Using Sensitivity Data in DICE to identify CIELO benchmarks, and the Nuclear Data and Sensitivity Testing Tool

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Overview

- **Sensitivity Data in DICE (Database for ICSBEP)**
- **Searching For CIELO Benchmarks with DICE**
- **Tools for Iron**
- **Sensitivity * Perturbation =**
- **Nuclear Data and Sensitivity Testing Tool (NDaST)**

FYI: Sensitivity data tells you how much k_{eff} will change (%) if the nuclear data changes (%). [not discussing GPT at the moment…]

Fictional Example: I change the U^{238} fission cross section by 1% uniformly in energy. The sensitivity data tells me HMF-001 k_{eff} will change by 0.05% or 50 pcm.

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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

Script and examples given those wishing to compute their own sensitivity data; including S. van der marck (Data tester), J. Bess (ICSBEP Chair), T.Kozlowski (UAM). Also participated in comparison of sensitivity data across codes, spearheaded by E.Ivanov.

	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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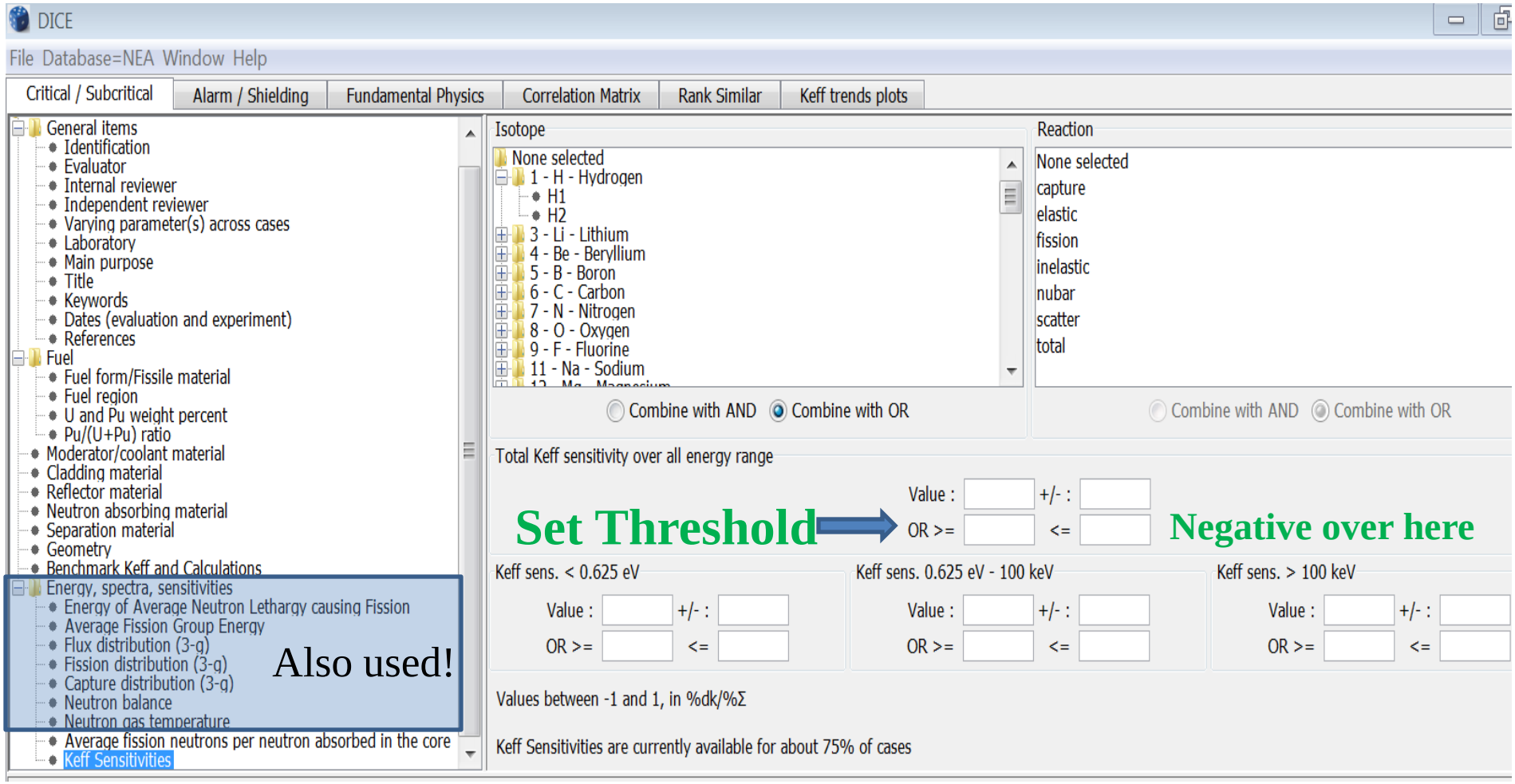
DICE k_{eff} Sensitivities Search

3 Group search, full 238 Group SDF's are stored and distributed. Thus you can do your own search in a different group structure…I'll even email you a script to do this if you ask me.



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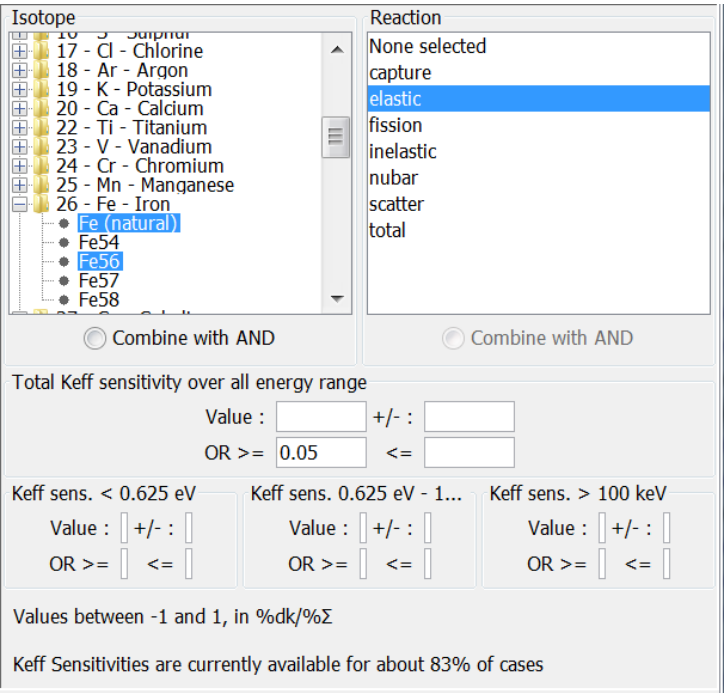
Example: Iron Elastic Scattering Sensitivity

Search → Results



Actually you don't even need the DVD to do this (just java)… google 'DICE ICSBEP'

Evaluation identification	Title
PU-MET-FAST-015	IRON-REFLECTED ARRAY OF PLUTONIUM FUEL RODS
PU-MET-FAST-026	SPHERICAL ASSEMBLY OF 239PU(δ, 98%) WITH 11.9-CM STEEL REFLECTOR
PU-MET-FAST-028	STEEL-REFLECTED SPHERICAL ASSEMBLY OF 239PU(δ, 89%)
PU-MET-FAST-032	STEEL-REFLECTED SPHERICAL ASSEMBLY OF 239PU(a, 88%)
PU-MET-FAST-045	CRITICAL EXPERIMENTS PERFORMED FOR LAMPRE, THE LOS ALAMOS MOLTEN PLUTON
PU-MET-INTER-002	ZPR-6 ASSEMBLY 10: A CYLINDRICAL PLUTONIUM/CARBON/STAINLESS STEEL ASSEMBI
HEU-MET-FAST-013	SPHERE OF HIGHLY ENRICHED URANIUM REFLECTED BY STEEL
HEU-MET-FAST-021	STEEL-REFLECTED SPHERICAL ASSEMBLY OF 235U(90%)
HEU-MET-FAST-043	HEU CYLINDERS AXIALLY REFLECTED BY STEEL
HEU-MET-FAST-072	ZEUS: FAST-SPECTRUM CRITICAL ASSEMBLIES WITH AN IRON - HEU CORE SURROUND
HEU-MET-FAST-075	ZPPR-20 PHASE C: A CYLINDRICAL ASSEMBLY OF U METAL REFLECTED BY BERYLLIUM (
HEU-MET-FAST-084	HEU METAL CYLINDERS WITH MAGNESIUM, TITANIUM, ALUMINUM, GRAPHITE, MILD S
HEU-MET-FAST-085	HIGHLY ENRICHED URANIUM METAL SPHERES SURROUNDED BY COPPER, CAST IRON,
HEU-MET-INTER-001	THE URANIUM/IRON BENCHMARK ASSEMBLY: A 235U(93%)/IRON CYLINDER REFLECTE
HEU-SOL-THERM-033	HIGHLY ENRICHED URANYL NITRATE IN ANNULAR TANKS WITH CONCRETE REFLECTI(
HEU-SOL-THERM-038	WINCO SLAB TANKS: TWO INTERACTING TANKS OF HIGHLY ENRICHED URANYL NITRA
HEU-SOL-THERM-044	CONCRETE-REFLECTED URANYL NITRATE SOLUTION CYLINDER CONTAINING PERIODI
HEU-COMP-INTER-003	REFLECTED URANIUM-HYDRIDE CYLINDRICAL ASSEMBLIES

