DICE 2014 and Integration with a Nuclear Data and Sensitivity Testing Tool (NDaST)

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NCSP TPR @ LLNL
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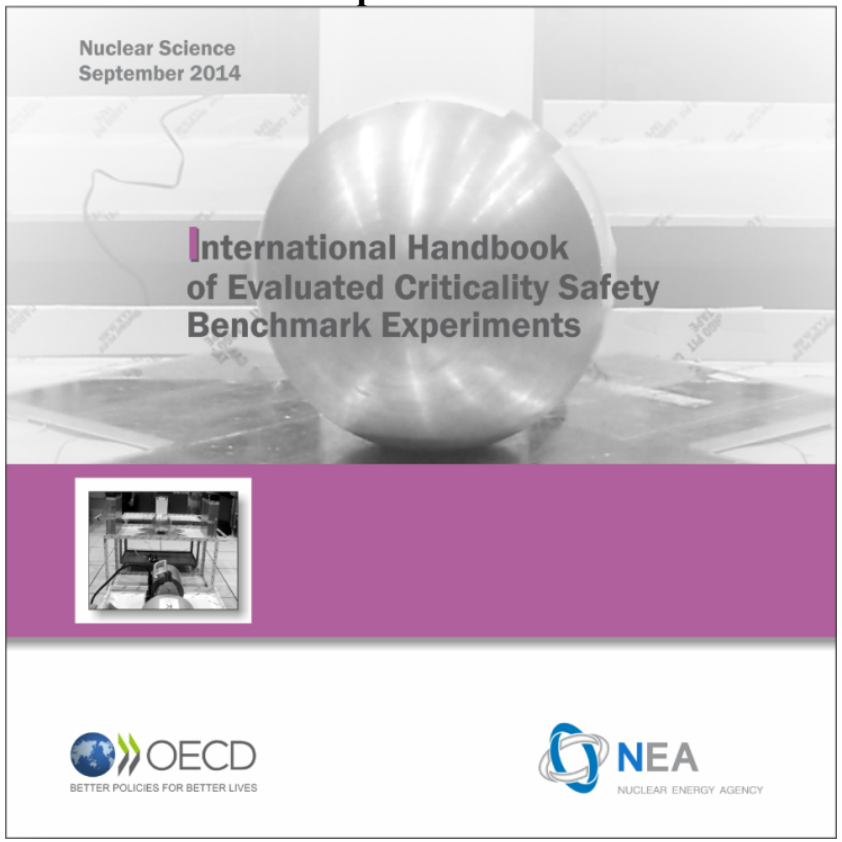
Overview

Handbook (est 1992/1995)

4839 Critical and Subcritical Benchmarks, Organized by Fissile Material, Form and Fission Spectrum



DATABASE for ICSBEP (DICE)

Answers How Efficiently Search the Handbook

- Distributed with Handbook since 2001
- Relational database
- User Friendly Way to Search
- This presentation describes major recent advances namely,

1) New Sensitivity Data

2) Tools using sensitivity data to identify useful benchmarks

3) Load your own k_{eff} data into DICE

4) Improved accessibility

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Methods to Find Relevant Benchmarks

Classic Benchmark selection approach:

Search based on material compositions

Search based on spectrum

Expert judgement

TABLE I: The benchmark cases containing significant amounts of certain elements.

Element	Benchmark cases
Be	hmf5, hmf41 (1,2), hmf58, hmf59, hmf66, hmf69, hmt22, pmf19, pmf21, pmf38, pmf44 (3), mmf7, umf5

HB Organized by Fissile Material, Physical Form and Fission Spectrum

HMF=HEU-MET-FAST

DICE

- Fuel
  - Fuel form/Fissile material
  - Fuel region
  - U and Pu weight percent
  - Pu/(U+Pu) ratio
- Moderator/coolant material
- Cladding material
- Reflector material
- Neutron absorbing material
- Separation material
- Geometry
- Benchmark Keff and Calculations
- Energy, spectra, sensitivities
  - Energy of Average Neutron Lethargy causing Fission
  - Average Fission Group Energy
  - Flux distribution (3-g)
  - Fission distribution (3-g)
  - Capture distribution (3-g)
  - Neutron balance

Improved Benchmark selection approach:

Above + Use sensitivity (%dk/%d∑)

Where to get the sensitivities for thousands of benchmark experiments?

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DICE Sensitivity Data….Recently Much Improved!

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

	THERM	INTER	FAST	MIXED
PU	525/608	4/10	114/121	9/9
HEU	664/895	21/32	383/403	75/84
IEU	142/180	5/21	31/43	7/23
LEU	1424/1612	0/0	1/1	5/5
U233	186/197	29/29	8/10	8/8
MIX	323/436	2/7	40/67	1/26
SPEC	0/0	0/0	4/20	0/0

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Searching by Sensitivity in DICE

3 Group search, full 238 Group SDF's are stored

DICE

File Database=NEA Window Help

Critical / Subcritical | Alarm / Shielding | Fundamental Physics | Correlation Matrix | Rank Similar | Keff trends plots

- General items
  - Identification
  - Evaluator
  - Internal reviewer
  - Independent reviewer
  - Varying parameter(s) across cases
  - Laboratory
  - Main purpose
  - Title
  - Keywords
  - Dates (evaluation and experiment)
  - References
- Fuel
  - Fuel form/Fissile material
  - Fuel region
  - U and Pu weight percent
  - Pu/(U+Pu) ratio
- Moderator/coolant material
- Cladding material
- Reflector material
- Neutron absorbing material
- Separation material
- Geometry
- Benchmark Keff and Calculations
- Energy, spectra, sensitivities
  - Energy of Average Neutron Lethargy causing Fission
  - Average Fission Group Energy
  - Flux distribution (3-g)
  - Fission distribution (3-g)
  - Capture distribution (3-g)
  - Neutron balance
  - Neutron gas temperature
  - Average fission neutrons per neutron absorbed in the core
  - Keff Sensitivities

Also used!

