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User Manual for GANDR GUI

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Abstract

GANDR GUI is a graphical computer code with the primary intention of generating input files for GANDR in a user-friendly way. The GANDR GUI is written in c++ and uses wxWidgets to construct graphical elements. Source code and binaries for Windows and Linux are available on the IAEA-NDS GitHub page. The provided binaries are statically compiled and don't need any external dependencies apart from the system libraries already present in Windows 10 and most Linux distributions. The GUI should compile on MacOS but was never tested by the developers.

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User Manual for GANDR GUI

Introduction and scope of the project

GANDR GUI is a graphical computer code with the primary intention of generating input files for GANDR, a long-term project for the **G**lobal **A**ssessment of **N**uclear **D**ata based on sensitivity and uncertainty analysis developed by D. W. Muir. This manual does not focus on the functionality and operation of GANDR but describes the usage of the GANDR GUI. To learn more about GANDR, the reader is advised to read the official documentation, available at the time of writing this manual at the website [16].

The main purpose of the GANDR GUI is to provide the user a friendly way to run GANDR evaluations. As of 2019, GANDR input is composed of 37 cards, each requiring multiple settings to be entered in a pre-defined text format. New input cards are added as additional functionality is developed. GANDR GUI is **not** able to generate all possible combinations of user input. Instead, it was designed to constrain the number of options available and guide the users through the most common use cases and to minimize the chance of errors.

Currently, most options are supported for the following modes of GANDR operation:

- Classic mode (imode=12)

- Standards mode (imode=10)

- Mixed mode (imode=11)

- Integral mode (imode=15)

GANDR GUI is built in a modular fashion, so new modes might be added.

This document describes the set-up of the environment required to work with the GANDR GUI and program operation.

Installation and environment set-up
GANDR GUI is statically compiled and does not require and dependencies to run besides GUI libraries that are normally present on the system. The program has been built and tested on Windows 10 and Ubuntu Linux, but it should work on any Linux distribution with support for GTK3 [16] library. GANDR GUI and all its build dependencies are available for Mac OS, so support can be added when an Apple computer becomes available to the developers.

Installation
Since the GUI is statically compiled, it does not require installation of any libraries besides GTK3 on Linux, which is already available on most distributions. The users can simply run the executable from any folder.

Environment set-up
GANDR GUI can use reaction definitions that are available in threshold files that are located on ZOTTVL [16] directory. Every time GANDR is started, it tries to read the location of the ZOTTVL folder from the system variable "ZOTTDIR". If the path is not available in the form of the system variable, GANDR opens a file dialog that the user can use to locate the directory.

If the directory is not specified, some functionality, like loading the default reaction definitions is not available, but the program can still be used.

Compiling the program on Linux

To re-compile GANDR GUI on Linux, the user needs to check-out the GANDR code with all its dependencies in a folder and run "make". The required external build dependencies are g++, GTK3 development libraries, wxWidgets 3 development libraries. The only internal build dependency is a header-only serialization library Cereal, which is distributed as a git submodule.

Compiling the program on Windows

This manual does not provide detailed instructions for building wxWidgets on Windows. The users first need to check-out and compile wxWidgets (available from [16]) as a static library. The next step is to create a Visual Studio 2017 project or use the one provided with GANDR GUI as a template and modify the path to the wxWidgets library.

Using the program

Basic program navigation

The main window of the GANDR GUI (Figure 1) is composed of a checked list of the currently defined GANDR runs and four buttons that allow the user to add runs, remove runs, add or modify the initialization run and generate GANDR output. Any run can be double-clicked to view and modify its properties.
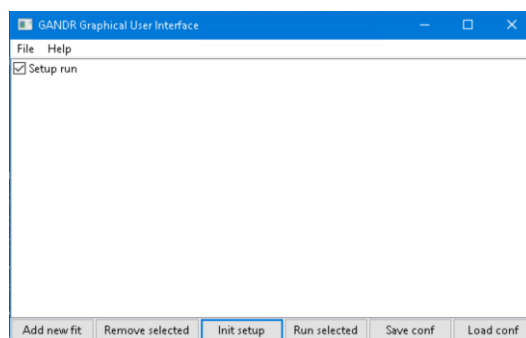

