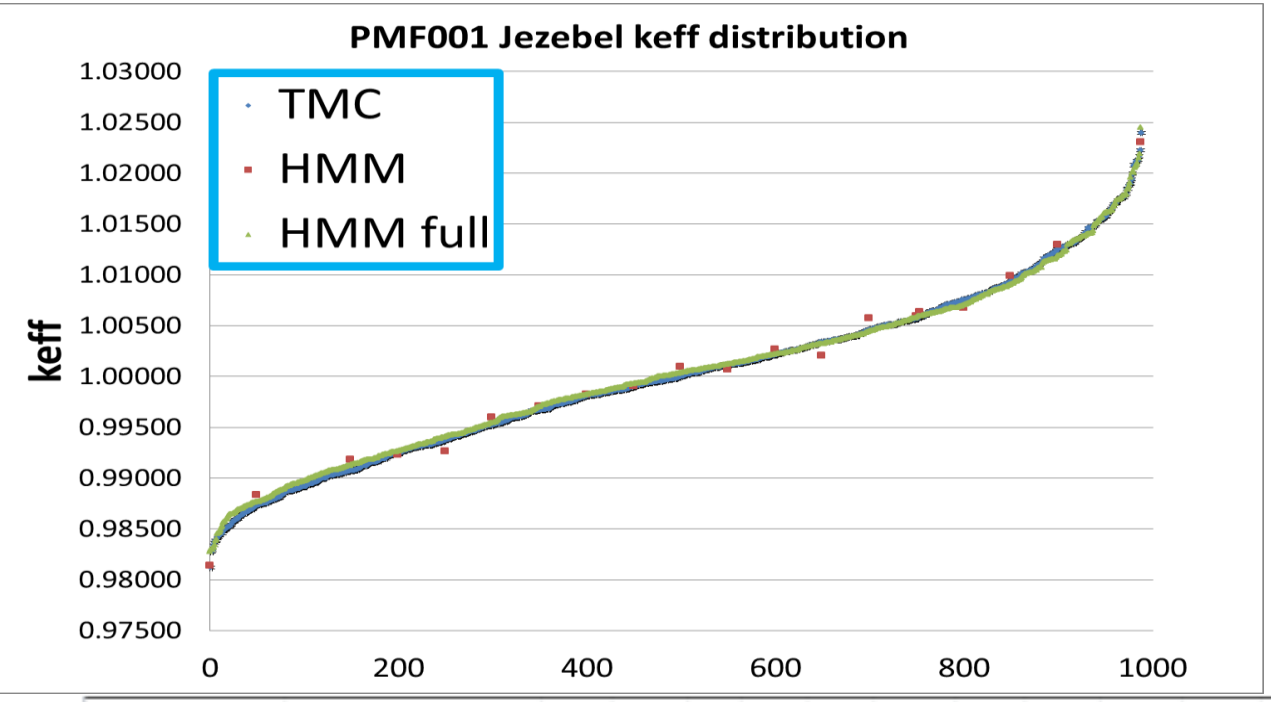
- Represented within any energy group structure required.
- Analytical or personal spectrum weightings may also be applied





- Multiple perturbations of the same nuclide-reaction can now be input for faster comparison with one single run
- NDaST now has a 'file upload' feature, to avoid needing to already have libraries held in a JANIS base.

Half Monte Carlo Method (HMM) Results

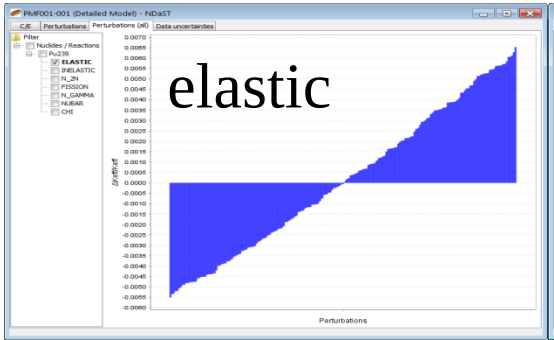


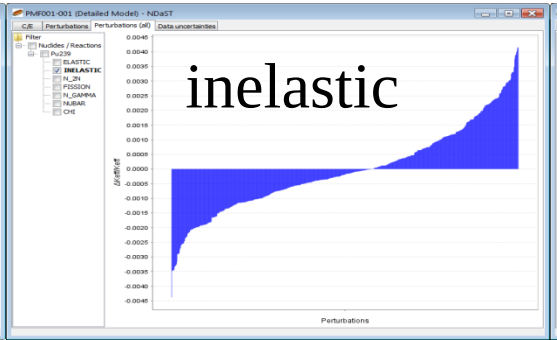
k_{eff} distribution, sorted lowest k_{eff} to highest, plotted with the HMM k_{eff} predictions for 20 samples and full automated set

