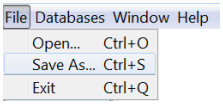
The Nuclear Data Sensitivity Tool (NDaST)
'How to' Beginner's Guide

Contents

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 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.



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.

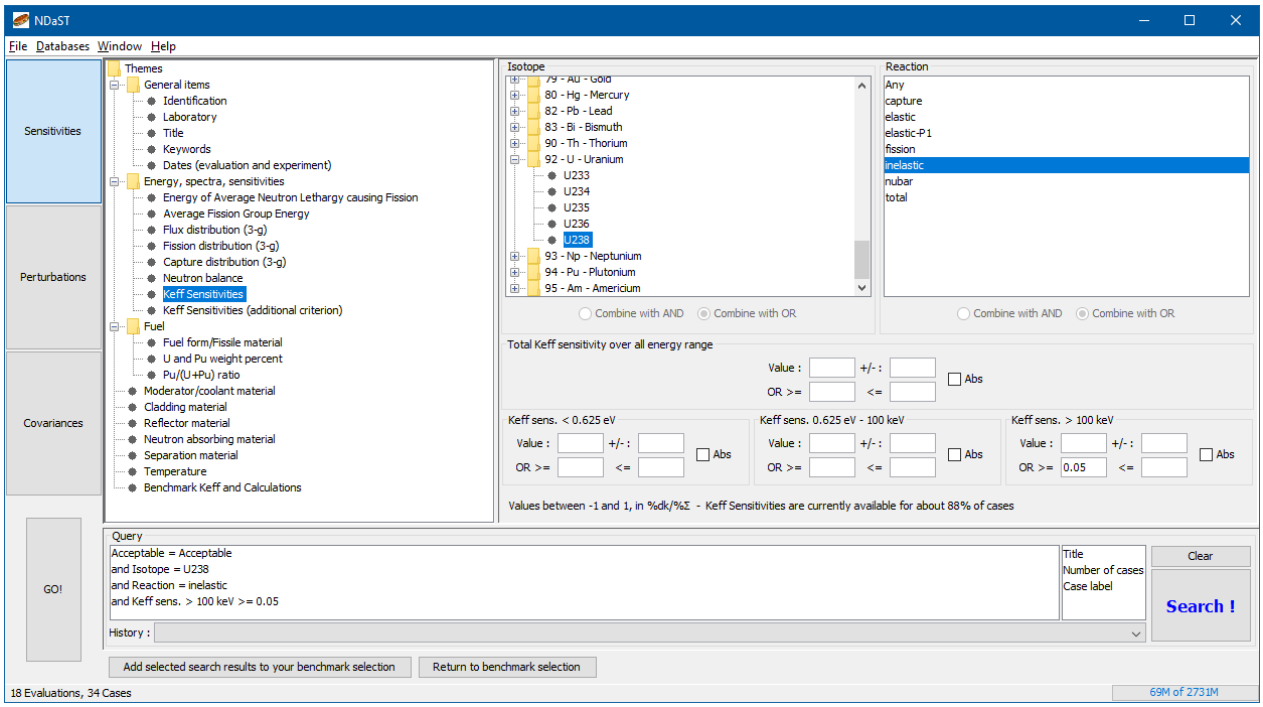


Figure 1 - Using DICE search to select keff sensitive benchmarks

- 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).

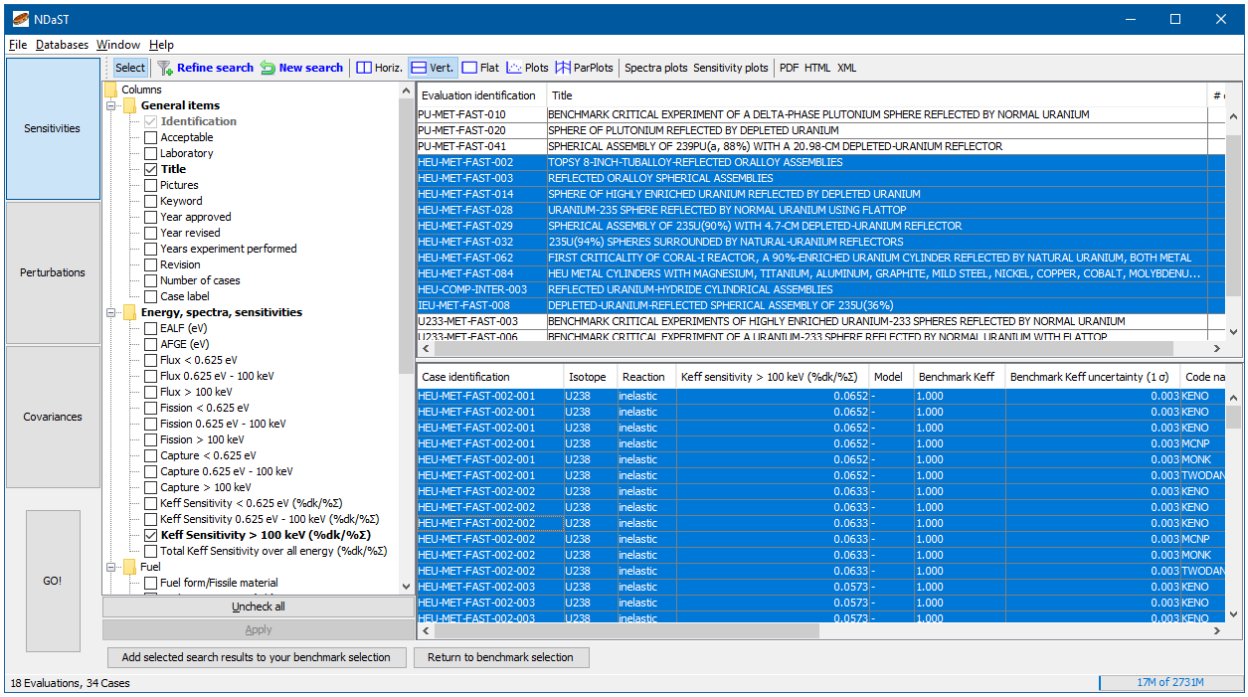
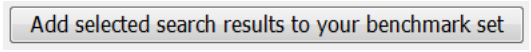
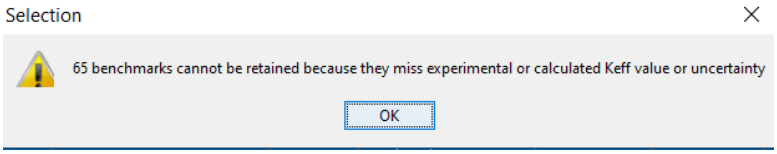


Figure 2 - Adding sensitive cases to NDaST benchmark set

- Click 'Add selected search results to your benchmark set' at bottom left of the panel. 

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:


- 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 

to the left of the corresponding row.

Return from this by clicking 'Ok' or '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:

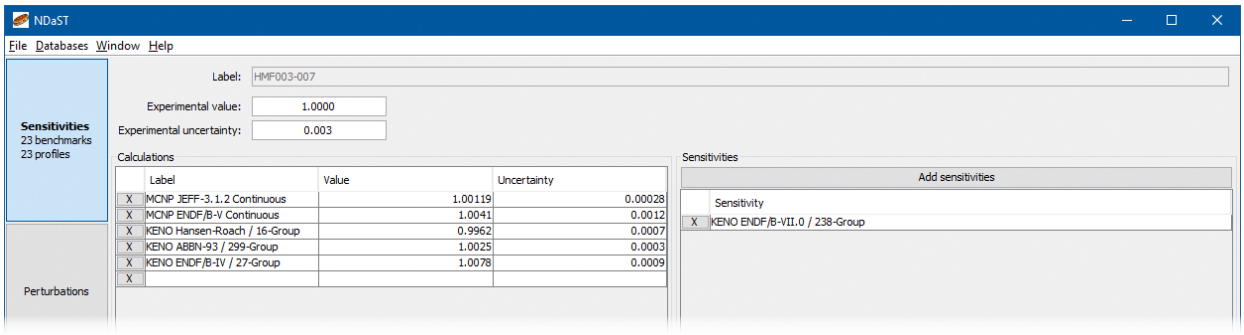
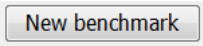


Figure 3 - Modify case experimental and computed results

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

- 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'. 

. A list of formats accepted is provided in the section 'NDaST Supported Files' later in this document.

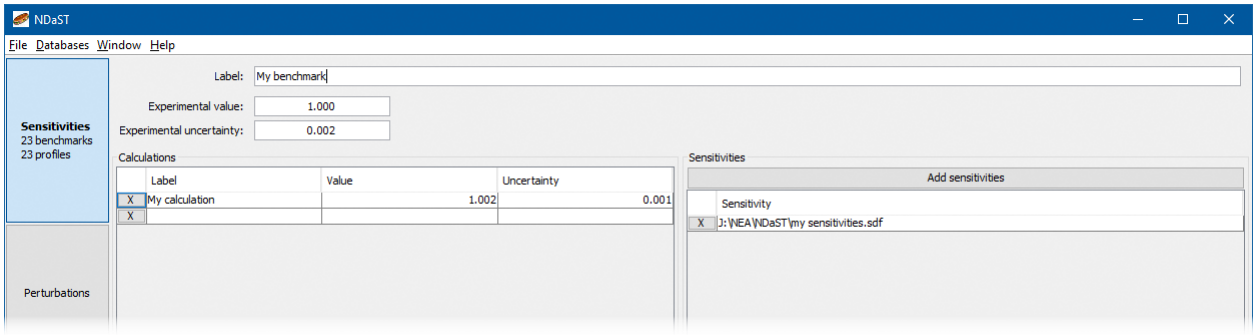


Figure 4 - Add new benchmark personal data

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.

