

ERYA v2.35 (ERYA/Profiling Tutorial)

# **ERYA Profiling**

## **User Guide & Tutorial**

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## Introducing ERYA Profiling

### Welcome!

ERYA Profiling is a software application designed to aid the analysis of thick samples, where the main task is to figure out what is their composition in terms of their elements and/or isotopes.

It is the natural evolution of the ERYA-Bulk program, where a more realistic physical model is applied.

The efficiency of the method implemented by this software depends highly of the physical model, experimental setup and measurement accuracy.

In general, the measurement of samples beamed by light particles are more precise when the sample had lighter elements than weighted ones, and this fact makes possible to use the excitation function of lighter elements by their gamma emissions to determine the composition of the sample.

Since it uses the gamma emissions of the sample's elements, it justifies why this analytical method is called PIGE (Particle Induced Gamma Emission).

This program avoids the problem-prone and time consuming tasks to evaluate the results, that once require several printed tables, and an huge man-powered tedious calculation task, now it gives the results in a matter of seconds.

ERYA-Bulk was developed at LibPhys-UNL, by the institution *Faculdade de Ciências e Tecnologia* (FCT) - *Universidade Nova de Lisboa* (UNL), on *Departamento de Física* (Physics Department), postal code address 2829-516 Caparica, Monte da Caparica, Portugal.

ERYA-Bulk was programmed by Vasco Manteigas ([vm.manteigas@campus.fct.unl.pt](mailto:vm.manteigas@campus.fct.unl.pt)), with advice from Micaela Fonseca ([micaelafonseca@fct.unl.pt](mailto:micaelafonseca@fct.unl.pt)), and Luís de Souto Martins, where the first one was the original programmer of the previous LabView ERYA version, and the second one implements the numerical routines of the first version of ERYA-Profiling, bundled on LabView version.

**Disclaimer:** All Software screen-shoots are made from the Windows version running on a Linux computer using the Wine compatibility layer. Some screen-shoots from Mac OS X version are provided for additional acquaintance.

## Physical Theory of Gamma Ray Emission Yield Analysis on Heterogeneous Samples

The program evaluate the stoichiometry composition of an heterogeneous sample, make by several layers, where each one composition can be made of several elements, by evaluate the nuclear reaction yield of each element. Since, in theory, the yields depends of their relative stoichiometry, it is possible to find the correct sample composition using this method.

On the homogeneous case, each individual yield could be evaluated from the following integral:

$$Y(E_0) = \epsilon_{\text{abs}}(E_y) n_p f_m f_i N_A A^{-1} \int_0^{E_0} \frac{\sigma(E)}{\epsilon(E)} dE \quad (1)$$

Where it depends from the Detector Efficiency ( $\epsilon_{\text{abs}}$ ) at the element gamma ray emission energy, the number of protons ( $n_p$ ), the element/isotope relative abundance ( $f_i$ ), the relative fraction mass ( $f_m$ ), the isotope/element atomic mass ( $A$ ) and Avogadro's Number ( $N_A$ ).

Both multiplied by the proper integral in function of energy, where depends from the element's cross-section excitation function ( $\sigma$ ) and the stopping power ( $\epsilon$ ). Each of relevant functions depends from the relative stoichiometry of the sample.

When the sample are heterogeneous, the integral is a little more complicated, since the the terms related to the relative stoichiometry now depends on the depth, or energy, where it turns to be:

$$Y(E_0) = \epsilon_{\text{abs}}(E_y) n_p N_A A^{-1} \int_0^{E_0} \frac{f_m(E) f_i(E) \sigma(E)}{\epsilon(E)} dE \quad (2)$$

And a more realistic model of energy dissipation require to take account of the energy loss of the beam. This require to model a distribution of the energy straggling dissipation, and another distribution related to the own detector's physics, where on on-line help is called, by convenience, the thermal distribution.

Since the energy variable can be spitted by the sum:

$$E = \bar{E} - \Delta E \quad (3)$$

Making a distinction of the average energy  $\bar{E}$ , and energy dispersion  $\Delta E$ , the integral in (2), can now be written:

$$Y(E_0) = \epsilon_{\text{abs}}(E_y) n_p N_A A^{-1} \int_0^{E_0} \int_E^{\infty} \frac{f_m(E) f_i(E) F(\bar{E}) \sigma(\bar{E})}{\epsilon(E)} dE d\bar{E} \quad (4)$$

Where the cross-section on ERYA-Profiling is now an integrable function along the dispersion distribution  $F$ . And since the actual distribution is the convolution of a thermal and a straggling one, the integral (4) is now a triple integral:

$$Y(E_0) = \epsilon_{\text{abs}}(E_y) n_p N_A A^{-1} \int_0^{E_0} \int_E^\infty \int_{\bar{E}}^\infty \frac{f_m(E) f_i(E) F_T(\bar{E}') F_S(\bar{E} - \bar{E}') \sigma(\bar{E})}{\epsilon(E)} dE d\bar{E} d\bar{E}' \quad (5)$$

In order to simplify (5) to be reasonable to implement the numerical integration of the yields, the program make the following simplifications:

- The sample are sliced by several layers with a constant depth  $x$ , where the stoichiometry can be constant of each element, then the yield of an element is the sum of all partial yields respective to each layer, this replace the energy integration, by a sum of partial yields:

$$Y(E_0) = \sum_{L=1}^N Y_L(\bar{E}_L) \quad (6)$$

And the average energy at the current layer  $\bar{E}_L$  are a constant along the main terms of the integral, leaving the integral of the distributions separated, since:

$$Y_L(E_L) = \epsilon_{\text{abs}}(E_y) n_p f_m(\bar{E}_L) f_i(\bar{E}_L) N_A A^{-1} \int_{x_0}^{x_1} \int_{y_0}^{y_1} \frac{F_T(x) F_S(y-x) \sigma(\bar{E}_L - y) \Delta \bar{E}_L}{\epsilon(\bar{E}_L)} dx dy \quad (7)$$

Where the double integral domain  $x = [-3\Omega_T, 3\Omega_T]$ ;  $y = [\lambda_0, \lambda_{0.995}]$  are truncated along the 3-sigma approximation of the relevant distributions.

The thermal distribution is a Gaussian Distribution, truncated at 3-sigma, where it is numerically trivial to evaluate. However, the straggling is modeled by a Vavilov Distribution, which require additional numerical routines to handle properly.

A full discussion of the numerical Vavilov Distribution is out of scope of this manual, but some additional information can be retrieved on on-line help, and a full description are elucidated on the program bibliography.

Also notice that ERYA-Profiling evaluate a series of (6,7) integrals along a sequence of several energies, in order to evaluate a spectrum of yields in function of the initial energy.

## What's New on ERYA Profiling?

This application was a full rewrite of a previous LabView program that handles the PIGE database management, and an additional program that made the numerical profiling of the sample.

With the new ERYA-Profiling, all code is integrated on a single program.

ERYA Profiling is now fully implemented on C++ language, while the core framework, including the Graphic User Interface, are derived from a cross-platform library called wxWidgets.

wxWidgets is an open-source framework inspired from the Microsoft Foundation Classes, and compliant with the Standard Template Library, while extends to be compatible to several operating systems and computer architectures, easing the port to several systems.

The new ERYA Profiling (Emitted Radiation Yield Analysis) are available natively for Windows, Linux and Mac OS X, and several modern computer architectures, since it runs on 32-bit and 64-bit CPU, either Intel or ARM.

Binary packages are available for Windows, Linux and Mac OS X Intel x86-64 versions. Linux packages for ARM machines, such as the ARM mini-computers like the Raspberry Pi 3, Pine 64 or Kirin are also available. The supported Linux distributions are Debian 9 Stretch, or any derivative of this distribution, like Ubuntu 18.04 LTS.

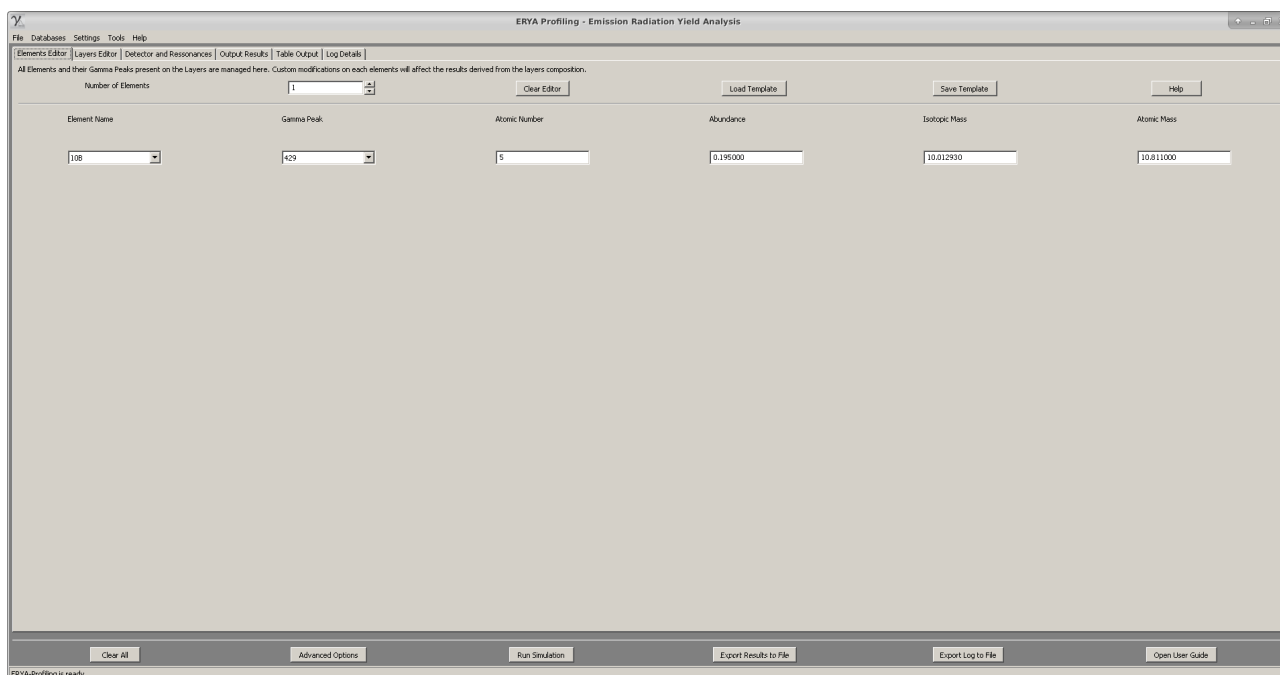
If you are interested to contribute to maintain the wxWidgets ERYA Profiling source-code, or any issue related to the program use, please contact the programmer by it's e-mail.

The standard package contains a Database with over 100 elements and isotopes, the 1977 and 1991 Ziegler Parameters, and a sample Detector profile. Both of this three files can be edited by the user, and later on next manual section, it will detail the recommended steps to edit safely the Databases.

The software can export the original LabView ERYA Databases, and convert them to the native wxWidgets ERYA Database format, saving countless hours of manual workarounds to export the databases. Even this feature are maintained for legacy support, all conversion features will be described on the *LabView Export* chapter.

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### The new ERYA-profiling Main Program User Interface...



Like the previous ERYA-Bulk companion program, ERYA-Profiling shares the following core features:

1. A new unified Database format for the Elements, Detector and Ziegler Parameters, that use the standard XML document format, and inter-changeable between the wxWidgets ERYA-Bulk and ERYA-Profiling.
2. An on-line help, although simple, which explain the main program features, and major tasks.
3. New file filter imports of IBANDL files, ASCII source files and Excel 2007 Xlsx files, where the user can get more quickly the data, and convert to the desired native data structures.
4. The whole GUI was written from scratch, and use the new wxWidgets objects which make more easy to handle data, and implement a more concise work-flow. And also simplifies the porting to several operating systems.

More details can be obtain from the ERYA-Profiling own on-line help system.

## Quick Start!

To install ERYA-Profiling it is very simple...

- Select the adequate package which matches your operating system and architecture, and download it to your computer. All packages require, by default design, to install on computer's local storage. Normally, the user just need to run the package installer that will move the asset files to the default protected program directory. Once installed, just open the menu entry of ERYA to run the application.

**Windows:** For Windows users, the wxWidgets libraries and GNU C++ Runtime Library are already bundled on the application installation package.

The Windows version package will install ERYA on the default Program Files folder, and will create an Start Menu entry.

**Linux:** The Linux version are normally available as a Debian package. Ubuntu or Mate distributions usually give a GUI tool to install packages, while Debian usually don't install such GUI tool by default. You need a Linux distribution compatible with Debian 9 Stretch, with backports repository enabled, or Ubuntu 18.04 LTS to install ERYA correctly.

As a general rule, open a Terminal application, and type the following commands to install ERYA:

```
$ sudo apt-get update && sudo apt-get dist-upgrade (Update manually your system)
```

```
$ sudo dpkg -i eryaprofiling_2.25-5_amd64.deb (64-bit Intel)
```

```
$ sudo dpkg -i eryaprofiling_2.25-5_i386.deb (32-bit Intel)
```

```
$ sudo apt -f install (To install the library dependencies.)
```

Note: If sudo command not work as devised, as more likely to happen on the Debian 9 systems, use "su" instead to open a root shell. Then repeat the same commands without the "sudo", since it was already a root session.

**Attention:** On Debian 9 Stretch, enable the Debian backports repositories beforehand, in order to install the updated wxWidgets libraries, by editing the /etc/apt/source.list file, merging the following line, as root:

```
> deb http://deb.debian.org/debian stretch-backports main contrib non-free
```

And then install the required libraries:

```
$ sudo apt -t stretch-backports -f install (Replace stretch by your current Debian Version)
```

**Mac OS X:** For Macintosh users, please update your computer software to a more recent version. Versions of Mac OS X up to 10.10 and 10.11 are reported to work fine.



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In order to install ERYA, once downloaded to your computer, just extract the zip file and then copy the ERYA-Bulk.app to the Applications folder.

**Other Linux Systems:** If you have a Linux mini-computer using an ARM processor, select the 32-bit *armhf* package, or the 64-bit *arm64* package. This will install ERYA using the same procedure as described on “Linux” previous section, that is:

```
$ sudo dpkg -i eryaprofiling_2.25-6_armhf.deb (32-bit ARM)
```

```
$ sudo dpkg -i eryaprofiling_2.25-6_arm64.deb (64-bit ARM)
```

```
$ sudo apt -f install (To install the library dependencies.)
```

**Note:** Only recent ARM mini-computer boards support 64-bit binaries! The Raspberry 3 model support both the 32-bit and the 64-bit versions, but require to install the Debian 9 Stretch *arm64* version to work on 64-bit.

