<u>The Nuclear Data Sensitivity Tool (NDaST)</u> <u>'How to' Beginner's Guide</u>

Contents

The Nuclear Data Sensitivity Tool (NDaST)	1
'How to' Beginner's Guide	1
Basics	2
Sensitivities Panel	3
Perturbations Panel	7
Method 1: Manually add perturbations	8
Method 2: Paste perturbations from a list	8
Method 3: Use automated Calculate ratios function	9
Preserve Cross Sections During Perturbations	12
Covariances Panel	14
Search covariances	14
Select Library	15
All isotopes	15
From Sensitivity	16
Own covariances file	17
Analytic Covariances	17
Visualising and storing selected covariances	18
Advanced Panel	19
Launch Prompt and Option to Compute Off-Diagonals	20
Output Results Window	22
XML File Headings	30
NDaST Supported Files	31
NDaST Command Line	32

Basics

The software is laid out in three main 'panels' - Sensitivities Sensitivities , Perturbations Perturbations and Covariances Covariances. The first of these is compulsory. The second two are optional, but either one must be populated with some input data in order to launch a valid calculation using the 'Go' GO! button. There is also an optional Advanced panel that is not required.

The option to save or open data from single or multiple panels simultaneously File Databases Window Help is accessed via the 'File -> Open / Save As' menu. Data is saved to a readable XML formatted file (.ndast extension); see section 'XML File Headings' for a summary of the format.

Open... Ctrl+O Save As... Ctrl+S Exit Ctrl+Q

Sensitivities Panel

In this panel, mandatory data needs to be added in order to provide the cases (responses) for which the subsequent calculations will be carried out. There are two ways in which this can be done:

1. Complete a valid DICE DICE search or IDAT IDAT search search (via buttons to the top left), returning cases that meet the supplied search criteria. A recommended method of searching, is by use of the 'keff sensitivities' search dialogue; search for 3 energy group sensitivity limits for given isotope(s) and reaction(s). An example for U235 inelastic scattering is shown in Figure 1. It is likely this search will be directed towards the nuclear data perturbations under investigation.



Figure 1 - Using DICE search to select keff sensitive benchmarks

• After performing a search, highlight rows from the Case (bottom) table returned from the search, see Figure 2. Note that these may be populated by highlighting rows from the Evaluation (top) table. In both cases, hold down the Control key or use a mouse left-click-drag in order to select multiple rows (or press Ctrl-A to select all).



Figure 2 - Adding sensitive cases to NDaST benchmark set

Click 'Add selected search results to your benchmark set' at bottom left of the panel.
 Add selected search results to your benchmark set
 Note that this returns the data for all computed results (from the stored code and nuclear data library combinations) even if only one row from the case is highlighted. Note: if you have selected benchmarks that do not contain a sensitivity profile, you will see a warning message such as: Selection

65 benchmarks cannot be retained because they miss experimental or calculated Keff value or uncertainty	
ОК	

• Returning to NDaST, you will now see one row per selected Case. The number of calculations and sensitivity files returned from the database is indicated in this row.

These calculation and sensitivities data can be accessed for modification by double-clicking on the row and editing the data shown in the subsequently displayed tables.

- Add personal calculation results and sensitivity data to the corresponding tables.
- Remove calculations or sensitivities by clicking the cross button is to the left of the corresponding row.

Return from this by clicking 'Ok' or 'Cancel'. Ok Cancel

This step (1.) can be repeated multiple times, until the desired benchmark set is created. Otherwise, or in addition, the following step can be carried out:

						—	×
ndow <u>H</u> elp							
Label:	HMF003-007						
Experimental value:	1.0	000					
Experimental uncertainty:	0.0	03					
Calculations				Ser	nsitivities		
Label		Value	Uncertainty		Add sensitivities		
X MCNP JEFF-3.1.2 Cont	tinuous	1.00119	0.00028		Sensitivity		
X MCNP ENDF/B-V Contin	nuous	1.0041	0.0012	X	KENO ENDE/B-VII. 0. / 238-Group		
X KENO Hansen-Roach /	16-Group	0.9962	0.0007				
X KENO ABBN-93 / 299-G	Group	1.0025	0.0003				
X KENO ENDF/B-IV / 27-0	Group	1.0078	0.0009				
X							
	Label: Experimental value: Experimental uncertainty: Calculations Label X MCNP JEFF-3. 1.2 Coni X MCNP JEFF-3. 1.2 Coni X MCNP ENDF/B-V CML X KENO ABBN-93 / 299-C X KENO ABBN-93 / 299-C X KENO ABBN-93 / 299-C	ndow Help Label: HMF003-007 Experimental value: 1.00 Experimental uncertainty: 0.00 Calculations Label X MCNP JEFF-3.1.2 Continuous X MCNP JEFF-3.1.2 Continuous X MCNP JEFF-3.1.2 Continuous X MCNP JEFF-3.1.2 Continuous X MCNO ENDF/B-1V / 27-Group X MENO ENDF/B-1V / 27-Group X MENO ENDF/B-1V / 27-Group	ndow Help Label: HMF003-007 Experimental value: 1.0000 Experimental uncertainty: 0.003 Calculations Label Value X MCNP ERF-3.1.2 Continuous X MCNP ERF-3.1.2 Continuous X MCNP ERF-8/W Continuous X MCNP ENDF-8/W (27-Group X MCNP ENDF-8/W (27-Group X MCNP ENDF-8/W (27-Group) X MCNP ENDF-8/W (27-Group	Indow Help Label: HPF003-007 Experimental value: 1.0000 Experimental uncertainty: 0.003 Calculations Calculations X MCNP EFF-3.1.2 Continuous 1.00119 X MCNP EFF-B.1.2 Continuous 1.00119 X MCNP EFF-B.1.2 Continuous 1.00119 X MCNP EFF-B.4.1 / 16-Group 0.9962 X MCNP EFF-B.4.1 / 27-Group 0.0025 X MCNP EFF-B.4.1 / 12-Group 0.9962 X MCNP EFF-B.4.1 / 12-Group 0.9962 X MCNP EFF-B.4.1 / 12-Group 0.0003 X MCNP EFF-B.4.1 / 12-Group 0.0003 X MCNP EFF-B.4.1 / 12-Group 0.0003	ndow Help Label: IMF003-007 Experimental value: 1.0000 Experimental uncertainty: 0.003 Calculations X MCNP EFF-3.1.2 Continuous 1.0019 0.00028 X MCNP EFF-3.1.2 Continuous 1.0019 0.00028 X MCNP EFF-8/P.4 Continuous 1.0019 0.00028 X MCNP EFF-8/P.4 Continuous 1.0014 0.0012 X MCNP EFF-8/P.4 Continuous 1.0014 0.0012 X MCNP EFF-8/P.4 Continuous 1.0025 0.0003 X MENO Harsen-Roach / 15-Group 0.9952 0.0003 X MENO HARSEN-83/29-Group 1.0025 0.0003 X MENO FINDF/B-1V / 27-Group 0.0009 X MENO FINDF/B-1V / 27-Group 0.0009	Indow Help Label: HMF003-007 Experimental value: 1.0000 Experimental value: 0.003 Calculations Calculations X MCNP ERF-5.1.2 Continuous 1.0019 X MCNP ERF-5.1.2 Continuous 1.0019 X MCNP ERF-6.1.2 Continuous 1.0041 X MCNP ERF-6.1.2 Continuous 1.00425	 ndow Help

Figure 3 - Modify case experimental and computed results

2. Use the 'New Benchmark' button at the top left. New benchmark

- Provide a case label and an experimental value with an uncertainty (suggested default values if there isn't one are 1.000 ± 0.000).
- Complete the left hand table with computed result(s) you have obtained from personal calculation(s).
- Point the software to at least one sensitivity file, containing data in a valid format and return from this by clicking 'Ok' or 'Cancel'.
 Ok Cancel
 A list of formats accepted is provided in the section 'NDaST Supported Files' later in this document.