- 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.

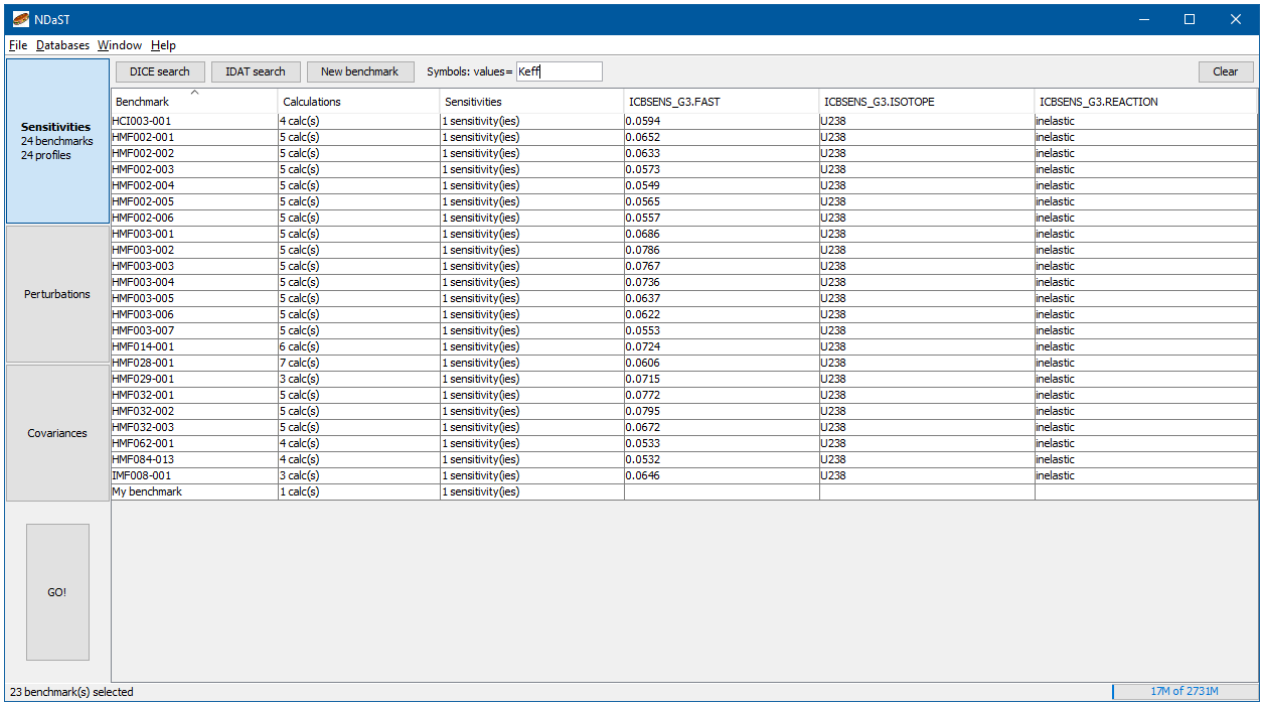


Figure 5 - Main sensitivity panel summarising benchmark set

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*:

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

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.

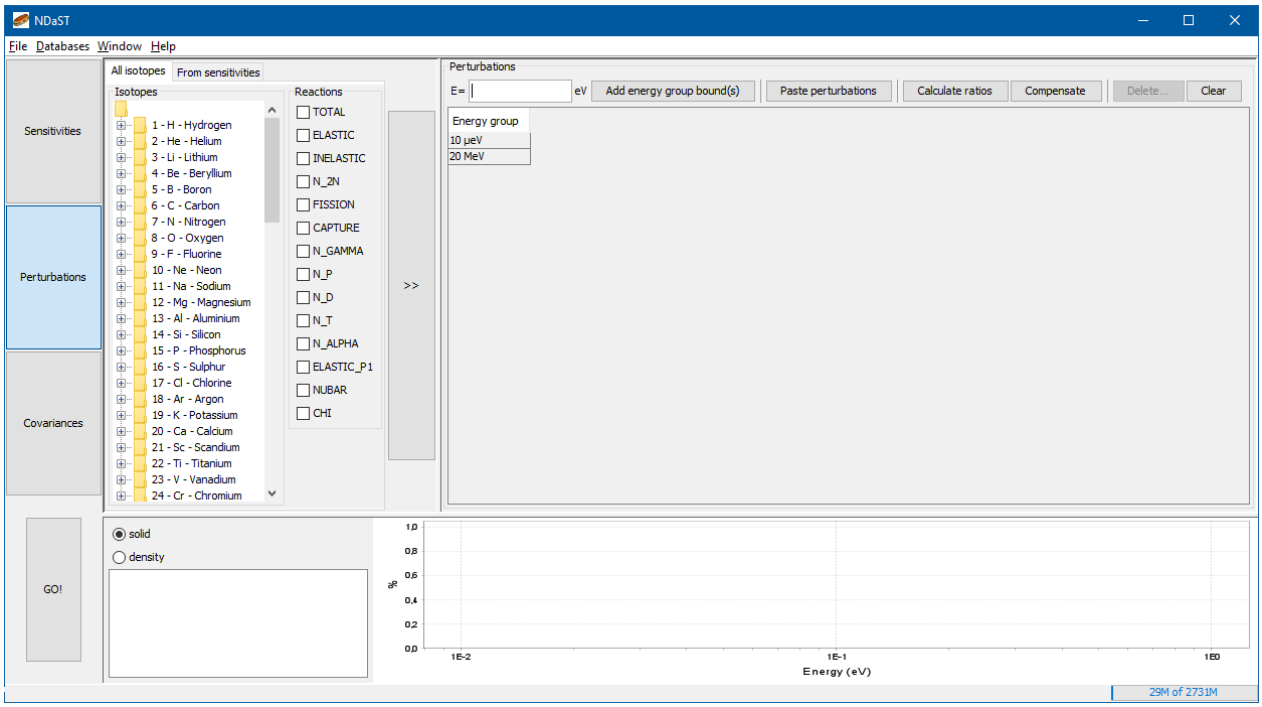


Figure 6 - Add nuclide-reaction column to perturbation table

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.

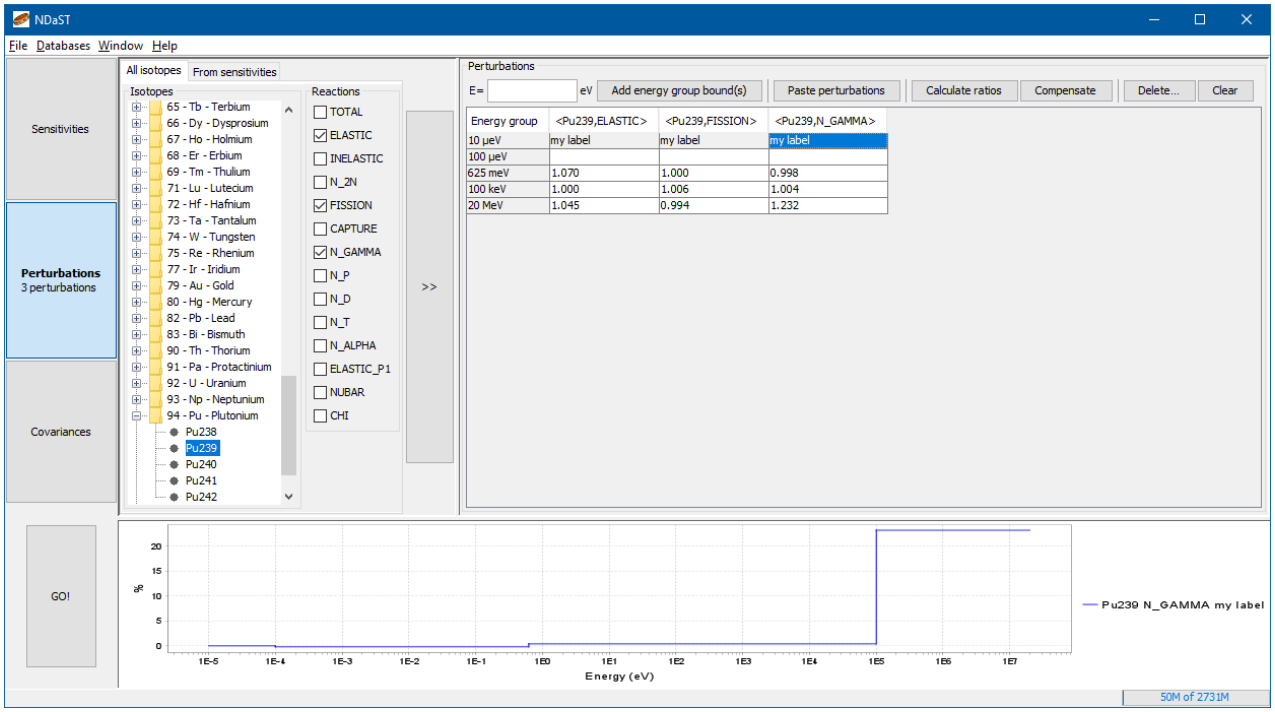


Figure 7 - Add energy band row and perturbation ratio to table

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.