Thermal/Intermediate/Fast/Total

Case identification	Isotope	Reaction	Keff sen...	Keff sen...	Keff sen...	Total K...
HEU-MET-INTER-001-001	Fe (natural)	elastic	-0.00011	0.02834	0.14435	0.17258
HEU-MET-INTER-001-001	Fe (natural)	elastic	-0.00011	0.02834	0.14435	0.17258
HEU-MET-INTER-001-001	Fe (natural)	elastic	-0.00011	0.02834	0.14435	0.17258
HEU-MET-INTER-001-001	Fe (natural)	elastic	-0.00011	0.02834	0.14435	0.17258
HEU-MET-INTER-001-001	Fe (natural)	elastic	-0.00011	0.02834	0.14435	0.17258
PU-MET-FAST-015-001	Fe (natural)	elastic	0	0.00741	0.1435	0.15091
PU-MET-FAST-026-001	Fe56	elastic	0	0.00499	0.11646	0.12145
MIX-MET-INTER-003-001	Fe56	elastic	-0.00008	0.02824	0.09205	0.12021
PU-MET-FAST-028-001	Fe56	elastic	0	0.00503	0.11054	0.11558
PU-MET-INTER-002-001	Fe56	elastic	-0.00004	0.03585	0.07886	0.11467
HEU-MET-FAST-085-003	Fe56	elastic	0	0.00697	0.09838	0.10535
SPEC-MET-FAST-014-001	Fe (natural)	elastic	0	0.00508	0.09818	0.10326
SPEC-MET-FAST-014-001	Fe (natural)	elastic	0	0.00508	0.09818	0.10326
SPEC-MET-FAST-014-001	Fe (natural)	elastic	0	0.00508	0.09818	0.10326
HEU-MET-FAST-021-001	Fe56	elastic	0	0.00564	0.09299	0.09863
IEU-MET-FAST-005-001	Fe56	elastic	0	0.00744	0.08338	0.09082
HEU-MET-FAST-013-001	Fe56	elastic	0	0.00407	0.06921	0.07328
HEU-SOL-THERM-044-004	Fe56	elastic	0.00468	0.03531	0.03254	0.07253
HEU-COMP-INTER-003-0...	Fe56	elastic	0.00009	0.02457	0.0472	0.07187
HEU-MET-FAST-072-003	Fe56	elastic	-0.00062	0.01469	0.05739	0.07147
HEU-MET-FAST-072-001	Fe56	elastic	0	0.00862	0.05755	0.06617
PU-MET-FAST-032-001	Fe56	elastic	0	0.00234	0.06304	0.06538
HEU-SOL-THERM-033-003	Fe (natural)	elastic	0.00196	0.0318	0.03131	0.06507
HEU-MET-FAST-084-007	Fe56	elastic	0	0.00349	0.0607	0.06419

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Exercise: Use DICE to find good benchmarks for Fe56 testing.

Q: Would you find the same benchmarks as the existing test suites?

Q: Given the same ‘loose’ question, would two people involved with ICSBEP come up with similar benchmarks?

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Fun Exercise: Use DICE to find Fe56 benchmarks…compare to current testing suite

Eval-Case	Hill	Dyrda	Kahler	Trkov	KAPL	Eval-Case	Hill	Dyrda	Kahler	Trkov	KAPL
ALARM-CF-FE-SHIELD-001		X[10]				IMF006-001				X	
FUND-IPPE-VDG-MULTI-TRANS-001		X[10]			X	LCT001[5]			*LCT017		
HCI003-004		X			X	LCT002[5]			*LCT010		X
HCT014-001		X				LCT007[5]					X
HCT014-002		X				LCT008[5]					X
HMF013-011			X[4]	X		LCT010[5]	X		X[3]		X
HMF021-001	X	X	X[4]	X	X	LCT017[5]	X		X[3]		
HMF024-001			X[4]	X		LCT037[5]					X
HMF033-001			X[3]			LCT042-001				X	
HMF034-003	X[2]		X[3]		X	LCT042-002				X	
HMF043-?	X[2]		X[3]			LCT043-?				X	
HMF085-003	X	X				LCT045-007	X				
HMF087-001	X[2]		X[3,4]	X		LMT015-?				X	
HMF088-001			X[4]	X		LST001[5]					X
HMF088-002			X[4]	X		LST003[5]					X
HMI001-001	X	X[9]		X		LST004[5]					X
HMM006-001	X					LST007[5]					X
HMM018-002		X				LST016[5]					X
HMT013-001	X[1]	X		X		MCF001-001				X	
HMT015-001				X		MCF005-001				X	
HST001-001					X	MCF006-001				X	
HST024-001		X				MMF011-001					X
HST024-002		X				MMF011-002					X
HST032-001					X	MMI003-001	X				
HST038[5]	X	X				PMF015-001	X	X[9]		X	
HST042-006					X	PMF025-001			X[4]	X	
HST044-004		X[11]				PMF026-001	X	X	X[4]	X	
HST044-031		X[11]				PMF028-001	X	X	X[4]	X	
ICT009-001		X				PMF032-001			X[4]	X	
IMF005-001	X			X	X	PMF045-007		X			
						PMI002-001	X			X	
						SPECMF014-001	X	X[9]			

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Table of Benchmarks With Total 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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Missing Stuff + Limitations

- 1st order
- Not All Cases
- Used SCALE 238 Group Energy structure
- Reactions (Not all are loaded into database)
- Angular Sensitivity
- Correlations required for reactivity effect benchmarks (just launched a task force within ICSBEP for these)

Next step

Lofty Goal: Given a new evaluation, give evaluators a tool to tell how the changes they've made will impact integral benchmarks…**in under 30 seconds**.

- Nuclear Data and Sensitivity Testing Tool

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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. Summer beta version. Contact james.dyrda@oecd.org to be become a beta user.

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Nuclear Data Sensitivity Tool (NDaST) Flowchart

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

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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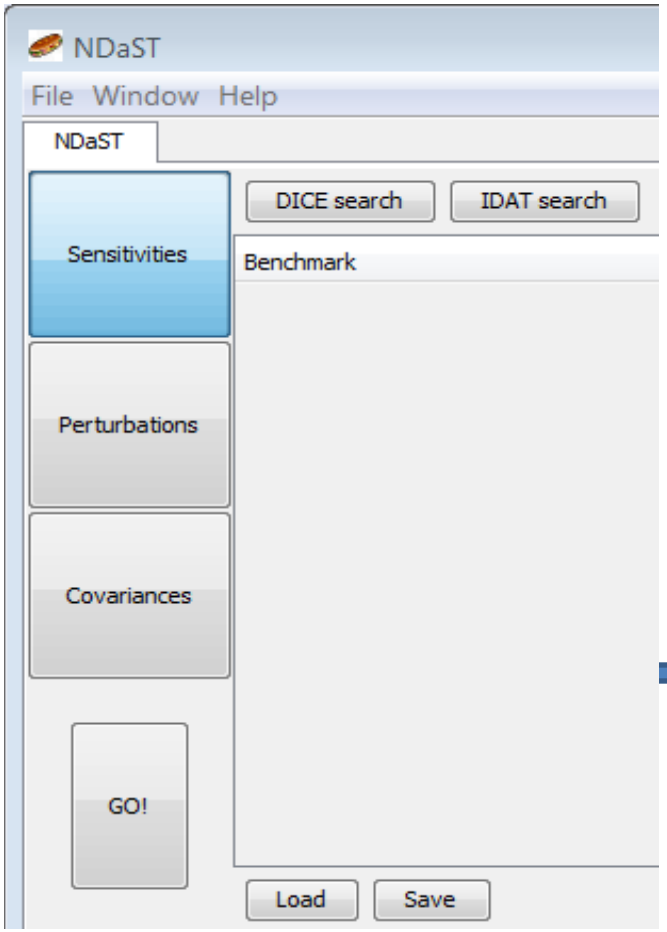
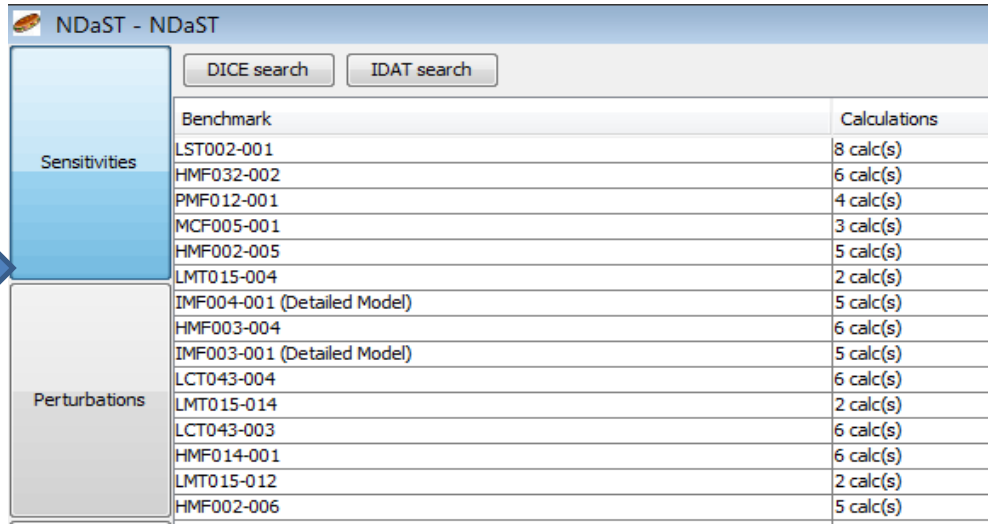
Panel 1: Select Benchmark Sensitivity Data

Currently can select benchmarks via DICE and IDAT criteria.
Finalised search options are undergoing refinement.



- Save/load customised benchmark list e.g. CIELO, CSEWG
- Enable sending/sharing of datasets for inter-comparisons (xml files)
- Load personal case results & sensitivity data