Isotope

- None selected
- 1 - H - Hydrogen
  - H1
  - H2
- 3 - Li - Lithium
- 4 - Be - Beryllium
- 5 - B - Boron
- 6 - C - Carbon
- 7 - N - Nitrogen
- 8 - O - Oxygen
- 9 - F - Fluorine
- 11 - Na - Sodium

Combine with AND / Combine with OR

Reaction

- None selected
- capture
- elastic
- fission
- inelastic
- nubar
- scatter
- total

Combine with AND / Combine with OR

Total Keff sensitivity over all energy range

Value : +/- :

OR >= <=

Set Threshold

Keff sens. < 0.625 eV

Value : +/- :

OR >= <=

Keff sens. 0.625 eV - 100 keV

Value : +/- :

OR >= <=

Keff sens. > 100 keV

Value : +/- :

OR >= <=

Values between -1 and 1, in %dk/%Σ

Keff Sensitivities are currently available for about 75% of cases

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DICE Plotting of Be Sensitivity > 0.005 for HMF

Can also read as 100 pcm/1% change in Σ

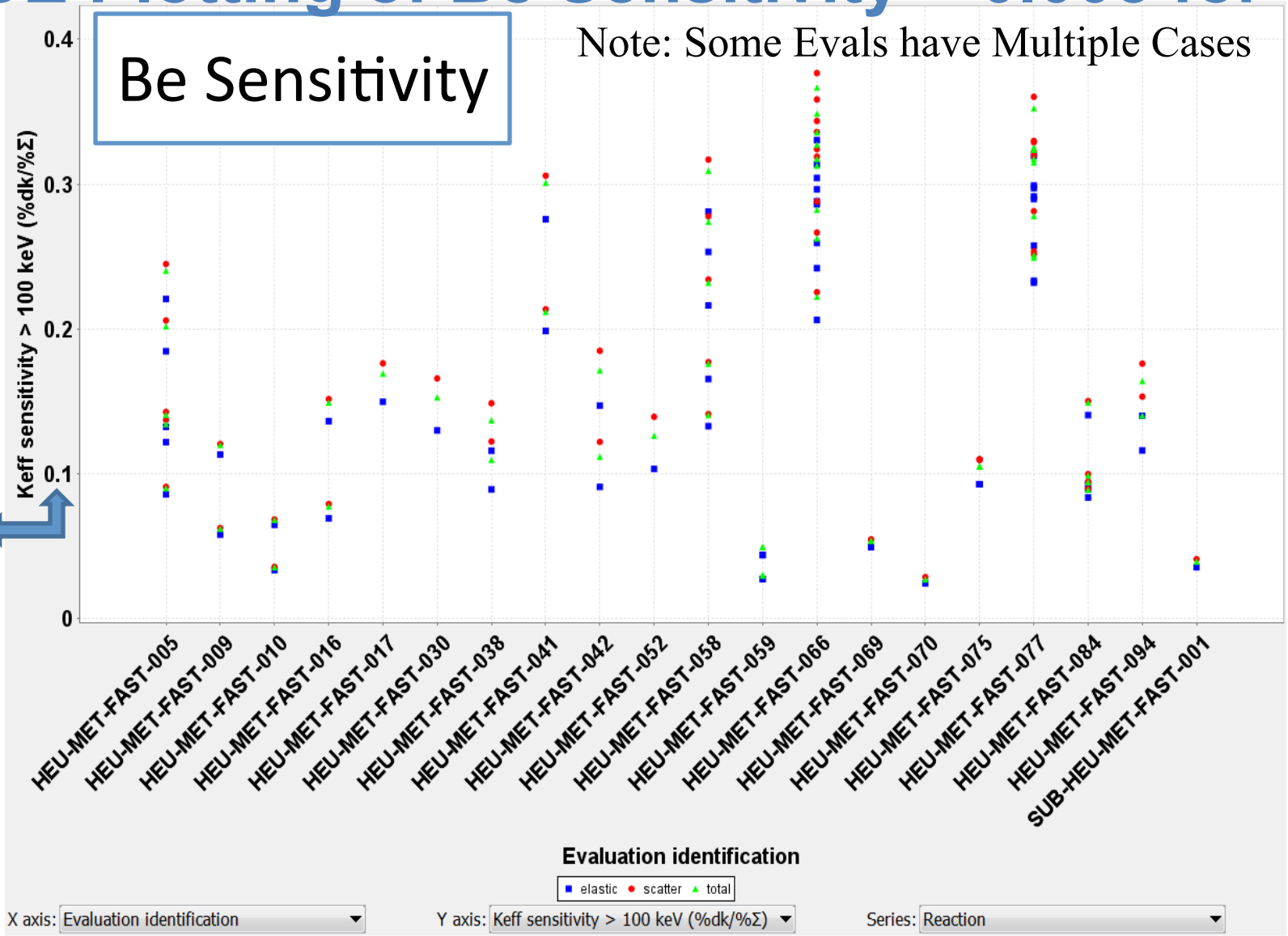

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Table of Benchmarks With Sensitivity Above Threshold