🥖 NDaST							-	×
<u>F</u> ile <u>D</u> atabases <u>W</u>	indow <u>H</u> elp							
	Label:	My benchmar	k					
	Experimental value:	1.0	00					
Sensitivities	Experimental uncertainty:	0.0	02					
23 profiles	Calculations				Se	nsitivities		
	Label		Value	Uncertainty		Add sensitivities		
	X My calculation		1.002	0.001		Sensitivity		
	X					J:\WEA\WDaST\my sensitivities.sdf		
Perturbations								

Figure 4 - Add new benchmark personal data

Option (2.) can also be completed multiple times, as needed. Using the delete key on a row from the Sensitivities panel will remove the entire entry from the benchmark set.

Finally:

• Save this list using the 'File -> Save As' menu.

values=	
---------	--

• Ensure that there is a text entry in the 'Symbols' box (values=) at the top of the panel. If this has been filled automatically, it may be edited to suit your preference; it is used to label output data post-execution. A label is required for both the experiment and the calculation.

🌌 NDaST								- C	ı x
<u>File</u> <u>D</u> atabases	<u>N</u> indow <u>H</u> elp								
	DICE search	IDAT search	New benchmark	Symbols: values= Keff					Clear
	Benchmark	Cal	lculations	Sensitivities	ICBSENS_G3.FAST	ICBSENS_G3.ISOTOPE	ICBSENS_G3.REACT	TION	
Sensitivities	HCI003-001	4 ca	alc(s)	1 sensitivity(ies)	0.0594	U238	inelastic		
24 benchmarks	HMF002-001	5 ca	alc(s)	1 sensitivity(ies)	0.0652	U238	inelastic		
24 profiles	HMF002-002	5 ca	alc(s)	1 sensitivity(ies)	0.0633	U238	inelastic		
	HMF002-003	5 ca	alc(s)	1 sensitivity(ies)	0.0573	U238	inelastic		
	HMF002-004 5 calc(s) HMF002-005 5 calc(s)		lc(s)	1 sensitivity(ies)	0.0549	U238	inelastic		
			1 sensitivity(ies)	0.0565	U238	inelastic			
	HMF002-006 5 calc(s)		1 sensitivity(ies)	0.0557	U238	inelastic			
	HMF003-001	5 ca	lc(s)	1 sensitivity(ies)	0.0686	U238	inelastic		
	HMF003-002	5 ca	alc(s)	1 sensitivity(ies)	0.0786	U238	inelastic		
	HMF003-003	5 ca	alc(s)	1 sensitivity(ies)	0.0767	U238	inelastic		
	HMF003-004	5 ca	alc(s)	1 sensitivity(ies)	0.0736	U238	inelastic		
Perturbations	HMF003-005	5 ca	lc(s)	1 sensitivity(ies)	0.0637	U238	inelastic		
	HMF003-006	5 ca	lc(s)	1 sensitivity(ies)	0.0622	U238 inelastic			
	HMF003-007	5 ca	lc(s)	1 sensitivity(ies)	0.0553	U238	inelastic		
	HMF014-001	6 ca	lc(s)	1 sensitivity(ies)	0.0724	U238	inelastic		
	HMF028-001	7 ca	lc(s)	1 sensitivity(ies)	0.0606	U238	inelastic		
	HMF029-001	3 ca	alc(s)	1 sensitivity(ies)	0.0715	U238	inelastic		
	HMF032-001	5 ca	alc(s)	1 sensitivity(ies)	0.0772	U238	inelastic		
	HMF032-002	5 ca	alc(s)	1 sensitivity(ies)	0.0795	U238	inelastic		
Covariances	HMF032-003	5 ca	alc(s)	1 sensitivity(ies)	0.0672	U238	inelastic		
Covariances	HMF062-001	4 ca	alc(s)	1 sensitivity(ies)	0.0533	U238	inelastic		
	HMF084-013	4 ca	lc(s)	1 sensitivity(ies)	0.0532	U238	inelastic		
	IMF008-001	3 ca	lc(s)	1 sensitivity(ies)	0.0646	U238	inelastic		
	My benchmark	1 ca	lc(s)	1 sensitivity(ies)					
GO!									
23 benchmark(s) se	elected							17M of 2	731M

Figure 5 - Main sensitivity panel summarising benchmark set

Perturbations Panel

This panel is filled with data representing perturbations to a nominal 'original' set of nuclear data. It is in the form of ratios, such that for example a +1% increase is represented by a perturbation factor of 1.01.

Completing this panel will initiate a calculation of the effect of these perturbations on the cases supplied in the Sensitivities panel. Linearity is assumed such that for response parameter R, sensitivities S and perturbations P:

$$\frac{\Delta R}{R} = S.\left(P-1\right)$$

These data are tabulated in the form:

- One column per nuclide-reaction
- One row per energy bound.

To add columns:

- Select one or several isotopes out of the collapsible tree to the top left (using the Ctrl key to make multiple selections).
- Select one or several reactions from the check-box list of reactions.
- Click the long double arrow (>>) button to add these nuclide-reaction combinations to the table at the top right.
- Any column may be removed from this table by clicking the top cell (containing the reaction heading) and hitting the 'Delete' key. There is first a confirmation prompt.



Figure 6 - Add nuclide-reaction column to perturbation table

To add perturbation factors to specified energy bounds, there are three supported options, depending on the complexity of the input needed:

Method 1: Manually add perturbations

- First, to add energy bound rows, type the values of the bounds into the energy (E=) box; several values can be listed at once, separated by semi-colons or spaces. Then click the 'add energy group bound(s)' Add energy group bound(s) button to the right of this.
- Unwanted values can be removed by selecting one or several energy groups and hitting the 'Delete' key. Note however, that the adjacent bounds will also change to keep all energy bounds contiguous.
- To add perturbation values, select a cell in the perturbations table at the bottom of the panel. Type in the desired ratio and hit the 'Enter' key. The perturbation may be labelled using the first row of the relevant column in the input table.



Figure 7 - Add energy band row and perturbation ratio to table

Method 2: Paste perturbations from a list

Select a cell from the required isotope-reaction column and click 'Paste perturbations'
 Paste perturbations
 to open a window containing instructions and a space to type/paste data.

- In the window, you must provide energy group bounds and perturbation values, in a two-column format, separated by tabs, spaces or semi-colons. These can be supplied in any order.
- Energies can either be given as a lower or upper energy bound as selected with the radio button. Either option will result in an assumed uppermost or lowest energy cut-off if not given. Chosen cut-offs may also be supplied as a line with a single value i.e., by omitting a perturbation value from beside it.
- The perturbation may be labelled using the text box at the bottom of the window. Click 'Ok' to register the values and return to the main panel.



Figure 8 - Paste perturbation dialogue window

Method 3: Use automated Calculate ratios function

This feature allows the user to perform mathematical manipulations on series of nuclear data, directly accessible from the JANIS database or personally loaded by the user. In the context of NDaST, a division operation to generate the ratio between two sets of data is the function used. To add a new entry via this method:

- Click the 'Calculate ratios' button Calculate ratios. Note that since this adds new columns to the perturbation input table, it does not matter which cell is selected.
- Once this opens up the 'Create perturbation from nuclear data' window, go through the dialogue from left to right, by selecting:
 - o Nuclear data evaluation(s) as numerators (i.e. new libraries)
 - Either from available 'JANIS libraries' or by importing 'Own files'

- Nuclear data evaluation (one only) to be denominator (i.e. old library)
 - Again, either from 'JANIS libraries' or by importing 'Own files'
- Nuclides from the available list of nuclides; this is populated with those found in common between numerators and denominator
- Reaction(s) from the fixed list of options; these will be added to the 'Selected' list on the far-right
- Finally, you will also need to assign an energy group structure and optionally, a spectrum weighting by clicking the respective buttons and choosing from the options supplied in the subsequent windows.
 - Options for group structure are: Uniform in log, File defined, or Single group.
 Each option involves a following specification via text input or file location. The default is 'Uniform in log' with 10 groups per decade, although increased accuracy has been seen with 100 or 1000 groups per decade.
 - Options for spectrum are: Constant, XY, PWR, General, Maxwellian and Fission. Again, each option requires subsequent specification for constant values, interpolation choice or file location. Defaults values are always provided in absence of user preference.
- Note that via the dropdown menu within the dialogue window, two mathematical methods are available to create the final spectrum weighted, energy-grouped cross-section (XS) ratios:
 - NDaST calculates energy groups for the ratios of continuous XS (i.e. the ratios are taken first, the groupings second) this is the default option.
 - NDaST calculates ratios of energy-grouped XS (i.e. the groups are made first, the ratios second) – this option can be selected to speed up calculation of ratios at the possible expense of XS feature resolution.