Figure 1 Main screen of the GANDR GUI

Initialization of GRID, reaction definitions and PENDF/covariance files

To add or edit the initialization run, click the "Init Setup" button on the main screen. Since the initialization run is always defined with "inopt=0", attempting to add another run when one is already defined will modify the existing one instead.
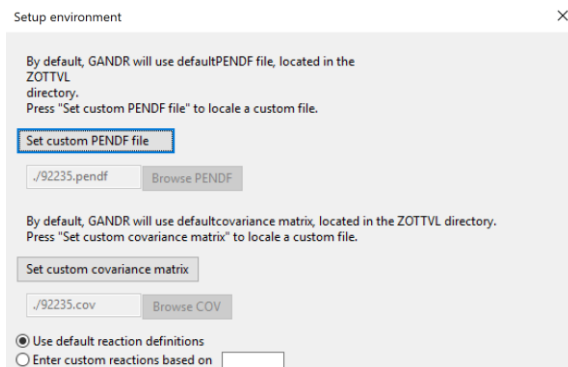
Figure 2 Controls used to define custom PENDF/covariance files and select an option to define custom covariances

Pressing the button opens a wizard (Figure 2) that takes the user through the process of run definition. On the first wizard page, the user can add a custom PENDF file by clicking the button labeled "Set custom PENDF file" and entering the path in the corresponding text entry box or by pressing the "Browse PENDF" button and invoking the file browse dialog. In a similar manner, the user can introduce a custom covariance matrix by pressing "Set custom covariance matrix" and specifying the file path.

If the user selects "Enter custom reactions", the next wizard page will display a table that can be used to define reactions. The reaction number entered in the text control will be used to load template reactions from a threshold file. In the table, the user can enter the reaction labels in the middle row and MT definitions separated by spaces in the right column.
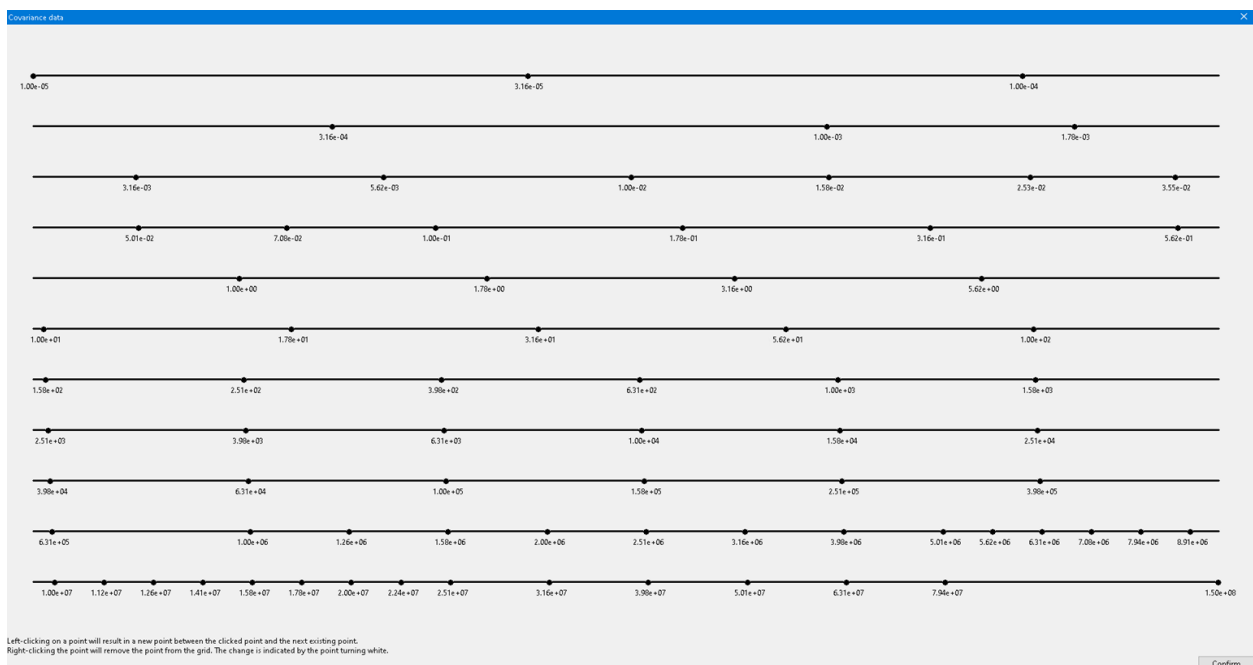

Figure 3 Dialog used to add and remove points from the 74-point GANDR grid

The last page of the wizard allows the user to select one of the predefined grids or define a custom grid. If an option to define custom grid is selected, a dedicated window (Figure 3) is opened that can be used to remove points from a default 74-point grid or add new points. Every black point represents one energy point on GANDR grid.