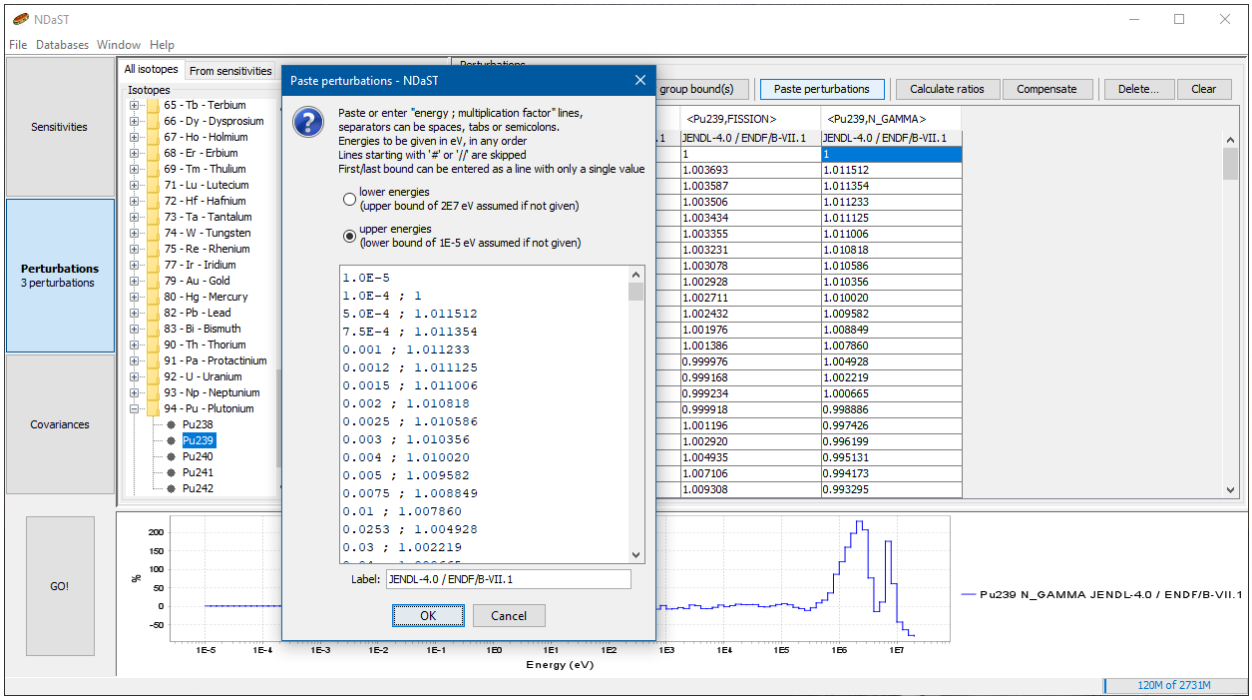


Figure 8 - Paste perturbation dialogue window

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 

. 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:
    - 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, #3[1]… 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.

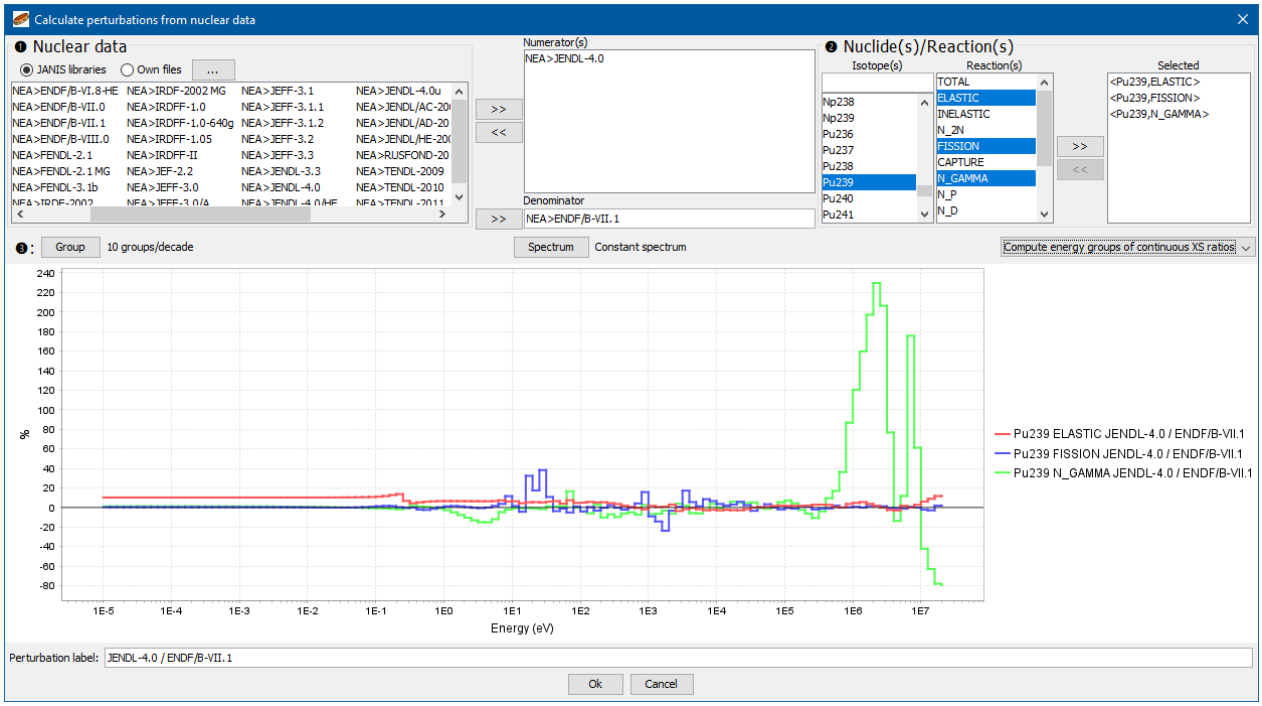


Figure 9 - Create perturbation from nuclear data dialogue window

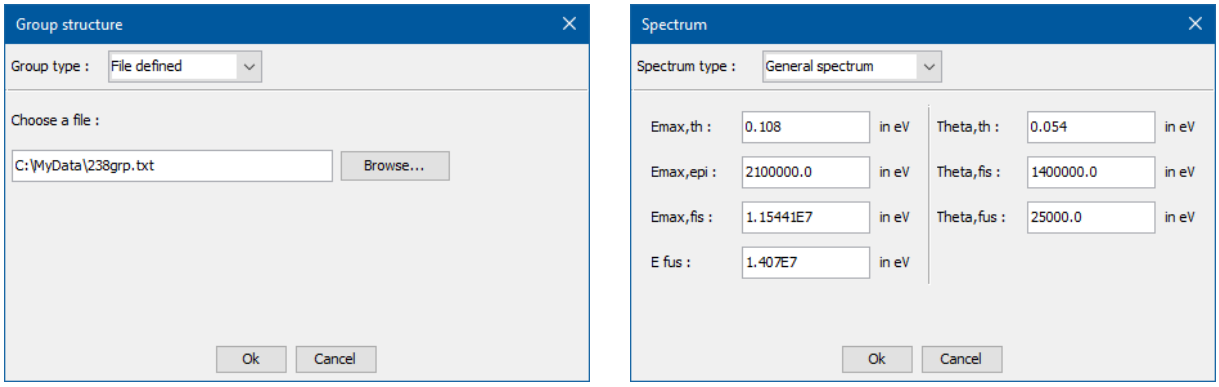


Figure 10 - JANIS ratio group structure and spectrum selection windows

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.

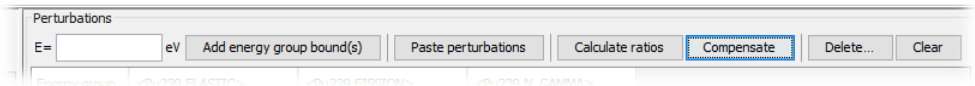


Figure 11 – Compensate button in the perturbations panel

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.

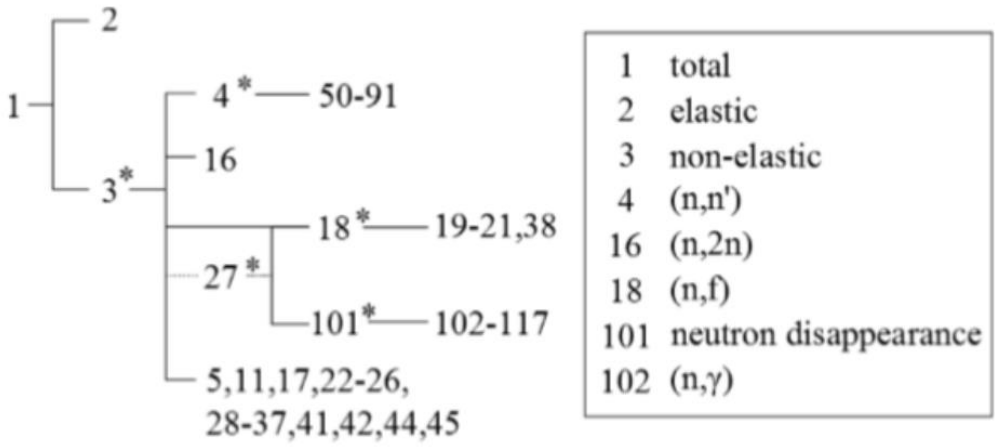


Figure 12 – ENDF/B Sum rules obeyed in compensate

In the example below, the JANIS ratio of the TENDL2017/TENDL2015 U235 Elastic cross-section 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.