The results of the above methods, tend to converge at a high number energy groups.

The perturbation(s) generated from the above criteria are shown below, plotting the percentage changes as a function of energy. The perturbations are automatically labelled based on the libraries selected, but may be edited in the textbox at the bottom of the window.

Multiple instances of the same nuclide-reaction pair are assigned an additional unique numerical identifier of the form #1, #2, #3¹... and so on. In this case the value for the nuclide-

¹ Note NDaST will assign all files read in a numerical identifier based on the sorted string associated with the file name, for this reason, files names should be given as: FILENAME00001, FILENAME00002, FILENAME00003...FILENAME00010, FILENAME00011 etc and not: FILENAME1, FILENAME2, FILENAME3...FILENAME10, FILENAME11 etc

reaction will be averaged in the main output, however the value of each instance will be still be available within the detailed results. This feature can be used with multiple random files to quantify the impact of each file, and later compute the skew and kurtosis of the resultant changes in the response parameter.



• Click 'Ok' to register the values and return them to the main panel.

Figure 9 - Create perturbation from nuclear data dialogue window

Group structure X	Spectrum	×
Group type : File defined V	Spectrum type : General spectrum V	
Choose a file :	Emax,th : 0.108 in eV Theta,th : 0.054	in eV
C:\/MyData\238grp.txt Browse	Emax,epi : 2100000.0 in eV Theta,fis : 1400000.0	in eV
	Emax,fis : 1.15441E7 in eV Theta,fus : 25000.0	in eV
	E fus : 1.407E7 in eV	
Ok Cancel	Ok Cancel	

Figure 10 - JANIS ratio group structure and spectrum selection windows

Instructions on how to use the computations feature within JANIS itself, may also be found in the documentation at the links below:

https://www.oecd-nea.org/janis/help/

https://www.oecd-nea.org/janis/janis-4.0/documentation/janis-4.0 manual rev1.pdf

https://www.oecd-nea.org/janis/janis-4.0/documentation/janis-4.0 manual rev1.html# Toc371025654

Finally:

- Save this list using the 'File -> Save As' menu.
- You can now hit 'Go' GO! to launch all possible valid calculations. The numbers of cases and perturbations will be summarised by the launch script before processing.

Preserve Cross Sections During Perturbations

When performing a perturbation of a cross section, NDaST has the capability to adjust one or more partial cross sections to preserve a total cross section using the 'compensate' button.

Perturbations										
E=	eV	Add energy gro	up bound(s)	Paste per	turbations	Calculate r	atios Cor	npensate	Delete	Clear
Eperay group	<pu239.p< th=""><th>A ASTTON</th><th>ZPU239 EISSIO</th><th>NS</th><th><pu239 n.g<="" th=""><th>AMMAS</th><th></th><th></th><th></th><th></th></pu239></th></pu239.p<>	A ASTTON	ZPU239 EISSIO	NS	<pu239 n.g<="" th=""><th>AMMAS</th><th></th><th></th><th></th><th></th></pu239>	AMMAS				

Figure 11 – Compensate button in the perturbations panel

The user needs to first make a perturbation to a cross section. Subsequently, by clicking 'Compensate', a dialogue is prompted, with a checkbox allowing a cross section to be preserved, and an editable table that allows which reactions will be adjusted in order to preserve the selected cross section. The list of MT sum rules is shown below.



Figure 12 – ENDF/B Sum rules obeyed in compensate

In the example below, the JANIS ratio of the TENDL2017/TENDL2015 U235 Elastic crosssection was added as a perturbation. The compensation button was then activated, and the decision to preserve the total cross section, by adjusting the fission cross section was made. A reference library also needs to be selected to retrieve the total cross section values.



Figure 13- Using the compensation button to preserve the U235 total cross section by adjusting the U235 Fission cross section (after perturbing the U235 Elastic cross section using JANIS ratios)

Covariances Panel

Covariance data are supplied via a search is carried out by library, isotope and reaction MT in order to compile a custom list of data files from multiple available sources.

Completing this panel will initiate a calculation of the propagated relative uncertainty U_{R} , due to nuclear data covariance in the cases supplied in the Sensitivities panel. The linear propagation 'sandwich formula' is used with sensitivities *S*, and covariances *C*:

$$\frac{U_R}{R} = S.C.S^T$$

There are four options for adding covariance data, 'Search covariances', 'Select library', 'Own covariance files' and, 'Analytical covariances'



Search covariances

In order add covariance matrices, connect the required JANIS databases using 'Databases > JANIS' in the main menu, then click on 'Search covariances'.

- Select evaluated library(ies) to search for available data select multiple libraries by holding down the control key.
- Complete any of the following search parameters: Isotope Z, A, State or neutron reaction MT identifier.
 - TIP: valid entries can be typed with separating commas, e.g. type "2, 4, 18" to search against elastic scattering, inelastic scattering and fission reactions.
- Once completed hit the 'Search' Search button. Note that recent searches may be retrieved from the 'History' drop-down bar.
- The returned results are shown in a table beneath, in the format of one row per reaction-nuclide pairing. All required covariance matrix pairs should be highlighted, using the control key or a mouse-drag to make multiple selections.
- Only data in a valid format (BOXER) can be used by the code, so the user should ensure their selection meets this requirement. Note that cross-MT pairs are only shown once, according to the rule MT2>MT1. The code will automatically prepare the transpose matrix for the reverse MT pairing. Hit the 'Ok' button to return the selection back to the main panel.

		narticle		Library										Count
	Any incid	lent narticle	A	ENDE/B-VIT)	^	Format: SOXER	ENDF						Search
Sensitivities	Radioact	tive data		ENDE/B-VIL	,		Material #1					Material #2		Open resul
	Incident	neutron data		ENDF/B-VIII	0		7 . 02 (1) Uranium	0.1 teach as				7.		opennesu
Sensitivities	Incident	gamma data		FENDL-2.1		2: 92 (U) Uranium			=	2:		Save resu		
	Incident proton data		FENDL-3.1b		A: 235	 State 	·	~		A: V State: V	\sim	_		
	Incident	deuteron data		IRDFF-1.0			Describes #1					Deservice #2		Print
	Incident	triton data		IRDFF-1.0-6	40g		Reaction #1				□-	Reaction #2		
	Incident	He3 data	~	IRDFF-1.05		~	2,4,16,18,102			~			~	<u>R</u> eset
														Interrup
	History :												\sim	interrup
	Results													Maximi
erturbations	Search	Incident particle	Evalua	tion Form	at Material	1 ME1	MT1	Material?	ME2	MT2				<u>H</u> uxim
	NEA	Incident neutron data	ENDF/B-	II.1 BOXER	U235	ME=33	MT=1: (n.total)	U235	ME=33	MT=2 : (z.elast	ic)			
	NEA	Incident neutron data	ENDF/B-	II.1 BOXE	U235	MF=33	MT=1: (n.total)	U235	MF=33	MT=18 ; (z.fiss	on)			
	NEA	Incident neutron data	ENDF/B-V	II.1 BOXER	U235	MF=33	MT=1: (n,total)	U235	MF=33	MT=102 : (z,y)	· ·			
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=2 : (z,elastic)	U235	MF=33	MT=2 : (z,elast	ic)			
	NEA	Incident neutron data	ENDF/B-V	II.1 BOXER	U235	MF=33	MT=2 : (z,elastic)	U235	MF=33	MT=4: (z,n')				
	NEA	Incident neutron data	ENDF/B-V	II.1 BOXE	U235	MF=33	MT=2: (z,elastic)	U235	MF=33	MT=16: (z,2n)				
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=2: (z,elastic)	U235	MF=33	MT=17: (z,3n)				
Covariances	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=2 : (z,elastic)	U235	MF=33	MT=18: (z,fissi	on)			
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE		MF=33	MT=2 : (z,elastic)		MF=33	MT=102: (z,γ)				
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=4 : (z,n')	U235	MF=33	MT=4 : (z,n')				
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=16: (z,2n)	U235	MF=33	MT=16: (z,2n)				
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=18 : (z,fission)	U235	MF=33	MT=18: (z,fiss	on)			
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=18 : (z,fission)	U235	MF=33	MT=102 : (z,γ)				
	NEA	Incident neutron data	ENDF/B-\	II.1 BOXE	U235	MF=33	MT=102:(z,γ)	U235	MF=33	MT=102 : (z,γ)				

• Figure 14 - Search and select nuclear covariance data matrices

Select Library

All isotopes

All isotopes From sensitivities

Another method to choose covariances is to click on 'Select library'. Select library'.

isotopes' All isotopes From sensitivities tab allows the user to select isotope(s) and reaction(s) that are returned from selected library(s). The libraries can be prioritised such that if a covariance exist from the library with the highest priority is available it will be selected, while if a covariance is not present, the library with the next highest priority will used as a source for the covariance.