To add points, the user needs to click on existing points; an extra point will appear at the midpoint to the next existing point. To delate a point, it can be right clicked; the point will color white to indicate that the grid has been thinned.

Adding a "Classic" run

In the "Classic" mode, uncorrelated data are read from formatted files from the EXFOR data base. Additional uncertainty values can be added by the user. The "EXFOR" files are referred to throughout the text. They are actually simple text files obtained from a two-stage process from the actual EXFOR entries. Step-1 is conversion of EXFOR into the computational C4 format (available from the EXFOR web interface) and construction of the tabular text files that can be produced with the LSTTAB module of the ENDVER package [16]. GANDR also supports EXFOR files in the C5 format, but the GUI support for this option will be added in the future releases.

Figure 4 First screen of the "Add run wizard"

To add a new "Classic" run, use the "Add new fit" button on the main screen (Figure 1) to open the "Add run wizard", seen on Figure 4. Enter the "most negative adjustment permitted", select "EXFOR data and press "Next" to advance to the screen shown on Figure 5. The text box between the "most negative adjustment permitted" and the Next/Cancel buttons is reserved for a comment that will be added to the GANDR input.
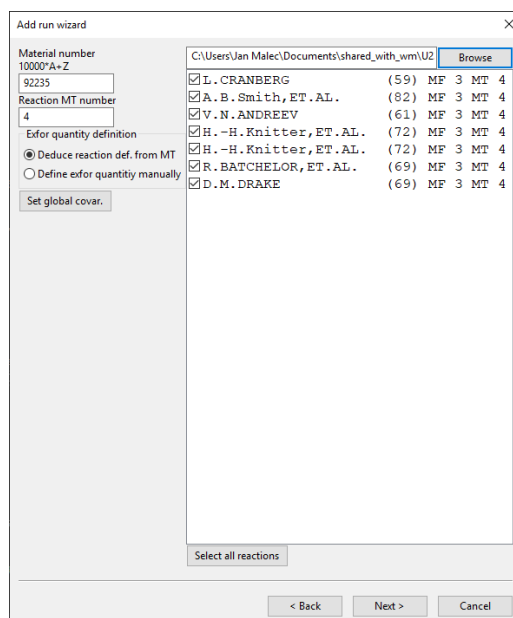
Figure 5 A screen used to select EXFOR data

The recommended way to find an EXFOR set by opening a dialog using the "Browse" button first. The EXFOR file will be automatically parsed and the experiments will be displayed in a list with checkboxes. The material AZ number and the Reaction MT number will be filled automatically. If they are not, that might mean that the EXFOR file could not be read or that it is improperly formatted. The user can use the checkboxes to include an experiment in the evaluation or exclude it from evaluation. The button titled "Select all reactions" will check all checkboxes. Double clicking an experiment will open a modal dialog (as seen on Figure 6) that can be used to add covariance data to the experiment. After the data is entered, the user can click "Confirm" to apply the changes. The "Set global covar." button can be used to override all local covariance data.
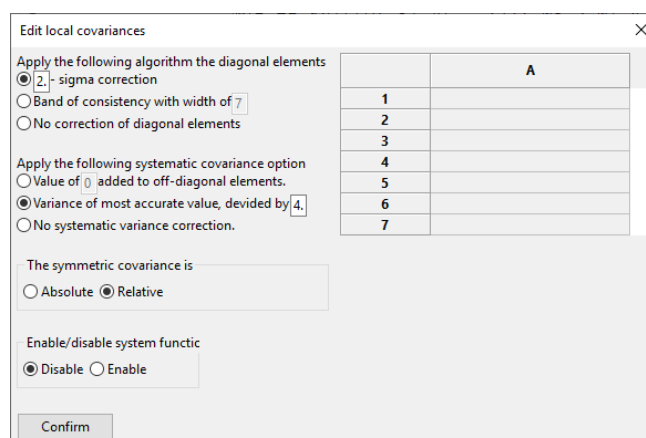