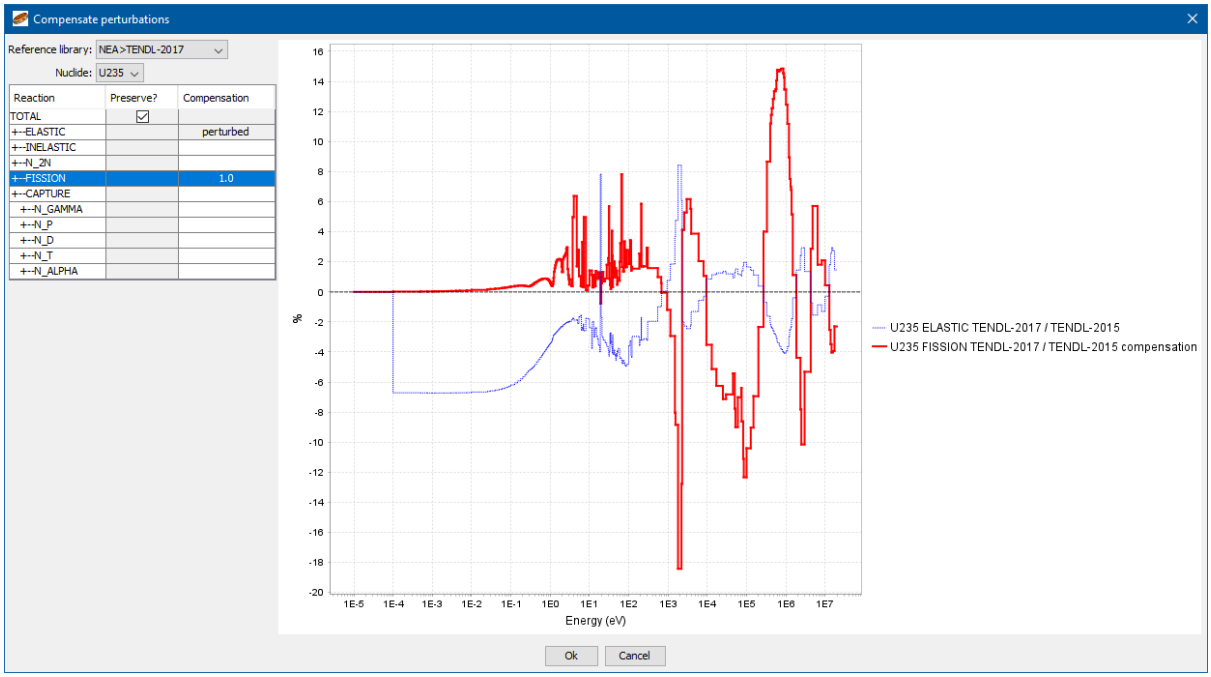


Figure 13- Using the compensation button to preserve the U235 total cross section by adjusting the U235 Fission cross section (after perturbing the U235 Elastic cross section using JANIS ratios)

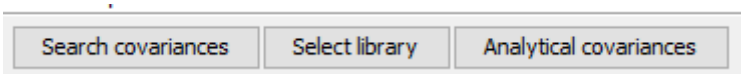
Covariances Panel

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.

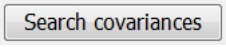
Completing this panel will initiate a calculation of the propagated relative uncertainty U_R, due to nuclear data covariance in the cases supplied in the Sensitivities panel. The linear propagation 'sandwich formula' is used with sensitivities *S*, and covariances *C*:

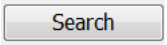
$$\frac{U_R}{R} = S.C.S^T$$

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

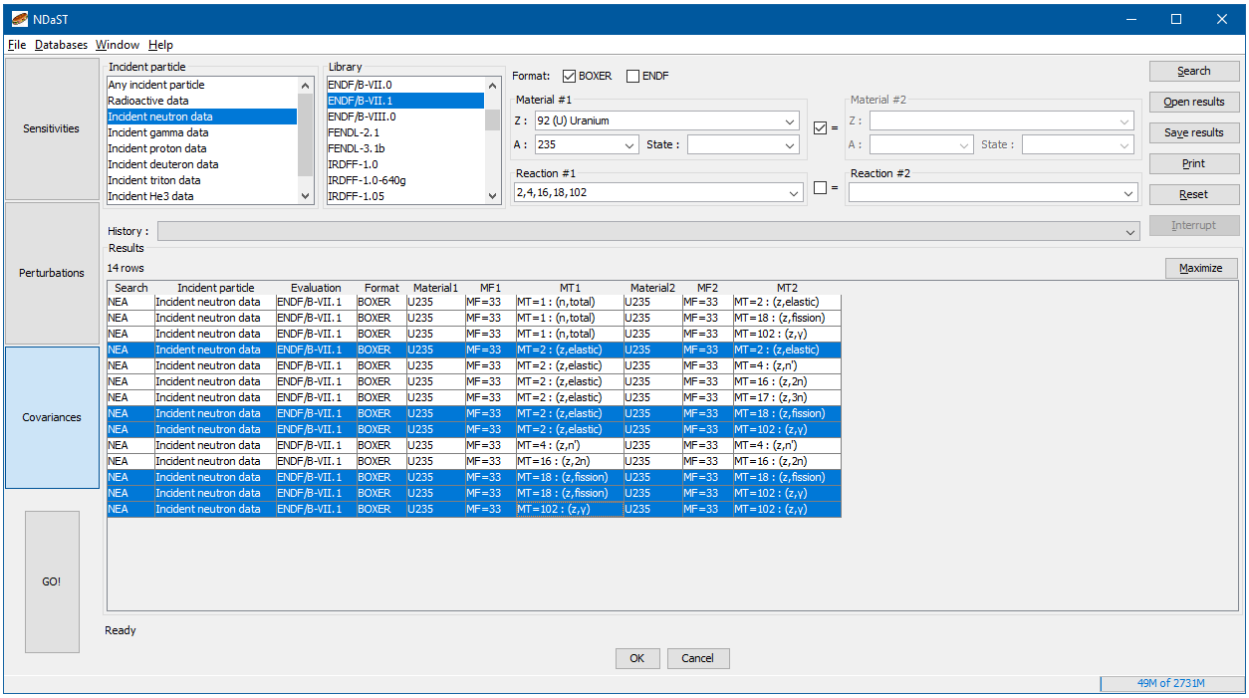


Search covariances

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' 

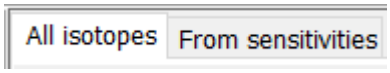
button. Note that recent searches may be retrieved from the 'History' drop-down bar.
- The returned results are shown in a table beneath, in the format of one row per reaction-nuclide pairing. All required covariance matrix pairs should be highlighted, using the control key or a mouse-drag to make multiple 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.

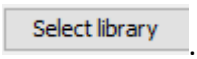


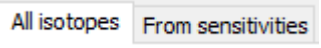
- **Figure 14 - Search and select nuclear covariance data matrices**

Select Library

All isotopes



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

. The 'All isotopes' 

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.

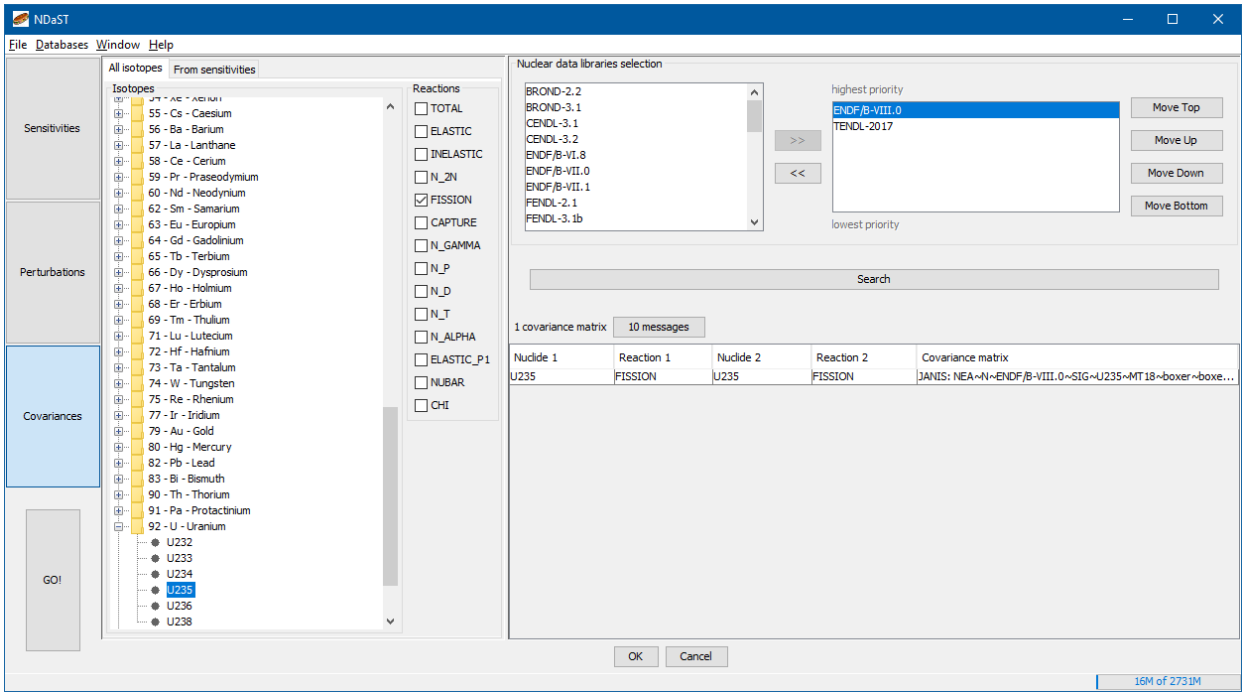
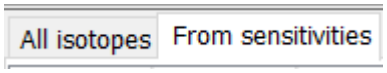


Figure 15 – Search covariances by library. U235 fission covariances are retrieved from ENDF/B-VIII.0 with highest priority, followed by TENDL2017.