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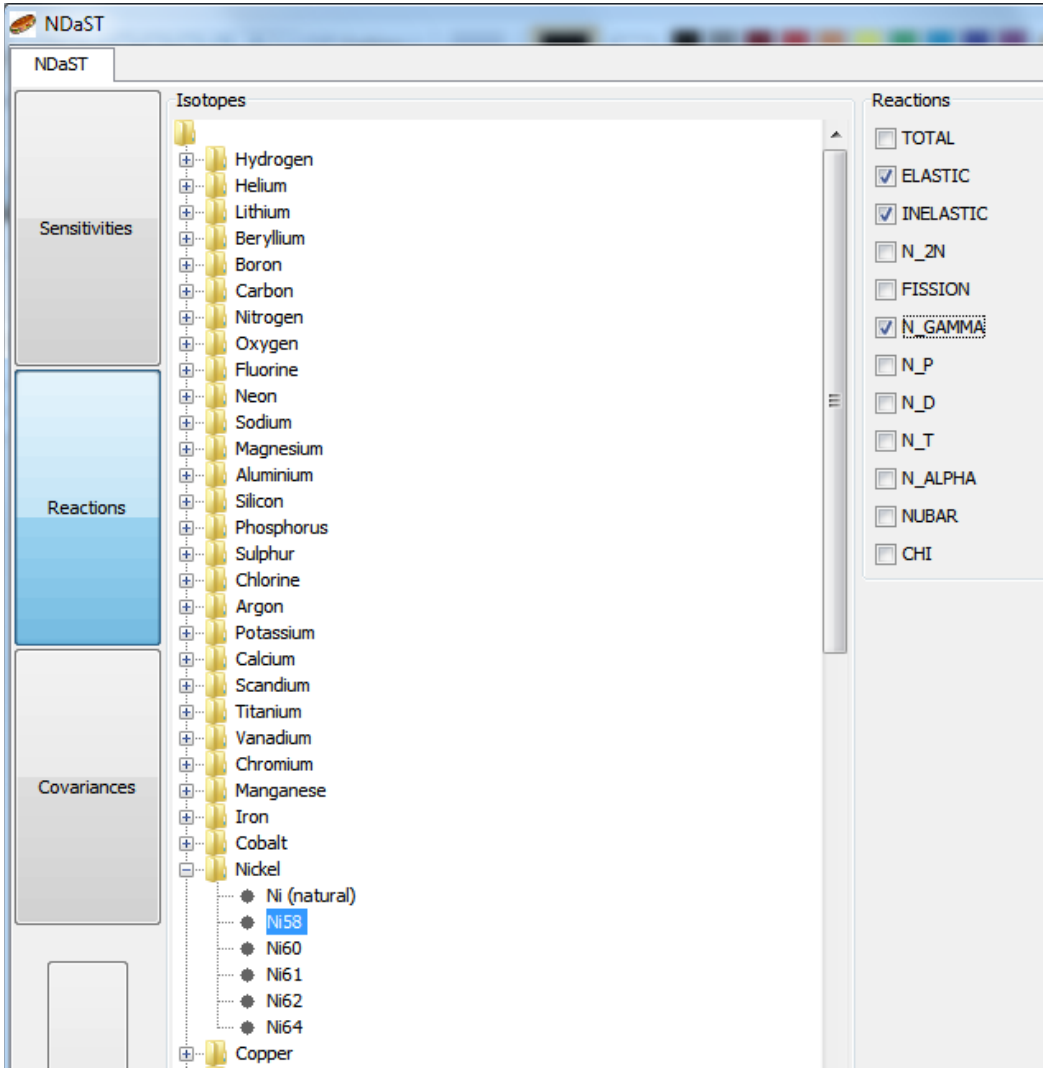
Panel 2: Isotope-Reaction-Energy Perturbations

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.0



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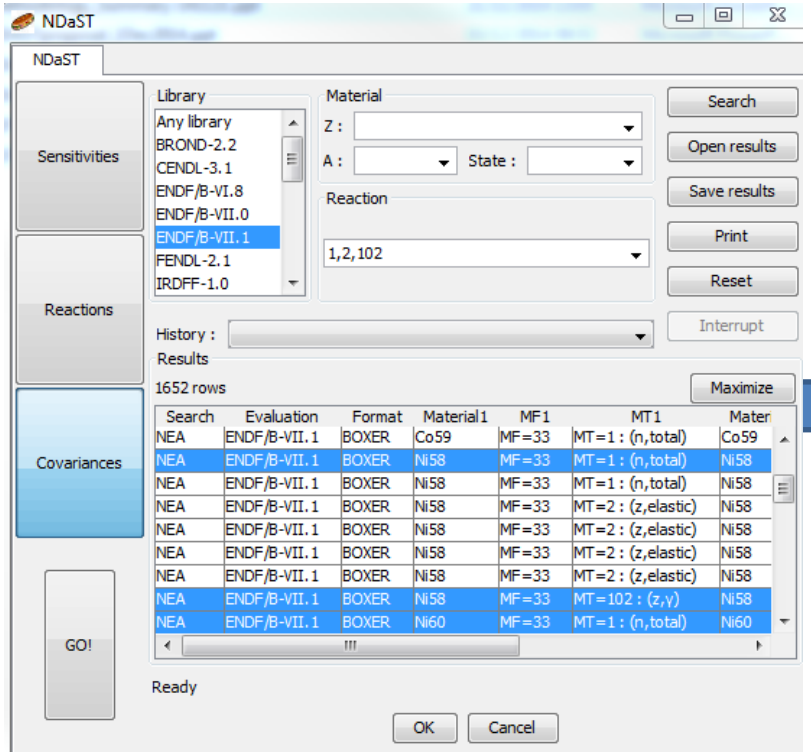
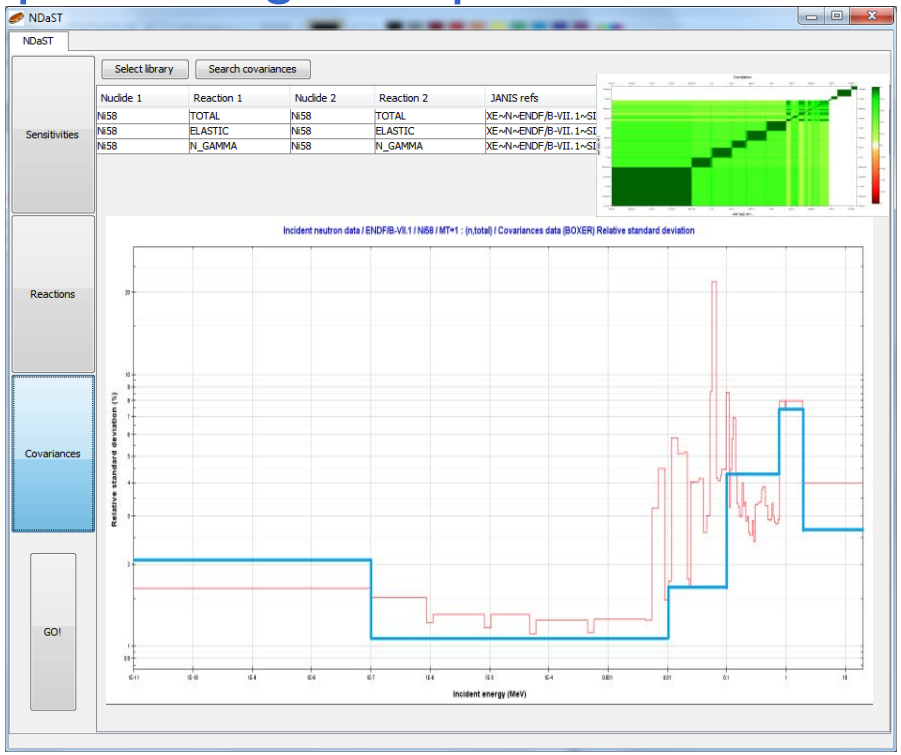
Panel 3: Select XS Covariance Data

Covariance data selected from JANIS for uncertainty propagation calculation

- Correlation plot
- Relative standard deviations plotted against perturbations





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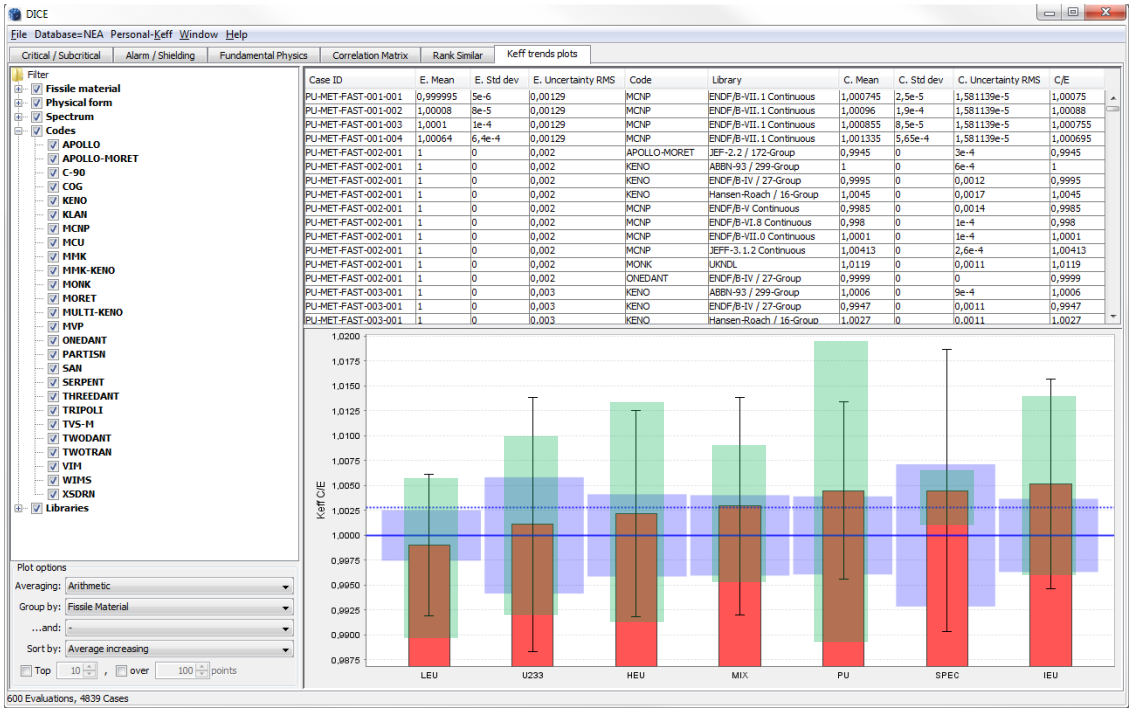
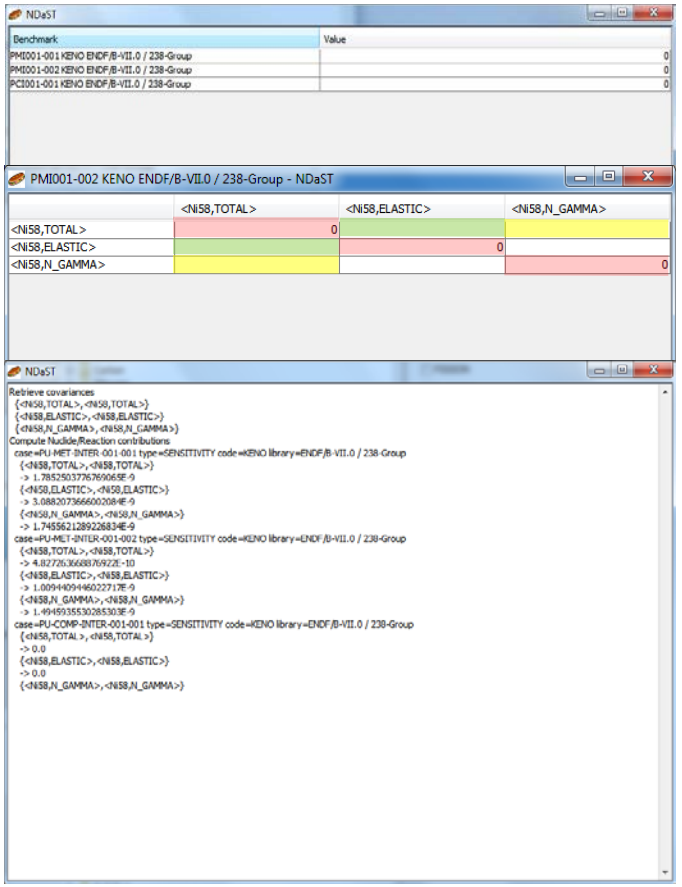
Output Windows and Plots