In the example shown in Figure 15, covariances from ENDF/B-VIII.0 will be searched and added with highest priority. If covariances are absent for the nuclide/reaction selected in ENDF/B-VIII.0, covariance data will then be retrieved from TENDL-2017. An arbitrary number of libraries can be added to the priority tree.



Figure 15 – Search covariances by library. U235 fission covariances are retrieved from ENDF/B-VIII.0 with highest priority, followed by TENDL2017.

From Sensitivity

All isotopes From sensitivities

Alternatively the 'From sensitivities' tab All isotopes' From sensitivities is similar to the 'All isotopes' but allows the user to select a subset of covariances depending on the value of the corresponding sensitivity coefficients. The list can be sorted by the maximum absolute value of the sensitivity profile or the integral of the absolute value of the sensitivity profile from all sensitivity profiles selected, allowing the user to select covariances from 'important' isotope reactions, potentially leading to significant speed-ups.

🌌 NDaST										– 🗆 X
<u>F</u> ile <u>D</u> atabases <u>W</u>	indow <u>H</u> elp)								
	All isotope	From sensitiv	/ities			Nuclear data libra	aries selection			
	Nuclide	Reaction	max(s)	Σ(s)	Filter	BROND-2.2		^	highest prior	ity
	Pu239	NUBAR	2,405e-1	9,5742e-1	TOTAL	BROND-3.1			ENDF/B-VIII	.0 Move Top
Sensitivities	Pu239	FISSION	1,8063e-1	6,612e-1	ELASTIC	CENDL-3.1				
147 benchmarks	Be9	ELASTIC	1,5081e-2	2,7361e-1		CENDL-3.2			>>	Move Up
159 profiles	HNat	ELASTIC	3,0711e-2	1,4681e-1	M INELASTIC	ENDF/B-VI.8				
	Th232	ELASTIC	1,0445e-2	1,0804e-1	□ N_2N	ENDF/B-VII.0			<<	Move Down
	U238	ELASTIC	1,3044e-2	8,662e-2	FISSION	ENDF/D-VII.1				
	Th232	INELASTIC	9,295e-3	7,4973e-2		FENDL-2.1				Move Bottom
	H1	ELASTIC	2,8896e-2	7,047e-2		LINDE-3.10		~	lowest priorit	ty
	Pu239	CHI	2,1147e-2	5,3178e-2	N_GAMMA					
	U238	NUBAR	1,6146e-2	5,0575e-2						
	U238	INELASTIC	7,8977e-3	4,4736e-2					Search	
Perturbations	U238	FISSION	1,2001e-2	3,6793e-2		L				
	Pu240	NUBAR	4,3103e-2	3,5193e-2						
	Pu239	ELASTIC	1,7251e-2	3,2851e-2		5 covariance matr	ices 17 messag	es		
	ZrNat	ELASTIC	2,3401e-3	3,2648e-2	N_ALPHA					
	Pu239	N_GAMMA	8,4125e-3	3,2565e-2	ELASTIC P1	Nuclide 1	Reaction 1	Nuclide 2	Reaction 2	Covariance matrix
	CuNat	ELASTIC	1,2912e-2	2,6235e-2		Pu239	FISSION	Pu239	FISSION	JANIS: NEA~N~ENDE/B-VIII.0~SIG~Pu239~MT18~boxer~box
	CNat	ELASTIC	1,3369e-2	2,61e-2		H1	FLASTIC	H1	FLASTIC	JANIS: NEA~N~ENDE/B-VIII.0~SIG~H1~MT2~boxer~boxer
	U238	N_GAMMA	3,677e-3	2,609e-2	CHI	Be9	ELASTIC	Be9	ELASTIC	JANIS: NEA~N~ENDF/B-VIII.0~SIG~Be9~MT2~boxer~boxer
Covariances	Pu240	FISSION	3,1906e-2	2,5361e-2		Th232	ELASTIC	Th232	ELASTIC	JANIS: NEA~N~ENDF/B-VIII.0~SIG~Th232~MT2~boxer~boxer
Covariances	H1	N_GAMMA	2,8202e-2	2,5154e-2	unsupported	U238	ELASTIC	U238	ELASTIC	JANIS: NEA~N~ENDF/B-VIII.0~SIG~U238~MT2~boxer~boxer
	Fe56	ELASTIC	9,2918e-3	2,4416e-2	Clear					
	IIITh 222	NL CAMMA	2 21140.2	12 2400-2						

Figure 16 – Selecting covariances matching the largest sensitivity profiles

Own covariances file

This option allows the user to directly import externally processed covariance data into NDaST. Currently covariance data of the format BOXER and COVERX are supported.

🥖 NDaST										- 0	×
<u>F</u> ile <u>D</u> atabases <u>V</u>	<u>V</u> indow <u>H</u> elp										
	Files				Covaria	nce matrices					
	Choose file(s) or drag them here				Selecte	ed	Nuclide 1	Reaction 1	Nuclide 2	Reaction 2	
	Files	Matrices	Supported	Selected			Ac225 (MAT8925)	MT1: TOTAL	Ac225 (MAT8925)	MT1: TOTAL	^
Sensitivities	INEAND-STINATE FILTENPOVED ENDERT 1 220-1-2225 hours (8)	20	copported (c c		\leq	Ac225 (MAT8925)	MT2 : ELASTIC	Ac225 (MAT8925)	MT2 : ELASTIC	_
	3: WEA WDaST DOXEL_TODER DOXER ENDERT 1 2380 (ac225.b0xer (*)	30		0 0		\checkmark	Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT4: INELASTIC	
	3: WEA WDaST Doxer_Tolder (BOXER-ENDERT, 1-238g (ac227.b0xer (*)	30		0 0			Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT51	
	J: (VEA (VDAST (poxer_folder (BOXER-ENDER) 7.1-238g (am240.boxer (*)	39		0 0			Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT52	
	J: WEA WUDAST VDOXET_FOIDER (BUXER-ENULFB7.1-2380 VDK248.DOXER (*)	24		6			Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT53	
	J: WEA WUDAST VDOXER_FOIDER VDOXER-ENUPED . 1-2380 (CT253.DOXER (*)	22		6			Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT54	
	J: WEA WDAST VDXer_folder (endfd / 1_HENDF \ac225.nendf	0					Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT55	
	J: WEA WDAST VDXer_folder (endfd / 1_HENDF \ac227.nendf	0					Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT56	
	J: WEA WDaST boxer_folder (endfb / 1_HENDF \am240.nendf	0					Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT57	
	J: WEA WDAST Vpoxer_folder (endfb / 1_HENDF \pk248.nendf	0					Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT58	
Perturbations	J: WEA WDaST (poxer_folder (endfb / 1_HENDF (cf253.hendf	0	(Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT59	
							Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT60	
							Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT61	
							Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT62	
							Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT63	
							Ac225 (MAT8925)	MT4 : INELASTIC	Ac225 (MAT8925)	MT64	
							Ac225 (MAT8925)	MT4: INELASTIC	Ac225 (MAT8925)	MT91	
						\checkmark	Ac225 (MAT8925)	MT16:N_2N	Ac225 (MAT8925)	MT16:N_2N	
							Ac225 (MAT8925)	MT17	Ac225 (MAT8925)	MT17	
						\checkmark	Ac225 (MAT8925)	MT18 : FISSION	Ac225 (MAT8925)	MT18 : FISSION	
Covariances							Ac225 (MAT8925)	MT37	Ac225 (MAT8925)	MT37	
							Ac225 (MAT8925)	MT51	Ac225 (MAT8925)	MT51	
							Ac225 (MAT8925)	MT52	Ac225 (MAT8925)	MT52	
							Ac225 (MAT8925)	MT53	Ac225 (MAT8925)	MT53	
							Ac225 (MAT8925)	MT54	Ac225 (MAT8925)	MT54	
							Ac225 (MAT8925)	MT55	Ac225 (MAT8925)	MT55	
<u>A</u> dvanced							Ac225 (MAT8925)	MT56	Ac225 (MAT8925)	MT56	
							Ac225 (MAT8925)	MT57	Ac225 (MAT8925)	MT57	
							Ac225 (MAT8925)	MT58	Ac225 (MAT8925)	MT58	
							Ac225 (MAT8925)	MT59	Ac225 (MAT8925)	MT 59	
							Ac225 (MAT8925)	MT60	Ac225 (MAT8925)	MT60	
							Ac225 (MAT8925)	MT61	Ac225 (MAT8925)	MT61	
							Ac225 (MAT8925)	MT62	Ac225 (MAT8925)	MT62	
							Ac225 (MAT8925)	MT63	Ac225 (MAT8925)	MT63	
COL							Ac225 (MAT8925)	MT64	Ac225 (MAT8925)	MT64	
<u>a</u> 0i							Ac225 (MAT8925)	MT91	Ac225 (MAT8925)	MT91	
							Ac225 (MAT8925)	MT102 : N_GAMMA	Ac225 (MAT8925)	MT102 : N_GAMMA	<
							Ac227 (MAT8931)	MT1: TOTAL	Ac227 (MAT8931)	MT1: TOTAL	~
						-					
			<u>A</u> dd s	elected covariance	e matrices	<u>C</u> ancel					
										57M of 2731	M