From Sensitivity



Alternatively the 'From sensitivities' tab  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.

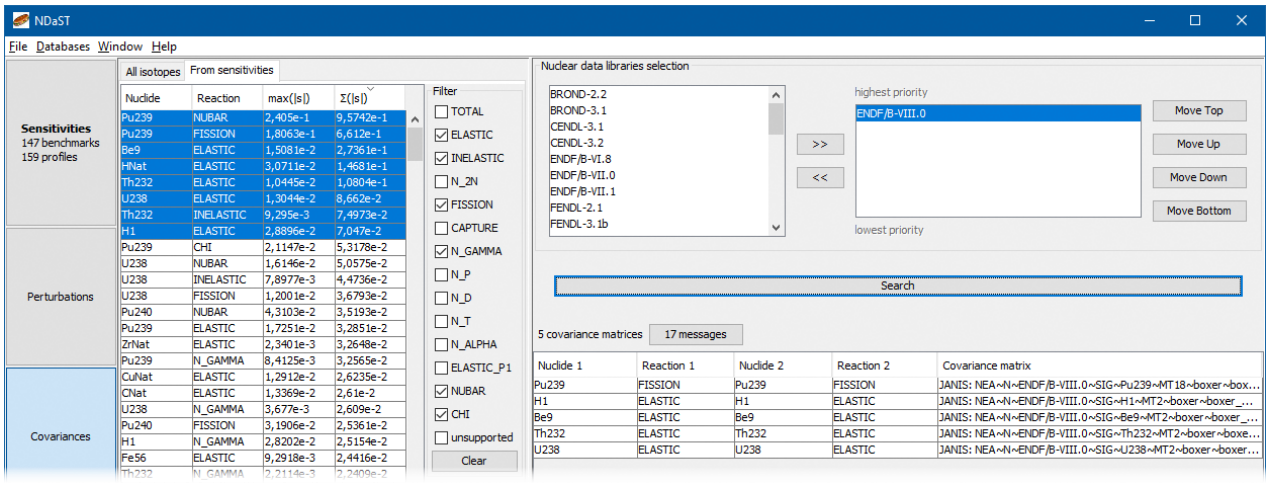


Figure 16 – Selecting covariances matching the largest sensitivity profiles

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.

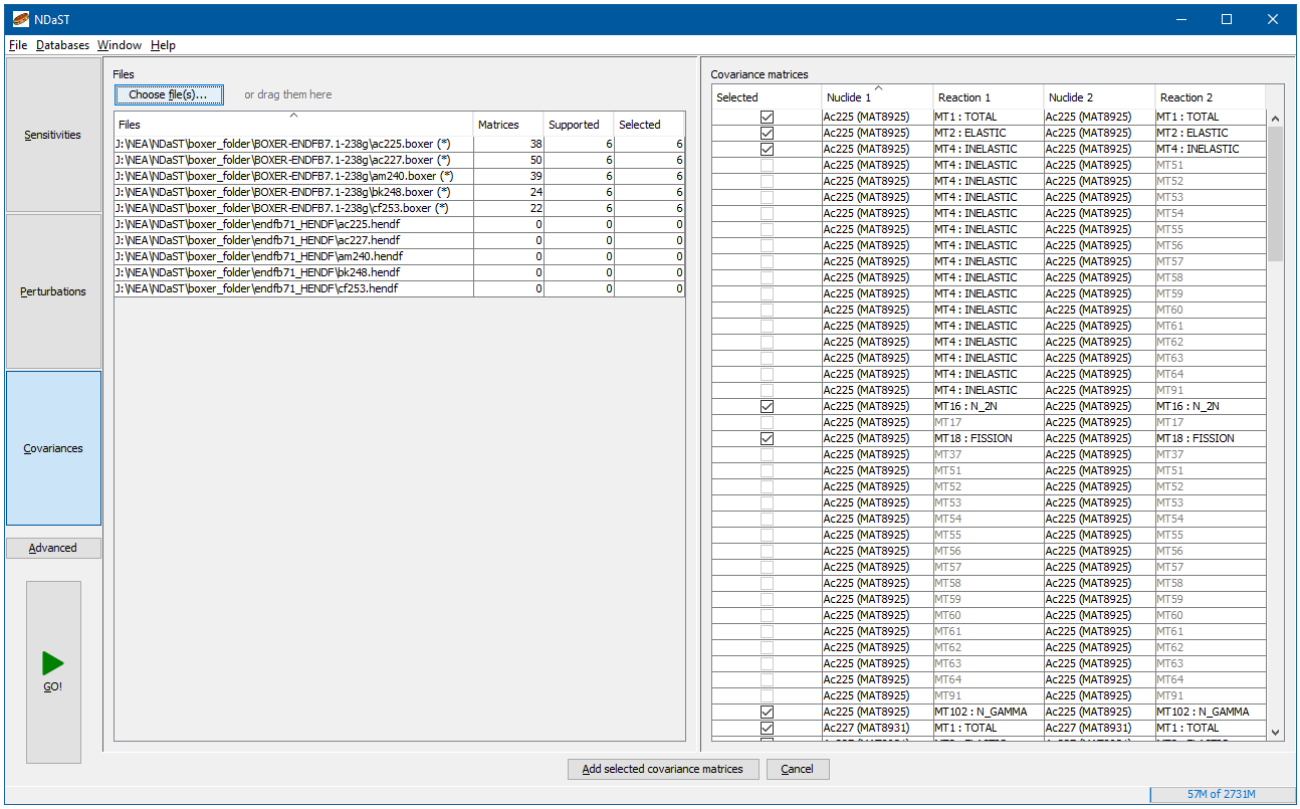


Figure 17: Example of importing a Covariance Matrix

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.

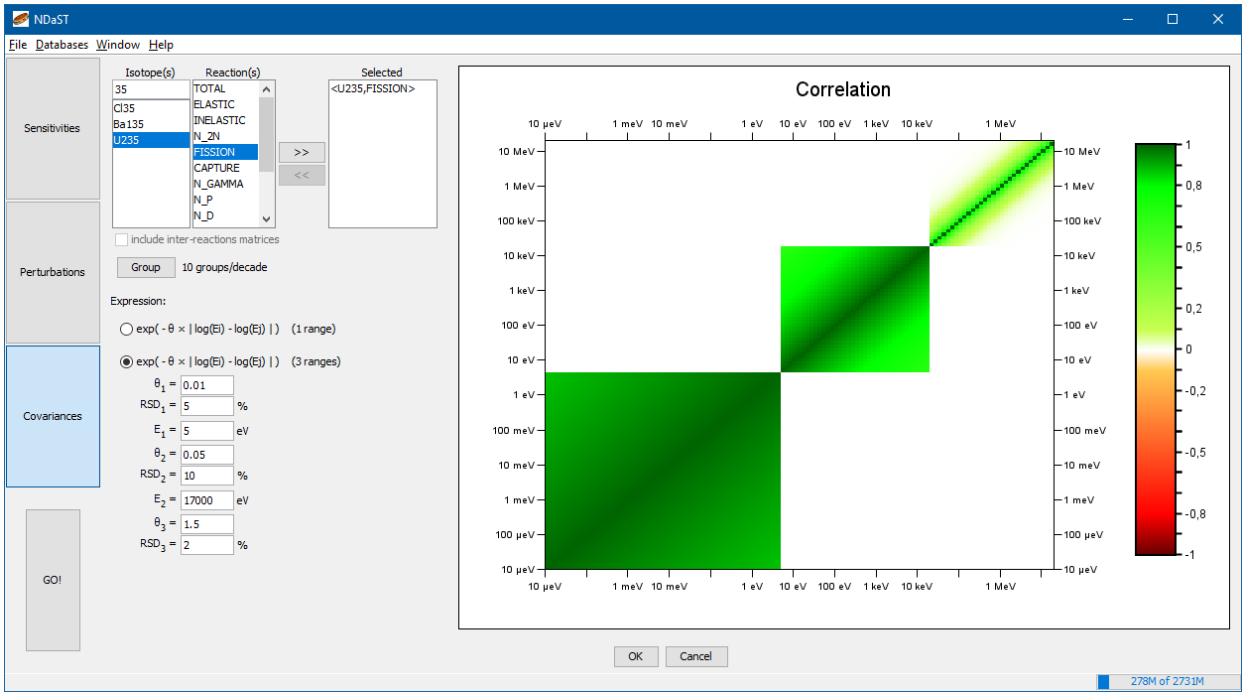


Figure 18- Example of an Analytic Covariance Matrix

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.