Since ERYA-Profiling require several computation time to handle all numerical simulations, consider to use a powerful computer to handle the task. Linux ARM real capable computers are the ones with 64-bit CPU such as the Snapdragon Series 800.

### **Additional warnings on Linux Versions:**

All Linux versions requires a X11 Window Server to run, or any windowing system capable to use the Xlib/GTK toolkit. Normally, all supported distributions will install and configure the base dependencies, and don't require any user manual configuration.

The program itself don't require more than a standard video display driver.

### **Starting ERYA-Profiling:**

- On Windows, select Start > ERYA-Profiling, and ERYA-Profiling main icon.

(On Windows 10, type ERYA on search-box to grab the launcher quicker)

- On Linux, select the icon from Programs > Education/Science > ERYA-Profiling.

(The real category can vary according to the default's Desktop Manager of your Linux distribution.)

- On Mac OS X, open the Applications folder from Finder, and then find and click on ERYA-Profiling icon to start the program.

### **Removing ERYA-Profiling:**

- On Windows, select the uninstaller icon, or from "Control Panel">"Program and Features", select the ERYA-Profiling group, and follow the instructions.

- On Linux, open a terminal application and type the following command as root:

```
$ sudo apt-get remove eryaprofiling
```

- On Mac OS X, simply delete the "ERYA-Profiling" program from "Applications" folder on Finder.

- Consult the table on next "Initial Setup" section, to find and delete the local profile folder, if necessary to clean the remaining vestiges.

## Initial Setup

At first run, the ERYA will create a configuration file, where the default Databases are defined.

It will trigger an wizard to guide the user, in order to select the default databases, and some program settings. Once made a correct configuration, ERYA will load the configuration file to select and load automatically the database files.

The user can place the configuration file as a local or portable setting, as explained below:

Operating System	Windows	Linux	Mac OS X
Portable Setting	In the same program directory		
Local User Profile	C:\users\name\Local Settings\Application Data\ERYA-Profiling-Win64\*	/home/name/.ERYA-Profiling-Linux/*	/Users/name/Library/Application Support/ERYA-Profiling-OSX/*
Config Name	ERYA-Profiling-Win64.conf	ERYA-Profiling-Linux.conf	ERYA-Profiling-OSX.conf

**Warning!** Do not choose a Portable Setting if you install the program to a protected directory.

**Note:** A guided step-by-step setup for Windows and Mac OS X are displayed on the next session.

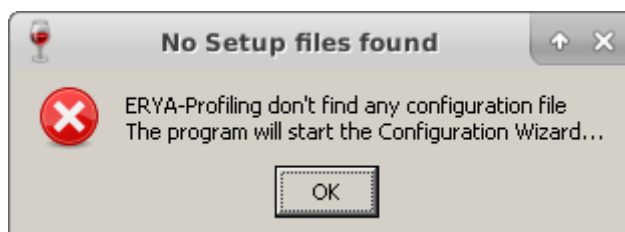
**Portable Setting:** Once the configuration file are written on the program directory, the setup is complete. Any change of core Detector, Elements and Ziegler will overwritten the original program ones, since you set the same working directory.

**Local User Profile Setting:** Once the profile folder are created, and the configuration file are written, a copy of Database, Ziegler and Detector files are created on the same local user profile folder. Any changes by the user will change, by default, the local copies, not the original ones on the program folder. At least you can save the original files as an informal backup.

**Note:** Once ERYA are correctly configured, the program should load the databases and display the main GUI without any errors, otherwise it may be necessary to read the Troubleshooting guide to try solve the problems.

### Initial Setup Step-by-Step

1. Once ERYA are started by the first time, the application will display a warning about absent configuration files. If you have installed before, it is highly recommended to delete first the local user profile folder has described by the table on the previous chapter, then repeat this step again.



2. It will start a wizard, guiding the user for the next steps. Just click on “Next” to go forward, or “Prev” to go back. The wizard will not make any real work until the user choose all obligatory settings.

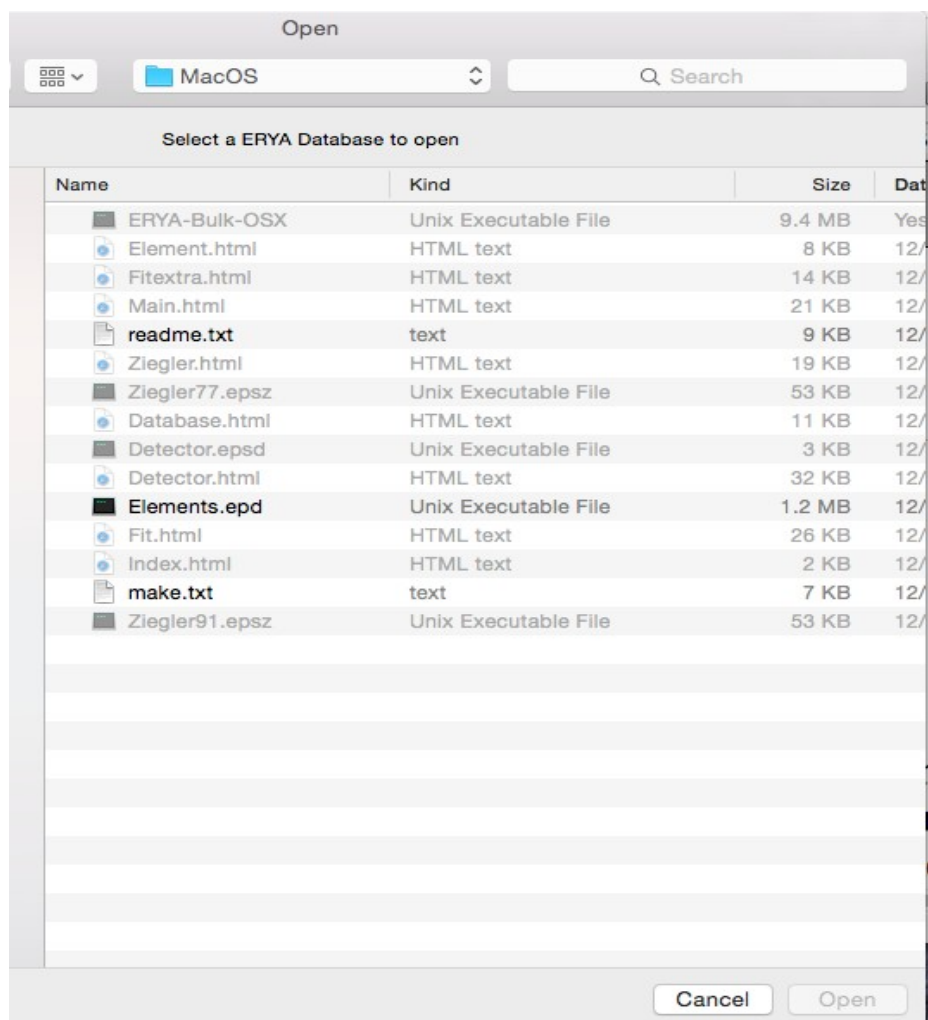


Notice that each wizard pages will ask to select a compatible database file.

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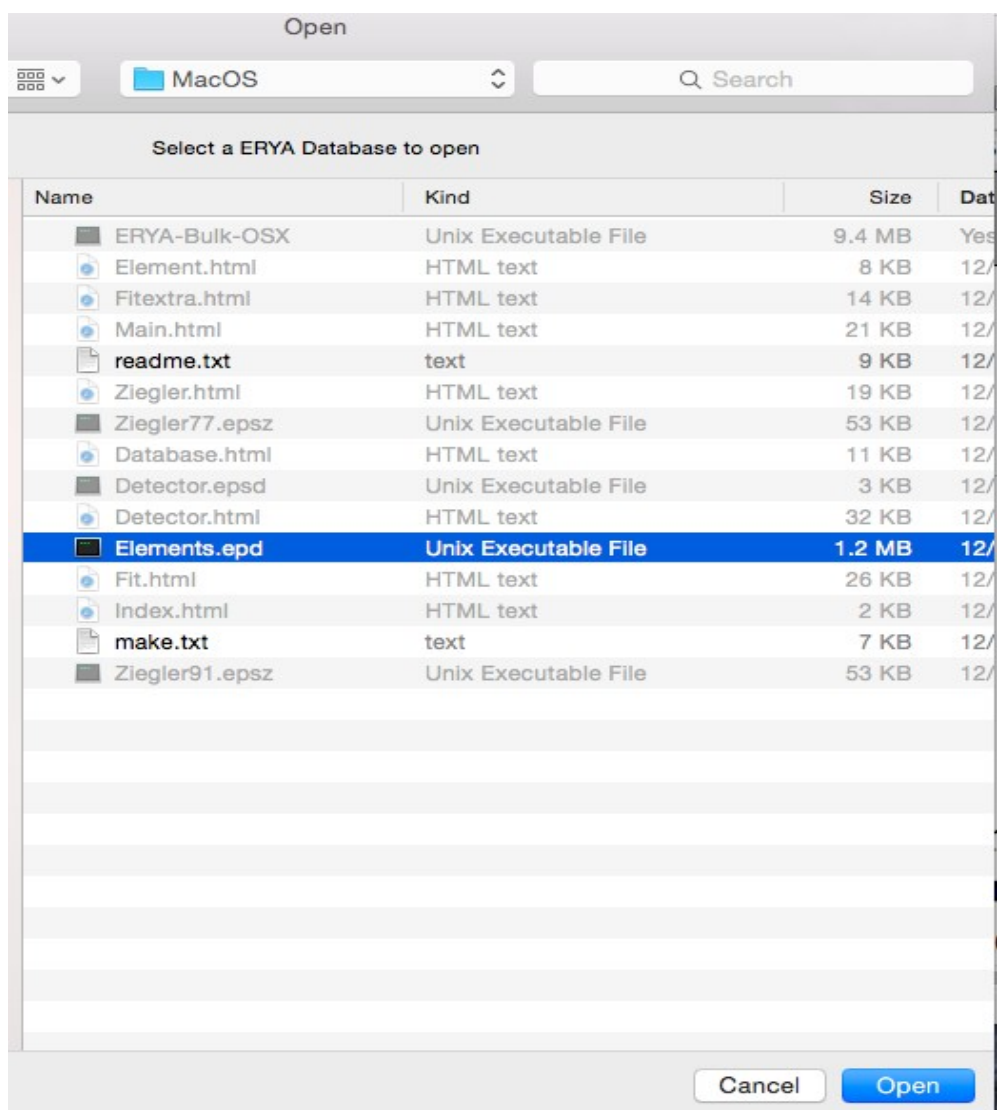
3. Now the program will ask from the ERYA's package, which file should be the default start-up Element Database. Since Windows and Linux standard dialogs are more easy to filter files to the supported extensions, just select the file with **epd** extension.

On Mac OS X, the standard dialog will display all files, but shades the incompatible ones:



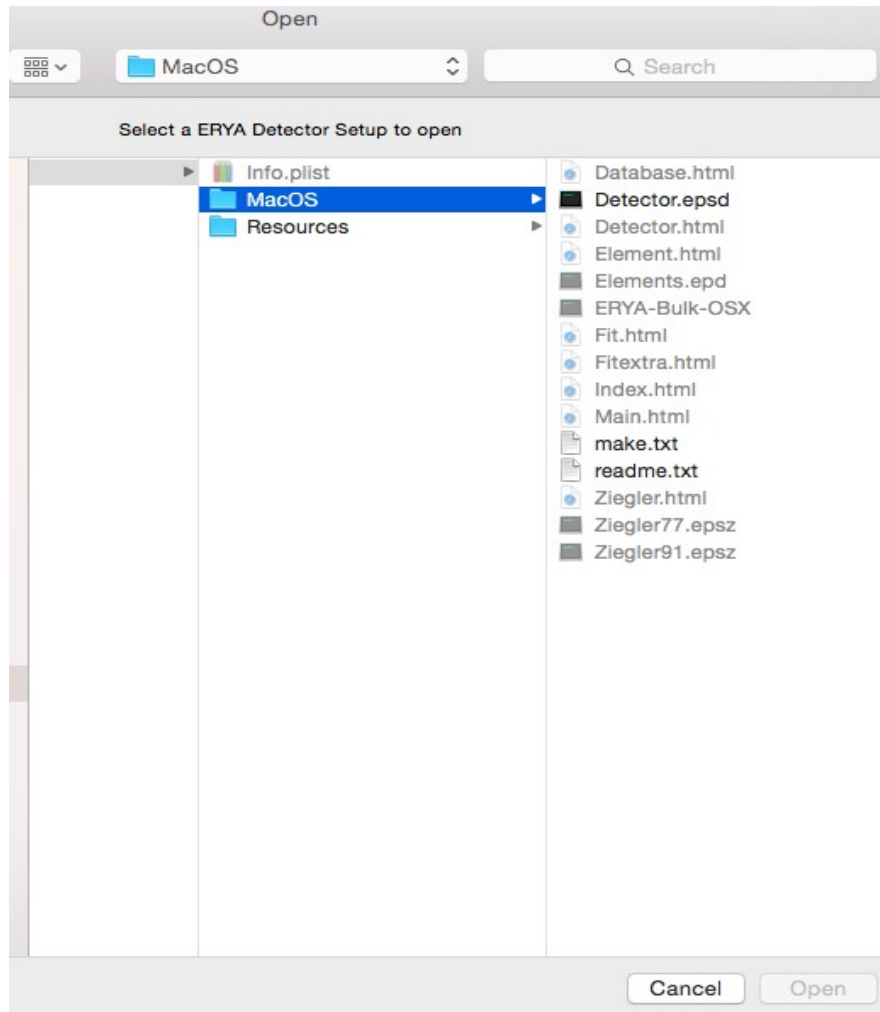
## ERYA v2.35 (ERYA/Profiling Tutorial)

And select the file with **epd** extension, as indicated:



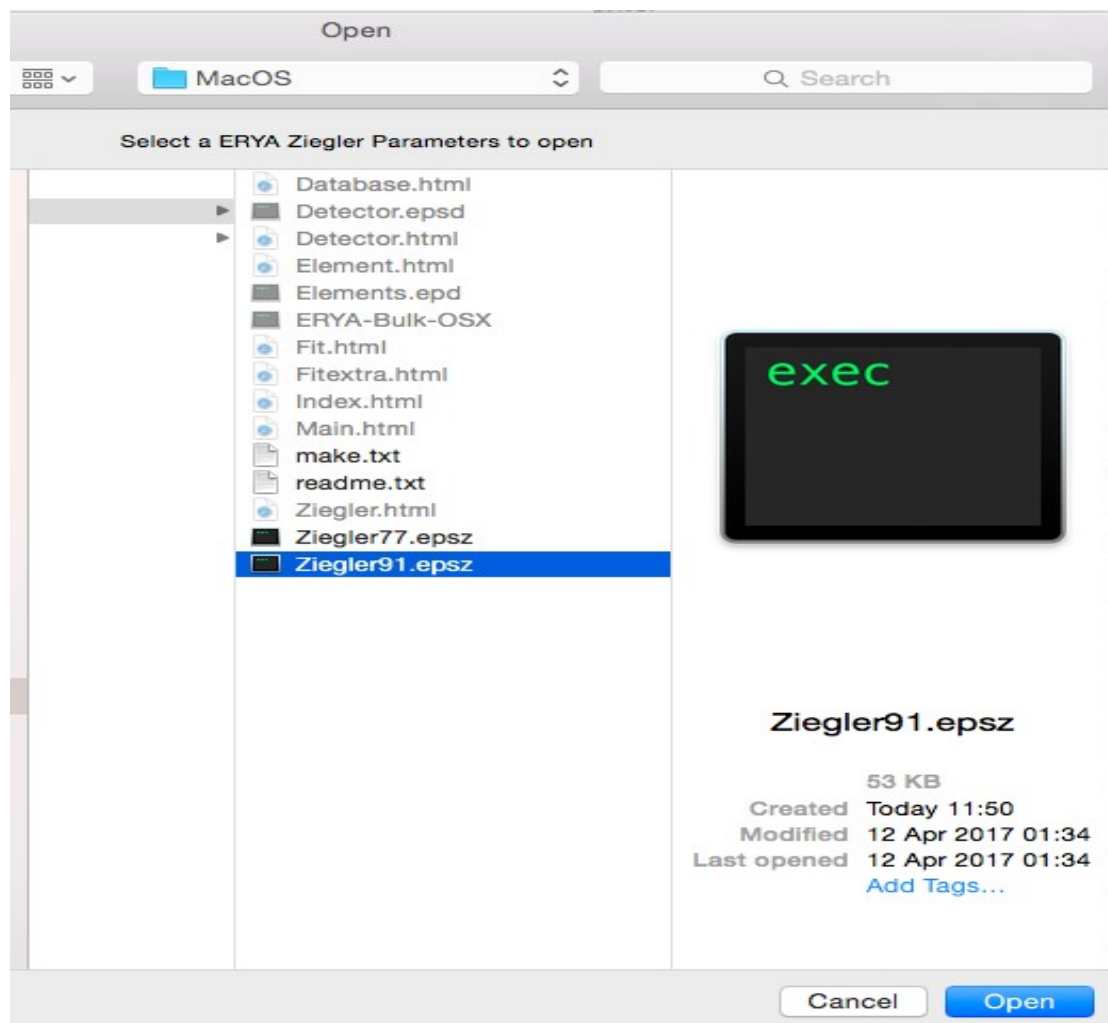
## ERYA v2.35 (ERYA/Profiling Tutorial)

4. The same logic will apply for the Detector Profile, and select the file with **epsd** extension:



## ERYA v2.35 (ERYA/Profiling Tutorial)

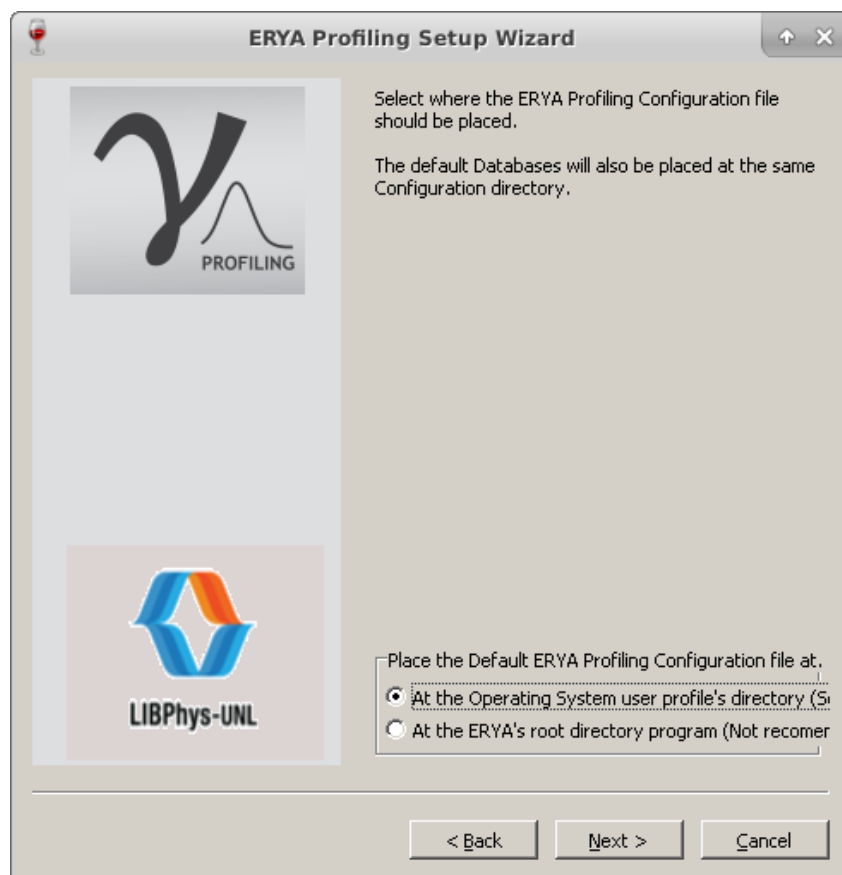
5. Finally, select the file for the Ziegler Parameters, with **epsz** extension, where it is recommendable to choose the most recent version:





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**6.** At the last page, the user can select the local (default) folder profile, providing by the default operating system's settings, or the root folder (the same of the main program). It is highly recommendable to select the local profile setting.



Once selected, click “Next” to read the final informations, and click on “Finish” to start the real configuration procedure.

**7.** The selected files are analyzed, and placed on the target directory.

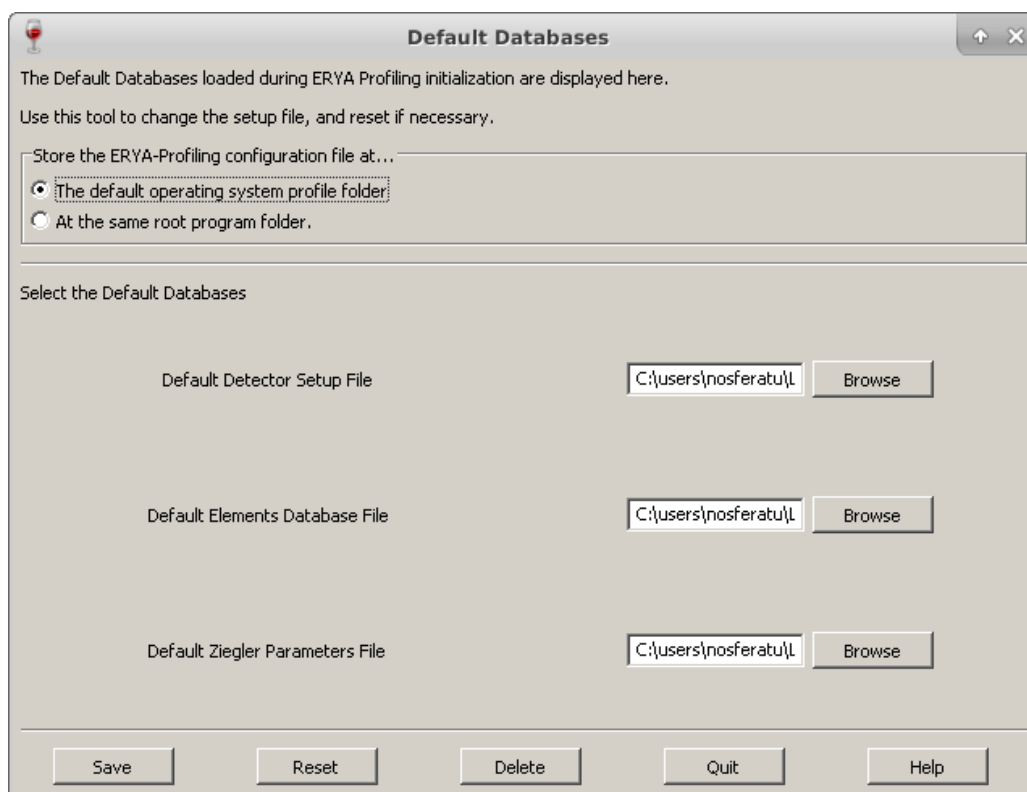
**8.** The configuration file are created, and the main GUI is loaded automatically. ERYA-Profiling are now ready to use, unless an error occurs (see the Troubleshooting section for additional details).

On next start-ups, the program will load the configuration file automatically, and the main GUI starts without additional user input.

## Changing Setup Settings

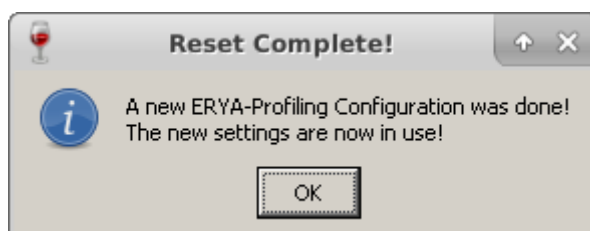
To change the Default Databases, you can use the built-in widget from Settings > Program Settings...

Where a new widgets opens, and the user can change the current settings, and update the new ones.



ERYA will check the new default databases, and update the configuration file, if successfully.

The program will warn the user when the new settings are updated, and can resume from it.



## Setup Troubleshooting Guide

1. In case of some error, whatever the motive, that makes ERYA warns about corrupted or non-existent databases, then program will start without any databases.

In this case you can use the Setup widget tool as explained before, and then select “Delete” to delete the wrong configuration file, where it will force ERYA to repeat the initial setup wizard again. The same can be made, by the Settings > Reset Settings menu option.

If necessary delete manually the user profile folder as detailed on “Initial Setup”, to force ERYA to start the initial setup routine again. Also, delete any configuration file on root program folder.

Avoid to use third-source database files to perform a clean installation, since it could be the source of problems.

2. If the ERYA warns that cannot write any file, even the configuration file, to the selected folder, this means you are trying to write on a protected folder that requires additional privileges.

ERYA-Profiling’s author recommends that in any circumstance, **you should not run ERYA-Profiling** with administrator privileges, since it is not necessary, and can make a mistake that could overwrite important operating system files unnecessarily by user’s own mistake.

3. The optimal screen size for ERYA is a FullHD screen (1080p), but can work on a 720p screen at minimum, and main window screen will create scroll bars in case when the screen don’t fit all the elements on the same time. If the other windows appear cropped, then you need to increase the screen resolution.

## Explore the Database Management Tools

### Detector Efficiency

One of the essential Databases needed to ERYA operate is the Database Efficiency profile file.

To manage the Detector profile, open the widget from Databases>Detector Efficiency, and then should open the following dialog panel:

Input the desired algebraic function that models your detector efficiency:

fxvar = E, fyvar = F: a3=-2078.4, a2=-312.84, a1=5.006, a0=0.001: x=1/E, F=a3\*x^3+a2\*x^2+a1\*x+a0

Or export a file, and edit the following table:

	Energy (keV)	Absolute Efficiency
1	3451.152	0.002234752
2	3272.99	0.002316666
3	3253.416	0.002326201
4	3201.962	0.002351812
5	2598.458	0.002726009
6	2034.755	0.00326954
7	2015.181	0.003293695
8	1771.351	0.003637642
9	1408.011	0.004360555
10	1360.25	0.004482848
11	1298.6	0.00465329
12	1238.282	0.004835545
13	1212.95	0.004917178
14	1175.102	0.005045307
15	1112.116	0.005276634
16	1087	0.005375862
17	1037.84	0.005583019
18	964.131	0.005930237
19	867.388	0.006467974
20	846.772	0.006597056
21	778.903	0.00706562
22	688.678	0.007815736
23	443.976	0.011114434
24	411.115	0.011794414
25	383.859	0.012425139
26	367.789	0.012829216
27	356.014	0.013141918
28	344.275	0.0134686
29	302.858	0.01475321
30	276.404	0.01560384

Buttons: Import, Export, Copy, Paste, Clear, OK, Cancel, Help

The operation are straightforward, and a good useful documentation can be readied from the “Help” button.

In practice, this editor combines a text field, that expects that the user fill an algebraic expression that gives the Detector Efficiency in function of Energy, and a two-column table to fill any experimental values for the Detector Efficiency.

The origin of this dual configuration is mainly for compatibility with previous softwares.

Both fields can be filled, however ERYA will choose the by default the function field if it is correctly defined, ignoring the table.

Selecting the table option, the user should fill the highest number possible of experimental values, but the accuracy will be better if the energy range and number of values are higher, since the program will make a segmented linear interpolation along the values of the efficiency table.

### **Managing the Detector Efficiency profile file**

While it is possible to fill directly the detector's efficiency data by using the built-in spreadsheet editor, the user can also export any compatible experimental values from external files.

The native Detector Efficiency profile file is a XML file, where stores the experimental efficiency points, and the additional user defined efficiency function. This file had a **epsd** extension.

By other hand, it is possible to export and import the experimental efficiency (the custom function are discarded!) from or to an ASCII file, which requires to be a full numerical two columns of data, separated by a space or tab (Any decimal number should use the C-like standard, like 5.5), or even an Excel file.

The Excel file should be a simple sheet (or fill the first sheet only) with only two columns of numbers, and it is highly recommendable to avoid any cell formating, or attachments, but it is fine to add labels on the first row, which will be ignored.

The ERYA's Excel file filter only supports Excel 2007 and beyond version files (with **xlsx** extension), and only recognizes cells with names and numbers.

Any edition can be stored by using the "Export" button, and then choose the native XML (epsd), ASCII (txt) and Excel (xlsx). You should overwrite the Default Detector Profile, as you defined on initial setup and described on "Quick Setup" chapter, to make permanent changes.

Stored and additional Detector profiles can be loaded from the "Import" button, and it will overwrite the previous content.

By clicking "OK", the current edition will be used by ERYA program as a new default Detector Profile. Hitting "Cancel", any edition will be discarded.