Figure 17: Example of importing a Covariance Matrix

Analytic Covariances

The last option to provide covariance data is to use an analytic equation to provide covariance data. Such an approach has been taken in [2].

NDaST allows the user to use the same equation described in [2] to specify a 1 or 3 group analytic correlation matrix, with the relationship between submatricres specified by theta. The standard deviation (diagonal value) is specified in RSD. If the user chooses to specify a 3 energy group covariance, the energy boundaries can be adjusted.

² 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.



Figure 18- Example of an Analytic Covariance Matrix

Visualising and storing selected covariances

Each covariance matrix returned to the main panel can be viewed by highlighting it from the table at the top left. When selected, two plots are shown in the panel:

• A coloured correlation plot (ranging from -1 to 1) in the top right, displaying the correlation parameter *ρ*, for the given energy-to-energy (*i-j*) value, i.e.:

$$\rho_{i,j} = \frac{C_{i,j}}{\sqrt{C_{i,i} C_{j,j}}}$$

- A plot showing the relative standard deviation (matrix diagonal square-root) in plus/minus percent, against energy. If a perturbation has been supplied in the Perturbations panel, this is shown as a series against these axes. This can help compare the perturbation to the estimated magnitude of the standard deviation uncertainty.
 - TIP: use a left or right click mouse-drag to zoom in and out of either plot.
 - TIP: the plot can be saved, copied and adjusted using the right mouse-click.

Finally:

- Save this list using the 'File -> Save As' menu.
- You can now hit 'Go' GO! to launch all possible valid calculations. The numbers of cases and covariances will be summarised by the launch script before processing.

Advanced Panel

The advanced panel is optional, and is used to modify the matching of sensitivity profiles and covariance data when one exists by element vs. nuclide.

Depending on the nuclear data library, some cross sections are only available by element. While NDaST can handle both nuclide and elemental sensitivities, matching with a covariance library can result complexities.

The first case is where NDaST contains an elemental sensitivity, and either a perturbation or covariance for a particular isotope is given. The user can chose to treat the elemental sensitivity as equal to the isotopic sensitivity, but ticking the 'Subs by Element' checkbox. This can be a desirable approximation in cases such as Carbon, where one isotope has a large abundance. NDaST also allows the user to set a value for the abundance value where the user wishes that an elemental sensitivity be representative of the isotopic sensitivity, for example to perform this substitution whenever the isotopic abundance is over 99%.

The second case is where NDaST contains isotopic sensitivities, and either a perturbation or covariance for a particular element is given. The user can select which isotopic sensitivities are used for the sum. NDaST also allows the user to set a value of the total abundance that is used to select which isotopic sensitivities are used, prioritising those with the highest abundance until the specific abundance sum is achieved.

Note: Available DICE/IDAT databases used for the integral experiments contain a mixture of libraries, in particular the ABBN library, which has a large number of elemental sensitivities. Caution should be exercised when comparing these results across libraries, particular when computing uncertainty propagation by sandwich rule, or the C(k) metric described in the following section.

🌌 NDaST								– 🗆 X					
<u>F</u> ile <u>D</u> atabases <u>V</u>	file Databases Window Help												
	Isotope	z ^	A	State	Abundance	Subst. by ele	Sum for element	Restore <u>d</u> efaults Clear_					
	H1	1	. 1	0	99.9855	\checkmark		Tarta and data and the					
	H2	1	. 2	0	0.0145			isotopes/elements mapping					
Constituition	He3	2	. 3	0	0.0002			Configure here the default mapping done in NDaST between isotopes and elements.					
Sensitivities	He4	2	4	0	99.9998			Use the "Restore defaults" to revert to the default configuration or to apply this default configuration					
	Li6	3	6	0	4.85			before recomputing a .ndast file which was saved with a previous version (i.e. a version which was not					
	Li7	3	7	0	95.15	\checkmark		doing such mapping).					
	Be9	4	9	0	100	\checkmark		Use the "Clear" button to disable all mappings					
	B10	5	10	0	19.65								
	B11	5	11	0	80.35			Subst. by element					
	C12	6	12	0	98.94	\checkmark							
	C13	6	13	0	1.06			Sensitivity profiles given for elements will be used when looking for sensitivity profile for the isotopes					
	N14	7	14	0	99.6205	\checkmark	\checkmark	Selected in this column. For example : if a perturbation or covariance matrix for Si-28 (isotope) is selected, and a sensitivity profile					
Perturbations	N15	7	15	0	0.3795			is not found for Si-28 but a sensitivity profile for Si-0 (element) is given then use this elemental profile.					
_	016	8	16	0	99.757	\checkmark							
	017	8	17	0	0.03835			Select most abundant isotope of each element, with abundance ≥ 90 % Apply					
	018	8	18	0	0.2045								
	F19	9	19	0	100	\checkmark		Sum for element					
Ne20	Ne20	10	20	0	90.48	\checkmark		Sensitivity profiles for the selected isotopes are mandatory					
Ne21 10 21 Ne22 10 22	0.27			to allow NDaST computing a sensitivity profile for the element when needed (i.e. when a pertubation or									
	Ne22	10	22	0	9.25			covariance matrix for the element is used). Note that all isotopes of a given element will be summed, the selection here only indicates which ones are					
	Na23	11	. 23	0	100	\checkmark	\checkmark						
	Mg24	12	24	0	78.965			mandatory to compute such sum.					
<u>C</u> ovariances	Mg25	12	25	0	10.011			For example : for Zn if Zn-64, Zn-66, and Zn-68 are selected here and a perturbation or covariance matrix					
	Mg26	12	26	0	11.025			for Zn-U (element) is used:					
	Al27	13	27	0	100	\checkmark	\checkmark	• if sensitivity profiles are given for Zn-64, Zn-66, Zn-67, Zn-68, Zn-70 : these will be summed to					
	Si28	14	28	0	92.2545	\checkmark		compute a sensitivity profile for Zn-0					
	Si29	14	29	0	4.672			 if only sensitivity profiles are given for Zn-64, Zn-66 : no sum will be done and the profile will be 					
	Si30	14	30	0	3.0735			reported as missing					
<u>A</u> dvanced	P31	15	31	. 0	100	\checkmark							
	S32	16	32	0	94.85	\checkmark		Select isotopes to achieve an abundance sum ≥ 90 % Apply					
	S33	16	33	0	0.763								
	S34	16	34	0	4.365								
	S36	16	36	0	0.0158								
	CI35	17	35	0	75.8								
	Cl37	17	37	0	24.2								
	Ar36	18	36	0	0.3336								
601	Ar38	18	38	0	0.0629								
GOi	Ar40	18	40	0	99.6035								
	K39	19	39	0	93.2581	\leq							
	K40	19	40	0	0.0117	<u> </u>							
	K41	19	41	0	6.7302	<u> </u>							
	Ca40	20	40	0	96.941								
	Ca42	20	42	0	0.647		<u> </u>	۶ 					
								153M of 2731M					

Figure 19: Advanced Panel, table of Isotope abundance and whether an elemental sensitivity can be substituted for an isotope and whether the isotopic sensitivities can be summed to form the elemental sensitivity.

