

# **Status of the Nuclear Data Sensitivity Tool (NDaST)**

**Ian Hill**

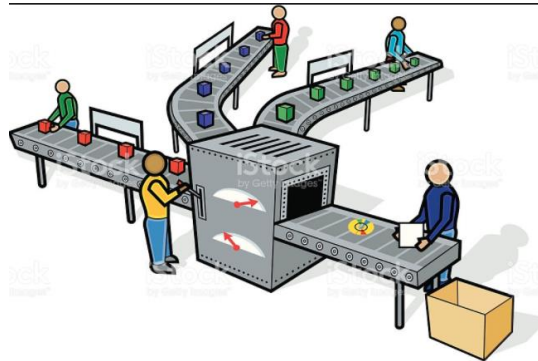
**Division of Nuclear Science and Education**

**WPEC SG46  
March 15<sup>th</sup> 2022**

## 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>



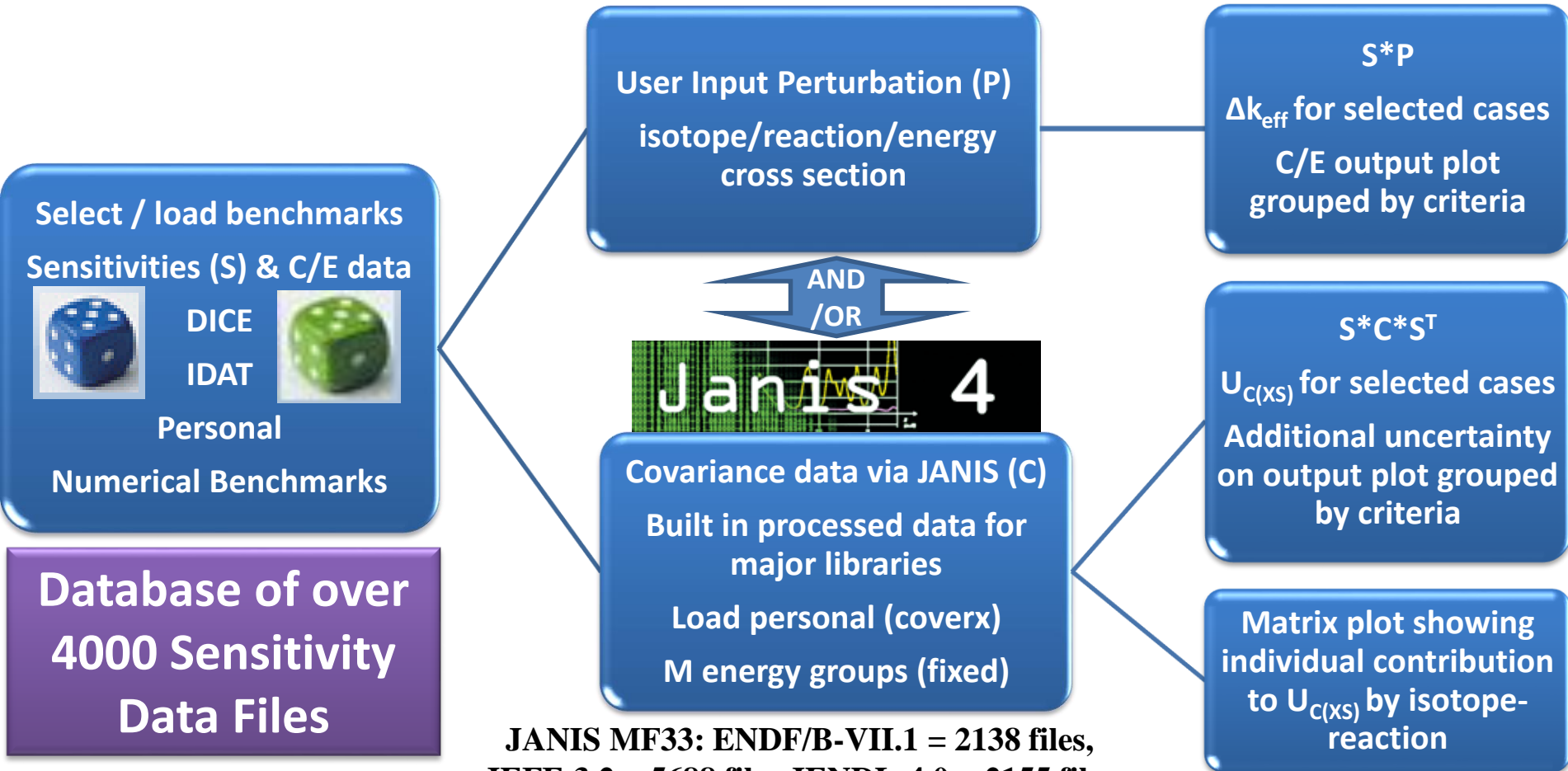
**Industrial engineering**: is a branch of [engineering](#) which deals with the optimization of complex [processes](#), [systems](#), or [organizations](#). **Industrial engineers** work to eliminate waste of time, money, materials, person-hours, machine time, energy and other resources that do not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