### **Deprecated Features:**

Albeit deprecated, it is also possible to copy the table contents to a text or spreadsheet file. Just select the contents, and click "Copy", and then paste to your text editor. The reverse is simpler, click on the first target cell, and then click "Paste". If necessary, clear the built-in table by clicking "Clear". Since this feature is more a hit-and-miss regarding to formating, the clipboard feature is not recommended, and it's deprecated.

## Custom Efficiency Function

The optional algebraic efficiency function is the new ERYA feature, and it is just a input line box to the user code a custom function, overriding the table interpolation.

Taking the following example, as a good starting point:

**fxvar = E, fyvar = F: a3=-2078.4, a2=-312.84, a1=5.006, a0=0.001:**

**x=1/E, F=a3\*x^3+a2\*x^2+a1\*x+a0**

It represents, symbolically, the following function:

$$\epsilon_{\text{abs}}(E_y) = 0.001 + 5.006 E_y^{-1} - 312.84 E_y^{-2} - 2078.4 E_y^{-3}$$

In reality this feature are a very simple programming language built into ERYA, implemented as an interpreter, and an extensive explanation are described on Detector's on-line help (Click "Help" to open).

Basically the user should define the function variables (accepts one dependent *fyvar* and one independent *fxvar* ), and optionally, but highly recommended, any number of numerical constants.

Finally, it should write the algebraic function, in a manner much similar to Fortran, C or Basic (The Built-in language is more similar to Simple Basic, but restricted to algebraic expressions.).

Each major section should be separated by colons (:), and any sequence of variables should be separated by commas (,).

Any expression should be any algebraic formula assigned to a variable by the equal (=) sign.

Any function variables and constants should be declared first, before use them to the algebraic function! (Or you get a declaration error, which can be triggered by clicking "OK", since it will make a full syntax check before update the current Detector profile.)

To simplify the function, it is possible to make a chain of functions, separated by commas (,), as long all relevant variables and partial functions are previously declared. Like the own example already shown, by defining a compound function by the variable *x* as *x=1/E*, the main function can be written as a normal polynomial.

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### Ziegler Parameters

Like the Detector counterpart, the Ziegler Parameter widget follows the same layout and functions. The ERYA accepts the 1977 and 1991 Ziegler model, and both of them are hard-coded on the ERYA code. This editor manages the experimental parameters required by this model. It is also possible to use the SRIM interpolation tables, or define a custom macro similar to the Detector widget.

The Ziegler Editor are opened from Databases > Ziegler Parameters

	Element	A-1	A-2	A-3	A-4	A-5	A-6	
1	H	0.0128116	0.00533047	0.651042	0.531902	1959.010	1.188700	598.26
2	He	0.3117870	0.00499529	0.118546	0.920917	984.843	1.082230	554.38
3	Li	0.6445030	0.00500368	0.866544	0.567488	962.900	1.015660	1620.3
4	Be	0.9535610	0.00507406	1.304500	0.590300	1945.120	1.057030	326.95
5	B	1.5315100	0.00488520	2.567600	0.423246	1738.880	1.032080	1829.4
6	C	2.4028900	0.00491497	2.491010	0.414939	1858.360	1.015810	2504.1
7	N	3.3100700	0.00495744	0.540621	0.779940	1104.150	0.967848	2235.3
8	O	0.9727060	0.00500390	1.351020	0.549900	1254.280	0.968356	5093.2
9	F	0.6904080	0.00462723	0.326749	1.105200	1301.900	0.943525	47.037
10	Ne	0.2812350	0.00459698	0.525630	0.878183	1158.300	0.938564	10.160
11	Na	2.1535200	0.00440847	2.309230	0.606001	1332.240	0.943478	735.11
12	Mg	3.4298300	0.00436897	2.393770	0.554737	1140.290	0.929844	2107.4
13	Al	0.0389096	0.00454168	4.279750	0.478838	1316.420	0.934106	565.57
14	Si	1.3310100	0.00443533	1.522620	0.775843	1227.020	0.914146	1091.1
15	P	5.7811900	0.00398281	0.324072	1.227690	673.459	0.865731	123.61
16	S	0.6117410	0.00446376	3.381010	0.542907	1160.670	0.912049	14031.
17	Cl	1.1530700	0.00447333	4.204640	0.538231	1301.130	0.902702	4923.0
18	Ar	1.7040800	0.00447609	2.750720	0.583835	2713.930	0.953183	2035.7
19	K	2.6026500	0.00432185	1.568110	0.864656	556.393	0.844750	120.01
20	Ca	0.5365550	0.00440846	3.227060	0.602927	500.851	0.833450	1766.3
21	Sc	1.7187000	0.00436934	4.602850	0.516212	1601.600	0.914664	6341.6
22	Ti	0.1464030	0.00484558	5.540140	0.455903	1763.460	0.919014	3951.9
23	V	4.2123800	0.00400130	3.798580	0.482892	2416.970	0.936204	7735.9
24	Cr	0.6978810	0.00430794	2.286300	0.784069	967.872	0.857874	17.852
25	Mn	0.5927430	0.00431334	1.406250	0.968261	1426.420	0.881488	14.400
26	Fe	0.0283155	0.00354506	0.564961	1.241110	1527.810	0.881848	25.949
27	Co	0.2695450	0.00432088	2.242490	0.764706	1243.910	0.867051	23.491
28	Ni	3.6823400	0.00437139	1.521460	0.736656	1470.860	0.874909	251.68
29	Cu	2.1540300	0.00432278	2.693900	0.523003	1717.270	0.893617	2099.3
30	Zn	0.5318470	0.00382833	0.675606	1.066470	1008.480	0.826099	35.893
31	Ga	6.9197300	0.00401198	0.522284	0.974708	899.033	0.821636	371.58

When a new parameters file are loaded, the ERYA will try to figure out the difference from the 1977 and 1991 Ziegler models, by counting the number of nonzero columns, but the user can override the program own guess by selecting the desired version from the pull-down menu located above the spreadsheet editor.

Is also the only Database where the ERYA-Profiling differs slightly from the ERYA-Bulk, since on this program, it contains 16 columns, due to the extra “Element Density” and “Bloch Parameter”.

The other controls are very similar, in terms of features, of the Detector widget. Like the Detector, it is possible to copy and paste from a compatible text or spreadsheet file.

The native Ziegler Parameters file is a XML file with **epsz** extension. If the user desires, it is possible, like the Detector widget, to import and export the current built-in table content to a text file or an Excel file.

### **Cautions between ERYA-Bulk and ERYA-Profiling Ziegler's Databases**

Both programs use the same XML based *epsz* file, but had a slight difference: the ERYA-Profiling had two additional columns for the density and mean ionization constants.

This means, that if ERYA-Bulk reads the ERYA-Profiling Ziegler's database it will discard the two unused columns (and save it will rebuild as the expected ERYA-Bulk version).

And ERYA-Profiling when read the ERYA-Bulk version will add a filler value "1" to all densities, and "10" for all mean ionization parameters.

On previous LabView ERYA profiling, those columns are two additional text files, since it use the same binary Ziegler file from the LabView ERYA, and on this new program, the extended Ziegler database combine all former files.

To avoid manual merging, considerer to use the "Tools" > "LabView Import" wizard described on the *LabView Import Tools* chapter.

It's possible to export and import the Ziegler's parameters using an Excel *xlsx* file, but avoid to share between programs, to avoid unexpected results.

### **Using the SRIM tables**

If you want to use the SRIM tables for the stopping-power, select the option from the top right scroll-box. When selecting the SRIM tab, it is possible to switch between the interpolation tables for each selected element. The number on scroll-box is the element's atomic number.

When the user select the "Import" button when the SRIM tab is active, ERYA will parse the Stopping-Power table created by the SRIM® software, and place automatically the values on the correct atomic number table.

The ERYA's **epsz** database file will store the SRIM interpolation tables along the Ziegler's Parameters.

### **Converting from other formats**

ERYA's Ziegler widget can import at read-only level, the binary LabView Ziegler's Parameters file (and add two placeholder values for density equal "1", and Bloch Parameter equal "10"), and the ASCII SRIM's Stopping Power output file.

Even both formats had the same "ASCII txt" extension, ERYA had the filter libraries to handle the different formats automatically.

Pure numerical ASCII and Excel *Xlsx* files can be imported, but requires the user take care to the current context. When the current select tab are the Ziegler spreadsheet, any imported file requires



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to be with 14 or 16 columns. Otherwise, with the SRIM tab active, the user should elect manually the correct atomic number, before import the file that should had two columns of numerical data.

Either way, when the program read the Ziegler's file, the element's name column are replaced to their chemical symbol, since the program had an hard-coded dictionary to this task.

When the user export the tables, it will extract the selected SRIM table or Ziegler table to a text file format, composed by two or 16 columns of numerical data.

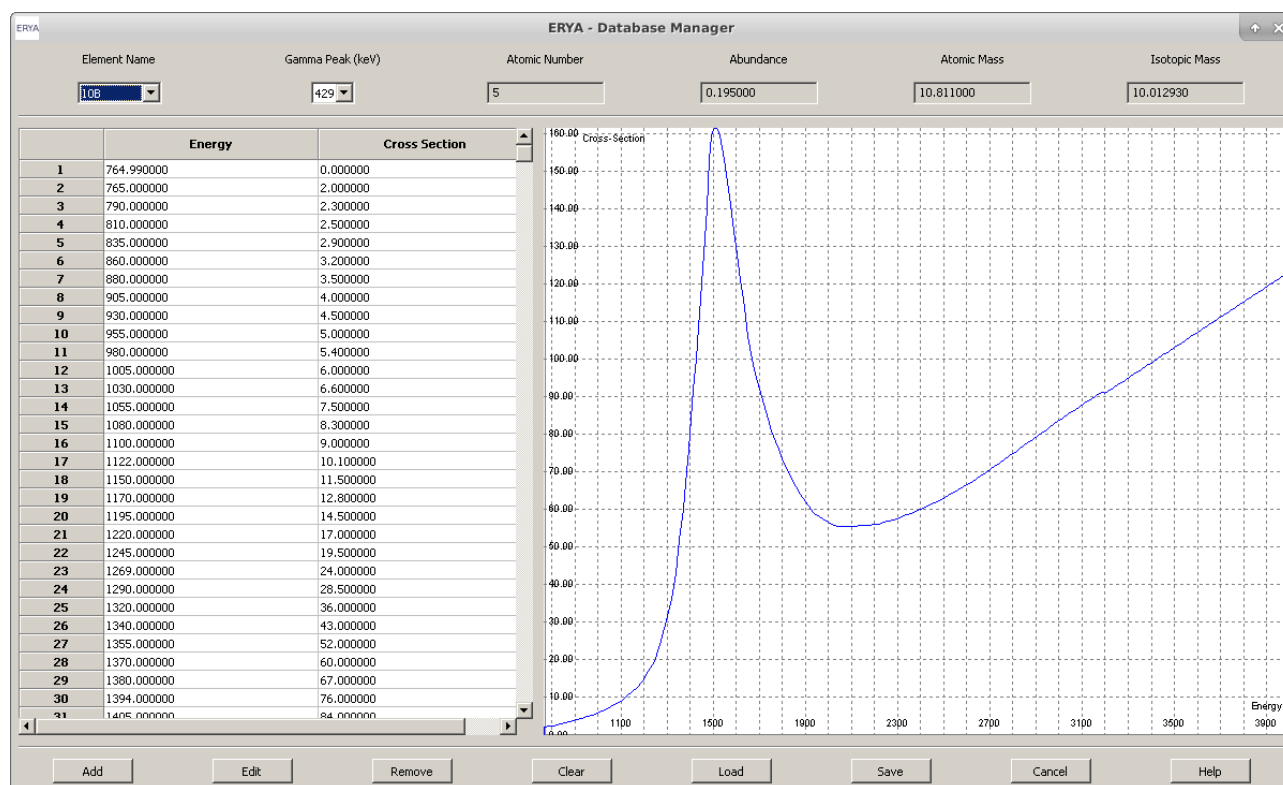
The same import and export logic are also applied to Excel Xlsx files.

Further details can be readied from the on-line help widget, by clicking on "Help" button.

## Element Database

For major convenience, the physical characteristics of several elements/isotopes are handled by the Database Manager widget.

To open the Database Manager, just open the Databases > Elements menu:



Using this tool, it is possible to handle one database at time (normally the default database).

By clicking on “Element Name” pull-down box, the selected element/isotope will refresh the “Gamma Peak” pull-down box, and then the user can select the available gamma emission peak from the same element. For each Element/Gamma pair, a read-only Energy/Cross-Section table and graphical plot will be drawn. Up to four global element physical proprieties will also be displayed.

The real interest here, is the possibility to add or edit elements to the database.

Selecting any element from the list, then the select and displayed Element can be removed (click on “Remove”), or edited (“Edit”).

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It will open a new dialog, and now the Element contents can be changed:

	Energy	Energy Error	Cross Section	Cross Section Error
1	764.990000	0	0.000000	0
2	765.000000	0	2.000000	0
3	790.000000	0	2.300000	0
4	810.000000	0	2.500000	0
5	835.000000	0	2.900000	0
6	860.000000	0	3.200000	0
7	880.000000	0	3.500000	0
8	905.000000	0	4.000000	0
9	930.000000	0	4.500000	0
10	955.000000	0	5.000000	0
11	980.000000	0	5.400000	0
12	1005.000000	0	6.000000	0
13	1030.000000	0	6.600000	0
14	1055.000000	0	7.500000	0
15	1080.000000	0	8.300000	0
16	1100.000000	0	9.000000	0
17	1122.000000	0	10.100000	0
18	1150.000000	0	11.500000	0
19	1170.000000	0	12.800000	0
20	1195.000000	0	14.500000	0
21	1220.000000	0	17.000000	0
22	1245.000000	0	19.500000	0
23	1269.000000	0	24.000000	0
24	1290.000000	0	28.500000	0
25	1320.000000	0	36.000000	0
26	1340.000000	0	43.000000	0
27	1355.000000	0	52.000000	0
28	1370.000000	0	60.000000	0
29	1380.000000	0	67.000000	0
30	1394.000000	0	76.000000	0
31	1405.000000	0	84.000000	0

**Note:** The same widget are displayed when the user click on “Add”, but it will open a blanked dialog.

### Other Database Manager Options

The other Database Manager available controls is the option that can delete the entire Database from memory (“Clear”), or load(“Load”) from and save(“Save”) to a file which should contains the source database related to the Element Database.

Like the other essential files, the native ERYA Database is a XML file with extension **epd**, but support other file formats for compatibility reasons.