- Results panel showing individual results of C/E or $\Delta k_{eff}/k_{eff}$ XS uncertainty and a grouped trend plot





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

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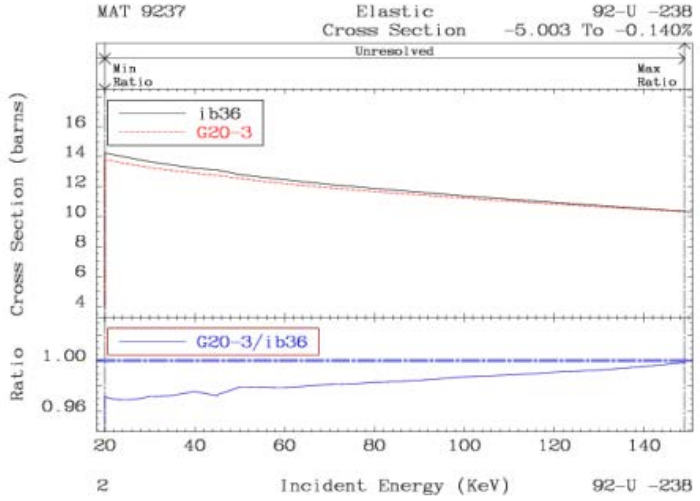
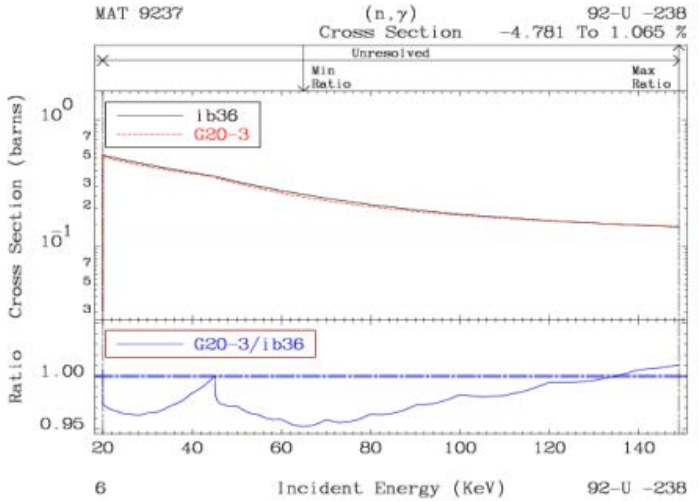
Example: ^{238}U CIELO

- Testing of integral benchmark experiments to iterations of the evaluated data
- https://www-nds.iaea.org/CIELO/
  - A. Trkov (IAEA), “Benchmarking of the CIELO ^{238}U Evaluated Data File”, December 2014
- CIELO Files U238ib36 and U238ib36ur
  - amendments to URR cross section 20 keV – 149 keV





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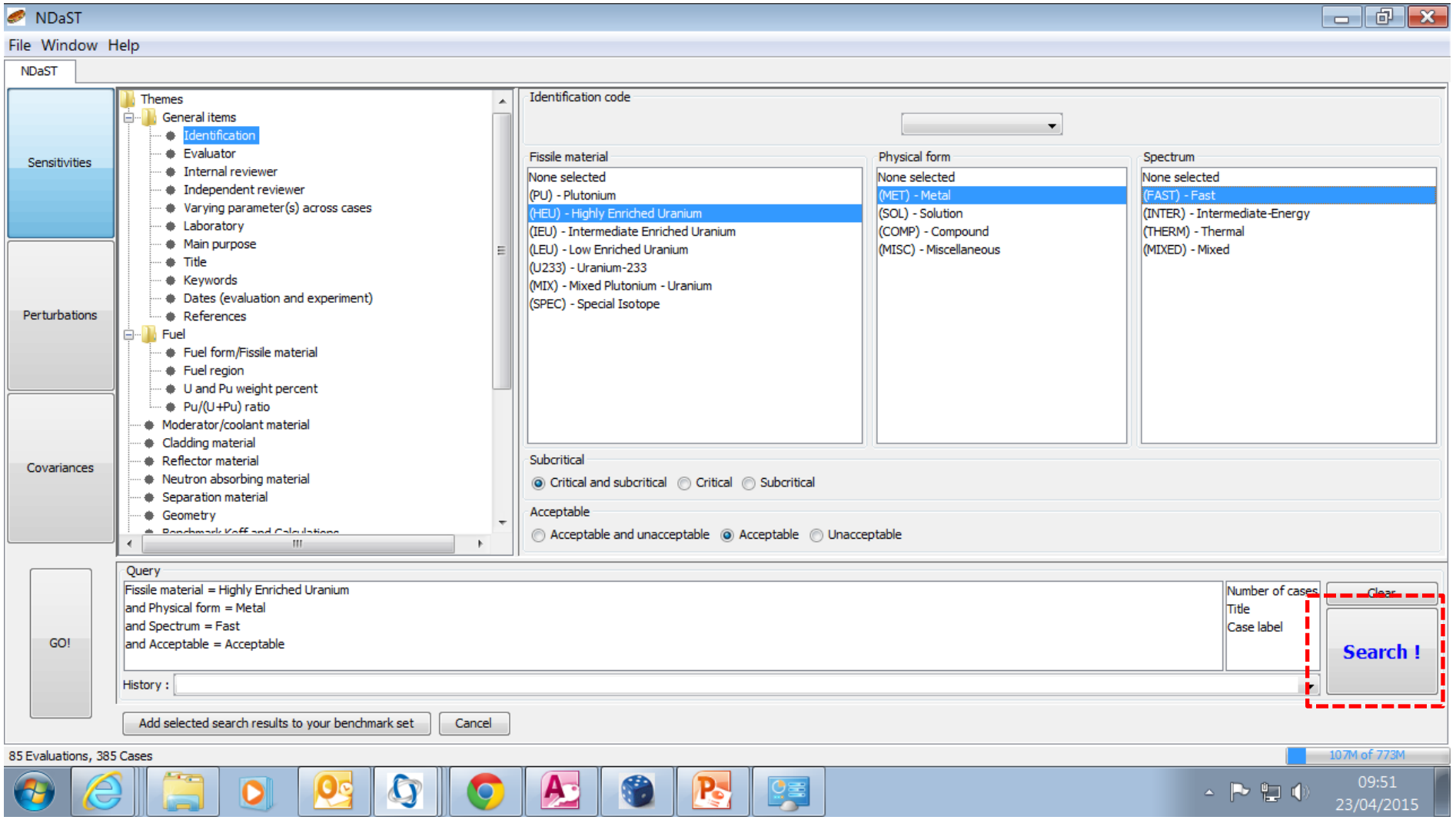
Simple Benchmark Selection



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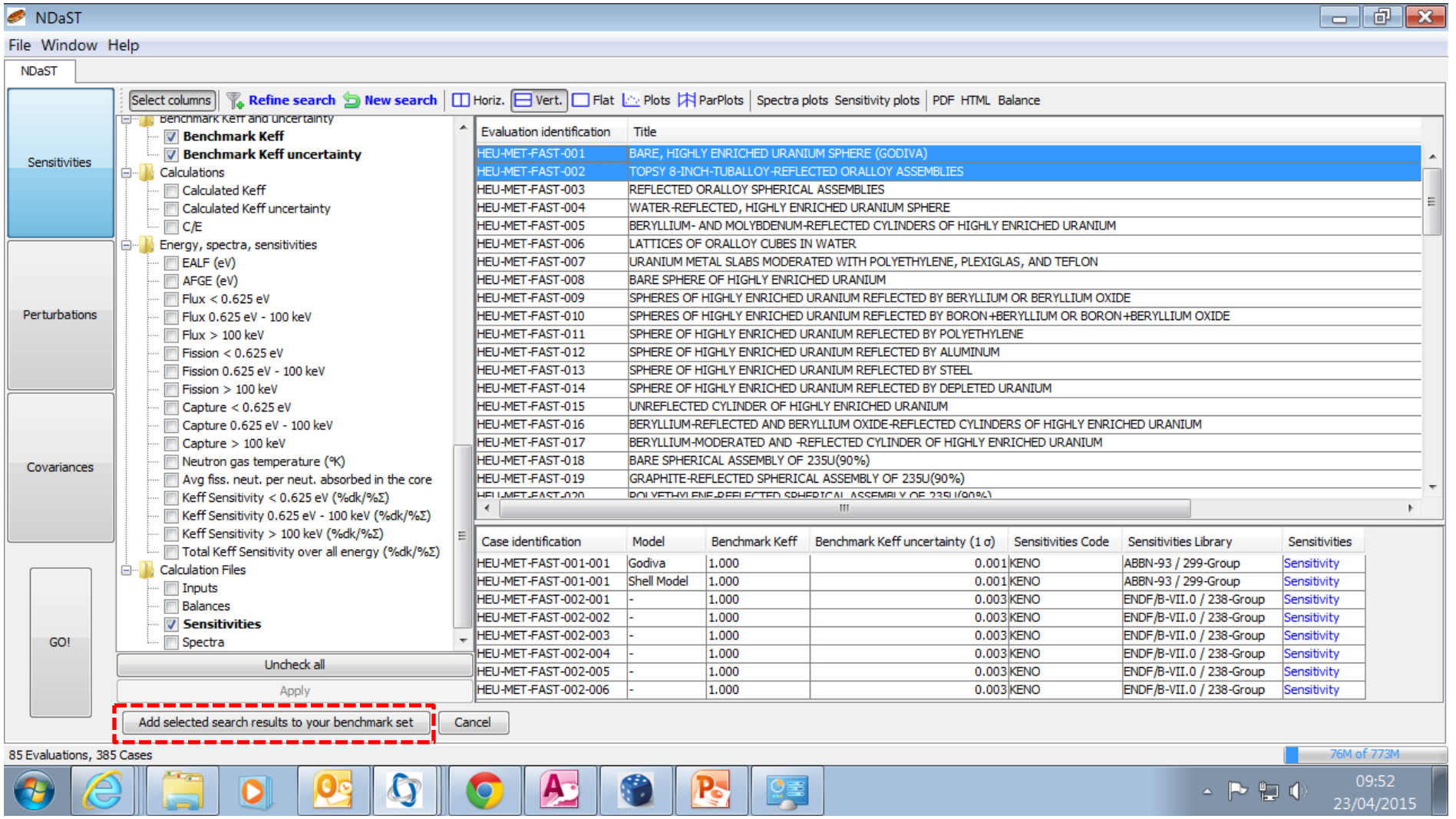
Addition of Benchmarks to Set