Figure 6 Dialog used to add local covariance data

If the option "Define EXFOR quantity manually" in the checkbox titled "EXFOR quantity definition" is selected, a modal window with a list of all GANDR reactions will appear. The user can use check boxes to define the EXFOR quantity as a combination of GANDR reactions.
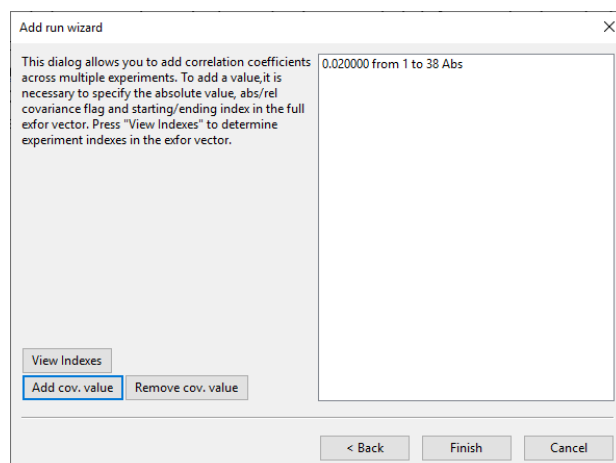
Figure 7 Screen used to add correlation coefficients across multiple experiments

The next screen, shown on Figure 7, allows adding the correlation coefficients across multiple experiments. Using the recommended workflow, the user first opens a table (Figure 8) listing data indexes and energy ranges for all the experiments by selecting "View Indexes" and adding the values using the "Add cov value" button while keeping the index table open for reference.

Figure 8 Data indexes for selected experiments

Like all list elements, the covariance data items on the table in Figure 7 can be double clicked to bring up an editing dialog. To remove covariance data, select an item in the table from Figure 7 and press "Remove cov. value". Note that currently GANDR only supports adding of covariance data between neighboring experiments.

Press "Finish" to complete the run definition. After successful completion, a new run will appear in the main window (Figure 1).

Adding an "Standards" run

Begin by opening a new instance of "Add run wizard" from the main screen (Figure 1). On the first wizard page (Figure 4), enter the "most negative adjustment permitted", select "Standards data" and advance to the next screen by pressing "Next".

In the second screen press "Browse" to open a file dialog and select the file containing data in an ENDF format. The file will be read and parsed by GANDR GUI in order to store reaction data used in the next steps.
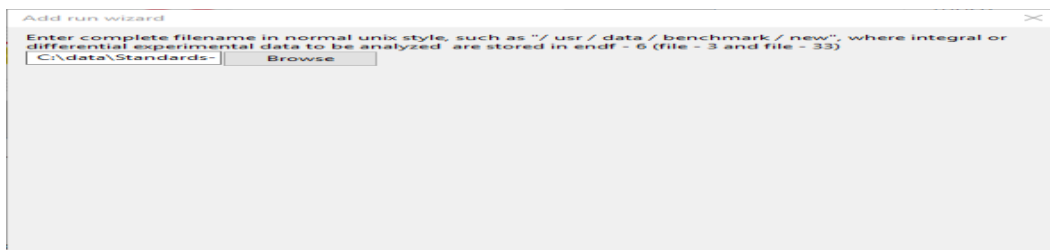
Figure 9 The "Browse" button opens a file dialog used to load data in ENDF format

After pressing next, the user is presented with a new wizard page (Figure 10) with a list of experiments and two buttons "Add experiment" and "Remove experiment". Pressing "Add experiment" opens a new wizard that allows the user to add new materials to the evaluation.
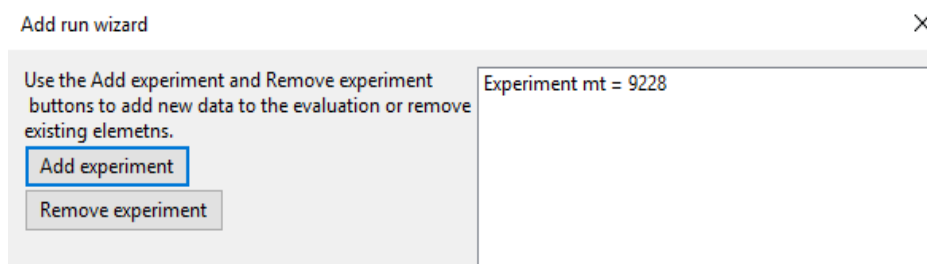