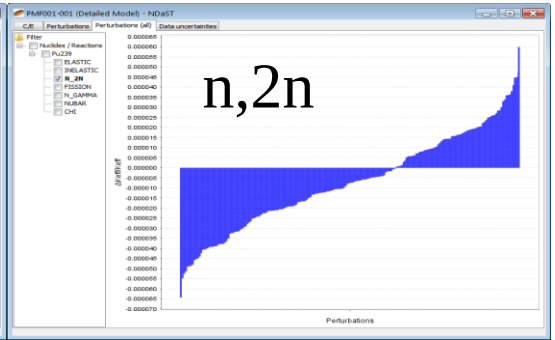
Example breakdown by reaction for 20 sample cases

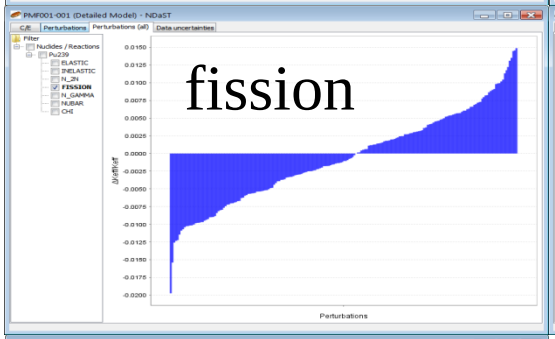
	Delta keff (pcm)																			
	Case Number																			
	24	34	38	170	431	436	455	476	494	527	558	591	643	670	680	710	738	772	782	993
Elastic	606	-217	-157	-441	513	59	-520	59	216	-47	606	-222	-490	-348	42	364	629	-481	393	-253
Inelastic	110	252	-19	75	-190	139	119	132	384	-9	-130	219	1	-206	81	-192	69	-14	-143	-45
N,2N	-3	-1	-4	-3	-4	1	-6	1	2	-6	-3	-4	-3	-3	-4	-4	-1	-6	-7	2
Fission	-800	120	780	566	1488	486	-272	485	-877	16	827	-940	-974	-537	541	-1258	-767	314	-486	-367
N,Gamma	-29	3	13	22	19	-30	-27	-30	10	-18	-22	-10	21	-42	-51	-28	-22	23	5	34
nubar	-249	113	126	-27	610	225	-175	-48	-189	138	-221	272	-428	-2	-230	315	482	-200	221	207
Chi	144	-129	-187	-219	-254	-15	-62	-129	-76	-130	111	-208	-117	-154	130	-61	55	59	95	1
Total	-221	141	552	-27	2183	865	-943	470	-530	-56	1170	-893	-1989	-1291	508	-864	444	-305	79	-421