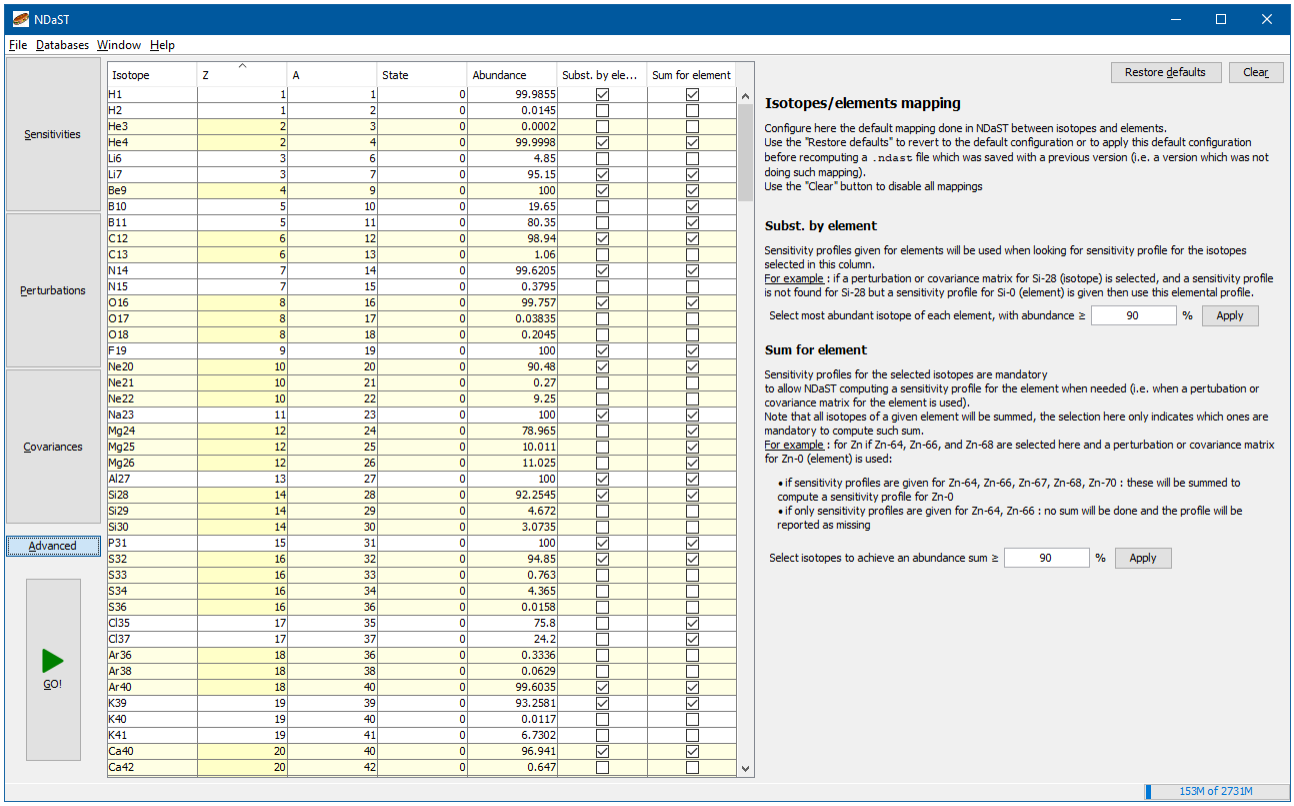


Figure 19: Advanced Panel, table of Isotope abundance and whether an elemental sensitivity can be substituted for an isotope and whether the isotopic sensitivities can be summed to form the elemental sensitivity.

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.

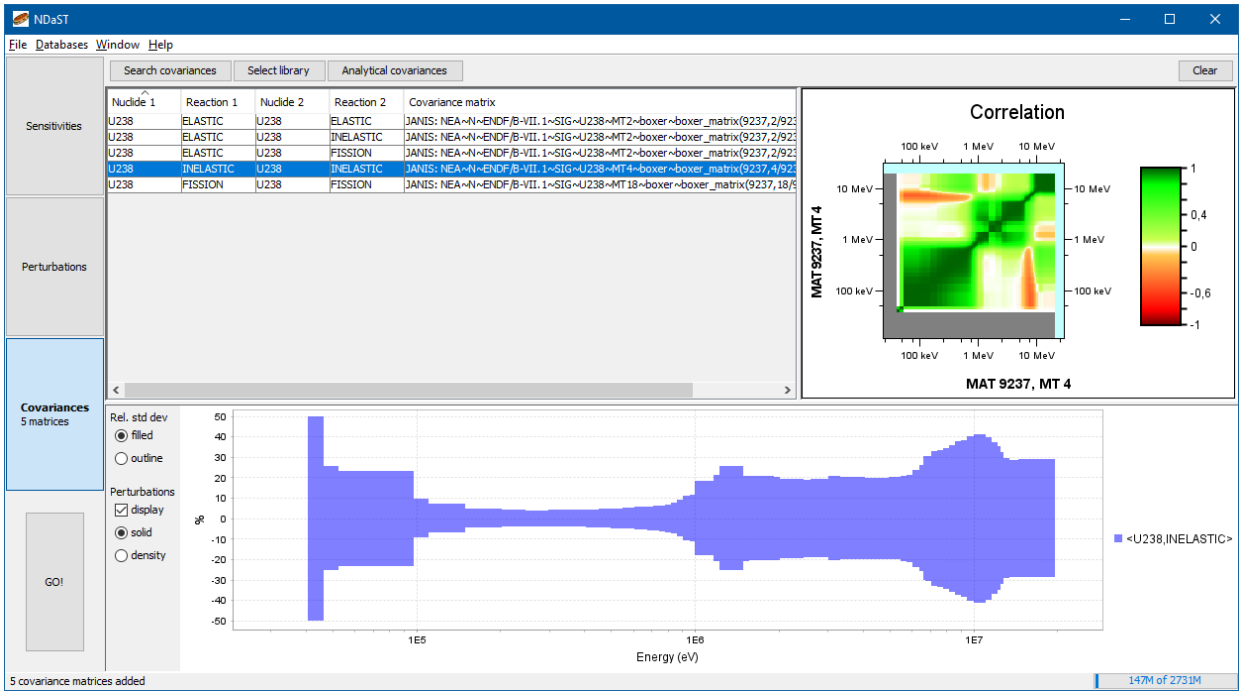


Figure 20 - Main covariance panel displaying matrix plots

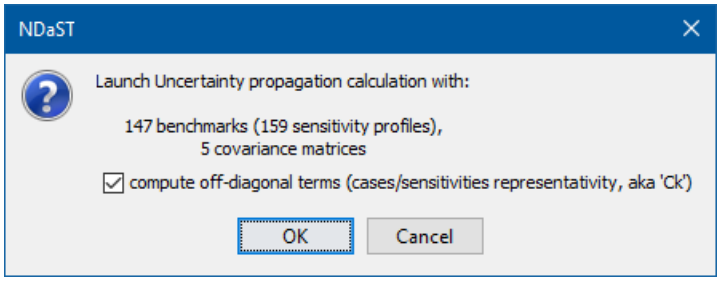


Figure 21 - Launch prompt with off-diagonal computation option

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.

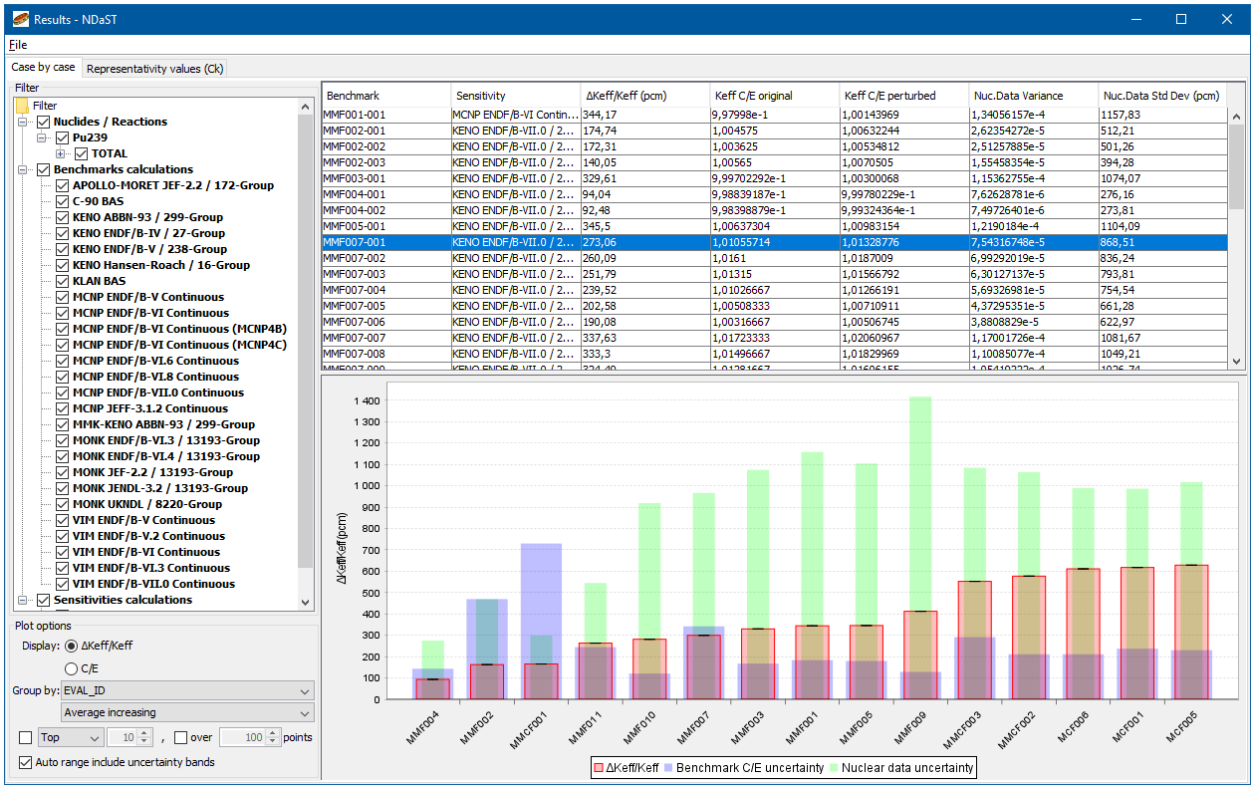


Figure 22 – Standard output window layout with expanded 'filter tree'