Element or Isotope	Threshold(pcm/%∑)	Benchmark Cases
Deuterium	>100	HST001(1-2), HST004(3-6),HST020(1-5), HCI006(6), HCT017(1-9), HCM002(7,10,11,20), LMT001(1),LMT002(1-12), LMT015(1-22)
Fe	<-100 >100	**PMF015**(1),**PMF026**(1),**PMF028**(1),**PMI002**(1),**HMF021**(1),**HMF085**(3),**HMI001**(1), **IMF005**(1),**MMI003**(1),**SPECMF014**(1),**HMI001**(1)
Cu	>100	**PMF013**(1),**HMF072**(1-3),**HMF073**(1),**HMF085**(1-2),**HMI006**(1-4),**IMF020**(2,4-5)
Gd^{157}	<-100	**PST034**(3-6),**HST014**(3),**HST016**(2,3),**LCT005**(3,4,9-11), **LCT052**(1-6),**MST006**(4-6),**MST007**(3-7),**MMCT004**(4-6)
W	<-50 and >50	**HMF060**(1),**HMF067**(1-2),**HMF070**(1-3),**IMF014**(2),**PMF005**(1),**HMF003**(8-11), **HMF049**(3),**HMF050**(1),**HMF084**(14),**HMF085**(6)

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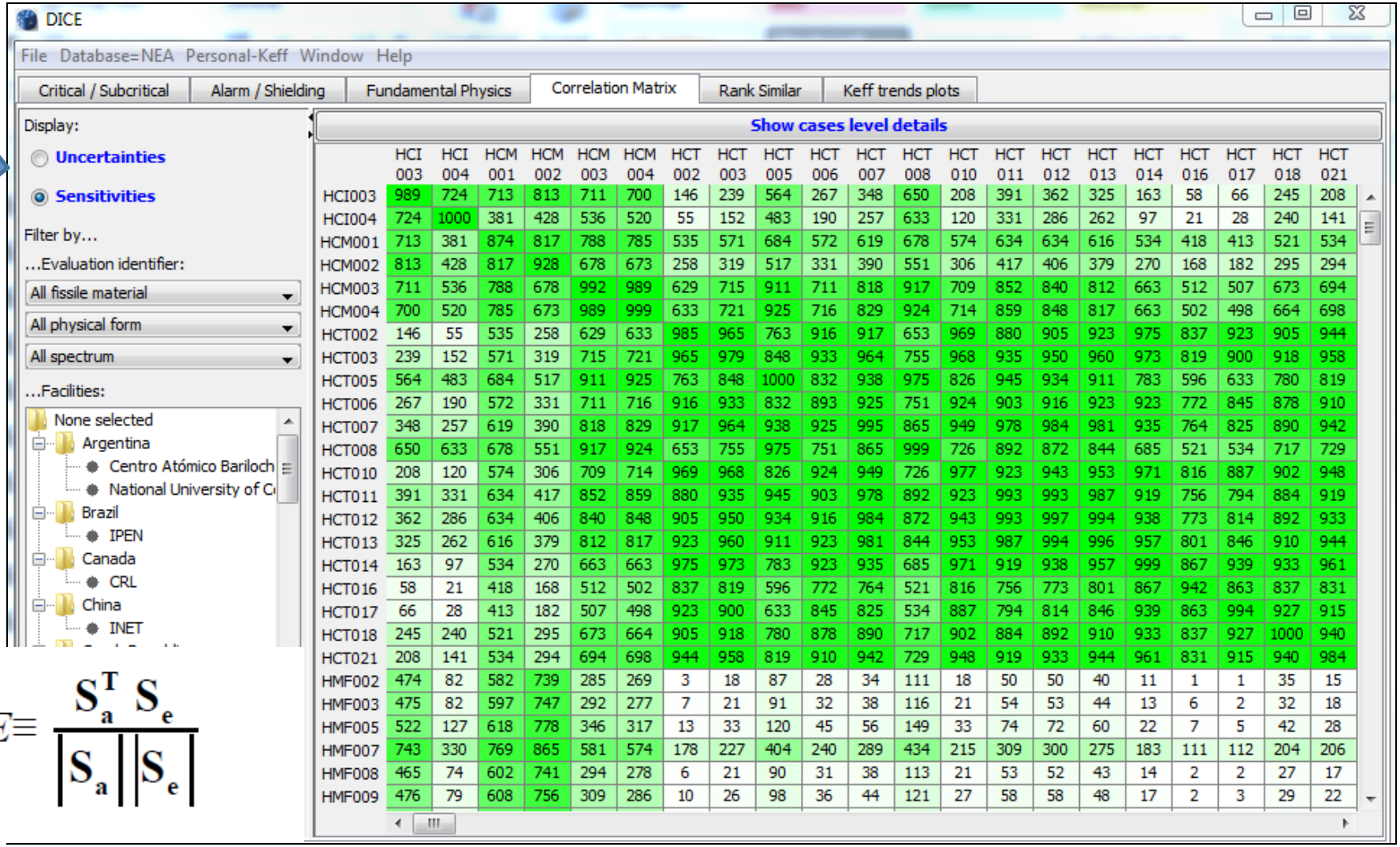
Cosine Similarity Matrix by Evaluation