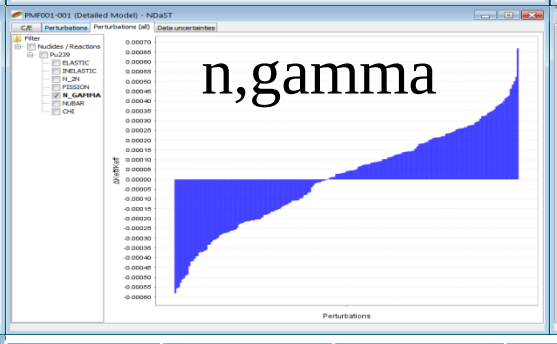
Delta k_{eff} Distributions by Reaction

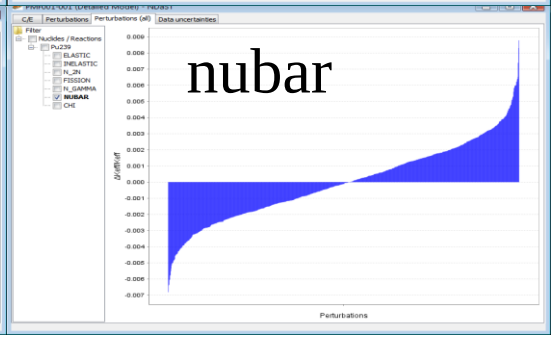


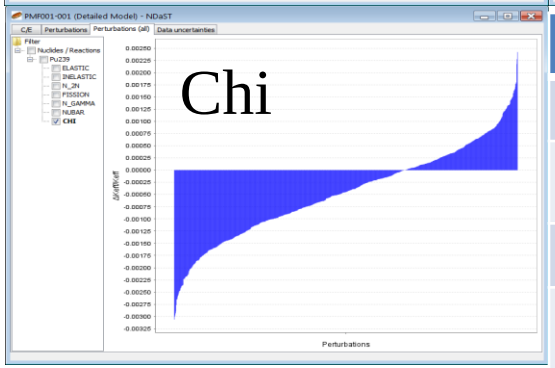






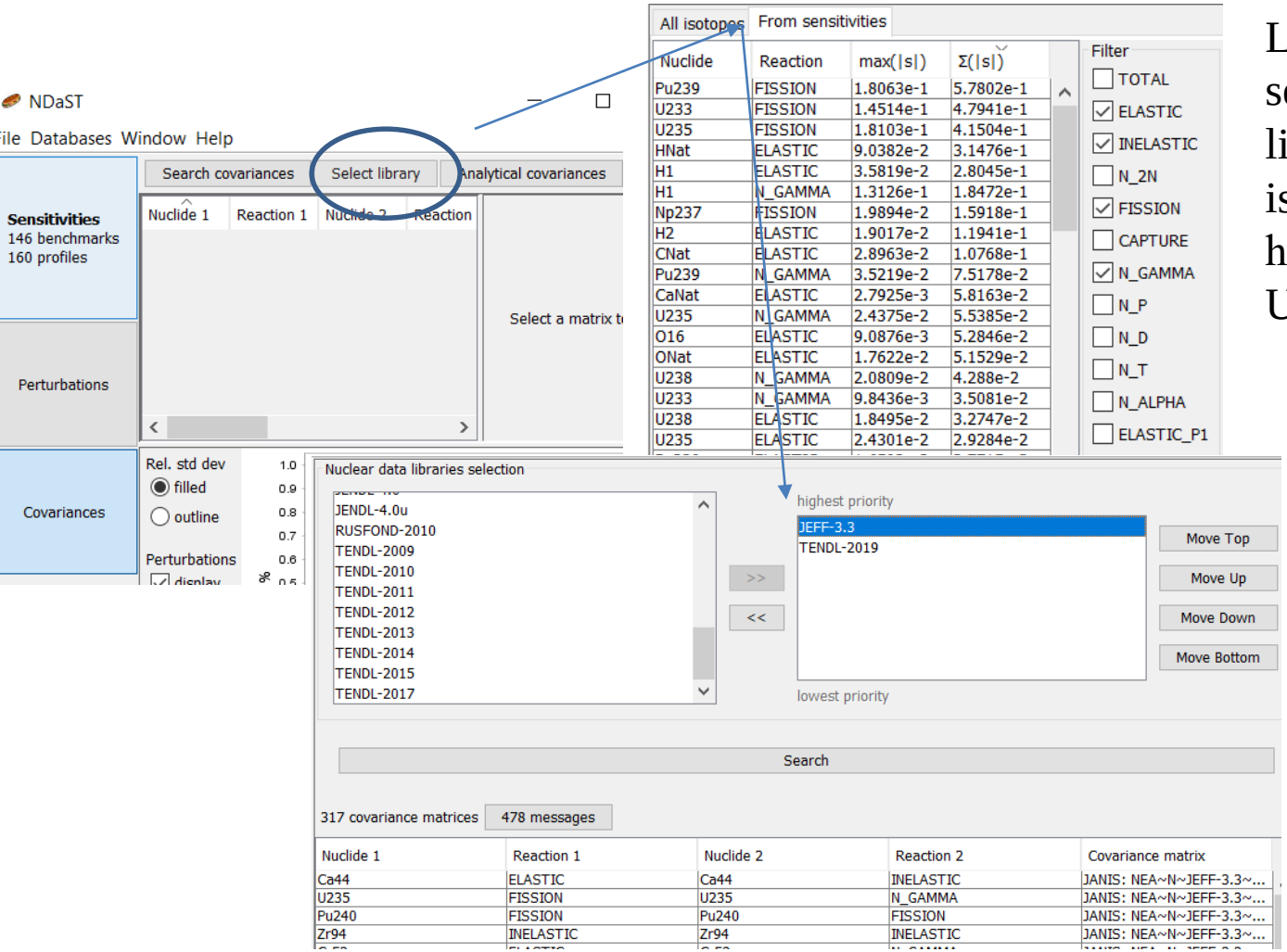






	elastic	inelastic	n,2n	fission	n,gamma	nubar	chi
Mean	0.00014	-0.00004	-0.00001	-0.00064	0.00001	-0.00002	-0.00046