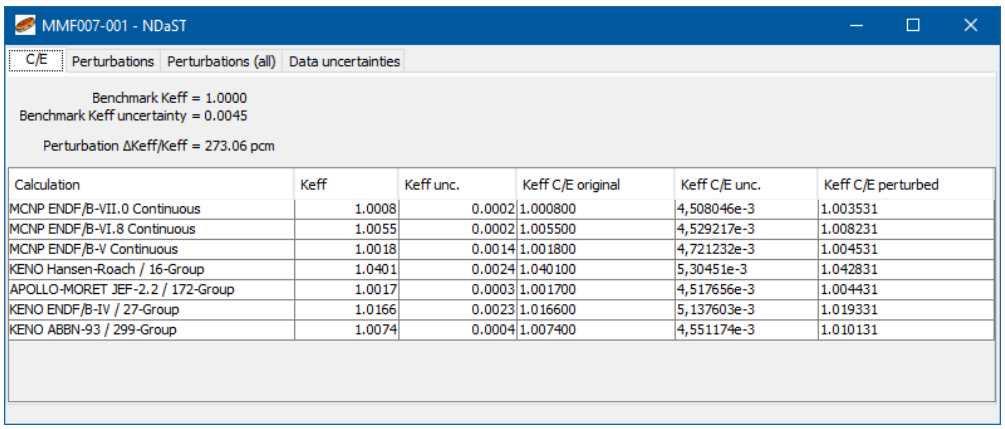


Figure 23 - Detail pop-up showing C/E tab

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).

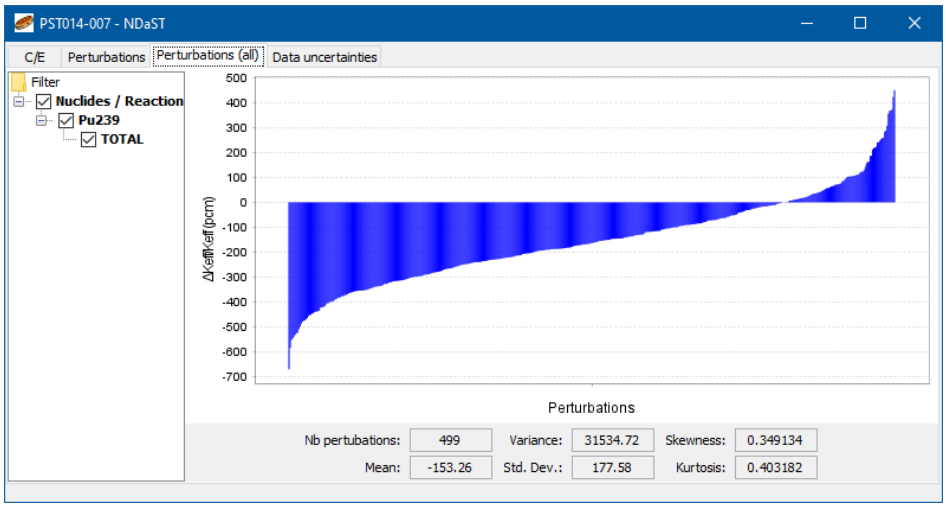


Figure 24 - Detail pop-up showing distribution of all individual perturbations

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.

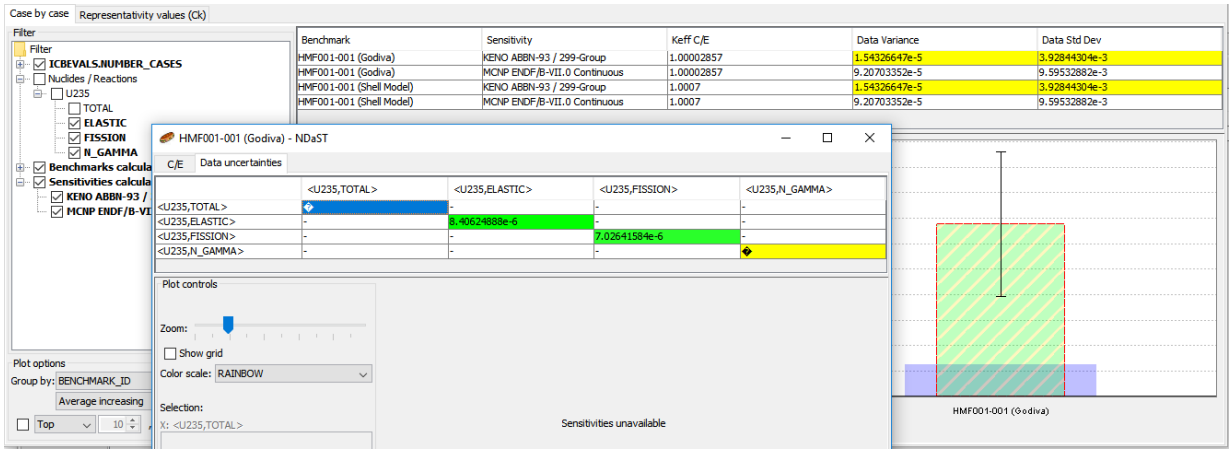


Figure 25 - Output with yellow banding / shading denoting missing sensitivity data

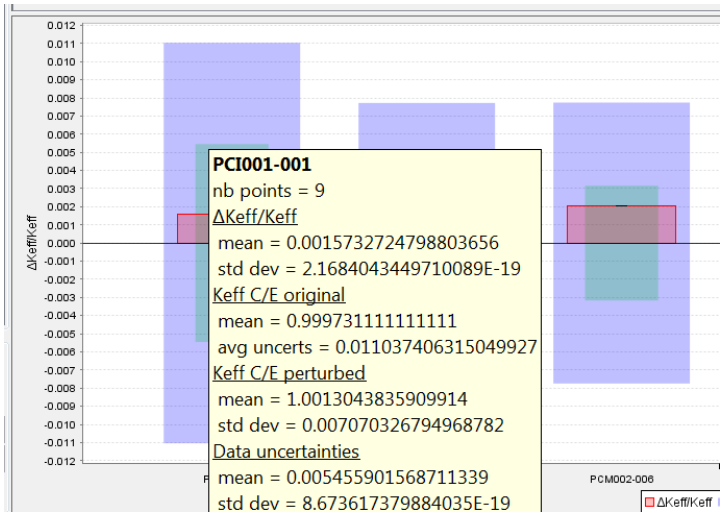


Figure 26 - Plot with active tool-tip

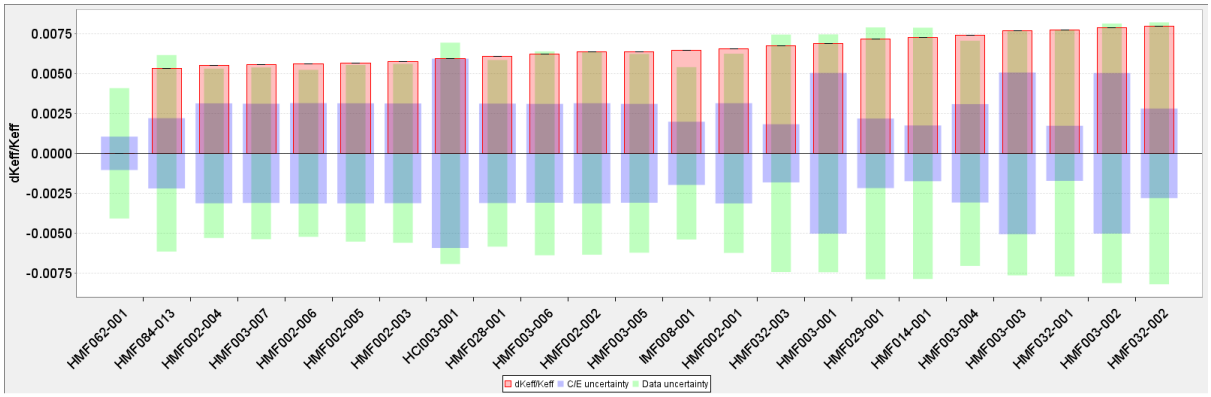


Figure 27 - Delta k_{eff} output plot

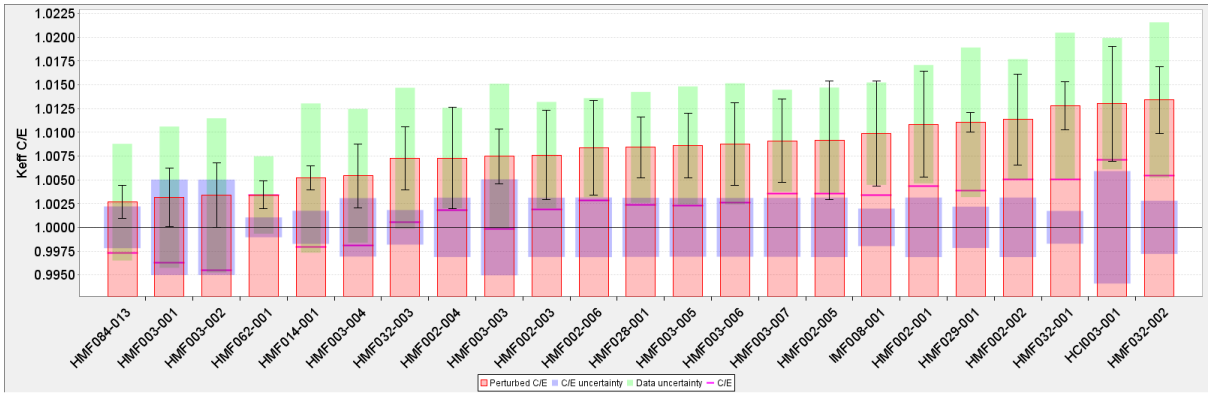


Figure 28 - C/E k_{eff} output plot

- 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.
  - 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

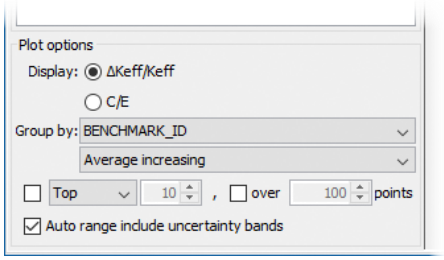


Figure 29 - Display options for output plots

- 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 nuclide-reaction 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 re-position 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.