## Nuclear Data Sensitivity Tool (NDaST) Flowchart

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



XML and GUI



**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]

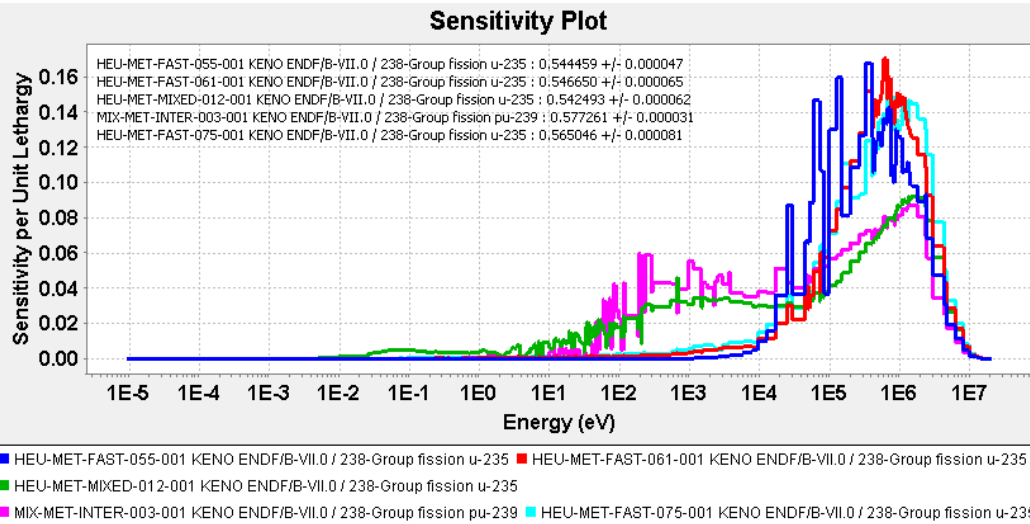
- Sensitivity dot product to characterise similarity.
- Covariance Data Available [JANIS]**
- All major libraries have BOXER files with MF32/MF33 processed. (~30 libraries with covariances, ~40 libraries)
  - Users can add MF31. In the future these will be available
  - No MF34. Will come in the future.
  - Supports user entered BOXER / COVERX files
  - Supports some versions of the SCALE covariance library

## Load Own Covariance

The screenshot shows a Windows File Explorer window titled "Open" with a close button in the top right corner. The address bar shows the current location is "BOXER-ENDFB7.1-238g". The left sidebar contains navigation options: "Recent Items", "Desktop", "Documents", "This PC", and "Network". The main pane displays a grid of files, all with the ".boxer" extension. The files are arranged in five columns and ten rows. At the bottom of the window, the "File name:" field is empty, and the "Files of type:" dropdown is set to "All supported files (\*.endf; \*.pendf; \*.hendf; \*.boxer; \*.coverx; \*.zip; \*.gz; \*.gzip)".

File Name	File Name	File Name	File Name	File Name
ac225.boxer	b11.boxer	cf246.boxer	cm243.boxer	cr53.boxer
ac226.boxer	be9.boxer	cf248.boxer	cm244.boxer	cs133.boxer
ac227.boxer	bi209.boxer	cf249.boxer	cm245.boxer	cs135.boxer
ag109.boxer	bk245.boxer	cf250.boxer	cm246.boxer	er166.boxer
al27.boxer	bk246.boxer	cf251.boxer	cm247.boxer	er167.boxer
am240.boxer	bk247.boxer	cf252.boxer	cm248.boxer	er168.boxer
am241.boxer	bk248.boxer	cf253.boxer	cm249.boxer	er170.boxer
am242m.boxer	bk249.boxer	cf254.boxer	cm250.boxer	es251.boxer
am243.boxer	bk250.boxer	cm240.boxer	co59.boxer	es252.boxer
au197.boxer	c0.boxer	cm241.boxer	cr50.boxer	es253.boxer
b10.boxer	ce141.boxer	cm242.boxer	cr52.boxer	es254.boxer