St. dev.	0.00344	0.00145	0.00002	0.00648	0.00025	0.00238	0.00093
Skew	0.12074	0.34519	0.11337	0.05432	-0.17265	0.18915	-0.03932
Kurt.	-1.20829	0.10658	-0.45525	-0.38844	-0.60157	0.02513	-0.22921

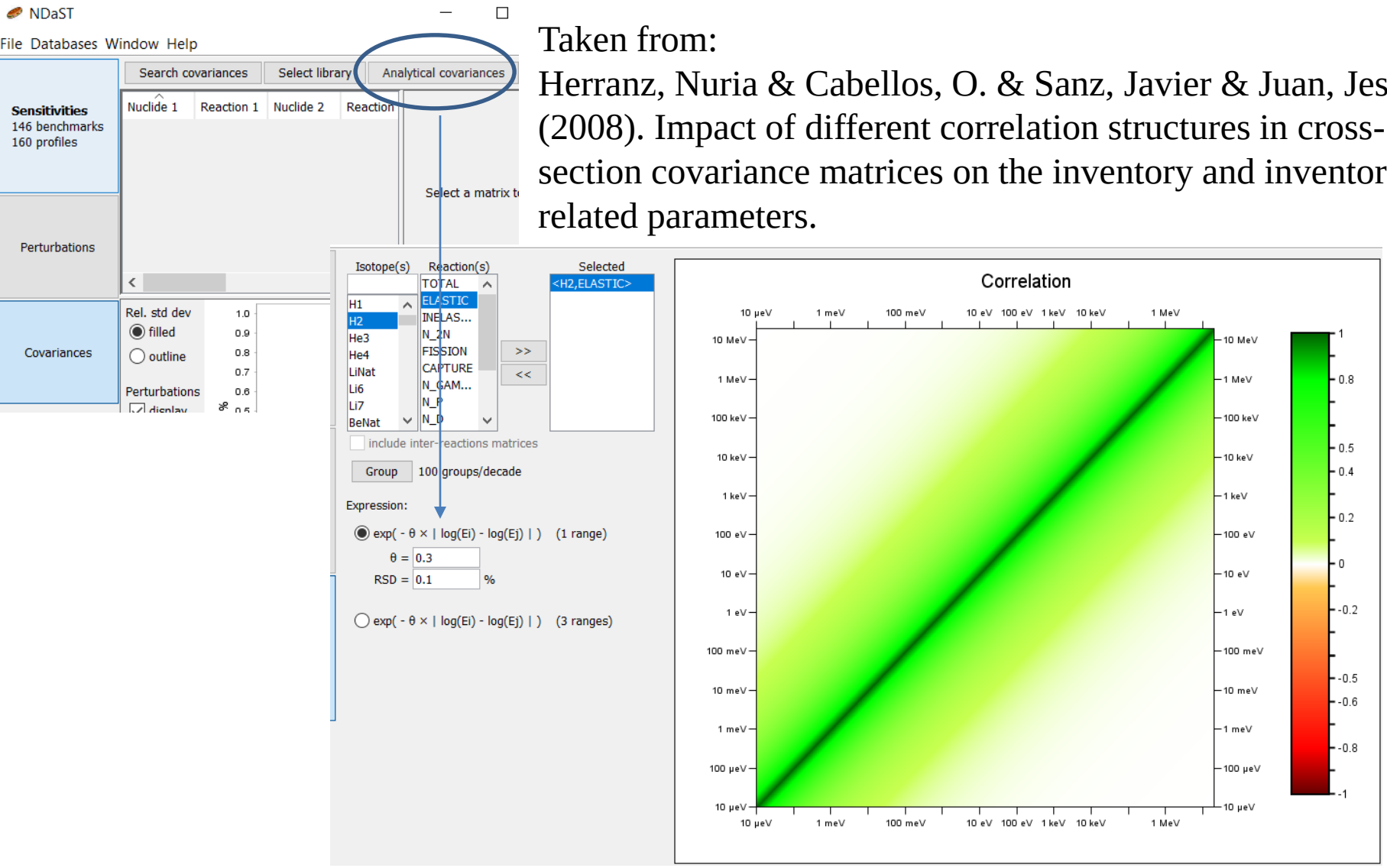
New Functionality to Search Covariance Data