Correlations between uncertainties and between sensitivities



	HCI 003	HCI 004	HCM 001	HCM 002	HCM 003	HCM 004	HCT 002	HCT 003	HCT 005	HCT 006	HCT 007	HCT 008	HCT 010	HCT 011	HCT 012	HCT 013	HCT 014	HCT 016	HCT 017	HCT 018	HCT 021
HCI003	989	724	713	813	711	700	146	239	564	267	348	650	208	391	362	325	163	58	66	245	208
HCI004	724	1000	381	428	536	520	55	152	483	190	257	633	120	331	286	262	97	21	28	240	141
HCM001	713	381	874	817	788	785	535	571	684	572	619	678	574	634	634	616	534	418	413	521	534
HCM002	813	428	817	928	678	673	258	319	517	331	390	551	306	417	406	379	270	168	182	295	294
HCM003	711	536	788	678	992	989	629	715	911	711	818	917	709	852	840	812	663	512	507	673	694
HCM004	700	520	785	673	989	999	633	721	925	716	829	924	714	859	848	817	663	502	498	664	698
HCT002	146	55	535	258	629	633	985	965	763	916	917	653	969	880	905	923	975	837	923	905	944
HCT003	239	152	571	319	715	721	965	979	848	933	964	755	968	935	950	960	973	819	900	918	958
HCT005	564	483	684	517	911	925	763	848	1000	832	938	975	826	945	934	911	783	596	633	780	819
HCT006	267	190	572	331	711	716	916	933	832	893	925	751	924	903	916	923	923	772	845	878	910
HCT007	348	257	619	390	818	829	917	964	938	925	995	865	949	978	984	981	935	764	825	890	942
HCT008	650	633	678	551	917	924	653	755	975	751	865	999	726	892	872	844	685	521	534	717	729
HCT010	208	120	574	306	709	714	969	968	826	924	949	726	977	923	943	953	971	816	887	902	948
HCT011	391	331	634	417	852	859	880	935	945	903	978	892	923	993	993	987	919	756	794	884	919
HCT012	362	286	634	406	840	848	905	950	934	916	984	872	943	993	997	994	938	773	814	892	933
HCT013	325	262	616	379	812	817	923	960	911	923	981	844	953	987	994	996	957	801	846	910	944
HCT014	163	97	534	270	663	663	975	973	783	923	935	685	971	919	938	957	999	867	939	933	961
HCT016	58	21	418	168	512	502	837	819	596	772	764	521	816	756	773	801	867	942	863	837	831
HCT017	66	28	413	182	507	498	923	900	633	845	825	534	887	794	814	846	939	863	994	927	915
HCT018	245	240	521	295	673	664	905	918	780	878	890	717	902	884	892	910	933	837	927	1000	940
HCT021	208	141	534	294	694	698	944	958	819	910	942	729	948	919	933	944	961	831	915	940	984
HMF002	474	82	582	739	285	269	3	18	87	28	34	111	18	50	50	40	11	1	1	35	15
HMF003	475	82	597	747	292	277	7	21	91	32	38	116	21	54	53	44	13	6	2	32	18
HMF005	522	127	618	778	346	317	13	33	120	45	56	149	33	74	72	60	22	7	5	42	28
HMF007	743	330	769	865	581	574	178	227	404	240	289	434	215	309	300	275	183	111	112	204	206
HMF008	465	74	602	741	294	278	6	21	90	31	38	113	21	53	52	43	14	2	2	27	17
HMF009	476	79	608	756	309	286	10	26	98	36	44	121	27	58	58	48	17	2	3	29	22

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

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Accessibility of DICE

Order ICSBEP Handbook

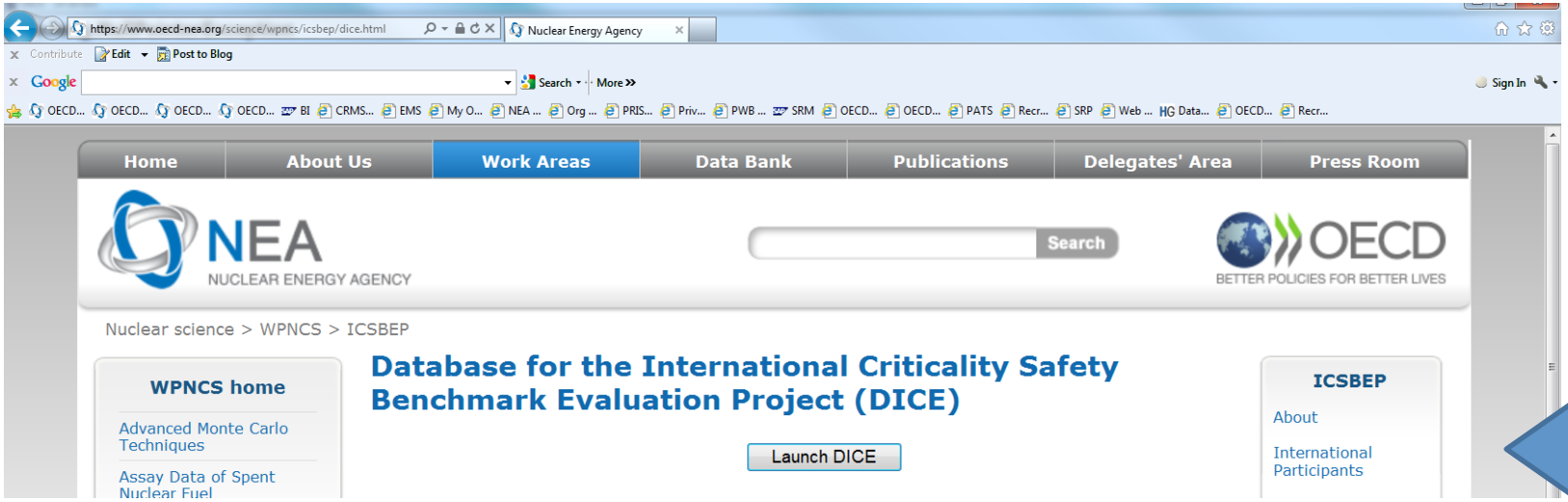
https://www.oecd-nea.org/science/wpncs/icsbep/order.html

and it comes with DICE and all of the data!

Or Now

Webstart Version

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



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Integrating Sensitivity Data With Nuclear Data

Idea: Potential scoping tool that leverages sensitivity data to make rapid predictions of the integral responses to changes in nuclear data.