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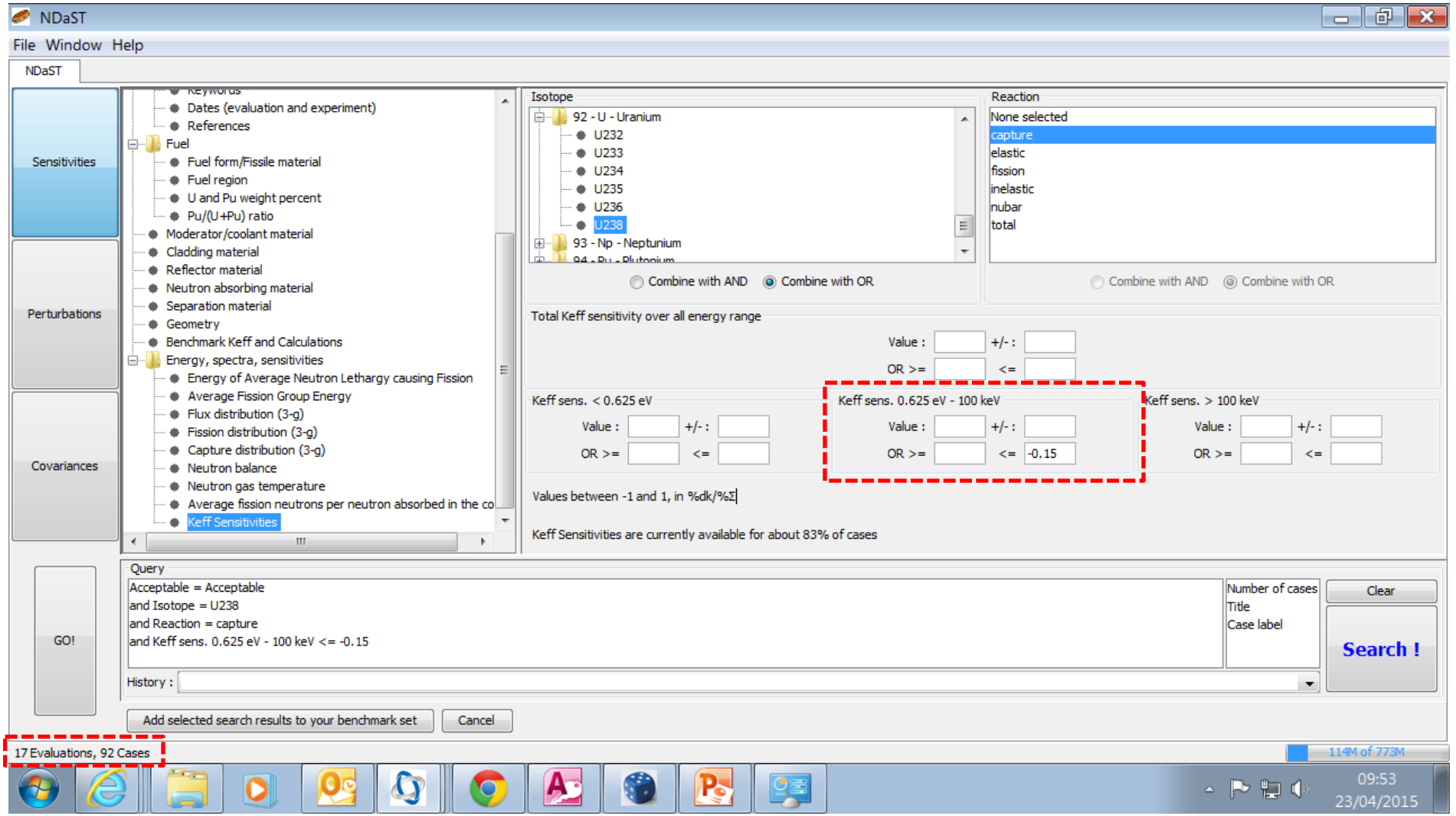
Sensitive Benchmark Search



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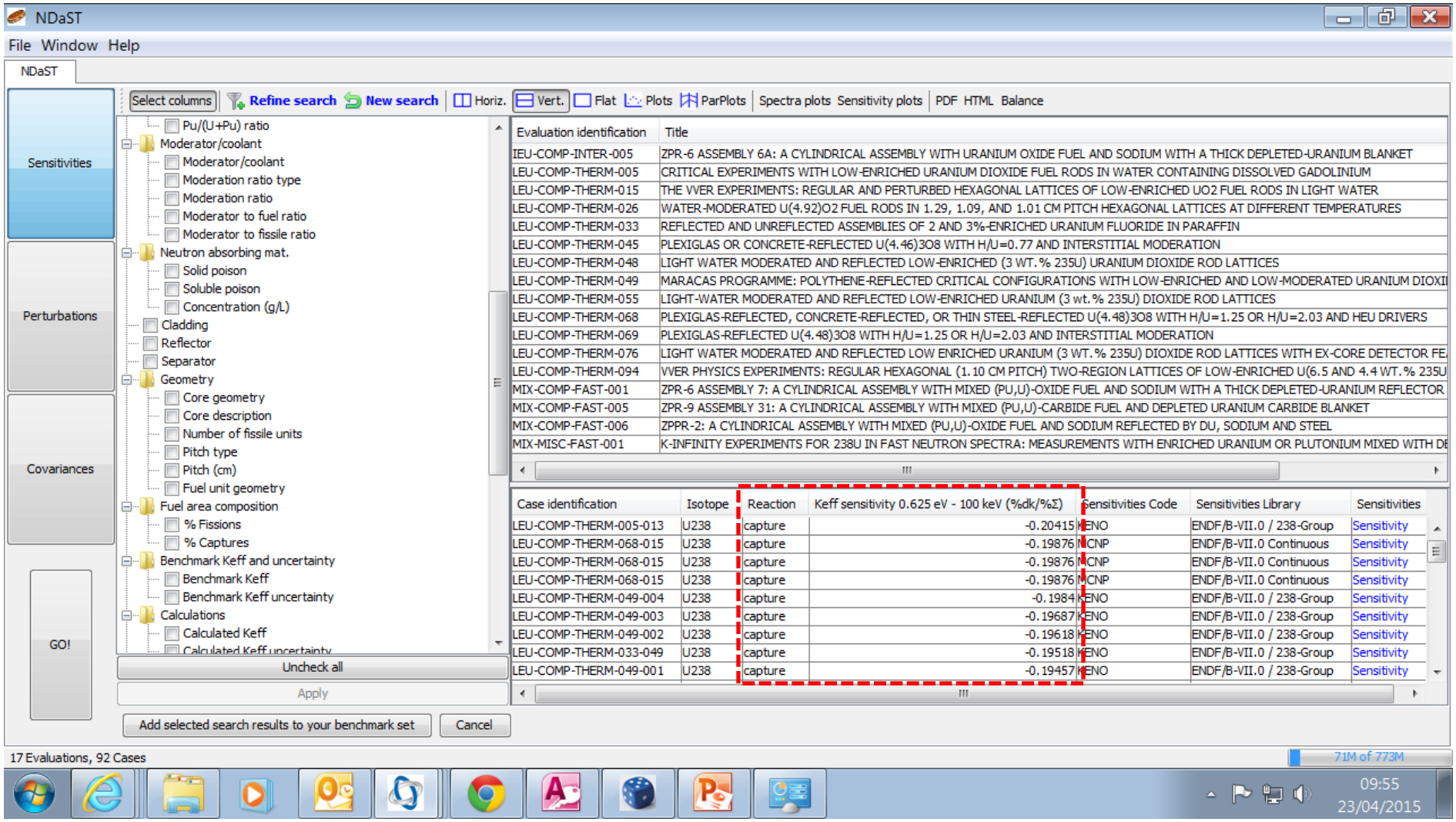
Filter in Order of Sensitivity



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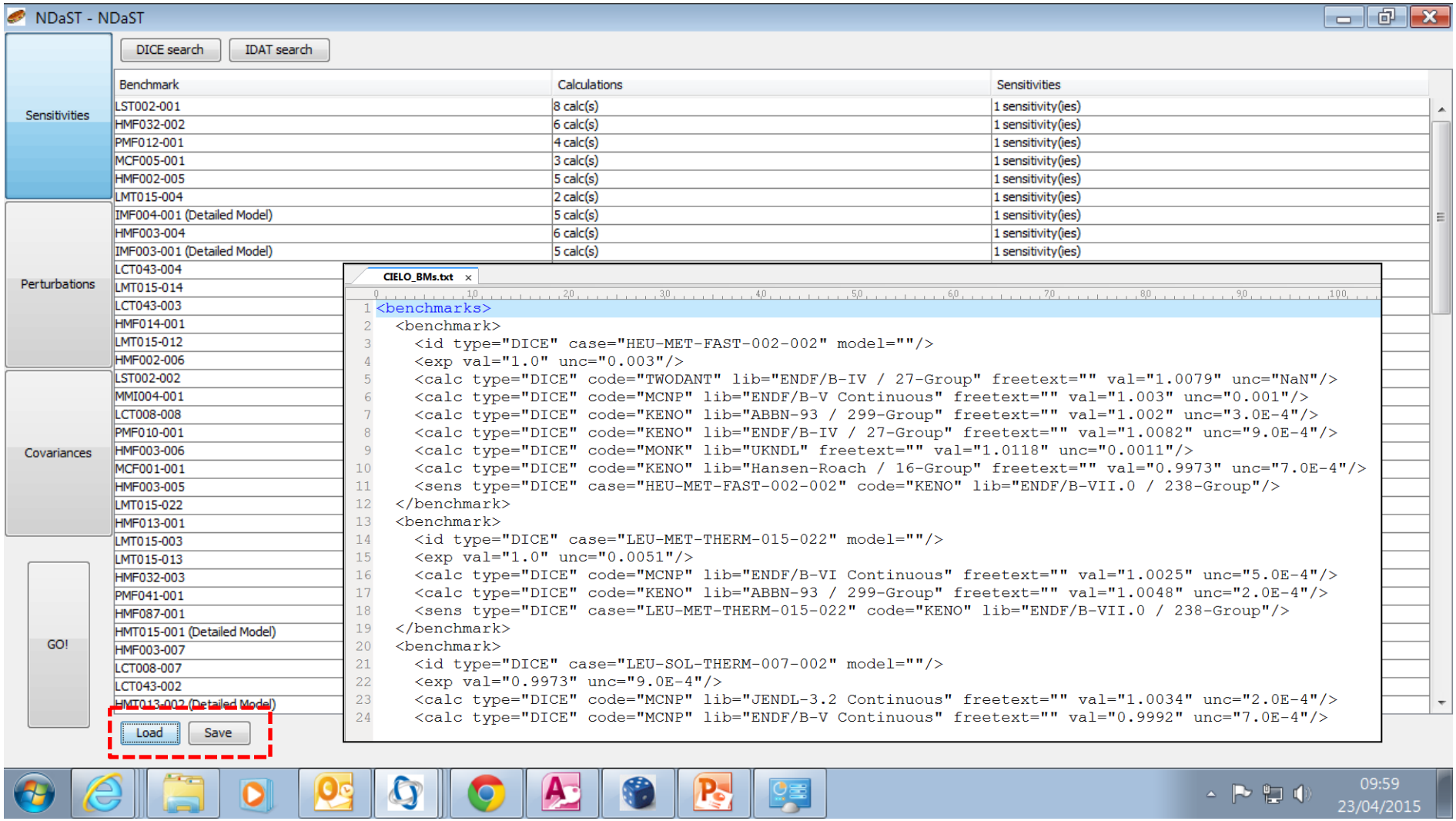
Save and Load Customised xml File