Looks through all the sensitivities and provides a list of which isotopes/reactions reactions have ‘high’ sensitivities
User can select top X

Based on priority list, NDaST will retrieve a covariance file for each selected isotope/reaction.

Analytic Covariance



Taken from:
Herranz, Nuria & Cabellos, O. & Sanz, Javier & Juan, Jesus. (2008). Impact of different correlation structures in cross-section covariance matrices on the inventory and inventory-related parameters.

NDaST can compute c(k) and they are dynamic

Results - NDaST

File

Case by case | Representativity values (Ck)

Filter

- Filter
- Nuclides / Reactions
  - H1
  - H2
  - CNat
  - O16
  - Cu63
  - Th232
  - U233
  - U235
    - ELASTIC
    - INELASTIC
    - FISSION
    - N_GAMMA
  - U238
    - ELASTIC
    - INELASTIC
    - FISSION
    - N_GAMMA
  - Np237
  - Pu239
  - Pu240
- Benchmarks calculations
- Sensitivities calculations
  - KENO ABBN-93 / 299-Group
  - KENO ENDF/B-VII.0 / 238-Group
  - KENO ENDF/B-VII.0 Continuous
  - MCNP ENDF/B-VI Continuous

	HMI006-001...	HMI006-002 ...	HMI006-003...	HMI006-004...	MMF001-001 ...	SMF008-001...	SMF008-001 (...
HMI006-001 KE...	1	0.9937	0.9711	0.924	0.3072	0.566	0.566
HMI006-002 KE...	0.9937	1	0.9915	0.959	0.3274	0.5968	0.5968
HMI006-003 KE...	0.9711	0.9915	1	0.9865	0.3562	0.6331	0.6331
HMI006-004 KE...	0.924	0.959	0.9865	1	0.409	0.6815	0.6815
MMF001-001 M...	0.3072	0.3274	0.3562	0.409	1	0.6335	0.6335
SMF008-001 (D...	0.566	0.5968	0.6331	0.6815	0.6335	1	1
SMF008-001 (Si...	0.566	0.5968	0.6331	0.6815	0.6335	1	1

Command Line: Potential to implement in pipeline

Current:

```
Usage: <input> <output> [OPTIONS]...
    <input>  : NDaST file with input parameters (sensitivities plus and/or covariances)
    <output> : NDaST file with input parameters and calculation results
  Options:
    -q,  --quiet        : suppress all messages except errors
    -od, --off-diagonal : compute off-diagonal terms (cases/sensitivities representativity,
aka 'Ck')
    -f,  --force        : allow overwriting output file
```

To be implemented (2022):