## DICE+IDAT With Proposed 7 Group Structure

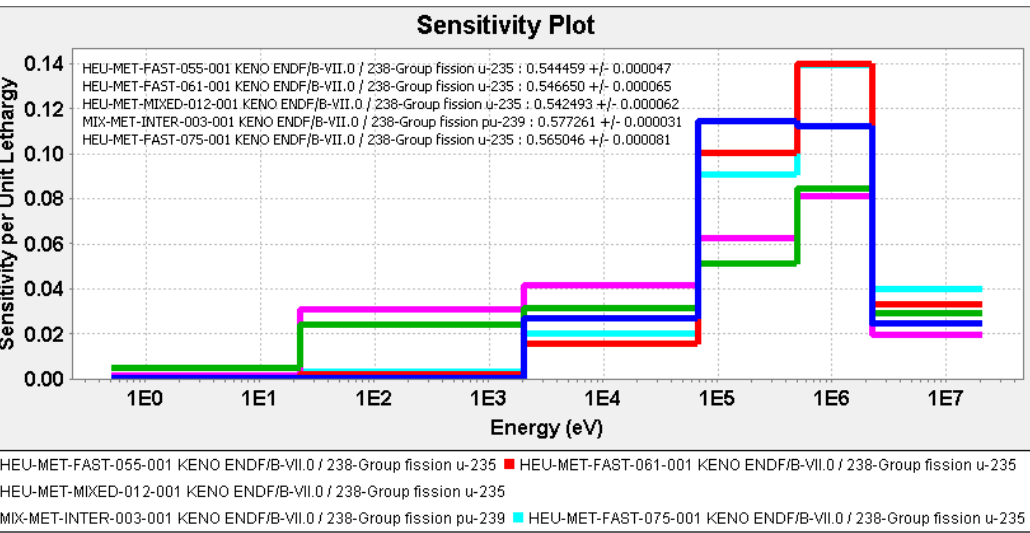


Representation  
 Per unit lethargy bin  
 SCALE 238-group  
 Plots Table  
 Clear  
 Load own data...  
 Lines width: [dropdown] Black & white  
 No comparison  Ratio  Difference

- k-40
- k-41
- li-6
- li-7
- mg-24
- mg-25
- mg-26
- mn-55
- n-14
- na-23
- o-16
- si-28
- si-29

Some ZPPR Fission Sensitivity Profiles

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



Representation  
 Per unit lethargy bin  
 7GWPECSG46.txt  
 Plots Table  
 Clear  
 Load own data...  
 Lines width: [dropdown] Black & white  
 No comparison  Ratio  Differ

- k-40
- k-41
- li-6
- li-7
- mg-24
- mg-25
- mg-26
- mn-55
- n-14
- na-23
- o-16
- si-28
- si-29

7GWPECSG46.txt

Format:

- Auto-detect
- ABBN
- TSUNAMI1D/SUSD3D
- TSUNAMI3D
- MCNP Output
- WPEC SG33
- Binary

File Edit Form

1.96403E+7  
 2.23130E+6  
 4.97871E+5  
 6.73795E+4  
 2.03468E+3  
 2.26033E+1  
 5.40000E-1

## Linking to representative benchmarks from various application

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

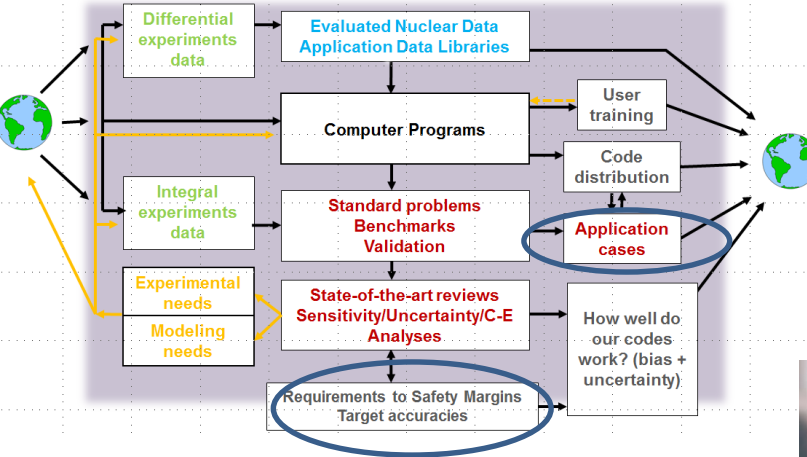
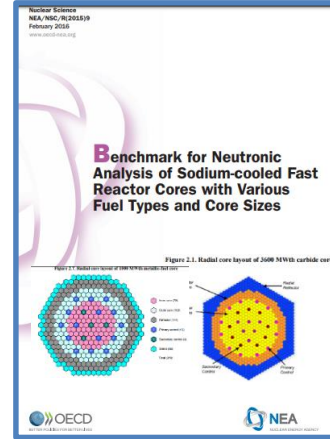
MIT  
Benchmark for Evaluation And Validation of Reactor Simulations