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Computation of Ratios in JANIS

TEMP N U238

File Tools Selected Help

Computed Computed

Incident neutron data / u238ib36ur_endf.zip / U238 / /

Incident en...	MT=2 : (z,e...	MT=102 : (...
	Computed	Computed
2e4	0.971467	0.973627
3e4	0.97174	0.964998
4e4	0.975812	0.984005
5e4	0.979184	0.972036
6e4	0.978773	0.958956
7e4	0.981423	0.958505
8e4	0.982838	0.96394
9e4	0.984505	0.972371
1e5	0.98742	0.982438
1.1e5	0.988619	0.981653
1.2e5	0.990871	0.99405
1.3e5	0.992707	0.995953
1.4e5	0.995375	1.005996
1.5e5	0.998682	1

Tabler

1st column values :

original values

interpolated values

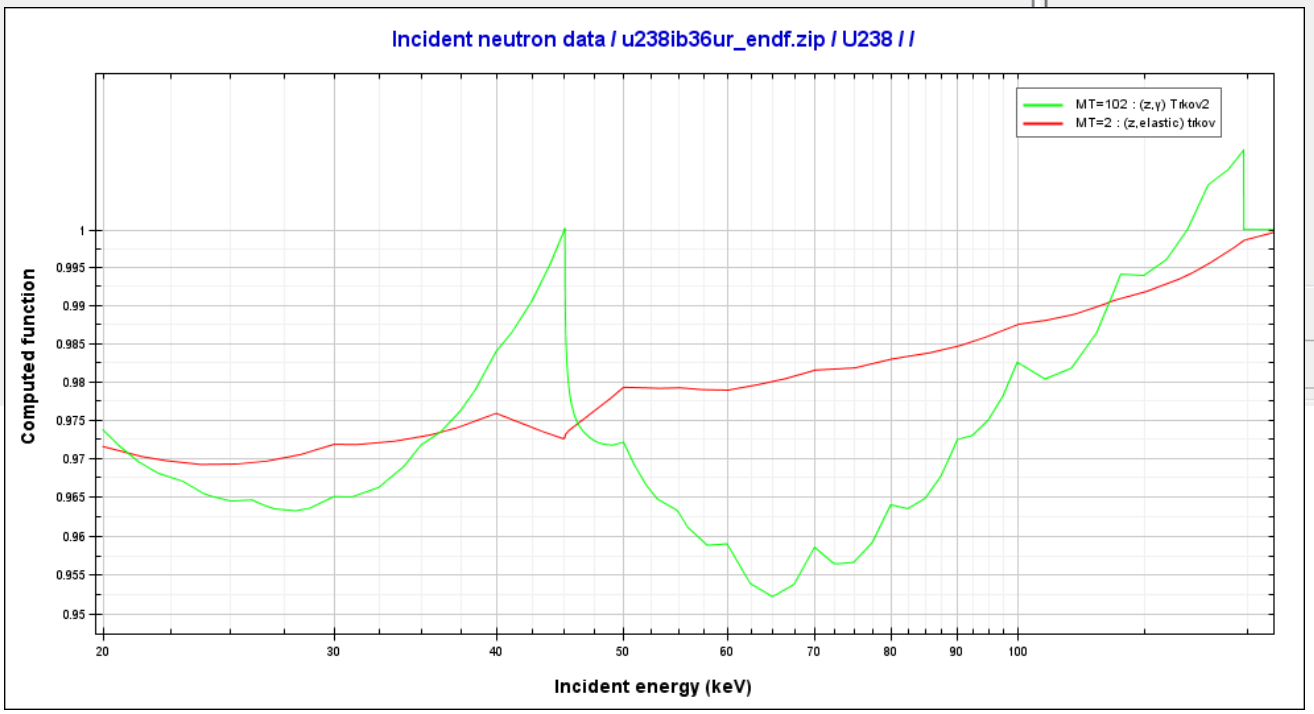
lin : step = 10 keV

log : per decade = 10

min= 20 keV

max= 150 keV

More...



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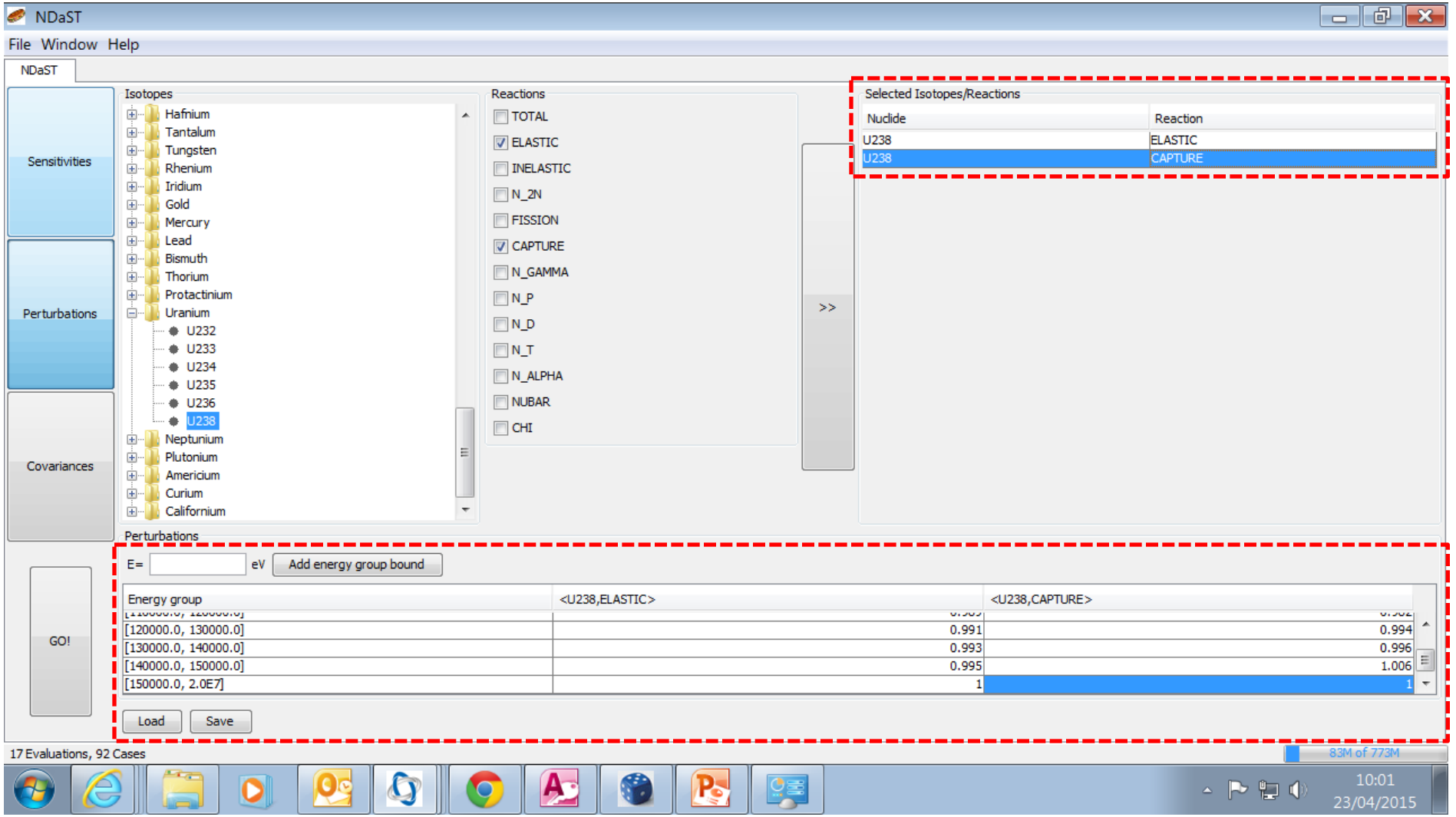
Addition of Reactions and Perturbations