ERYA have a read-only support to export the original LabView Database on binary form, and have a good compatibility to read the LabView ASCII Source Database files, and also write to the ASCII format, although it splits any elements with different gamma emission values to separated registers.

It is recommend to use the *LabView Import Tools* to handle conversions of LabView databases, even it can open by this tool directly, since all further LabView support are deprecated.

However it is not possible to use the LabView format as a default Database, since it will convert everything to the XML format.

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When the user choose to save a new or edited Database, ERYA will optimize the database structure and write a new copy, or overwrite it, to the user selected file. Then, the changed Database are reloaded to the main memory.

Additional details can be obtained from the “Help” button.

## Adding/Editing new Elements

When the user wants to edit or create a new element from scratch, using the cited controls from “Database Manager”, it should opens the new Element Editor.

Any element should have a name, a gamma peak emission value, and also the user should type their Atomic Number, Abundance and the Atomic and Isotopic Mass.

The element cross-section should could now be typed, by placing the energy/sigma pairs, and their experimental errors. The default units are the Energy in keV, and the cross-section in milibarn.

Normally, the cross-section are experimental values stored on several file sources, and it is very rare to manually type on the built-in sigma table editor.

It is possible to export the cross-section from a r33 file from IBANDL (where also fills the Element Name, and the Gamma Emission), from a ASCII file (usually in two-columns text files, but the cross-section are in barn.keV), and even from an Excel file (As long had a xlsx extension, and can have two or four columns, grouping the IBANDL and ASCII profiles.)

The user can save the current Element data to all three files, but have some caveats as explained on on-line help.

## A Basic Example: Magnesium-26

To explain the basic work-flow of create or editing Database’s Elements, we will show how to create a new element using an IBANDL file, and make a backup to a file, if you need to do so.

1. Go to IBANDL website at: <https://www-nds.iaea.org/exfor/ibandl.htm>
2. Select an nucleon, which can be any of the list, but choose a proton projectile (ERYA only support proton projectiles, or you give an unrealistic physical modulation). It is highly recommendable to filter data types by PIGE only, and select the ones with “mb” units format.

In this example save two or three samples with the highest number of cross-section points, where the target are the magnesium-26 isotope.

3. Save the relevant cross-section files as r33 files. (Click the “Save” button from the web-page.)
4. Start ERYA, then open the Database Manager, and finally, click “Add”.

The Element Editor widget, which should be blank, opens.

5. Select the relevant r33 files, from the “Import R33” button.

The ERYA will only display r33 files, if you select “IBANDL” files from the standard dialog window.

Select the adequate r33 file, and click “OK”. The program may ask to delete the main physical parameters located below the top window, and choose “Yes”, anyways.

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And it will fill the cross-section and some of the element's parameters.

In your example, the widget fills the following data, as display here:

	Energy	Energy Error	Cross Section	Cross Section Error
1	998	0.000	0.012	0.002
2	1098	0.000	0.000	0.000
3	1198	0.000	0.005	0.001
4	1299	0.000	0.000	0.000
5	1399	0.000	0.011	0.002
6	1499	0.000	0.012	0.002
7	1549	0.000	0.013	0.002
8	1599	0.000	0.000	0.000
9	1649	0.000	0.010	0.002
10	1699	0.000	0.006	0.001
11	1749	0.000	0.007	0.001
12	1799	0.000	0.000	0.000
13	1849	0.000	0.000	0.000
14	1899	0.000	0.013	0.003
15	1919	0.000	0.025	0.004
16	1939	0.000	0.036	0.005
17	1959	0.000	0.033	0.004
18	1979	0.000	0.063	0.006
19	1999	0.000	0.029	0.004
20	2019	0.000	0.092	0.008
21	2039	0.000	0.078	0.007
22	2059	0.000	0.076	0.007
23	2099	0.000	0.111	0.009
24	2119	0.000	0.128	0.010
25	2139	0.000	0.118	0.009
26	2159	0.000	0.169	0.012
27	2179	0.000	0.162	0.012
28	2199	0.000	0.150	0.012
29	2219	0.000	0.179	0.013
30	2239	0.000	0.215	0.015
31	2259	0.000	0.146	0.013

**6.** Using an isotope table, or an online reference material (even today the physical basic characteristics of several isotopes are available freely), fill the remaining gaps, like Abundance or the Isotopic Mass.

**7.** Click “Save”, and the new Database entry will be sorted and added.

The new element information will be displayed on Database Manager.

**8.** Repeat the steps 4 to 7 to add another entries.

**9.** Once return to the main Database Manager, click on “Save”, and select the current default Database file, if you want to make permanent changes, or choose another name, if you want to keep the custom database separated. (And save potential data losses!)

**10.** The new elements are now available to use.

### Additional Task:

When you successfully complete a new element profile, at step 6, you can click on “Export R33” to save the current data by the following three file formats:

1. Create a backup IBANDL file, while writes on “Comments” section the ERYA references, and the stored Elements physical characteristics.

The ERYA will assume, in some fields, that the cross-section represents an inelastic proton-nuclide collision, without changing the nuclear species, which can be incorrect, and requires a few additional manual editions of the resultant r33 file.

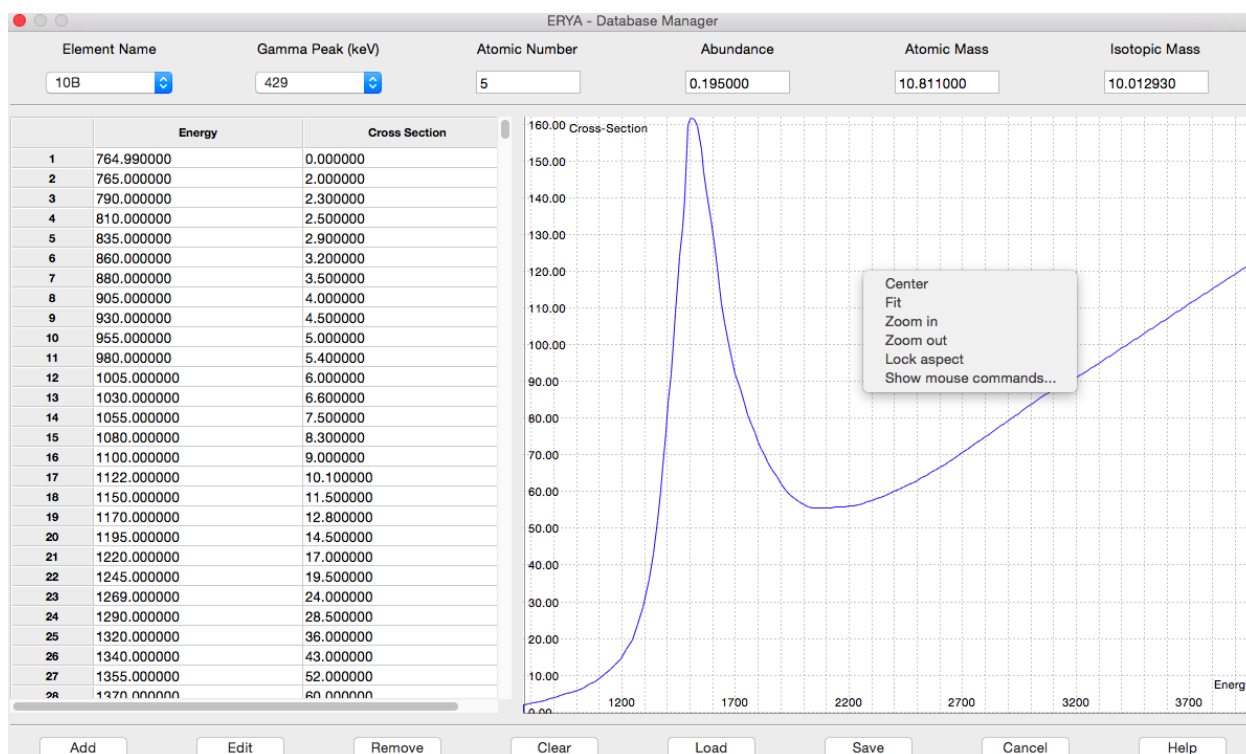
2. When the user choose to export as an ASCII file, only the cross-section are stored, and converted the cross-section column to barn.keV.

Every element name or physical references will be lost, and should choose this option only for compatibility purposes.

3. It is possible to store the cross-section table as an Excel file, where the user can choose a four-column version, or a two-column version where in the last option the cross-section are converted to barn.keV.

4. You can the graphic plot feature to zoom, fit or select a portion of the graphic by your convenience. The main commands are available by right-clicking the mouse over the plot.

You can select and drag the zoom window, while hold the left mouse button.



## Useful Utilities

### How to Export LabView Databases Safely

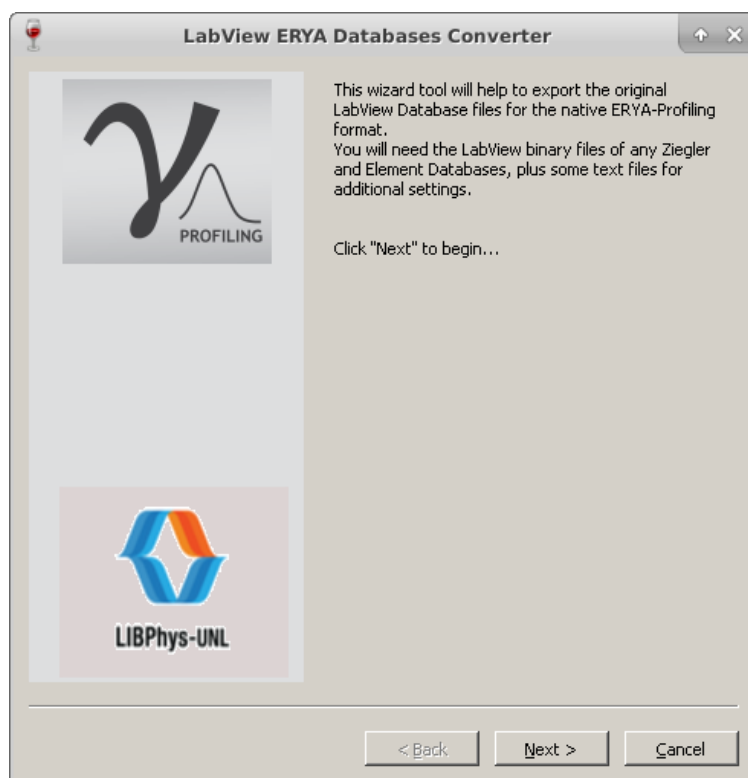
The original ERYA Profiling software package was a main program that use a GUI made with LabView Runtime, and additional working programs that makes the actual numerical simulation. The program package need five files to make them work, where ERYA-Profiling can export it.

It contains two binary files for the Elements Database, and Ziegler Parameters, and plain text files for the Detector, densities and mean ionization potential (also called as Bloch's Parameter).

Some LabView builds ever hard-codes the Detector efficiency function, and this require to fill manually the custom function text-box as described on the *Custom Efficiency Function* section of the Detector Profile widget.

If you ever needed to export the former databases, it is highly recommendable to use the following wizard tool available on Tools > Import ERYA LabView

1. Once selected the LabView Import Wizard, it should display the following wizard page:



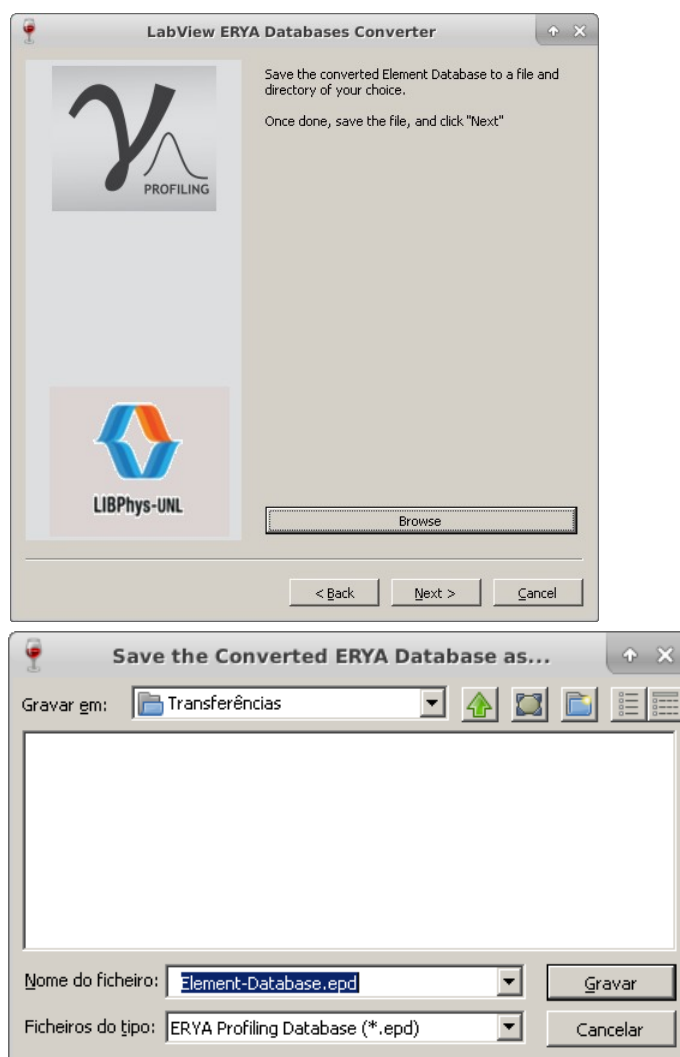


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2. On the next five pages, the program will ask to select a compatible file from the following components, as ever explained by own wizard's page:

- Element Database;
- Ziegler Parameters;
- Detector Efficiency;
- Element densities (can be a single column of values, as long are in the same atomic number order);
- Bloch's Parameters (can be a single column of values, as long are in the same atomic number order);

3. At this stage, the wizard will ask to use the define a series of three new files, using the same template, like this example:



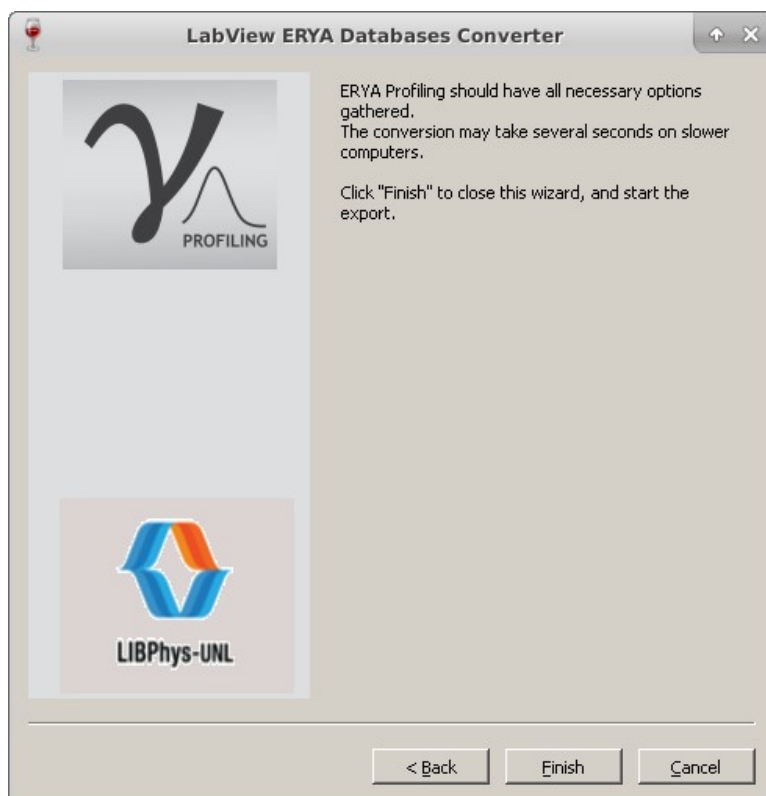
(Click on Browse button, then fill a name on an adequate folder, and click “Save”)

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4. Repeat the template from step 3 for the following files:

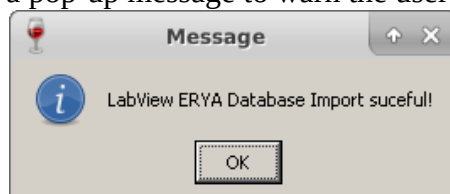
- Elements Database;
- Detector Efficiency;
- Ziegler Parameters;

5. Once reached the final wizard's page, as described below, click "Finish" to start the real conversion.



6. All previous databases are converted and written to the new three native format ERYA-Profiling formats. The process can take several seconds, where the Element's Database are analyzed, and sorted, taking the most time on the conversion procedure.