RELEASE rev. 2.0.2

MIT Computational Reactor Physics Group

April 11, 2018



### 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: FTR, the 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

IAEA TECDOC SERIES

IAEA-TECDOC-1742

Benchmark Analyses on the Control Rod Withdrawal Tests Performed during the PHÉNIX End-of-Life Experiments

ISBN 92-64-02316-X

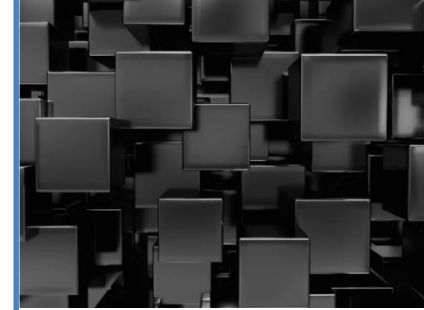
Burn-up Credit Criticality Benchmark

Phase II-D

PWR-UO<sub>2</sub> Assembly  
Study of Control Rod Effects on Spent Fuel Composition

Anne BARREAU  
Commissariat à l'énergie atomique  
France

Industry surrogate models/response functions



## 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

April 2015-2017

# Have I see it before?

[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

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.

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

And as parts of other presentations, example:

[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

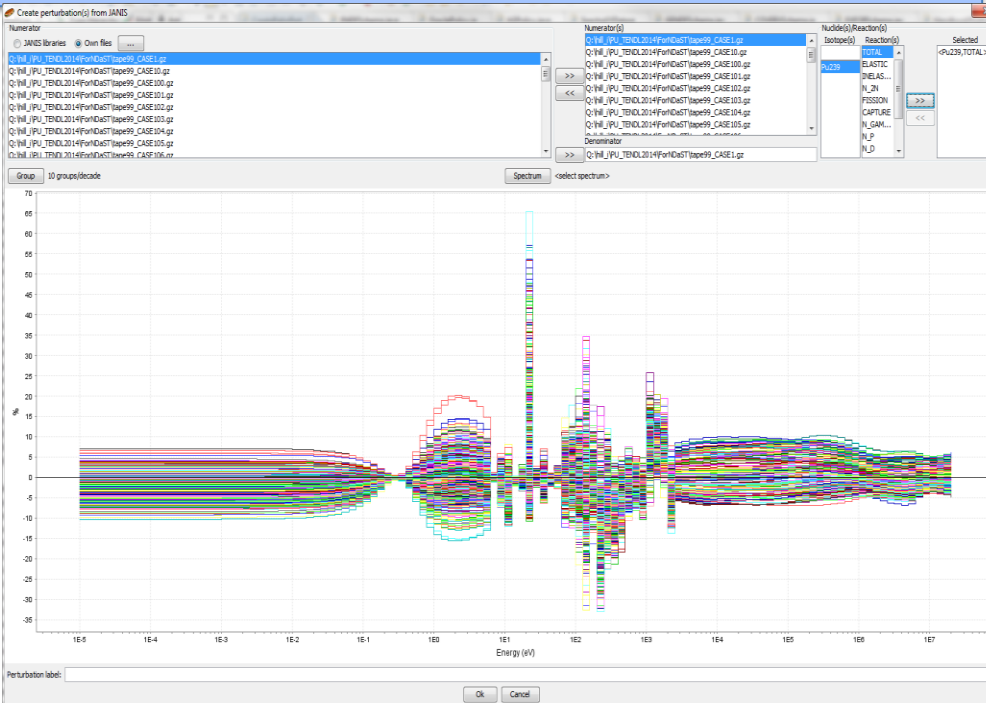
## NDaST: Automated JANIS Computations

- 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

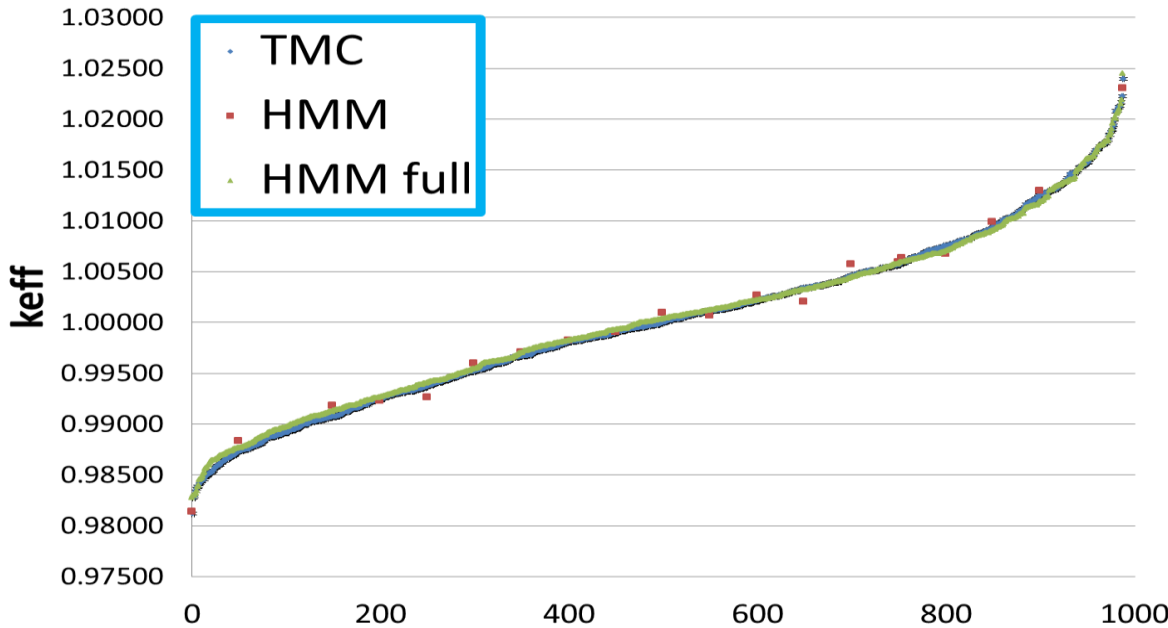
The screenshot shows the NDaST software interface. The 'Group structure' panel is active, showing a dropdown menu for 'Group type' with options: 'Uniform in log', 'Uniform in log', 'File defined', and 'Single group'. Below this, 'Lower energy' is set to 2.0E7 in eV and 'Upper energy' is set to 2.0E7 in eV. 'Subdivision' is set to 10.0 in groups/decade. The 'Spectrum' panel shows a dropdown for 'Spectrum type' with options: 'PWR spectrum', 'Constant spectrum', 'XY spectrum', 'PWR spectrum', 'General spectrum', 'Maxwellian spectrum', and 'Fission spectrum'. The 'PWR spectrum' option is selected. Other parameters include 'Emax,th' (0.054 in eV) and 'Emax,epi' (2100000.0 in eV). The 'Databases' window shows 'JANIS=(4)' selected with checkmarks for ENDF, JENDL, NEA, and JEFF.