- Changes and trends in Δk_{eff} for broad nuclear data perturbations
- Propagation of nuclear covariance data to benchmark C/E results

Integral Data Sources: Criticality (DICE), Reactor Physics (IDAT), Spent fuel (SFCOMPO), Numerical benchmarks, Shielding (SINBAD).

Nuclear Data: Evaluated nuclear covariance data files are accessible via the NEA JANIS application

A revival?

- Sensitivity analyses are successfully performed for decades
- NRG proposal: "3D uncertainty calculations with MCNP"
  A. Hogenbirk,
  S. van der Marck,
  JEF/DOC-1286,
  June 2009.

Conclusions NRG

- Automated 3D uncertainty calculations can easily be performed for all (benchmark) problems for which MCNP inputs exist
- Method works well for both shielding and k_{eff} benchmarks
- Method could be applied to exploit the large source of experimental benchmark data available
- Result: automated feedback to evaluator possible and hence reduced time for updated evaluation

JEFF Meeting, December 2010 OECD NEA – E. Dupont 3

Sensitivity/Uncertainty tools NRG

Status:

* Sensitivity/uncertainty tools were developed in the '70s and '80s
* No substantial recent developments
* Almost all tools based on deterministic methodology

5 years later, NDaST is now being developed, a Web (Java based) tool. Currently in alpha.

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Nuclear Data Sensitivity Tool (NDaST) Flowchart

Select / load benchmarks

Sensitivities (S) & C/E data

DICE

IDAT

Personal

Numerical Benchmarks

User Input Perturbation (P)

isotope/reaction/energy cross section

AND /OR

Janis 4

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

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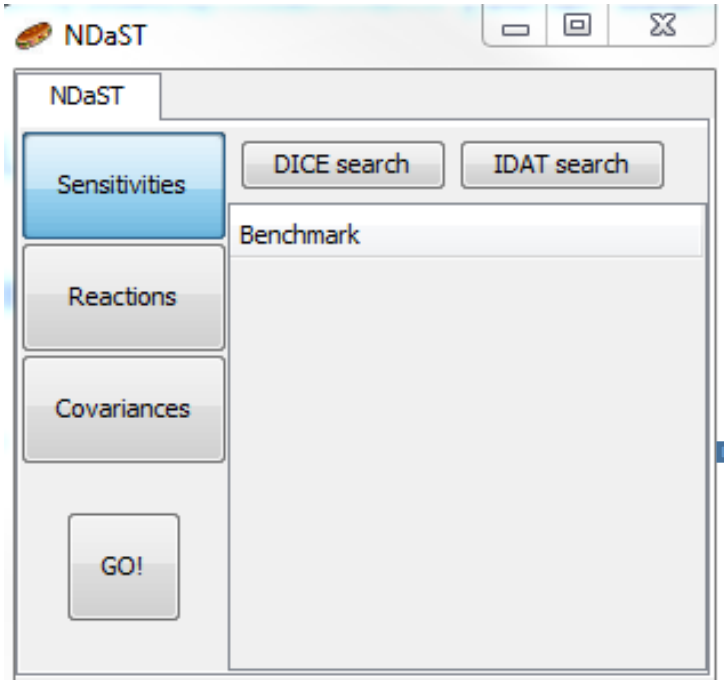
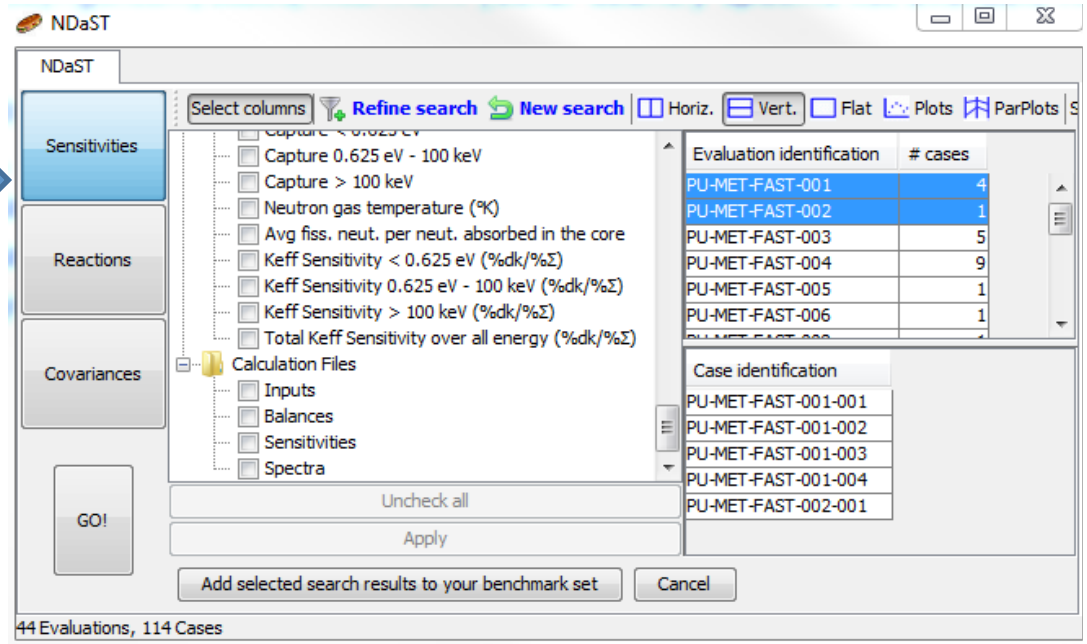
Panel 1: Select Benchmark Sensitivity Data

Currently can select benchmarks via DICE/IDAT criteria. Simplified search options are undergoing refinement.