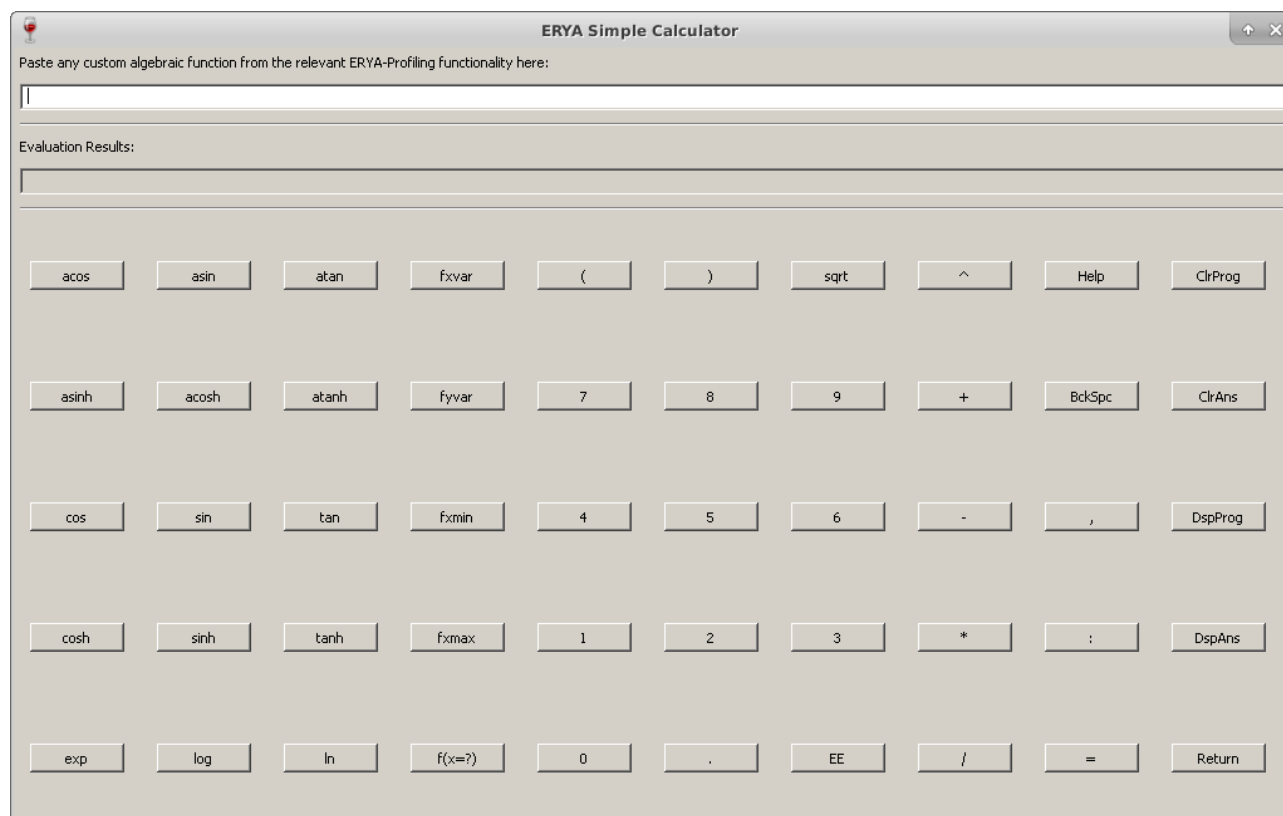
Once finished, it display a pop-up message to warn the user that the conversion was successful.



7. However, the new converted files will not substitute the original ones. You should use the Database Management tools to check each one, and use the *Setup Tool* to replace the converted databases as the new default ones.

## Using the ERYA Calculator

This widget is intended to serve as a debug tool for some advanced options that use the internal ERYA macro language, where the user can open a scientific calculator from “Tools” > “Calculator”



Either way, it can be used as a standard calculator anyway. Just fill any algebraic expression on first box, or input box, and then hit “Return” to evaluate numerically the expression on the second box.

Any syntax error will be displayed on the second box, also called output box.

It support a *direct mode*, and a *program mode*, where the difference is when the user defines a small program on the input box, more precisely a defined function, where can be:

$$\mathbf{fxvar = x , fyvar = y : a = 10 , b = 20 : a * x + b}$$

Or with a limited domain, as it is needed on the *Resonances* tab on the main menu interface:

$$\mathbf{fxvar = x , fyvar = y , fxmin = a , fxmax = b : a = 10 , b = 20 , g = a + b : g * x}$$

The variable names related to the *fxmin* and *fxmax* needed to be initialized, otherwise it use the default null values.

When the calculator is on *program mode*, it should hit the “f(x=?)” button, to fill a value, and it will display the result on output box.

More information are available on the on-line help.

### **SRIM Import Wizard**

In order to ease the import of several SRIM Stopping Power tables created by the SRIM software itself, an auxiliary wizard was created to batch the conversion of several tables at once.

The user need to select pure element stopping powers, where ERYA will only support the incident proton (hydrogen) beams. Once exported the outputs from the SRIM® software, just select the desired number of files, and follow the on-line instructions.

The wizard will also asks to get the Ziegler's parameters from several sources (including the current loaded on memory), and then a final native **epsz** file to output.

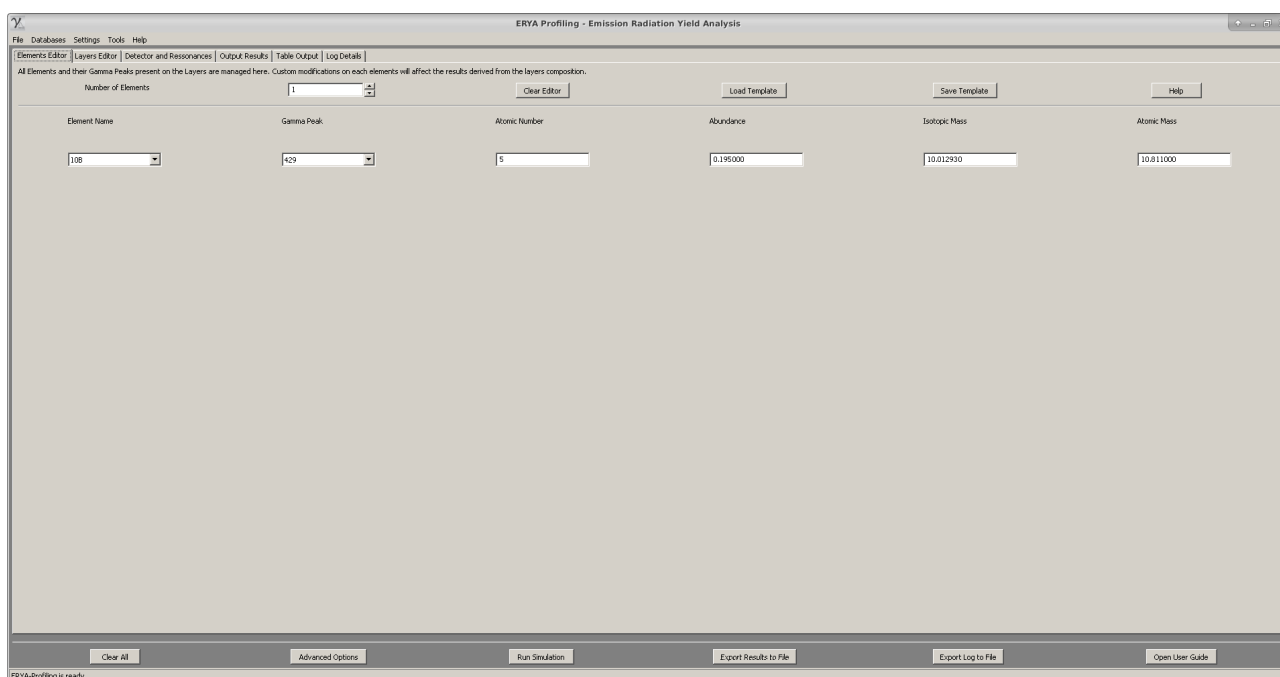
The whole batch conversion should be done in a matter of a couple of seconds, and only the valid SRIM files will be actually stored on the converted file.

## How to make a Profiling Analysis

The main purpose of ERYA - Profiling is to make a yield spectrum in function of energy, and the depth of the sample. Future improvements are under current discussion, so this chapter will detail the implemented features.

### Main Interface Features

If ERYA-Profiling was correctly configured, all default databases will load automatically on start-up, and wait for the user input, where it should be like this screen:



The program follow a modeled tabbed interface, where each tab had own functions and tools.

Database management are handled by the menu interface, as already described on previous chapters of this manual.

The bottom screen contains some buttons for the major tasks, and a status bar for some internal information, as will be briefly useful during the numerical evaluations.

The program require the user to fill the first three tabs, and then hit “Run Simulation” to start the simulation, where a percentage progress will be updated on the bottom status bar, since this process can take a long time to finish.

By clicking “Open User Guide”, it will display a resumed how-to tutorial of this current printed guide, with links for additional topics. Also each tab had own on-line help for additional information.

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### First Step: Define the Number of Elements

1. Select the “Elements Editor” tab, and select the number of Elements.
2. Once selected the adequate number of Elements, as notice that adding or removing won’t reset the remaining ones, change the Element Name from the pull-down inputs, and it will reload the Gamma Peaks pull-downs, and update the basic information from the Database.
3. Select the relevant Gamma Peak, as explained before.
4. Once selected all elements, if necessary, edit the basic Elements parameters, overridden the default values, without affecting the original values. This feature can be useful on samples with abnormal isotopic abundances, and avoid unneeded Databases editions.
5. The current elements selection will update the tables from other tabs, as it will detail later.

**Extra:** It’s possible to store the custom sample composition on a template file. It can be a normal Excel file, or a native XML based file with extension **epcs**. And loading the stored file, will fill the current “Elements Editor” tab without filling all over again.

Element Name	Gamma Peak	Atomic Number	Abundance	Isotopic Mass	Atomic Mass
25Mg	429	12	0.100000	24.985837	24.305000
27Al_F_0	344	13	1.000000	26.981500	26.981500
31P_ina	1264	15	1.000000	30.973800	30.973800
7Li_F	473	3	0.925000	7.016003	6.941000

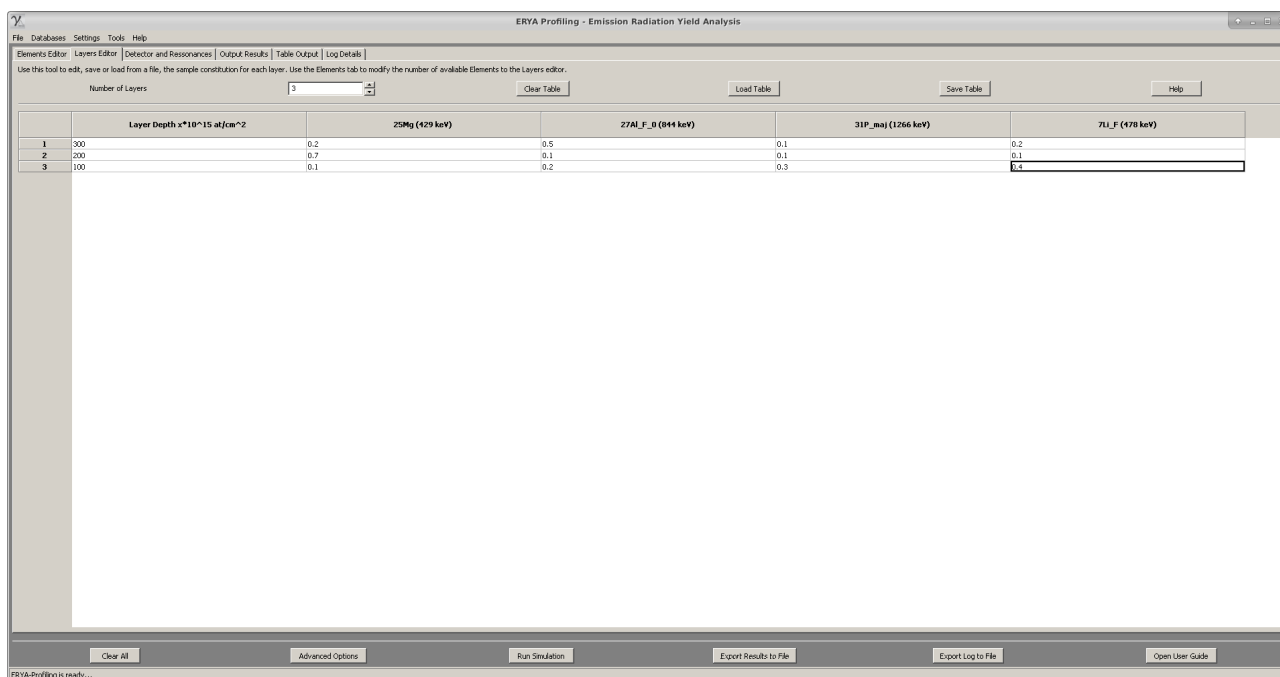
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### Second Step: Define the Number of Layers, and Detail their Composition

1. Select the “Layer Editor” tab, confirm the selected elements on the new table, and select the number of layers.
2. Define the depth of each layer on  $10^{15}$  at/cm<sup>2</sup> units, on the first column, and then the relative stoichiometry of each element. The program will make an internal renormalization during the main numerical simulation, then there’s no need to comply a manual input as long their sum should be equal to one, since the ERYA will fix without any additional user intervention.