- 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

PMF001 Jezebel keff distribution

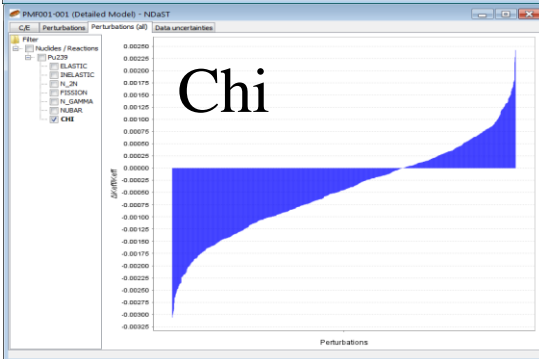
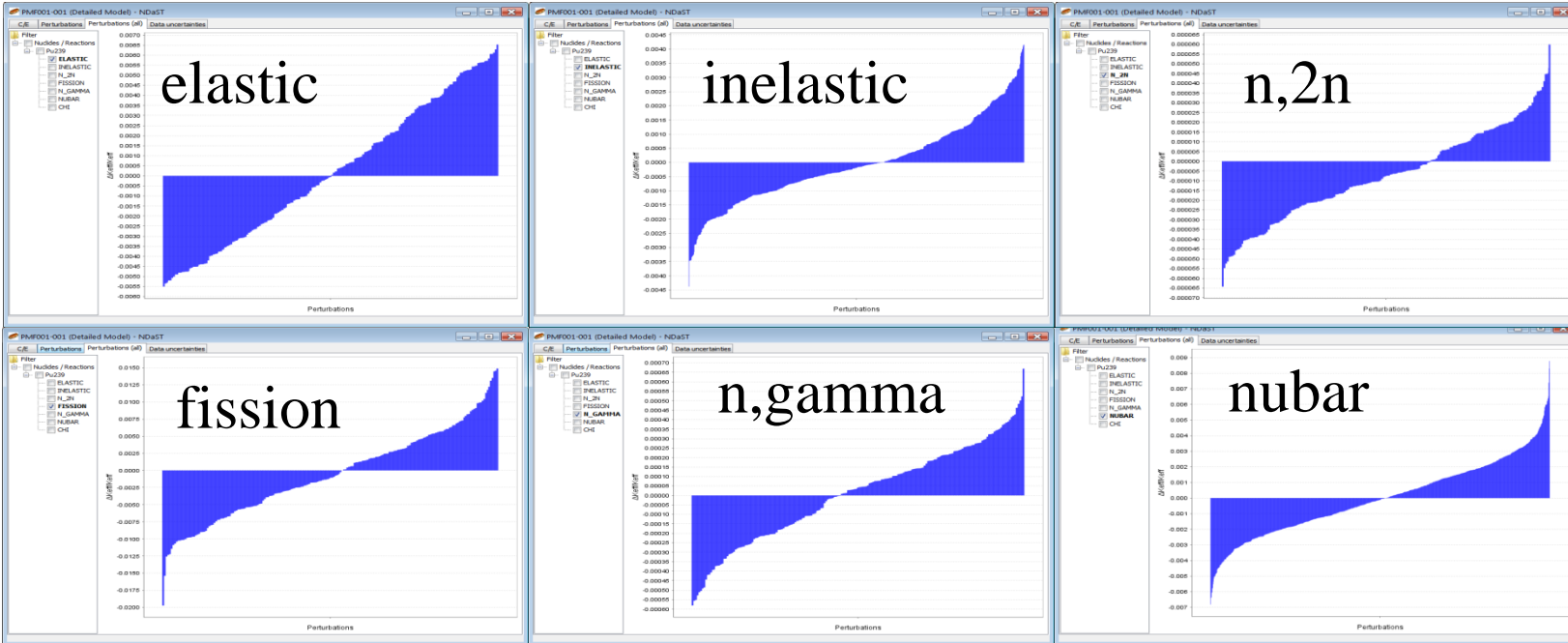


$k_{eff}$  distribution, sorted lowest  $k_{eff}$  to highest, plotted with the HMM  $k_{eff}$  predictions for 20 samples and full automated set

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 $k_{\text{eff}}$ 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

NDaST

File Databases Window Help

Sensitivities  
146 benchmarks  
160 profiles

Perturbations

Covariances

Search covariances **Select library** Analytical covariances

Nuclide 1 Reaction 1 Nuclide 2 Reaction 2

Select a matrix to

Nuclide	Reaction	max( s )	$\Sigma( s )$
Pu239	FISSION	1.8063e-1	5.7802e-1
U233	FISSION	1.4514e-1	4.7941e-1
U235	FISSION	1.8103e-1	4.1504e-1
HNat	ELASTIC	9.0382e-2	3.1476e-1
H1	ELASTIC	3.5819e-2	2.8045e-1
H1	N_GAMMA	1.3126e-1	1.8472e-1
Np237	FISSION	1.9894e-2	1.5918e-1
H2	ELASTIC	1.9017e-2	1.1941e-1
CNat	ELASTIC	2.8963e-2	1.0768e-1
Pu239	N_GAMMA	3.5219e-2	7.5178e-2
CaNat	ELASTIC	2.7925e-3	5.8163e-2
U235	N_GAMMA	2.4375e-2	5.5385e-2
O16	ELASTIC	9.0876e-3	5.2846e-2
ONat	ELASTIC	1.7622e-2	5.1529e-2
U238	N_GAMMA	2.0809e-2	4.288e-2
U233	N_GAMMA	9.8436e-3	3.5081e-2
U238	ELASTIC	1.8495e-2	3.2747e-2
U235	ELASTIC	2.4301e-2	2.9284e-2