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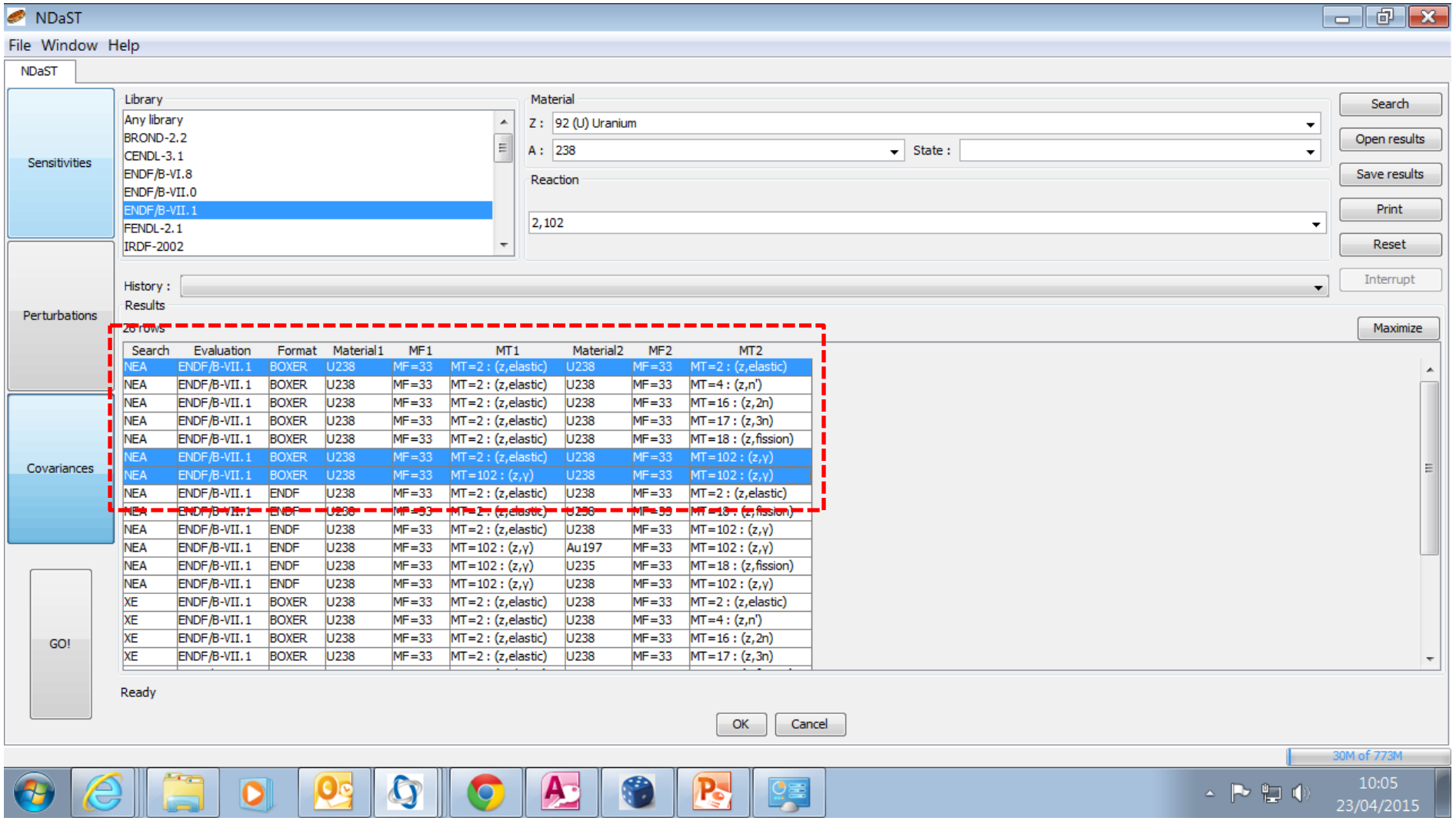
JANIS Covariance Search



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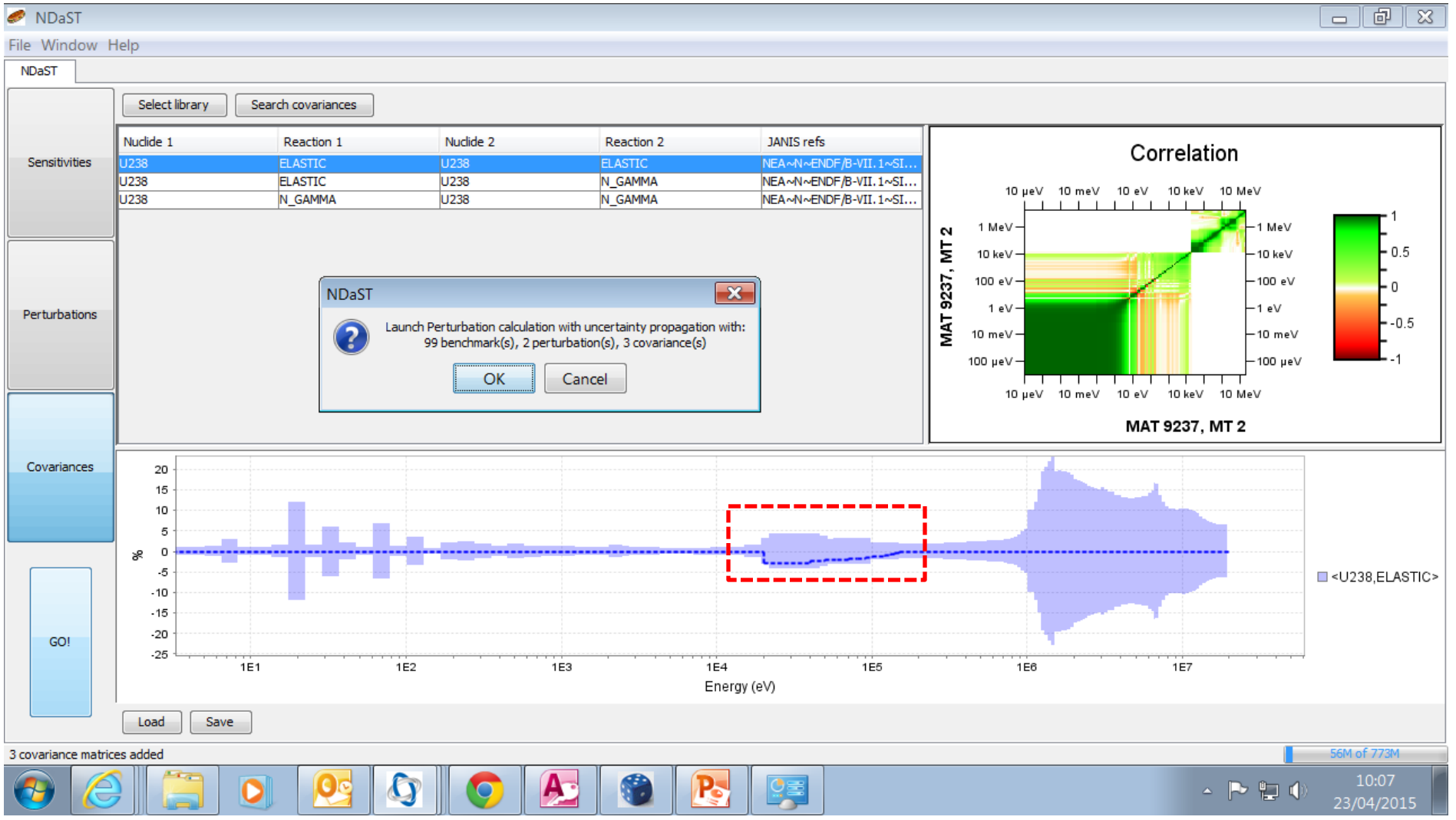
Visualisation of Covariance



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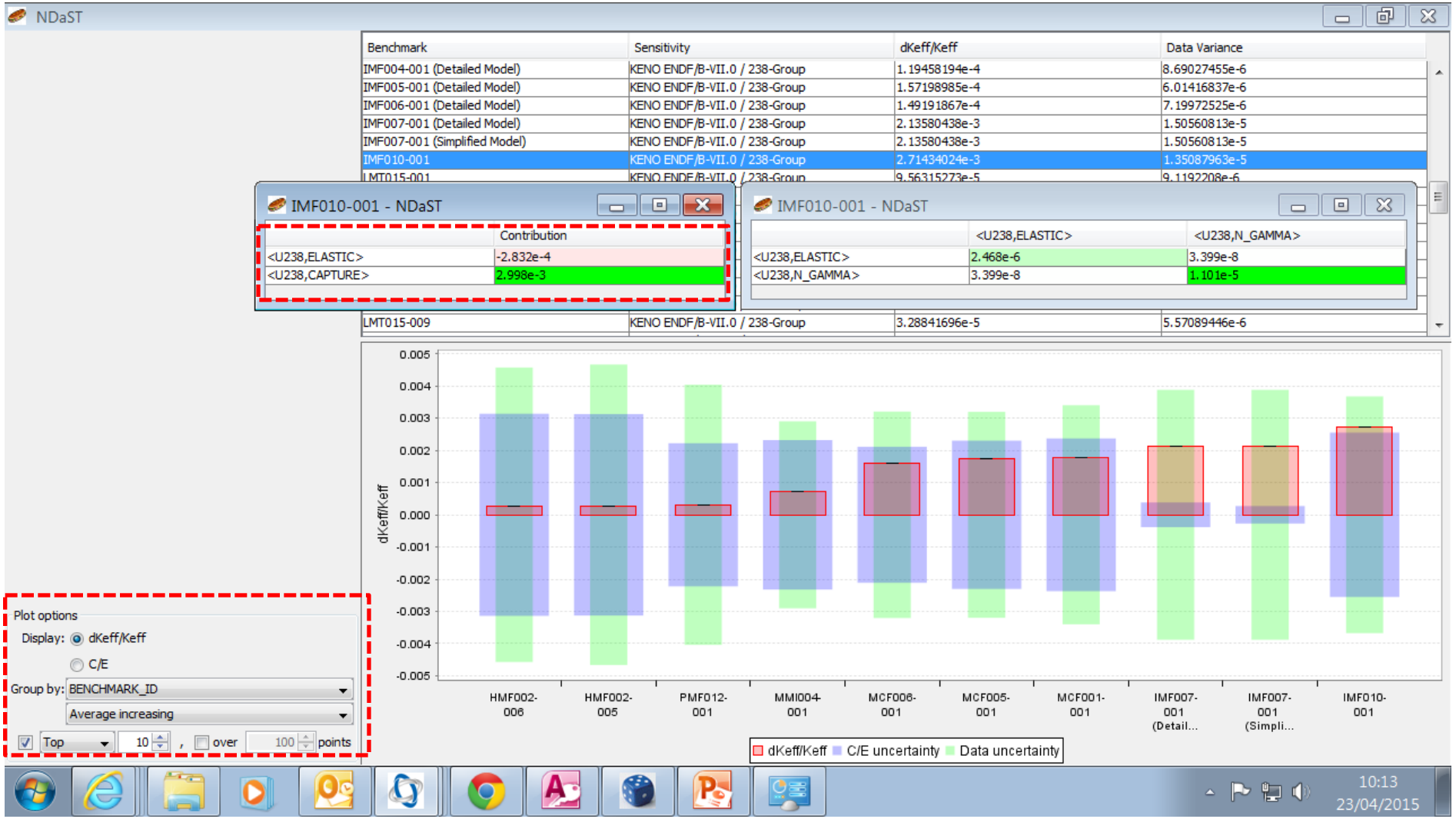
Delta k_{eff} Output and Plot