- » Save/load customised benchmark list e.g. CSEWG
- » Enable sending/sharing of datasets for inter-comparisons



Load personal case results & sensitivity data

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Panel 2: Isotope-Reaction-Energy Perturbations

Each isotope-reaction represented by a column with N energy group rows

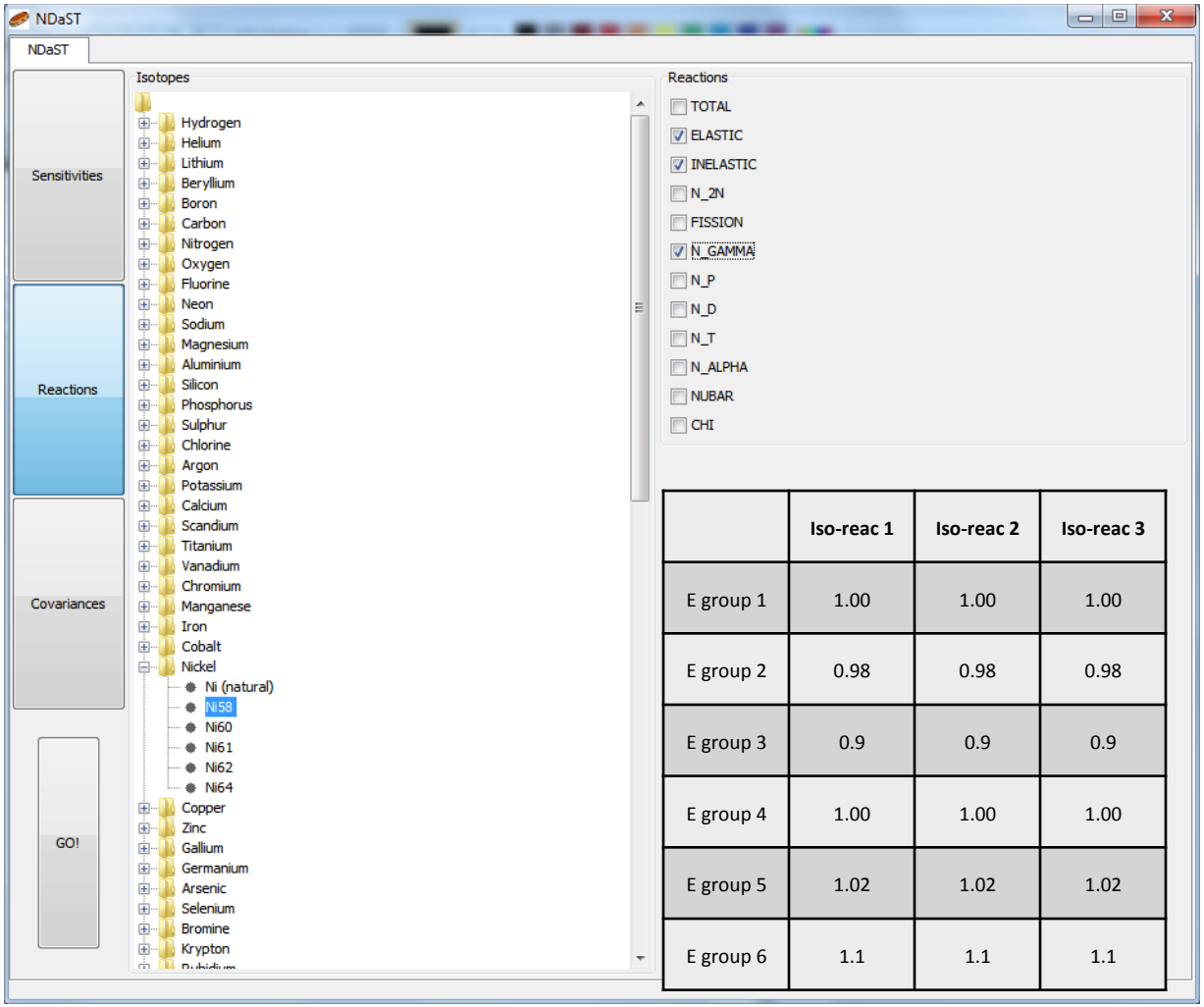
<u>Loading Options:</u>

-Manually

-Loaded from file

-Auto-computed by dividing 2 evaluated files (via JANIS)

Example: ENDF/B-VII.1/ ENDF/B-VII.2



	Iso-reac 1	Iso-reac 2	Iso-reac 3
E group 1	1.00	1.00	1.00
E group 2	0.98	0.98	0.98
E group 3	0.9	0.9	0.9
E group 4	1.00	1.00	1.00
E group 5	1.02	1.02	1.02
E group 6	1.1	1.1	1.1