Launch Prompt and Option to Compute Off-Diagonals

The tool will at this point summarise the number of calculations to be performed. In addition, if the number of cases is >1, the prompt window gives the option to tick a box to compute the off-diagonal uncertainty terms between all loaded cases, i.e. the complete covariance and correlation matrices. Covariances are calculated according to the standard single-case formula, but with *S* now a multi-columned matrix of all sensitivity vectors. Thus the covariance between cases *x* and *y* would be calculated as:

$$\frac{U_{R_{x,y}}}{R_{x,y}} = S_x. C. S_y^T$$

The associated inter-case correlations are known widely in the nuclear industry as ' C_k ' values or representativity factors and such terminology is therefore repeated in NDaST. They may be particularly useful for example, if a personal benchmark has been supplied as an 'application' case (see the 'New Benchmark' Section above); the results can inform the user on the degree of shared nuclear data uncertainty, given the similarity in sensitivity between the application and benchmark cases to the cross-sections involved.

- Note that this option can greatly increase the number of calculations to be performed, and as such should be used with caution when a large set of cases has been loaded.
- The additional data from these calculations are made available in a separate tab in the results output window, described in the following Section.



Figure 20 - Main covariance panel displaying matrix plots

NDaST	×
?	Launch Uncertainty propagation calculation with: 147 benchmarks (159 sensitivity profiles), 5 covariance matrices ✓ compute off-diagonal terms (cases/sensitivities representativity, aka 'Ck') OK Cancel

Figure 21 - Launch prompt with off-diagonal computation option

Output Results Window

Each time the software is launched, a new output results window is spawned. The user can therefore make minor modifications and view the difference side-by-side with a previous output. The basic output takes two forms:

- A numerical output table, giving the total perturbation, the original and perturbed mean C/Es and uncertainty (variance) values for each case on a row-by-row basis.
- A grouped plot showing the results as a trend against a number of different trending parameters.

If the option has been invoked, an extra tab for reviewing the calculated inter-case covariance / correlation matrices, or 'Representativity values (C_k) ', will also be made available. The nuclide-reaction and energy breakdown features described below for the basic 'Case by case' outputs, are equally available to those off-diagonal covariance data.

- 1. Numerical outputs:
 - Highlight data from any tables (including nuclide-reaction breakdowns) and copy to clipboard (press Ctrl-C) to export for post-processing.
 - Use the 'filter tree' to the left had side of the output window to exclude / include contributions to the table and plot. Reactions are nested in the tree below each of the nuclides. C/E data and sensitivity labels of the calculations are separated. Values are dynamically updated based on the current selection combination.
 - Left double mouse-click on an entry in the table to bring up the details behind as a new pop-up window. This contains separate tabs for:
 - Tabulated individual calculation C/E data (original and perturbed).
 - Tabulated Perturbation (delta) or Data uncertainty (variance) results, each broken down by the contributing nuclide-reaction pairs. These are colour coded by the magnitude from green (greatest +ve) to red (lowest –ve). They are also paired with a plot showing the result as a function of energy.
 - All perturbations shown as a bar plot this shows how the sum-total of the averages used in the main output window is composed of all nuclide-reaction contributions. The filter tree to the left can be used to include/exclude any values from the plot. When multiple entries for a nuclide-reaction are used, the bars are named according to the user supplied label, and are sorted by magnitude from lowest –ve to greatest +ve.

🏉 Results - NDaST							– 🗆 🗙
Eile							
Case by case Representativity values (Ck)							
Filter	Benchmark	Sensitivity	AKeff/Keff (ocm)	Keff C/E original	Keff C/E perturbed	Nuc Data Variance	Nuc Data Std Dev (ncm)
Filter ^	MME001.001	MCND ENDE /R VII Centin	244.17	0.07002+ 1	1.00142060	1 240E61E7e 4	1157.92
🖻 🔽 Nuclides / Reactions	MME002-001	KENO ENDE/B-VILO / 2	174 74	1 004575	1,00143909	2 623542726-5	512 21
🖃 🗹 Pu239	MME002-002	KENO ENDE/B-VII.0 / 2	172 21	1,003625	1,00534912	2,023342726-5	512,21
I TOTAL	MME002-002	KENO ENDE/B-VII.0 / 2	140.05	1,00565	1,0030505	1 554593546-5	304.28
🖻 🗹 Benchmarks calculations	MME003-001	KENO ENDE/B-VII.0 / 2	329.61	9.997022926-1	1,0070505	1,15362755e-4	1074.07
APOLLO-MORET JEF-2.2 / 172-Group	MME004-001	KENO ENDE/B-VIL 0 / 2	94.04	9 98839187e-1	9 99780229e-1	7 62628781e-6	276 16
	MME004-002	KENO ENDE/B-VIL 0 / 2	92.48	9 98398879e-1	9 99324364e-1	7 49726401e-6	273.81
KENO ABBN-93 / 299-Group	MME005-001	KENO ENDE/B-VII 0 / 2	345.5	1.00637304	1.00983154	1 2190184e-4	1104.09
KENO ENDF/B-IV / 27-Group	MME007-001	KENO ENDE/B-VII 0 / 2	273.06	1.01055714	1.01328776	7 54316748e-5	868.51
KENO ENDF/B-V / 238-Group	MME007-002	KENO ENDE/B-VII.0 / 2	260.09	1,0161	1.0187009	6.99292019e-5	836.24
KENO Hansen-Roach / 16-Group	MME007-003	KENO ENDE/B-VII.0 / 2	251.79	1.01315	1.01566792	6.30127137e-5	793.81
KLAN BAS	MME007-004	KENO ENDE/B-VILO / 2	239.52	1.01026667	1.01266191	5,69326981e-5	754.54
MCNP ENDF/B-V Continuous	MME007-005	KENO ENDE/B-VII.0 / 2	202.58	1.00508333	1.00710911	4.37295351e-5	661.28
MCNP ENDF/B-VI Continuous	MMF007-006	KENO ENDE/B-VII.0 / 2	190.08	1.00316667	1.00506745	3.8808829e-5	622.97
MCNP ENDF/B-VI Continuous (MCNP4B)	MMF007-007	KENO ENDF/B-VII.0 / 2	337.63	1.01723333	1.02060967	1.17001726e-4	1081.67
MCNP ENDF/B-VI Continuous (MCNP4C)	MMF007-008	KENO ENDF/B-VII.0 / 2	333.3	1.01496667	1.01829969	1,10085077e-4	1049.21
MCNP ENDF/B-VI.6 Continuous	MME007.000	VENO ENDER VIT O / 2	224.40	1.01091667	1.01606155	1.054102226.4	1026 74
MCNP ENDF/B-VI.8 Continuous							
MCNP ENDF/B-VII.0 Continuous	1 400						
MCNP JEFF-3.1.2 Continuous	1 200						
MINIK-KENO ABBN-93 / 299-Group	1 300						
MONK ENDF/B-VI.3 / 13193-Group	1 200						
MONK ENDF/B-VI.4 / 13193-Group	1 100						
MONK JEF-2.2 / 13193-Group	1.000						
MONK JENDL-3.2 / 13193-Group	1000						
	200						
VIP ENDE/B V 2 Continuous	5 800						
VIN ENDE/B VI Continuous	10 700						
VIN ENDE/B VI 2 Continuous	1 je 100						
VIP ENDE/B VII O Continuous	₹ ⁶⁰⁰						
Sensitivities calculations	500						
	400						
Plot options							
Display: () AKeff/Keff	300						
0.07	200						
OCE	100						
Group by: EVAL_ID ~	0						
Average increasing \checkmark	0	(a) fan *	an an	an an 10	00° 00°	an 400 600	°a, °a,
□ Top v 10 ÷ , □ over 100 ÷ points	MARC	white where w	with white white	white white	water whater what	it which were	MCL, MCL,
Auto range include uncertainty bands			□ ∆Keff/Keff 🔳 Ben	chmark C/E uncertainty	Nuclear data uncertai	nty	