**Extra:** It’s possible to store the table contents on an Excel file, or a native XML file with **epls** extension. This may make more easy to avoid manual inserted of a standard sample, by saving the initial values as template, and loading again.

Notice that loading templates on the “Layer Editor” will reload the “Element Editor” to the default values.



### **Extra Step: Using an Excel File or a ASCII file to Import a Template**

An additional option, inherited from the LabView ERYA program, was to fill a text file with a sample composition and export directly, instead to follow the manual steps of First and Second Steps.

On ERYA-Profiling, this feature was greatly improved, and warns the main issues of each option.

The major improvement was the Excel file import of a template, as it will detail here.

#### **1. Excel File Option:**

The Excel option had an additional advantage of the text import, since it is possible to use the first row as labels, and define directly the Elements and Gammas on their respective numerical columns.

Select any initial cell of an empty Excel file, but maintain a compact matrix of data, in order to avoid importation errors, due to a wrong matrix dimension.

On first column of the first row, write any word, since it will be the depth column, and then place the elements on the rightmost columns of the same row, the names and gammas. Normally, just use the pattern <Symbol> <Gamma>, separated by a space, like “19F 197” on a cell to represent the 197 keV gamma of the isotope 19F from the Database. Other variations are permitted, and are detailed on the on-line help reference.

Finally, write on the next adjacent rows, taking attention to assign correctly from each column, the depth and stoichiometry, like the built-in table editor from ERYA-Profiling.

Once written, save as Excel 2007 Xlsx File Format, and then use the “Load Table” to select the new created Excel File. It should extract the data and fill the “Element” and “Layer” editor automatically.

It is necessary to take care to not select a non-existent element or gamma, or the program will warn about a non-existent isotope from the current database, and the user should open the Excel file on your favorite spreadsheet program, and make the necessary corrections.

It's possible to export a pure numerical table on an Excel file, but require the user to define manually the number and names of all elements, making more prone to mistakes.

#### **2. ASCII File Option:**

In this case, create a numerical matrix separated by tabs and newlines, taking care to maintain a coherent number of columns. Also the user should define the number of Elements, and their names manually, before export the table.

A mistake can get an import error, or a garbled table, since the program doesn't know the expected matrix dimension beforehand.



## ERYA v2.35 (ERYA/Profiling Tutorial)

### Third Step: Define the Detector Parameters, and Resonances

1. To complete the necessary data to start a simulation, select the “Detector and Resonances” tab.
2. The user can now fill the main Detector physical parameters, and the number of energy samples, by defining a Energy Step along a Minimum and Maximum Energy sequence.
3. Optionally is possible to define a Lorentzian Resonance, or even a custom Function Resonance using the same ERYA macro language on *Detector Efficiency* or on *ERYA Calculator*, but require to use all four reserved keywords for a function to be valid, as it expects a defined resonance at a restricted domain of energies. The on-line help contains major details about the ERYA macro language syntax and examples.
4. Select the main resonance mode, using the bottom control, where the default is to ignore any custom resonance at all, or choose the Lorentzian or Custom Resonance function.

**Extra:** It's possible to save the current Detector and Resonance values on a XML file with **eprs** extension. Load it, will recover the stored values.

ERYA Profiling - Emission Radiation Yield Analysis

File Databases Settings Tools Help

Elements Editor Layers Editor Detector and Resonances Output Results Table Output Log Details

Configure the Detector main physical parameters here. Optionally, define the resonance model.

Clear Detector Clear Resonance Clear Custom Load Profile Save Profile Help

Detector Parameters

Beam Resolution (1eV) Temperature (K) Charge (nC) Energy Step (1eV) Minimum Energy (1eV) Maximum Energy (1eV)

1 300 1 1 2000 1010

Lorentzian Resonance Setup

Resonance Width (1eV) Resonance Peak (millibarn) Resonance Energy (1eV)

☐ Define a Limited Energy Range? Minimum Resonance Energy (1eV) Maximum Resonance Energy (1eV)

Custom Function Resonance Setup

Write down the algebraic function that models the resonance. When save the Detector profile, any custom function is also stored. Read the User Guide for more information.

Select Default Resonance

☒ Without Resonance (default)

☐ Select Lorentzian Resonance

☐ Select Custom Function Resonance

Clear All Advanced Options Run Simulation Export Results to File Export Log to File Open User Guide

ERYA-Profiling is ready...

### Additional Tip.

To save all contents of “Element Editor”, “Layers Editor” and “Detector and Resonance” tabs, along some additional values at once, use “File” > “Save” and save on a XML file with extension **epgs**.

When load a **epgs** file, with “File” > “Load”, it will load all three tabs contents automatically.

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### Last Step: Make the Simulation

Once everything done, according to the previous steps, hit the “Run Simulation” button, and if no error are reported, the simulation will begin, displaying the percentage on the bottom status bar:

The screenshot shows the ERYA Profiling - Emission Radiation Yield Analysis software interface. The window has a menu bar with File, Database, Settings, Tools, and Help. Below the menu bar is a tabbed interface with tabs for Elements Editor, Layers Editor, Detector and Resonances, Output Results, Table Output, and Log Details. The 'Detector and Resonances' tab is active, showing a configuration panel for the detector and resonance model. The panel is divided into three sections: Detector Parameters, Lorentzian Resonance Setup, and Custom Function Resonance Setup. The Detector Parameters section includes input fields for Beam Resolution (keV), Temperature (K), Charge (nC), Energy Step (keV), Minimum Energy (keV), and Maximum Energy (keV). The Lorentzian Resonance Setup section includes input fields for Resonance Width (keV), Resonance Peak (meV), Resonance Energy (keV), and checkboxes for 'Define a Limited Energy Range?' and 'Minimum Resonance Energy (keV)'. The Custom Function Resonance Setup section includes a text area for writing an algebraic function and a section for selecting the default resonance model. At the bottom of the window is a status bar showing 'Calculation Progress: ...54.247%'. The 'Run Simulation' button is highlighted in the bottom toolbar.

Detector Parameters					
Beam Resolution (keV)	Temperature (K)	Charge (nC)	Energy Step (keV)	Minimum Energy (keV)	Maximum Energy (keV)
3	300	1	1	2000	2010

Lorentzian Resonance Setup					
Resonance Width (keV)		Resonance Peak (meV)		Resonance Energy (keV)	
<input type="checkbox"/> Define a Limited Energy Range ?		Minimum Resonance Energy (keV)		Maximum Resonance Energy (keV)	

Custom Function Resonance Setup

Write down the algebraic function that models the resonance. When save the Detector profile, any custom function is also stored. Read the User Guide for more information.

Select Default Resonance

☒ Without Resonance (default)

☐ Select Lorentzian Resonance

☐ Select Custom Function Resonance

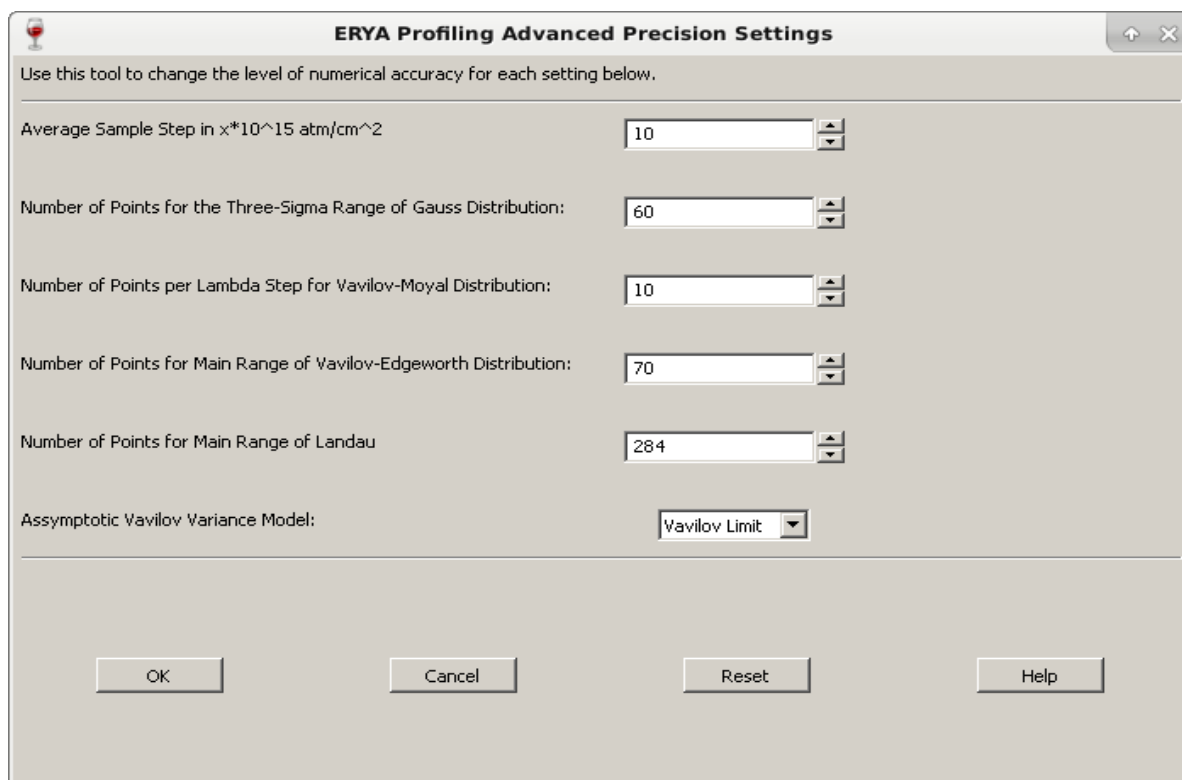
Clear All   Advanced Options   Run Simulation   Export Results to File   Export Log to File   Open User Guide

Calculation Progress: ...54.247%

Once finishes, the results are displayed on a graphic plot on “Output Results”, a numerical table of the same plot on “Table Output”, and a log of several intermediate values on the “Log Details” tab.

## Changing Accuracy Parameters (Optional)

If the user knows what are doing, it is possible to change the accuracy parameters by clicking the “Advanced Options” button on the bottom main page controls, which opens a simple widget:



The screenshot shows a window titled "ERYA Profiling Advanced Precision Settings". Inside, there is a text box that says "Use this tool to change the level of numerical accuracy for each setting below." Below this, there are five rows of settings, each with a label and a numeric input field with up/down arrows:

- Average Sample Step in  $x \cdot 10^{15} \text{ atm/cm}^2$ : 10
- Number of Points for the Three-Sigma Range of Gauss Distribution: 60
- Number of Points per Lambda Step for Vavilov-Moyal Distribution: 10
- Number of Points for Main Range of Vavilov-Edgeworth Distribution: 70
- Number of Points for Main Range of Landau: 284

At the bottom of the settings, there is a dropdown menu labeled "Assymptotic Vavilov Variance Model:" with "Vavilov Limit" selected. At the very bottom of the window, there are four buttons: "OK", "Cancel", "Reset", and "Help".

On most realistic scenarios, the user only change the Sample Step (Using  $10^{15} \text{ at/cm}^2$  units), where their range are from 1 to 1000 (default is 10). A smaller number on Sample Step may be needed with samples that contains sharp resonances, but it will increase the the simulation time.

Smooth cross-sections can be computed more fast, by choosing a greater Sample Step without losing much accuracy.

The next four parameters are related to the number of points of the intervals of integration related to the distributions, as explained on the brief theoretical chapter. The on-line reference contains some more detailed information.

The last option is to select between the Vavilov or Bohr Variance, applicable when all distributions goes to the Gaussian Limit. The numerical differences rarely make one to be great than the double of the other, and only on special contexts the evaluated yields will got a significant difference between the two modes.

### **Import Experimental Data**

Once the results are displayed on “Output Results”, mainly the graphical plot, it is possible to add additional plots of experimental data.

The current implementation only accept a single line per time, and only requires an Excel file with two columns of numerical data (the first row can be any labels, that will be ignored), or an ASCII filled with two tabbed columns of numerical data.

Then click on “Import Experimental Data”, and the correct file, and a new plot with a template name will be displayed, along the interpolated data on the “Table Output”.

To add another experimental data, simply repeat the same procedure again.

**Attention:** Notice that the experimental data, once plotted on the cited tab page, will also appears on the rightmost columns of the “Table Output” tab, but interpolated to match the energy spectrum created by the numerical simulation.

## **Saving Results**

ERYA Profiling provides three possible output files, as described below:

At first glance, it's possible to save the current graphic plot as an image image, using the “Save As Image” button from the “Output” tab page, and then select one of the four images types supported by this program.

If you zoom the image or crop the plot, when save the changed plot to the file, it will be stored as an image file as appear to be.

Using the “Table Output” and “Log Details” tabs pages buttons, it is possible to save the tables either by an ASCII text file, or an Excel file. Either way, the Excel format is more friendly for further data processing.

The log files of huge samples can creates tables with several thousands of lines, and ERYA-Profiling can take some minutes to save an Excel file with some hundred thousand rows.