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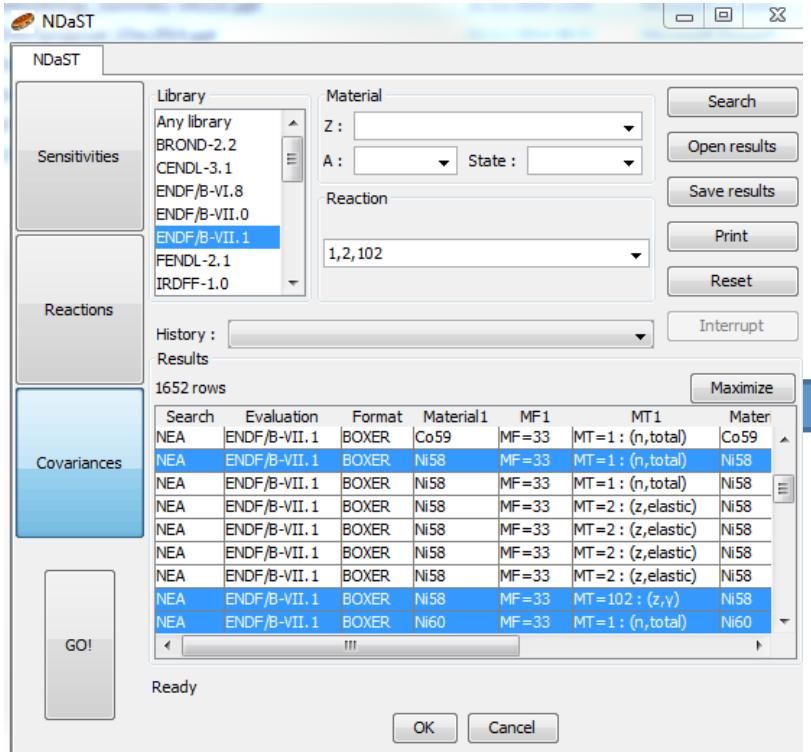
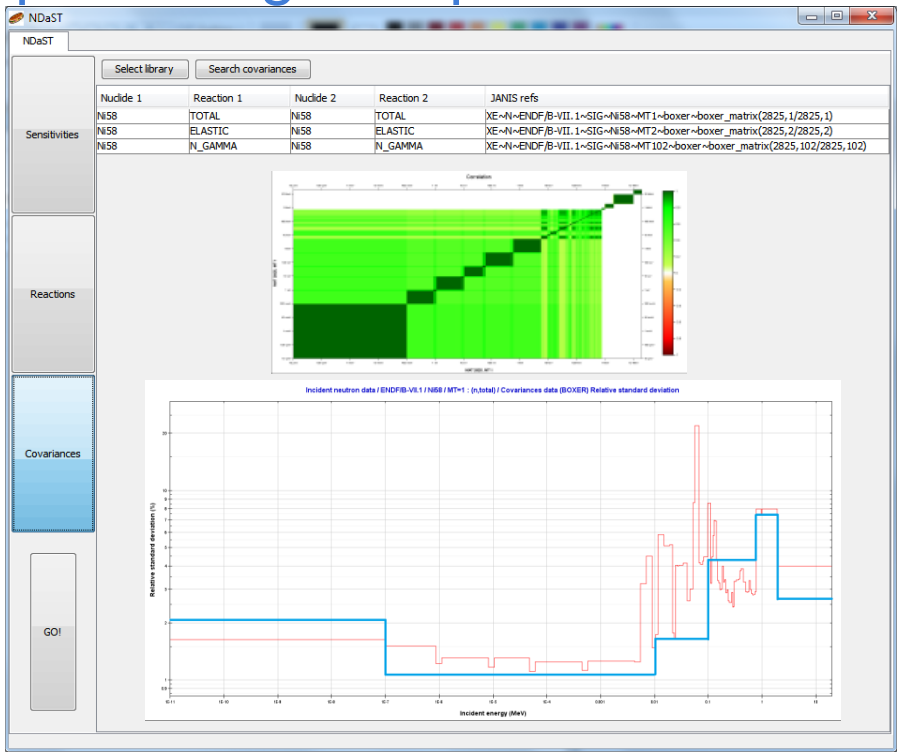
Panel 3: Select XS Covariance Data

Covariance data selected from JANIS for uncertainty propagation calculation

- Correlation plot
- Relative standard deviations plotted against perturbations





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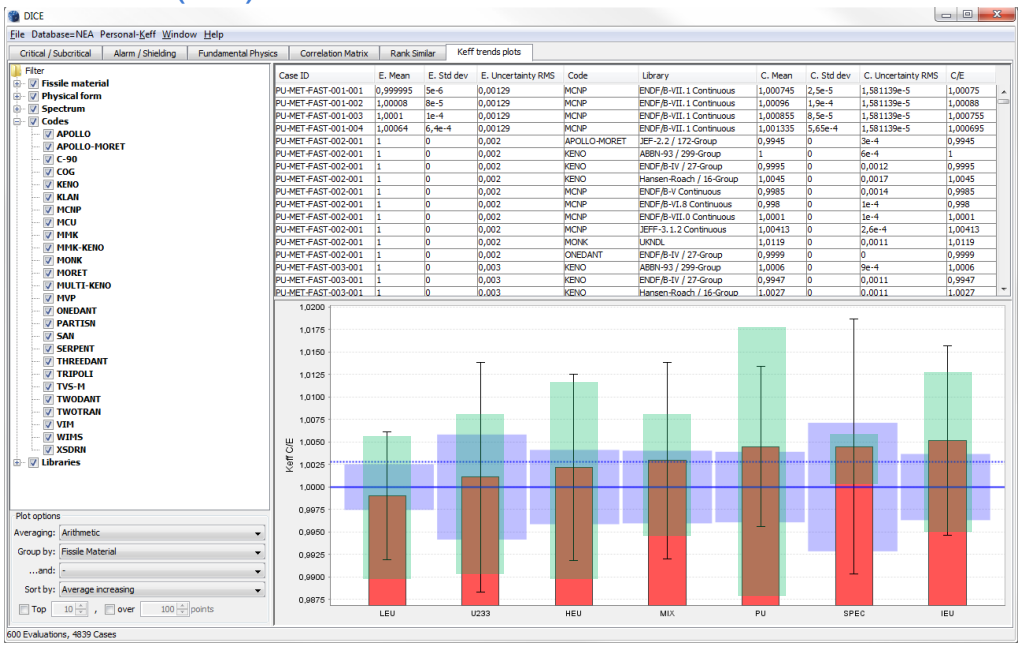
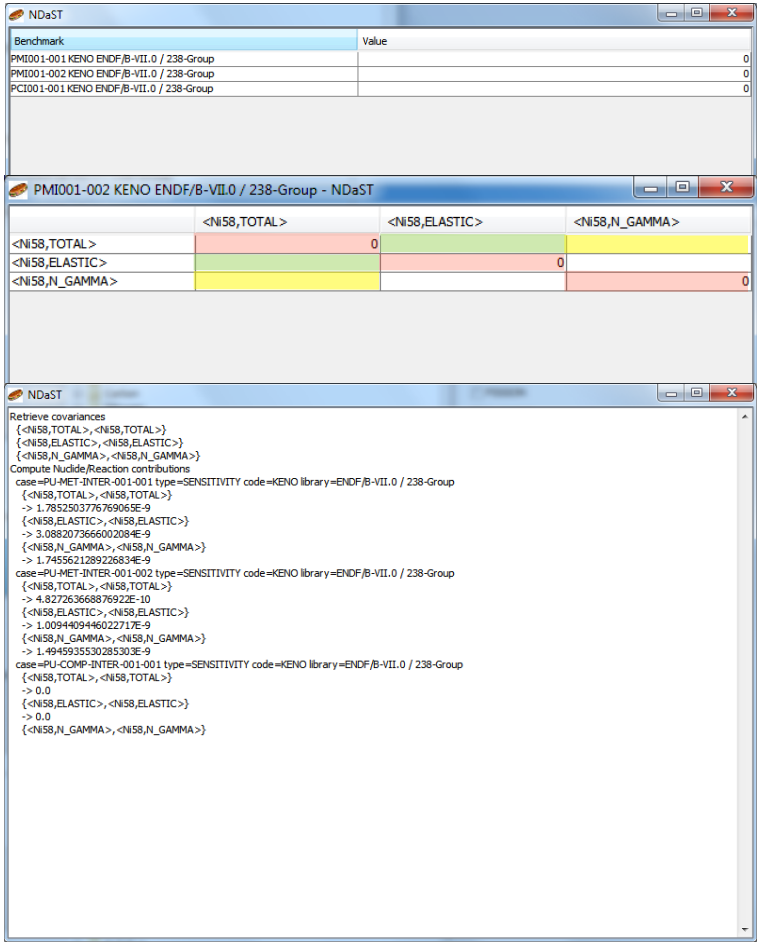
Output Panel