V

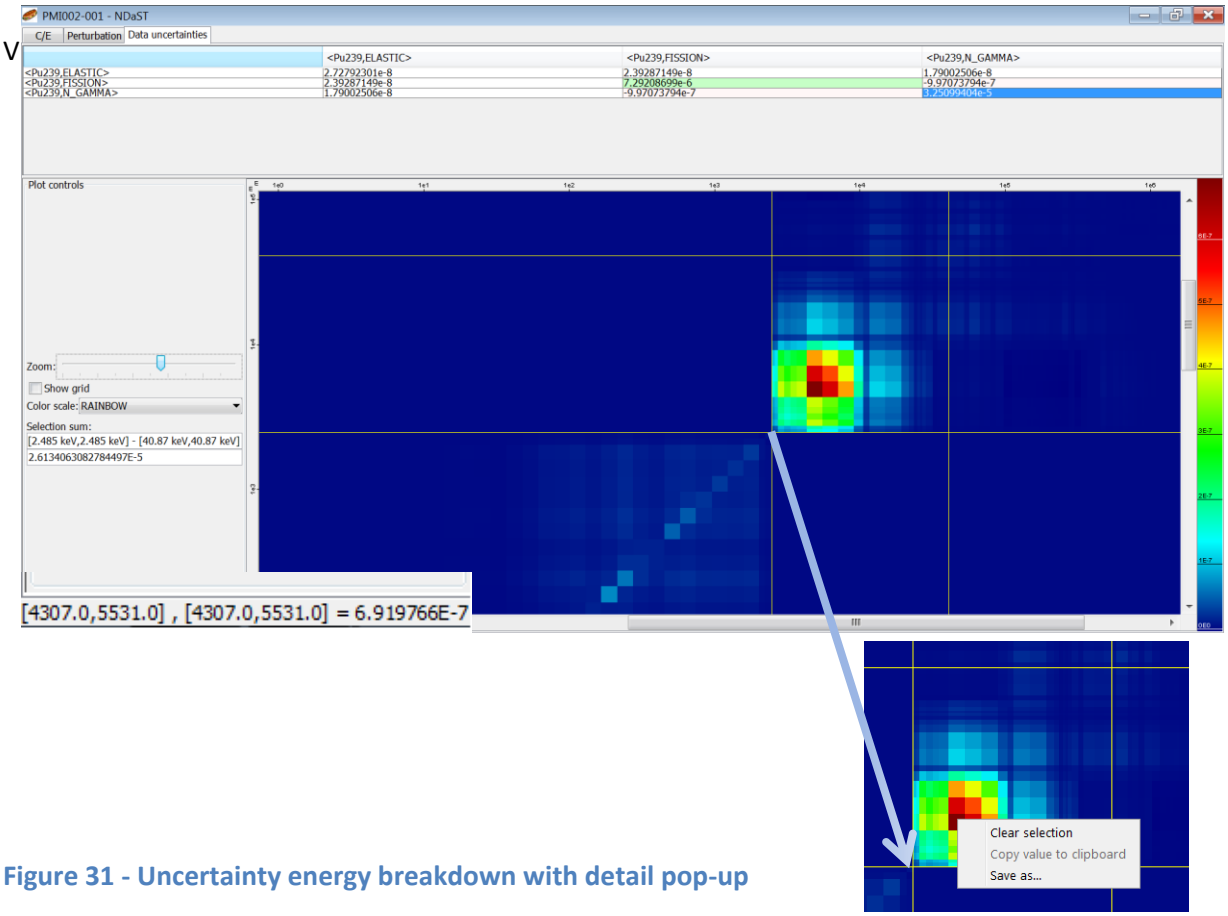
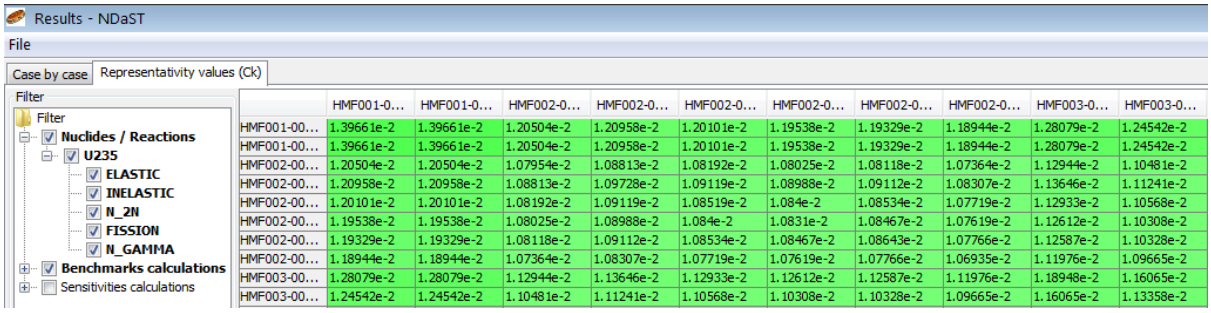


Figure 31 - Uncertainty energy breakdown with detail pop-up

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.
   - 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.



	HMF001-0...	HMF001-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF003-0...	HMF003-0...
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
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
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
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

	HMF001-0...	HMF001-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF002-0...	HMF003-0...	HMF003-0...
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
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
HMF003-00...	0.9937	0.9937	0.9967	0.9948	0.994	0.9921	0.9904	0.9929	1	0.9995
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

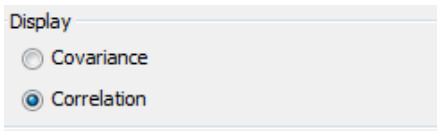
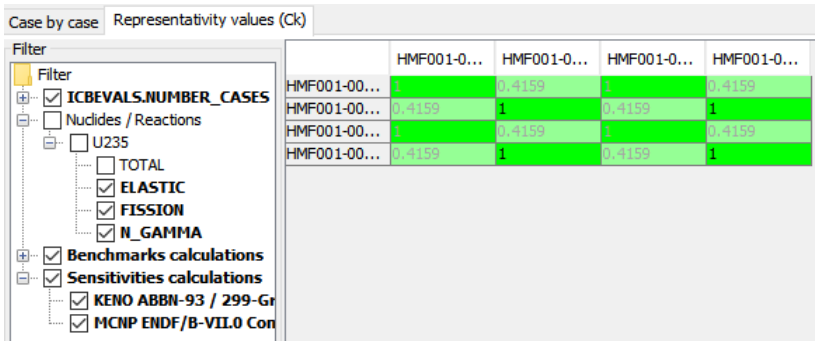


Figure 34 - Radio button to switch between covariance and correlation value displays



	HMF001-0...	HMF001-0...	HMF001-0...	HMF001-0...
HMF001-00...	1	0.4159	1	0.4159
HMF001-00...	0.4159	1	0.4159	1
HMF001-00...	1	0.4159	1	0.4159
HMF001-00...	0.4159	1	0.4159	1

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
→     →     →THIRD TIER

<?xml version="1.0" encoding="UTF-8" ?>
<ndast>
<params>
      <benchmarks symbolValue=" inp[t] " symbolDelta="Î” inp[t] ">
            <benchmark>
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OR          <id type="OWN" label=" inp[t] "/>
            <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] "/>
OR          <calc type="OWN" label=" inp[t] " val=" inp[n] "
            unc=" inp[n] "/>
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "
            lib=" inp[t] "/>
OR          <sens type="OWN" file=" inp[t] "/>
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            </benchmark>
      </benchmarks>
<perturbations>
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            <reaction> inp[t] </reaction>
            <emin> inp[n] </emin>
            <group emax=" inp[n] " mult=" inp[n] "/>
            </perturbation>
      </perturbations>
      <covariances>
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            <right z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
            </id>
```

```
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            </matrix>
      </covariances>
</params>
<results class="perturbations OR uncertainty OR combined-calc" >
      <perturbation>
            <benchmark>
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OR          <id type="OWN" label=" inp[t] "/>
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "
            lib=" inp[t] "/>
OR          <sens type="OWN" file=" inp[t] "/>
            <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] "/>
OR          <id type="OWN" label=" inp[t] "/>
            <sens type="DICE OR IDAT " case=" inp[t] " code=" inp[t] "
            lib=" inp[t] "/>
OR          <sens type="OWN" file=" inp[t] "/>
            <contrib>
            <covariance>
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            <right z=" inp[n] " a=" inp[n] " r=" inp[t] "/>
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            <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/

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

Sensitivity	TSUNAMI-B ASCII	TSAR	6.0, 6.1, 6.2
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 ndast@oecd-nea.org for assistance and/or to provide specific requests for future development of the feature.

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

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
```