Figure 10 Pressing "Add experiment" opens a new wizard, allowing the user to add new materials

Figure 11 portraits the first screen of the newly opened wizard asking for material number, reaction number and type of data to be fitted.
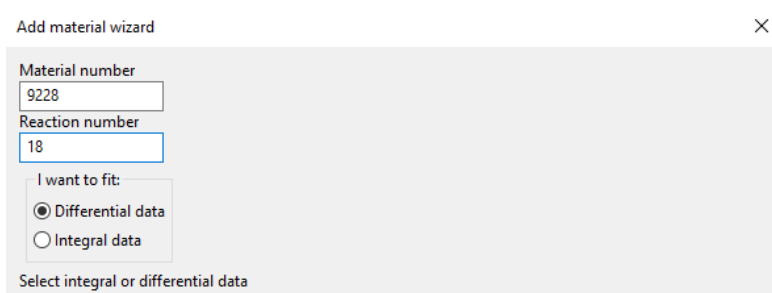

Figure 11 First screen of "Add material wizard" asking for material number, reaction number and type of data to be fitted

After proceeding to the second screen by pressing the button with label "Next", the user is asked to enter optional, additional covariance data. The interface (Figure 12) is similar to the one (Figure 7) used for adding covariance data to experiments in EXFOR format.
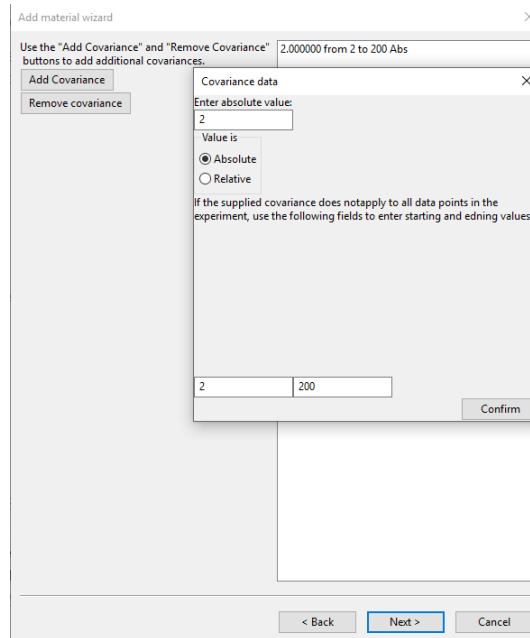
Figure 12 Additional covariance data is added to a list using a dialog

The button labeled "Add covariance" opens a modal dialog that can be used to enter the magnitude of the value, enter starting and ending data indexes and set covariance data nature by toggling between "Absolute" and "Relative" options in a radio box.
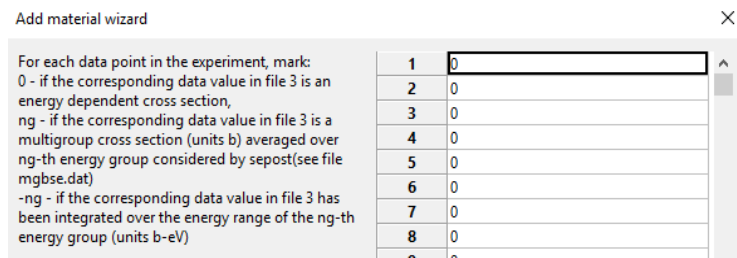