Figure 22 – Standard output window layout with expanded 'filter tree'

C/E Perturbations Perturbations (all)	Data uncertainties	5			
Benchmark Keff = 1.0000 Benchmark Keff uncertainty = 0.0045 Perturbation &Keff/Keff = 273.06 pcm					
Calculation	Keff	Keff unc.	Keff C/E original	Keff C/E unc.	Keff C/E perturbed
CNP ENDF/B-VII.0 Continuous	1.0008	0.0002	1.000800	4,508046e-3	1.003531
CNP ENDF/B-VI.8 Continuous	1.0055	0.0002	1.005500	4,529217e-3	1.008231
CNP ENDF/B-V Continuous	1.0018	0.0014	1.001800	4,721232e-3	1.004531
ENO Hansen-Roach / 16-Group	1.0401	0.0024	1.040100	5,30451e-3	1.042831
POLLO-MORET JEF-2.2 / 172-Group	1.0017	0.0003	1.001700	4,517656e-3	1.004431
ENO ENDF/B-IV / 27-Group	1.0166	0.0023	1.016600	5,137603e-3	1.019331
	1.0074	0.0004	1.007400	4,551174e-3	1.010131

Figure 23 - Detail pop-up showing C/E tab

- 2. Graphical output options:
 - Switch between 'Delta' and 'C/E' output views. In the first, the computed benchmark results are not used. In the second, the calculated perturbation 'delta' values are added to the computed benchmark results (i.e. those retrieved or input in the Sensitivities panel).
 - The following interpretations of the different bars on the outputs should be made:

- Red bar Average value of the Delta or C/E result for each grouped parameter. In addition (C/E output only), a red line shows the initial average value before perturbation.
- **Black error marker** Standard deviation of computed results (C/E output only) about the average.
- Blue bar Average experimental uncertainty for each grouped parameter.
- **Green bar** Average calculated nuclear data uncertainty *U_R*, for each grouped parameter.
- Hover the mouse pointer over any of the bars in a plot. This will bring up the 'tool-tip' window showing the quantitative values for all results in that particular grouping (i.e. red line and bar, blue bar, green bar and black error marker).



Figure 24 - Detail pop-up showing distribution of all individual perturbations

When sensitivity data matching a supplied covariance file are missing from an uncertainty propagation calculation, the following flags are made to those case results impacted:

- plots display bars/bands are striped yellow;
- table cells use a yellow background;
- a warning message is displayed in the related tooltips.







Figure 26 - Plot with active tool-tip







Figure 28 - C/E k_{eff} output plot

- The display options at the bottom left can be altered to:
 - Display the trend by various pre-determined grouping parameters.
 - Alter the order in which the grouped parameters are shown.
 - \circ $\;$ Limit the displayed results to only those of the upper or lower number N.
 - Limit the displayed results to only those with a minimum number of contained data points M.
 - Instruct plot Y axis auto range to consider or ignore uncertainty bands

Plot options	
Display:	
() C/E	
Group by: BENCHMARK_ID	~
Average increasing	~
□ Top ~ 10 🛓 , □ over	100 🌲 points
Auto range include uncertainty bands	

Figure 29 - Display options for output plots

- Plots can be saved, copied and adjusted using a single right mouse-click.
- Output results can also be saved from the 'File->Save As' menu of the output window. This can be in combination with any of the other panel data (sensitivities, perturbations or covariances) but must be in combination with sensitivities i.e. the cases selected as input to the first panel.



Figure 30 - Perturbation energy breakdown within detail pop-up

- 3. Viewing energy breakdowns:
 - For each of the perturbation or uncertainty results, the breakdown of each nuclidereaction contribution as a function of energy may be viewed. This is done by first double-clicking a row in the main output table to see the detail pop-up.
 - In the 'Perturbation' tab, select one or many of the nuclide-reaction rows in the table. The energy breakdown is then shown as a plot or table (on separate tabs) below. Each nuclide-reaction has a separate plot series or table column.
 - In the 'Data uncertainties' tab, select one single cell of the covariance table. The energy breakdown is then shown as an E×E colour plot below. The colour scale relative to the quantity within each energy group is displayed to the right. The following capabilities are also included:
 - Hovering the mouse pointer over the plot shows the cell co-ordinate and value in bottom left corner. Right click on the cell to place these co-ordinates and value in the computer clipboard memory.
 - Plots controls are available to the left (zoom, show gridlines and change colour scheme). Once zoomed in, the scroll-bars or mouse-wheel can be used to reposition the plot.
 - A rectangular region of the plot can be selected by dragging with the left mouse button. The co-ordinates and value of the region are shown in the two boxes beneath the plot controls.



Figure 31 - Uncertainty energy breakdown with detail pop-up

- 4. Inter-case covariance / correlation matrices:
 - From the main results output window select the 'Representativity values (C_k)' tab. This will shift from the standard the view (one benchmark case per row) to a complete matrix of all nuclear data uncertainties – each case representing both one row and one column.

Clear selection Copy value to cli

Save as..

- The radio button in the bottom left corner allows this table to be switched from the covariance, to the correlation matrix. Each of the diagonal values is thus represented by a value of 1, and each off-diagonal (inter-case) value represented in the range -1 to 1.
- Click any cell in either the covariance or correlation matrix to access the detailed table of data uncertainties broken down by each nuclide-reaction contribution and the energy breakdown plot described above.

When sensitivity data matching a supplied covariance file are missing from an off-diagonal uncertainty propagation calculation, the case results impacted are designated in the table with a grey font.

🖻 Results - NDaST											
File											
Case by case Representativity values	Case by case Representativity values (Ck)										
Filter		HMF001-0	HMF001-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF003-0	HMF003-0
Inter	HMF001-00	1.39661e-2	1.39661e-2	1.20504e-2	1.20958e-2	1.20101e-2	1.19538e-2	1.19329e-2	1.18944e-2	1.28079e-2	1.24542e-2
	HMF001-00	1.39661e-2	1.39661e-2	1.20504e-2	1.20958e-2	1.20101e-2	1.19538e-2	1.19329e-2	1.18944e-2	1.28079e-2	1.24542e-2
	HMF002-00	1.20504e-2	1.20504e-2	1.07954e-2	1.08813e-2	1.08192e-2	1.08025e-2	1.08118e-2	1.07364e-2	1.12944e-2	1.10481e-2
	HMF002-00	1.20958e-2	1.20958e-2	1.08813e-2	1.09728e-2	1.09119e-2	1.08988e-2	1.09112e-2	1.08307e-2	1.13646e-2	1.11241e-2
	HMF002-00	1.20101e-2	1.20101e-2	1.08192e-2	1.09119e-2	1.08519e-2	1.084e-2	1.08534e-2	1.07719e-2	1.12933e-2	1.10568e-2
FISSION	HMF002-00	1.19538e-2	1.19538e-2	1.08025e-2	1.08988e-2	1.084e-2	1.0831e-2	1.08467e-2	1.07619e-2	1.12612e-2	1.10308e-2
	HMF002-00	1.19329e-2	1.19329e-2	1.08118e-2	1.09112e-2	1.08534e-2	1.08467e-2	1.08643e-2	1.07766e-2	1.12587e-2	1.10328e-2
Benchmarks calculations	HMF002-00	1.18944e-2	1.18944e-2	1.07364e-2	1.08307e-2	1.07719e-2	1.07619e-2	1.07766e-2	1.06935e-2	1.11976e-2	1.09665e-2
	HMF003-00	1.28079e-2	1.28079e-2	1.12944e-2	1.13646e-2	1.12933e-2	1.12612e-2	1.12587e-2	1.11976e-2	1.18948e-2	1.16065e-2
Sensitivities calculations	HMF003-00	1.24542e-2	1.24542e-2	1.10481e-2	1.11241e-2	1.10568e-2	1.10308e-2	1.10328e-2	1.09665e-2	1.16065e-2	1.13358e-2