Filter

- TOTAL
- ELASTIC
- INELASTIC
- N\_2N
- FISSION
- CAPTURE
- N\_GAMMA
- N\_P
- N\_D
- N\_T
- N\_ALPHA
- ELASTIC\_P1

Nuclear data libraries selection

JENDL-4.0u  
RUSFOND-2010  
TENDL-2009  
TENDL-2010  
TENDL-2011  
TENDL-2012  
TENDL-2013  
TENDL-2014  
TENDL-2015  
TENDL-2017

highest priority

JEFF-3.3  
TENDL-2019

lowest priority

Move Top  
Move Up  
Move Down  
Move Bottom

Search

317 covariance matrices 478 messages

Nuclide 1	Reaction 1	Nuclide 2	Reaction 2	Covariance matrix
Ca44	ELASTIC	Ca44	INELASTIC	JANIS: NEA~N~JEFF-3.3~...
U235	FISSION	U235	N_GAMMA	JANIS: NEA~N~JEFF-3.3~...
Pu240	FISSION	Pu240	FISSION	JANIS: NEA~N~JEFF-3.3~...
Zr94	INELASTIC	Zr94	INELASTIC	JANIS: NEA~N~JEFF-3.3~...

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

NDaST

File Databases Window Help

Search covariances Select library Analytical covariances

Nuclide 1	Reaction 1	Nuclide 2	Reaction 2

Select a matrix to

Sensitivities  
146 benchmarks  
160 profiles

Perturbations

Covariances

Rel. std dev

filled	1.0
filled	0.9
filled	0.8
filled	0.7
filled	0.6
filled	0.5

Perturbations

display

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.

Isotope(s) Reaction(s) Selected

H1	TOTAL	
H2	ELASTIC	<H2,ELASTIC>
He3	INELAS...	
He4	N_N	
LiNat	FISSION	
Li6	CAPTURE	
Li7	N_GAM...	
BeNat	N_F	
	N_D	

include inter-reactions matrices

Group 100 groups/decade

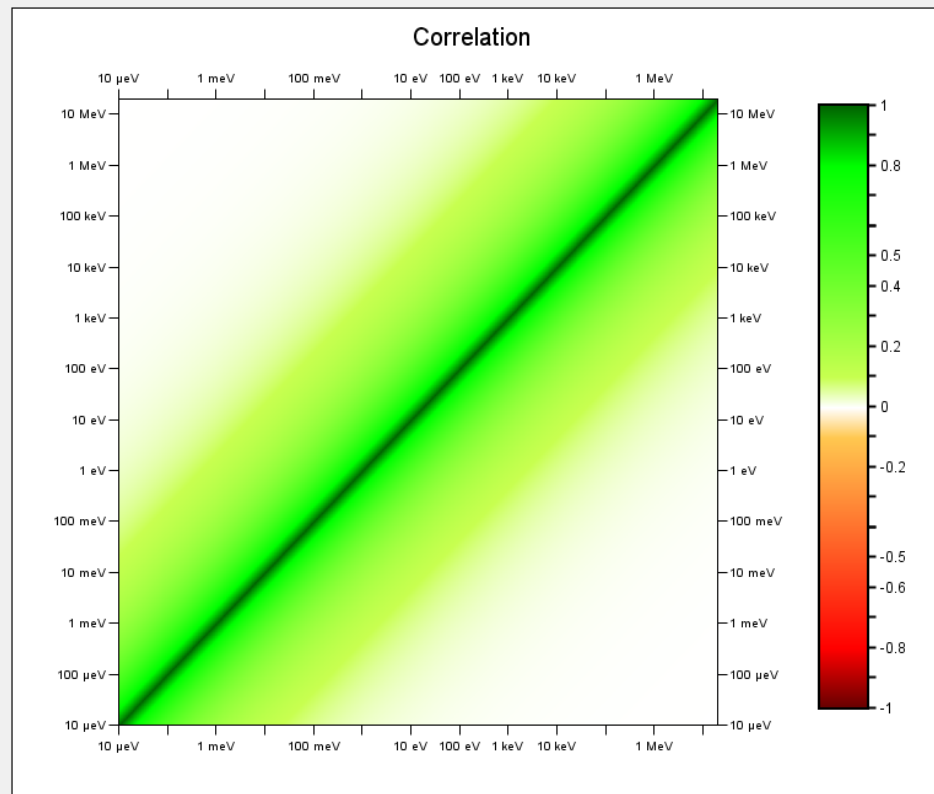
Expression:

$\exp(-\theta \times |\log(E_i) - \log(E_j)|)$  (1 range)

$\theta = 0.3$

RSD = 0.1 %

$\exp(-\theta \times |\log(E_i) - \log(E_j)|)$  (3 ranges)



## NDaST can compute $c(k)$ and they are dynamic

Results - NDaST

File

Case by case Representativity values (Ck)

Filter	HMI006-001...	HMI006-002 ...	HMI006-003...	HMI006-004...	MMF001-001 ...	SMF008-001...	SMF008-001 (...)
<input checked="" type="checkbox"/> Nuclides / Reactions							
<input checked="" type="checkbox"/> H1							
<input checked="" type="checkbox"/> H2							
<input checked="" type="checkbox"/> CNat							
<input checked="" type="checkbox"/> O16							
<input checked="" type="checkbox"/> Cu63							
<input checked="" type="checkbox"/> Th232							
<input checked="" type="checkbox"/> U233							
<input checked="" type="checkbox"/> U235							
<input checked="" type="checkbox"/> ELASTIC							
<input checked="" type="checkbox"/> INELASTIC							
<input checked="" type="checkbox"/> FISSION							
<input checked="" type="checkbox"/> N_GAMMA							
<input checked="" type="checkbox"/> U238							
<input checked="" type="checkbox"/> ELASTIC							
<input checked="" type="checkbox"/> INELASTIC							
<input checked="" type="checkbox"/> FISSION							
<input checked="" type="checkbox"/> N_GAMMA							
<input checked="" type="checkbox"/> Np237							
<input checked="" type="checkbox"/> Pu239							
<input checked="" type="checkbox"/> Pu240							
<input checked="" type="checkbox"/> Benchmarks calculations							
<input type="checkbox"/> Sensitivities calculations							
<input type="checkbox"/> KENO ABBN-93 / 299-Group							
<input type="checkbox"/> KENO ENDF/B-VII.0 / 238-Group							
<input checked="" type="checkbox"/> KENO ENDF/B-VII.0 Continuous							
<input checked="" type="checkbox"/> MCNP ENDF/B-VI Continuous							
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	0.6339	0.6339
SMF008-001 (D...	0.566	0.5968	0.6331	0.6815	0.6339	1	1
SMF008-001 (Si...	0.566	0.5968	0.6331	0.6815	0.6339	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.

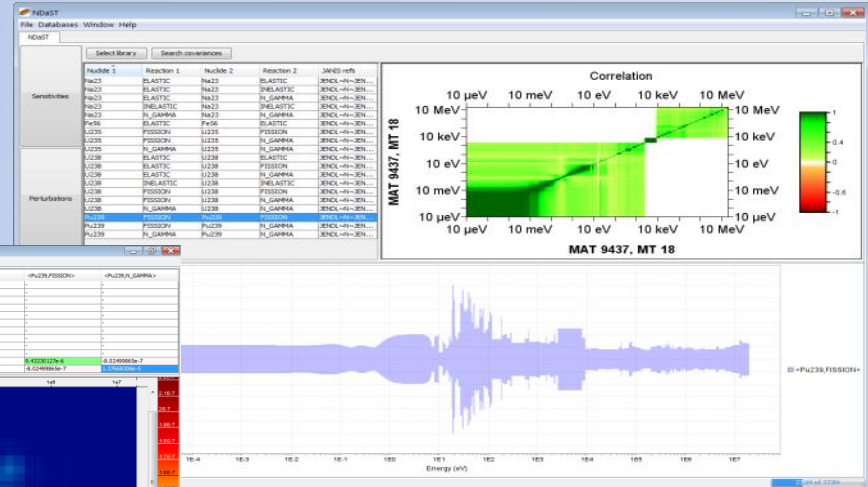


## Energy Dependence Breakdown

NDaST was previously able to display in its output the breakdown of either a perturbation (i.e.  $\Delta k_{\text{eff}}$ ) or uncertainty (covariance in  $k_{\text{eff}}$ ) 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](mailto:ndast@oecd-nea.org)