Figure 13 The "ng" parameter is set for each data point individually

If the user has chosen "Integral data" on the step displayed on Figure 11, the next wizard page produces, a table (Figure 13) with n elements, where "n" is the number of data points in the ENDF file. The user can assign a "ng" value to each data point. The meaning of the "ng" point is described in the wizard page on Figure 13 and in the GANDR documentation, found on the GANDR website [16]. When finished, the user can use the button labeled "Next" to advance to the last wizard page (as seen on Figure 14), that allows the user to add sensitivities to other materials. The same page follows the page used to add covariance data (Figure 12) if the user has selected "Differential data" in the first page of the "Add material wizard" (Figure 11)
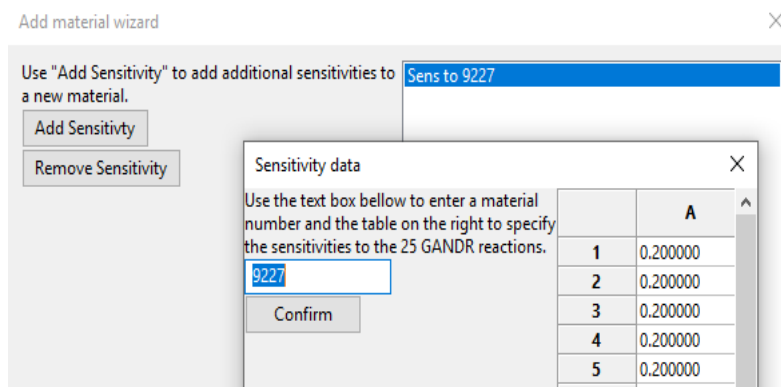
Figure 14 The last page of the "Add material wizard". It allows the user to add sensitivities to other materials.

Pressing the button titled "Add sensitivity" results in a modal dialog with a text entry button that must be used to enter the material number of the material our experiment is sensitive to and a table with 25 elements, where sensitivities to all 25 GANDR reactions can be entered. When all sensitivity data is entered in the dialog, the button with label "Confirm" can be used to add the sensitivity data to evaluation. Adding data will create a new element in the table displayed on the wizard page (Figure 14). The table entries can be double-clicked to view and edit sensitivity data. After pressing the button named "Finish", a new entry will be added to the table displayed on Figure 10, confirming successful addition.

If at least one experiment has been defined, pressing the button labeled "Finish" on the last page of the wizard (Figure 10), a new entry will appear on the table in the main window (Figure 1).

Mixed mode

The mixed mode allows the experimental data to be added in EXFOR format like in the "Classic" mode, but with the added capability of analyzing mixtures of materials, like in the "Standards" mode. The wizard is started by selecting "Add run wizard" on the main screen (Figure 1) and selecting "Mixture mode" on the first page of the "Add run wizard". The following wizard pages are a combination of pages from the "Classic" mode and "Standards" mode. Follow the instructions in chapters "Adding a "Classic" run" and "Adding an "Standards" run" to learn how the wizard is used.

Saving and loading configuration

GANDR GUI allows the user to save and load the entire configuration. The save/load system uses a serialization library named "Cereal" [16] to save all configuration parameters in a binary file and load it from a file in the same format.
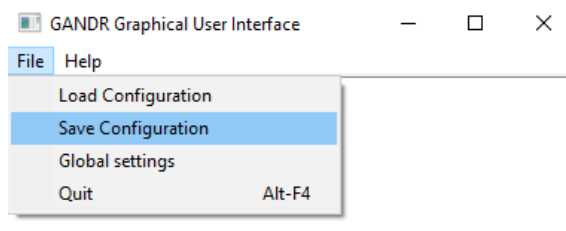

Figure 15 "Save configuration" and "Load configuration" options can be triggered from the "File" menu.

To save the current workspace, the user can select "Save configuration" option located in the "File" menu of the main screen (Figure 15) and use the dialog to specify file name. In a similar fashion, the user can select "Load Configuration" in the same menu to locate a save file.

After the configuration is loaded, the user can double click on any run in the list to open the corresponding wizard, where the parameters can be seen and edited.

The "Save configuration" and "Load configuration" options can also be accessed via

Running GANDR

In the Linux version, the user can use the button labeled "Run Selected" on the main screen (Figure 1) to write the selected runs in a file named "ganrun". And run the same file. If GANDR was started from a terminal window, that window will be used to display GANDR output.

On the same procedure will also cause a file named "ganrun" to be generated with the same contents as the Linux version, but GANDR will not be executed. The Windows version can be used to help the GANDR user prepare GANDR input and copy it later to a Linux computer capable of running GANDR. Care must be taken to modify all the paths in the GANDR input before transferring it to another computer.

References

1. GANDR documentation: https://www-nds.iaea.org/gandr/docs.html

2. GTK website: https://www.gtk.org

3. D.W. Muir, Global Assessment of Nuclear Data Requirements, Volume 2. The ZOTTVL Program.

4. https://github.com/wxWidgets/wxWidgets.git

5. Cereal GitHub page: https://github.com/USCiLab/cereal

6. https://www.iaea.org/resources/databases/endver