Figure 32 - Complete inter-case covariance matrix

🥔 Results - NDaST											
File											
Case by case Representativity values	s (Ck)										
Filter		HMF001-0	HMF001-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF002-0	HMF003-0	HMF003-0
Nuclides / Reactions	HMF001-00	1	1	0.9814	0.9771	0.9756	0.9719	0.9687	0.9733	0.9937	0.9898
	HMF001-00	1	1	0.9814	0.9771	0.9756	0.9719	0.9687	0.9733	0.9937	0.9898
	HMF002-00	0.9814	0.9814	1	0.9998	0.9996	0.999	0.9983	0.9993	0.9967	0.9987
	HMF002-00	0.9771	0.9771	0.9998	1	1	0.9997	0.9993	0.9999	0.9948	0.9974
	HMF002-00	0.9756	0.9756	0.9996	1	1	0.9999	0.9996	0.9999	0.994	0.9969
TISETON	HMF002-00	0.9719	0.9719	0.999	0.9997	0.9999	1	0.9999	1	0.9921	0.9955
	HMF002-00	0.9687	0.9687	0.9983	0.9993	0.9996	0.9999	1	0.9998	0.9904	0.9942
	HMF002-00	0.9733	0.9733	0.9993	0.9999	0.9999	1	0.9998	1	0.9929	0.996
Sopoitivition calculations	HMF003-00	0.9937	0.9937	0.9967	0.9948	0.994	0.9921	0.9904	0.9929	1	0.9995
Bill Sensitivities calculations	HMF003-00	0.9898	0.9898	0.9987	0.9974	0.9969	0.9955	0.9942	0.996	0.9995	1

Figure 33 - Complete inter-case correlation matrix

Display	
Covariance	
Orrelation	

Figure 34 - Radio button to switch between covariance and correlation value displays

Case by case Representativity values	(Ck)				
Filter		HMF001-0	HMF001-0	HMF001-0	HMF001-0
	HMF001-00	1	0.4159	1	0.4159
ILBEVALS.NUMBER_CASES	HMF001-00	0.4159	1	0.4159	1
	HMF001-00	1	0.4159	1	0.4159
	HMF001-00	0.4159	1	0.4159	1
FISSION					
N_GAMMA					
🗄 🖂 Benchmarks calculations					
Sensitivities calculations					
KENO ABBN-93 / 299-Gr					
MCNP ENDF/B-VII.0 Con					

Figure 35 - Inter-case correlations with grey font denoting missing sensitivities

XML File Headings

The following headings and sub-headings demonstrate the contents (in this case blank) of a '.ndast' XML formatted file. This is the file saved or loaded, from / to the NDaST program, and contains everything needed to define a specific calculation(s) and results.

The fields can be directly modified by the user, however invalid input e.g. to nuclide z,a combinations or reaction names will cause an error; hence, it is advised to begin by editing a pre-existing file and to take extreme care (save an edited file under a different name). Note also that only the <params> section is required, and that part(s) can be generated separately and later "merged", with either 'File > Open' inside the application or using an external script / program.

Text (inp[t]) or numerical (inp[n]) input required is indicated as necessary. The 'third tier' of headings are repeated sequentially to provide the complete set of data.

```
→FIRST TIER
     →SECOND TIER
\rightarrow
           →THIRD TIER
<?xml version="1.0" encoding="UTF-8" ?>
<ndast>
<params>
      <benchmarks symbolValue=" inp[t] " symbolDelta="Î" inp[t] ">
            <benchmark>
            <id type="DICE OR IDAT" case=" inp[t] " model=" inp[t] "/>
            <id type="OWN" label=" inp[t] "/>
OR
            <exp val=" inp[n] " unc=" inp[n] "/>
            <calc type="DICE OR IDAT " code=" inp[t] " lib=" inp[t] "
            freetext=" inp[t] " val=" inp[n] " unc=" inp[n] "/>
            <calc type="OWN" label=" inp[t] " val=" inp[n] "
OR
            unc=" inp[n] "/>
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "</pre>
            lib=" inp[t] "/>
            <sens type="OWN" file=" inp[t] "/>
OR
            <category key=" inp[t] ">= inp[t] or inp[n] </category>
            </benchmark>
      </benchmarks>
<perturbations>
            <perturbation label=" inp[t] ">
            <nuclide z=" inp[n] " a=" inp[n] "/>
            <reaction> inp[t] </reaction>
            <emin> inp[n] </emin>
            <group emax=" inp[n] " mult=" inp[n] "/>
            </perturbation>
      </perturbations>
      <covariances>
            <matrix>
            <id>
            <left z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
            <right z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
            </id>
```

```
<refs> inp[t] </refs>
            </matrix>
      </covariances>
</params>
<results class="perturbations OR uncertainty OR combined-calc" >
      <perturbation>
            <benchmark>
            <id type="DICE OR IDAT" case=" inp[t] " model=" inp[t] "/>
OR
            <id type="OWN" label=" inp[t] "/>
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "</pre>
            lib=" inp[t] "/>
            <sens type="OWN" file=" inp[t] "/>
OR
            <contrib>
            <nuclide z=" inp[n] " a=" inp[n] "/>
            <reaction> inp[t] </reaction>
            <val> inp[n] </val>
            </contrib>
            </sens>
            </benchmark>
      </perturbation>
      <uncertainty>
            <benchmark> MAY ALSO BE NESTED FOR OFF-DIAGONAL UNCERTAINTIES
            <id type="DICE OR IDAT" case=" inp[t] " model=" inp[t] "/>
            <id type="OWN" label=" inp[t] "/>
OR
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "</pre>
            lib=" inp[t] "/>
            <sens type="OWN" file=" inp[t] "/>
OR
            <contrib>
            <covariance>
            <left z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
            <right z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
            </covariance>
            <val> inp[n] </val>
            </contrib>
            </sens>
            </benchmark>
      </uncertainty>
</results>
</ndast>
```

NDaST Supported Files

Example files can be found at https://www.oecd-nea.org/ndast/example-files/

Туре	Format	Code	Version/option
Sensitivity	Binary		-
Sensitivity	TSUNAMI-B	SCALE	6.0, 6.1, 6.2
	ASCII		
Sensitivity	WPEC SG33		-
Sensitivity	TSUNAMI-B	MCNP6.2	6.2
	ASCII		KOPTS KSENTAL=TSUNAMI-B

Sensitivity	TSUNAMI-B	TSAR	6.0, 6.1, 6.2
	ASCII		
Sensitivity	ABBN ASCII	MMK-KENO	-
Covariance	BOXER	NJOY	99*
Covariance	COVERX	AMPX*	Library Distributed with SCALE

NDaST Command Line

A basic command line feature exists in NDaST. Users of this feature are requested to contact <u>ndast@oecd-nea.org</u> for assistance and/or to provide specific requests for future development of the feature.

The features requires to download all the JARs locally (<u>http://www.oecd-nea.org/ndast/webstart/NDaST_all_jars.zip</u>).

After downloading the jars the feature can be used as in the example below:

C:\Temp\NDaST_cmdline>java -cp NDaST.jar org.nea.ndast.app.cmdline.NDaSTCmdLine

```
Input or output file missing
```

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

For example:

C:\Temp\NDaST_cmdline>java -cp NDaST.jar org.nea.ndast.app.cmdline.NDaSTCmdLine my_input.ndast my_results.ndast -od