Refinement of Sensitive Benchmarks

ICSBEP Evaluation ID	Experiment Name	Sensitivity File	Delta-k/k	ND Uncertainty
IMF010-001	ZPR-6/9(U9)	KENO ENDF/B-VII.0 / 238-Group	0.00271	0.00368
IMF007-001 (Detailed Model)	Big Ten	KENO ENDF/B-VII.0 / 238-Group	0.00214	0.00388
IMF007-001 (Simplified Model)	Big Ten	KENO ENDF/B-VII.0 / 238-Group	0.00214	0.00388
MCF001-001	ZPR-6/7	KENO ENDF/B-VII.0 / 238-Group	0.00178	0.00340
MCF005-001	ZPR-9/31	KENO ENDF/B-VII.0 / 238-Group	0.00175	0.00320
MCF006-001	ZPPR-2	KENO ENDF/B-VII.0 / 238-Group	0.00160	0.00321
MMI004-001	ZPR-3/53	KENO ENDF/B-VII.0 / 238-Group	0.00071	0.00290

Cases shown with a >50 pcm effect due to this specific perturbation

- Energy breakdown also to be developed and included
- Cases to be run by rigorous calculation can be refined / minimised
- Allows analysis of competing effects at low computational cost
- An extra level of QA / checking has been performed

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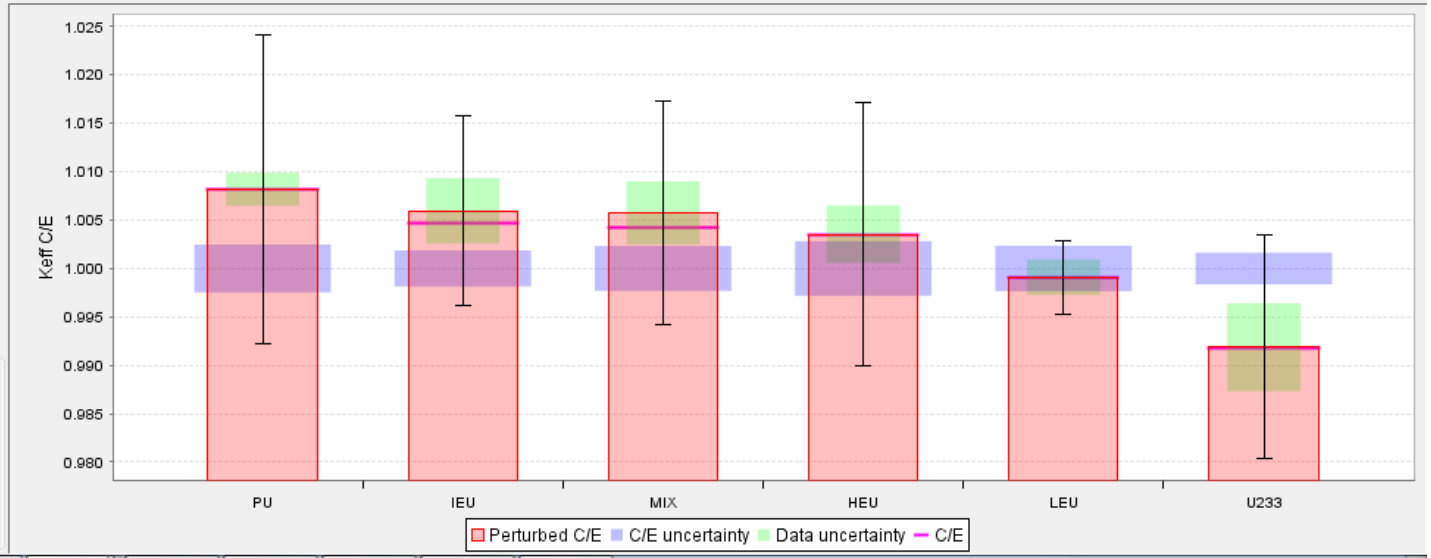
C/E Output Plot by Fissile Material

NDaST

Benchmark	Sensitivity	dKeff/Keff	Data Variance
IMF004-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.19458194e-4	8.69027455e-6
IMF005-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.57198985e-4	6.01416837e-6
IMF006-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.49191867e-4	7.19972525e-6
IMF007-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	2.13580438e-3	1.50560813e-5
IMF007-001 (Simplified Model)	KENO ENDF/B-VII.0 / 238-Group	2.13580438e-3	1.50560813e-5
IMF010-001	KENO ENDF/B-VII.0 / 238-Group	2.71434024e-3	1.35087963e-5
LMT015-001	KENO ENDF/B-VII.0 / 238-Group	9.56315273e-5	9.1192208e-6
LMT015-002	KENO ENDF/B-VII.0 / 238-Group	9.33693996e-5	9.12223259e-6
LMT015-003	KENO ENDF/B-VII.0 / 238-Group	9.37243754e-5	8.97314307e-6
LMT015-004	KENO ENDF/B-VII.0 / 238-Group	9.19485123e-5	9.04722604e-6
LMT015-005	KENO ENDF/B-VII.0 / 238-Group	9.2052567e-5	8.98066114e-6
LMT015-006	KENO ENDF/B-VII.0 / 238-Group	9.02603637e-5	9.05713507e-6
LMT015-007	KENO ENDF/B-VII.0 / 238-Group	9.03176989e-5	9.10123008e-6
LMT015-008	KENO ENDF/B-VII.0 / 238-Group	3.09194485e-5	5.53230246e-6
LMT015-009	KENO ENDF/B-VII.0 / 238-Group	3.28841696e-5	5.57089446e-6



Plot options
Display: dKeff/Keff
C/E
Group by: EVAL_ID_FISSILE_MATERIAL
Average decreasing
Top 10 , over 100 points

10:17
23/04/2015

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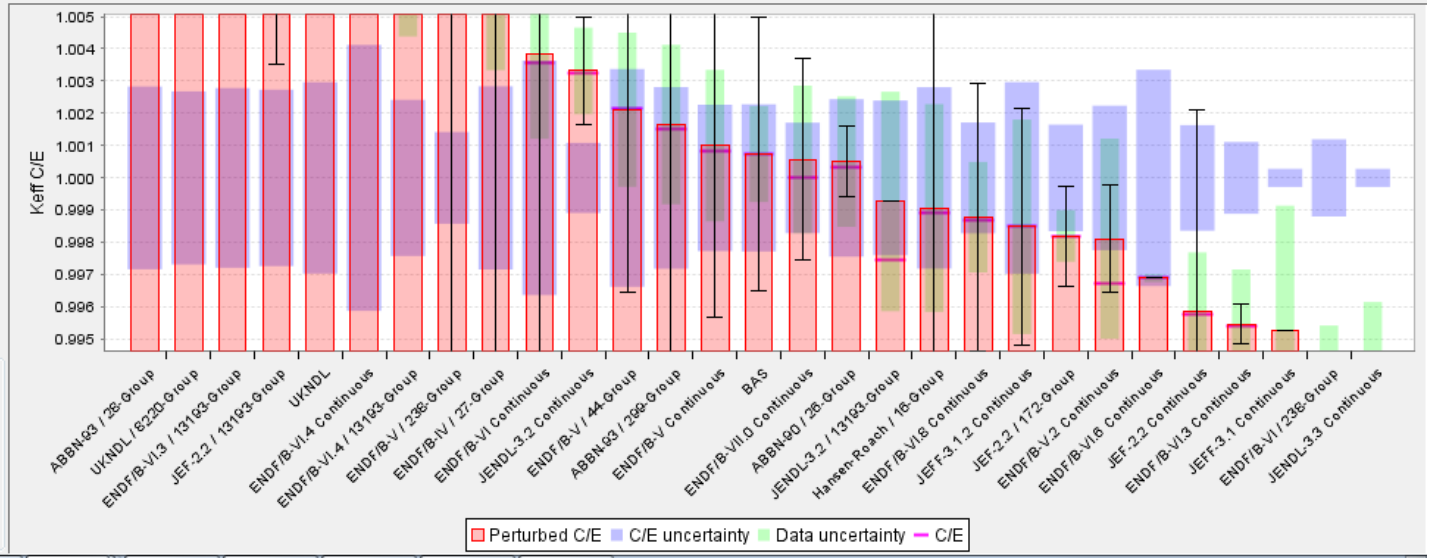
C/E Output Plot by Data Library

NDaST

Benchmark	Sensitivity	dKeff/Keff	Data Variance
IMF004-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.19458194e-4	8.69027455e-6
IMF005-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.57198985e-4	6.01416837e-6
IMF006-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	1.49191867e-4	7.19972525e-6
IMF007-001 (Detailed Model)	KENO ENDF/B-VII.0 / 238-Group	2.13580438e-3	1.50560813e-5
IMF007-001 (Simplified Model)	KENO ENDF/B-VII.0 / 238-Group	2.13580438e-3	1.50560813e-5
IMF010-001	KENO ENDF/B-VII.0 / 238-Group	2.71434024e-3	1.35087963e-5
LMT015-001	KENO ENDF/B-VII.0 / 238-Group	9.56315273e-5	9.1192208e-6
LMT015-002	KENO ENDF/B-VII.0 / 238-Group	9.33693996e-5	9.12223259e-6
LMT015-003	KENO ENDF/B-VII.0 / 238-Group	9.37243754e-5	8.97314307e-6
LMT015-004	KENO ENDF/B-VII.0 / 238-Group	9.19485123e-5	9.04722604e-6
LMT015-005	KENO ENDF/B-VII.0 / 238-Group	9.2052567e-5	8.98066114e-6
LMT015-006	KENO ENDF/B-VII.0 / 238-Group	9.02603637e-5	9.05713507e-6
LMT015-007	KENO ENDF/B-VII.0 / 238-Group	9.03176989e-5	9.10123008e-6
LMT015-008	KENO ENDF/B-VII.0 / 238-Group	3.09194485e-5	5.53230246e-6
LMT015-009	KENO ENDF/B-VII.0 / 238-Group	3.28841696e-5	5.57089446e-6



Plot options
Display: dKeff/Keff
C/E
Group by: CALC_LIB
Average decreasing
Top/Bot. 17 , over 100 points

10:20
23/04/2015

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Summary

- ✓ 4011 cases (>80%) have 3 group sensitivity data and full sensitivity profiles within DICE – many also in IDAT
- ✓ Useful tool for identifying possible benchmarks, complements existing methods
- ✓ An open web-based JAVA tool named NDaST is being developed to take advantage of these data – beta testers welcomed!
- ✓ Complement to full testing calculations e.g. via the NEA Nuclear Data Evaluation Cycle (NDEC)
- ✓ Enable rapid scoping of changes to nuclear data and to propagate nuclear covariance data uncertainties

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