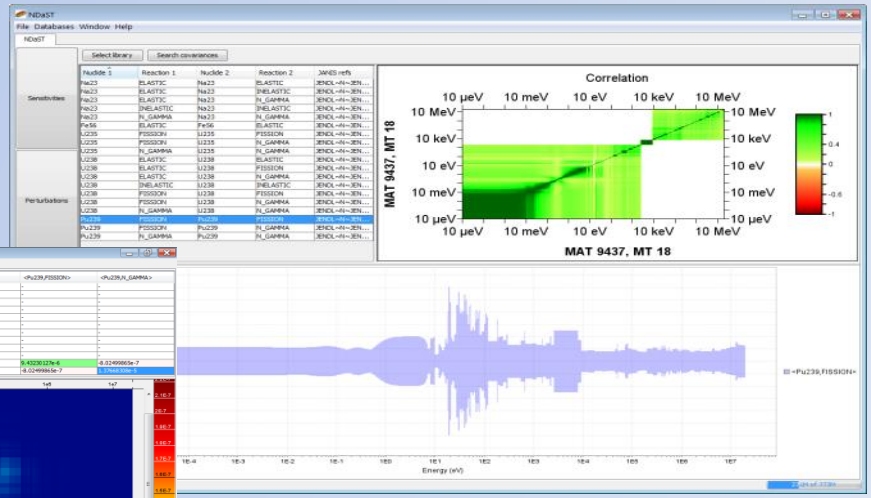
- Numerator and denominator, being either JANIS references or “file” references
  - group structure for ratios
  - Weighting spectrum for ratios

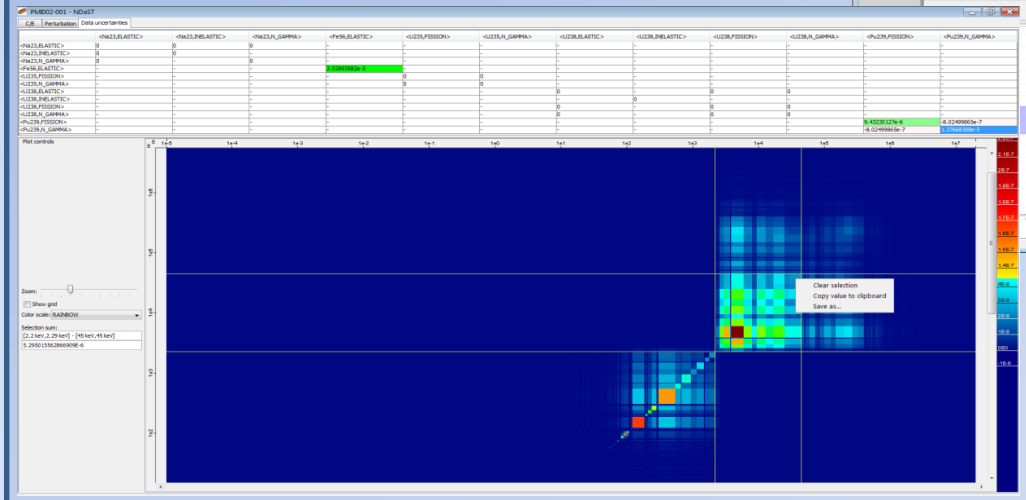
NDaST is a combination of GUI tools, not surprisingly its first port of call wasn’t to be designed for pipelines that didn’t/don’t exist.
GUI tools have been necessary to trouble shoot suspicious results. Linear perturbation theory, and the number of options depending on the exact code/library/benchmarks/covariance isn’t a oiled machine.

Energy Dependence Breakdown

NDaST was previously able to display in its output the breakdown of either a perturbation (i.e. Δk_{eff}) or uncertainty (covariance in k_{eff}) calculation as a function of the contributing nuclide-reaction pairings.
However, limitation to this degree of detail does not allow a deeper analysis of which energy regions constitute the greatest or smallest values within the total for that nuclide-reaction.

But the problem was the memory size of such a fine level of detail (~1000s of energy groups, ~100s of benchmarks, ~10s of nuclide-reaction pairs); noting that energy covariance matrices are large, square and often not very sparse.
The solution implemented was for the software to interactively relaunch the calculation specifically when clicked on by the user for a given nuclide-reaction pair.





In order that totals over different ranges of energy can be quickly computed and displayed, region selection bars may be used over the breakdown plot, which is colour-coded by magnitude.

Conclusion

Lots of potential for NDaST to integrate with other data sources, tools.

Complexity is still an issue.

Look for more training resources in 2022.

The person power for NDaST is extremely low, 0.2 FTE, and 70 % of this is simple maintenance (ensure compatibility with JANIS,DICE,IDAT) and outreach (such as this presentation).

Contact: ndast@oecd-nea.org