- Results panel showing individual results of C/E or ΔC/E $U_{C(XS)}$ and a grouped plot



Case ID	E. Mean	E. Std dev	E. Uncertainty RMS	Code	Library	C. Mean	C. Std dev	C. Uncertainty RMS	C/E
PU-MET-FAST-001-001	0,999995	5e-6	0,00129	MCNP	ENDF/B-VII.1 Continuous	1,000745	2,5e-5	1,581139e-5	1,00075
PU-MET-FAST-001-002	1,00008	8e-5	0,00129	MCNP	ENDF/B-VII.1 Continuous	1,00096	1,9e-4	1,581139e-5	1,00088
PU-MET-FAST-001-003	1,0001	1e-4	0,00129	MCNP	ENDF/B-VII.1 Continuous	1,000855	8,5e-5	1,581139e-5	1,000755
PU-MET-FAST-001-004	1,00064	6,4e-4	0,00129	MCNP	ENDF/B-VII.1 Continuous	1,001335	5,65e-4	1,581139e-5	1,000695
PU-MET-FAST-002-001	1	0	0,002	APOLLO-MORET	JEF-2.2 / 172-Group	0,9945	0	3e-4	0,9945
PU-MET-FAST-002-001	1	0	0,002	KENO	ABBN-93 / 299-Group	1	0	6e-4	1
PU-MET-FAST-002-001	1	0	0,002	KENO	ENDF/B-IV / 27-Group	0,9995	0	0,0012	0,9995
PU-MET-FAST-002-001	1	0	0,002	KENO	Hansen-Roach / 16-Group	1,0045	0	0,0017	1,0045
PU-MET-FAST-002-001	1	0	0,002	MCNP	ENDF/B-V Continuous	0,9985	0	0,0014	0,9985
PU-MET-FAST-002-001	1	0	0,002	MCNP	ENDF/B-VI.8 Continuous	0,998	0	1e-4	0,998
PU-MET-FAST-002-001	1	0	0,002	MCNP	ENDF/B-VII.0 Continuous	1,0001	0	1e-4	1,0001
PU-MET-FAST-002-001	1	0	0,002	MCNP	JEFF-3.1.2 Continuous	1,00413	0	2,6e-4	1,00413
PU-MET-FAST-002-001	1	0	0,002	MONK	UKNDL	1,0119	0	0,0011	1,0119
PU-MET-FAST-002-001	1	0	0,002	ONEDANT	ENDF/B-IV / 27-Group	0,9999	0	0	0,9999
PU-MET-FAST-003-001	1	0	0,003	KENO	ABBN-93 / 299-Group	1,0006	0	9e-4	1,0006
PU-MET-FAST-003-001	1	0	0,003	KENO	ENDF/B-IV / 27-Group	0,9947	0	0,0011	0,9947
PU-MET-FAST-003-001	1	0	0,003	KENO	Hansen-Roach / 16-Group	1,0027	0	0,0011	1,0027



- Grouped metrics also available
  - C/E mean, st. dev., chi-square

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Summary

Major changes in DICE capabilities, not widely known

- ✓ 4011 cases have 3 group sensitivity data in DICE
- ✓ Search and trending benchmark based on sensitivity
- ✓ Load personal database of k_{eff} calculations
- ✓ Nuclear Data Sensitivity Tool is being developed
- ✓ Enable rapid scoping of changes to nuclear data and covariance data

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Thanks for your attention

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