### Some Useful Tips

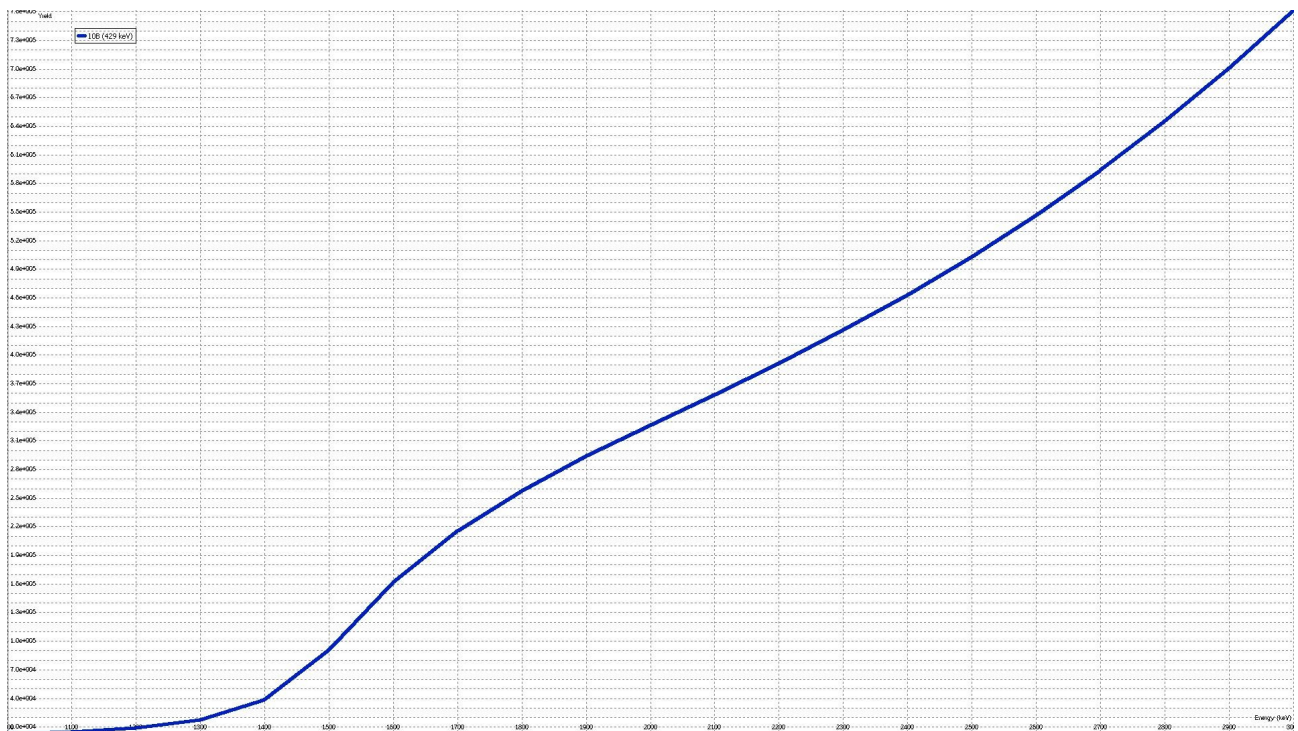
- Use the built-in tools described on this tutorial, when applied to the first three tabs, to fill the sample composition. It's much better than export from text or Excel files.
- Save all samples as **eggs** files from the "File" > "Save As", in order to create a collection of master samples. This is useful to use test different stoichiometries, once the file are load by the program, avoiding to fill everything manually. Instead, only a few values are changed at all.
- If the elements belonging to a sample have a smooth cross-section, increase the Sample Step, on the "Advanced Options" button. This will reduce the computation time.
- On samples with elements that have sharp resonances, reduce the Sample Step, in order to avoid loss of accuracy.

**Example: A Sampling with a smooth cross-section: 10-Boron**

- Fill a single layer with a single element with 3 million units of depth.
- Increase the Sample Step up to 1000. Later change the asymptotic model from Vavilov to Bhr
- Use a beam resolution of 3 keV, with 300 K, along a energy spectrum from 1000 to 3000, with 100 keV Step.
- If necessary, save the two experiments as **epgs** files, just in case to avoid manual typesetting for each experiment.
- Start the simulations.

## Results brief analysis:

The simulated yields for Bohr and Vavilov limits, respectively, on a gross sample are almost indistinguishable:





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The differences are less than 0.5%, and the plot are almost the same on the two models.

The tables are placed by the same order, first the Vavilov limit, then the Bohr limit.

	Energy (keV)	10B (429 keV)
1	1000.000000	2717.228415
2	1100.000000	5274.544323
3	1200.000000	9601.553814
4	1300.000000	17922.758726
5	1400.000000	38615.154252
6	1500.000000	90365.577384
7	1600.000000	160144.869170
8	1700.000000	213775.193351
9	1800.000000	256027.441638
10	1900.000000	292138.246598
11	2000.000000	324802.368436
12	2100.000000	356764.333349
13	2200.000000	389811.209142
14	2300.000000	424459.115374
15	2400.000000	461457.276585
16	2500.000000	501314.893491
17	2600.000000	544471.656737
18	2700.000000	591373.382015
19	2800.000000	642486.716552
20	2900.000000	698059.382653
21	3000.000000	758273.208885

	Energy (keV)	10B (429 keV)
1	1000.000000	2740.925196
2	1100.000000	5318.580543
3	1200.000000	9681.677921
4	1300.000000	18071.251579
5	1400.000000	38930.729757
6	1500.000000	91174.020336
7	1600.000000	162052.541618
8	1700.000000	216420.103288
9	1800.000000	258642.115446
10	1900.000000	294678.120413
11	2000.000000	327258.665583
12	2100.000000	359137.273657
13	2200.000000	392146.413576
14	2300.000000	426832.124868
15	2400.000000	463896.784290
16	2500.000000	503860.147319
17	2600.000000	547173.008336
18	2700.000000	594266.135610
19	2800.000000	645629.219719
20	2900.000000	701483.722185
21	3000.000000	762041.969388

**Example: A Sampling with a thin AlTi layer**

- Fill two layers layer with two elements: 150 units of pure Aluminum, and 200 units of pure Titanium. Here, the units are the depth in  $10^{15}$  at/cm<sup>2</sup>, as already acquainted.

**Note:** To do this, create two elements, and then two layers.

On the first layer, select 150 units for the depth, then a relative stoichiometry of “1” for Aluminum, and “0” for Titanium.

Finally, on the second layer, select 200 units for the depth, then a relative stoichiometry of “0” for Aluminum and “1” for Titanium.

- If necessary, reduce the Sample Step to 10. Also, make two experiments for the Vavilov and Bohr limits.

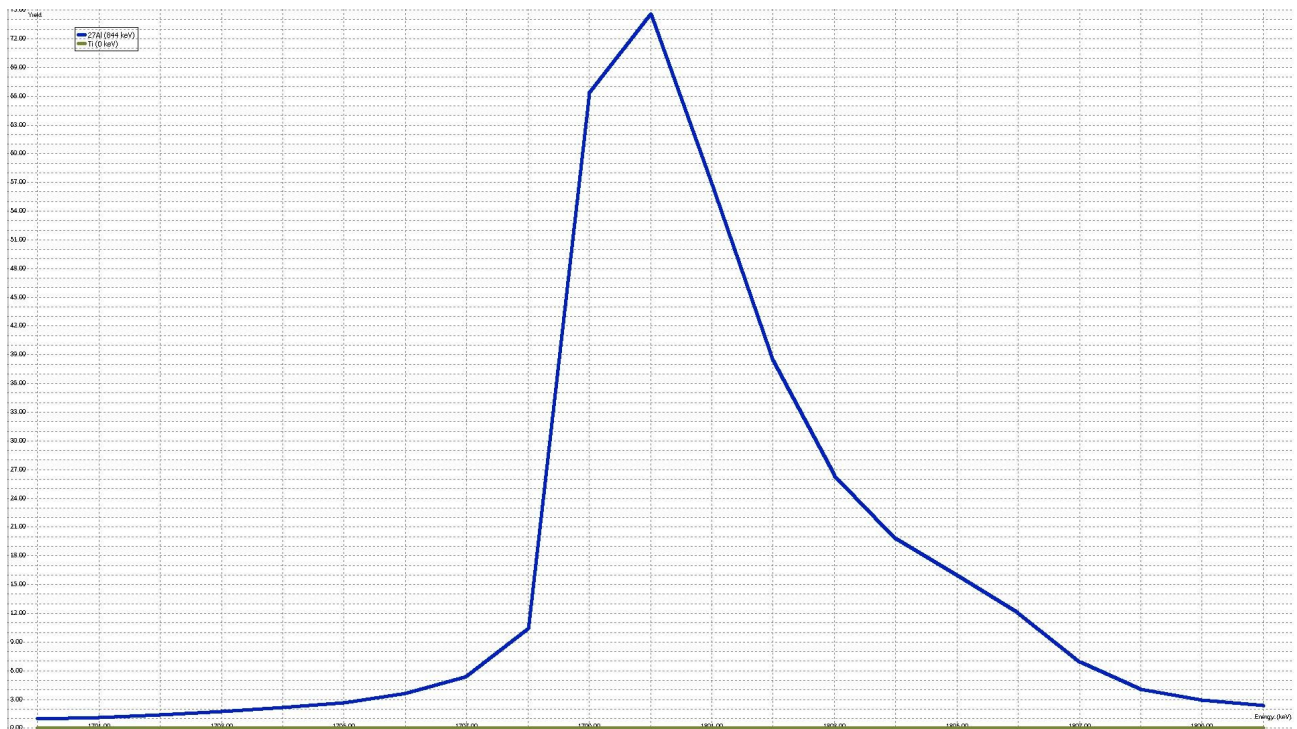
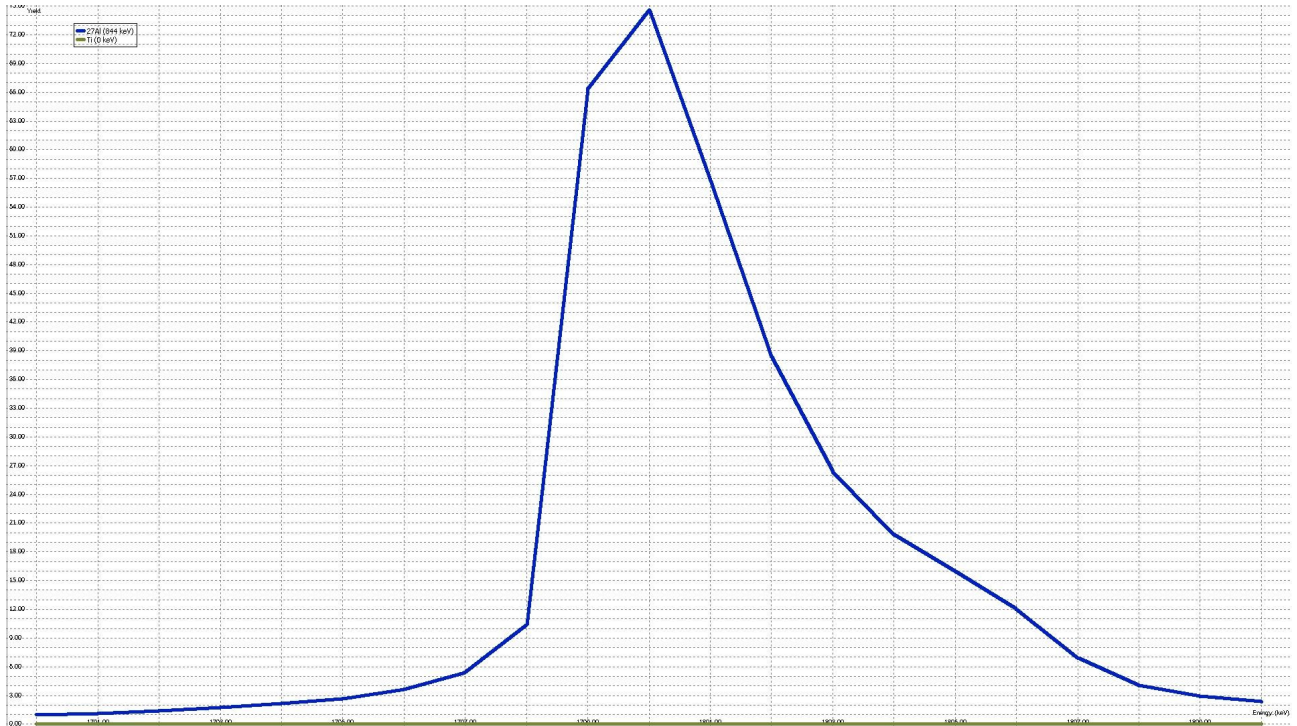
- Use a beam resolution of 3 keV, with 300 K, 1 $\mu$ C, along a energy spectrum from 1790 to 1810, with 1 keV Step.

- Start the simulations. (and notice that the incident beam will never be totally absorbed...)

- Once complete, try to reduce the Energy Step to a smaller value, like 0.1 keV, in order to obtain a better plot of the resonance at 1800 keV. (It leave here as an exercise.)

### Brief visualization of the Results:

Like the previous example, it will display the yield spectrum plot, first using the Vavilov limit, then the Bohr model:



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And the numerical tables follows the same order: first, Vavilov, then, Bohr.

	Energy (keV)	27Al (844 keV)	Ti (0 keV)
1	1790.000000	1.030773	0.000000
2	1791.000000	1.162767	0.000000
3	1792.000000	1.438590	0.000000
4	1793.000000	1.799537	0.000000
5	1794.000000	2.209915	0.000000
6	1795.000000	2.650835	0.000000
7	1796.000000	3.674698	0.000000
8	1797.000000	5.426299	0.000000
9	1798.000000	10.370724	0.000000
10	1799.000000	66.359140	0.000000
11	1800.000000	74.613382	0.000000
12	1801.000000	56.802435	0.000000
13	1802.000000	38.367960	0.000000
14	1803.000000	26.345006	0.000000
15	1804.000000	19.756846	0.000000
16	1805.000000	15.915519	0.000000
17	1806.000000	12.011785	0.000000
18	1807.000000	6.889559	0.000000
19	1808.000000	4.039940	0.000000
20	1809.000000	2.896744	0.000000
21	1810.000000	2.340699	0.000000

	Energy (keV)	27Al (844 keV)	Ti (0 keV)
1	1790.000000	1.030773	0.000000
2	1791.000000	1.162767	0.000000
3	1792.000000	1.438590	0.000000
4	1793.000000	1.799537	0.000000
5	1794.000000	2.209915	0.000000
6	1795.000000	2.650835	0.000000
7	1796.000000	3.674698	0.000000
8	1797.000000	5.426299	0.000000
9	1798.000000	10.370724	0.000000
10	1799.000000	66.359140	0.000000
11	1800.000000	74.613382	0.000000
12	1801.000000	56.802435	0.000000
13	1802.000000	38.367960	0.000000
14	1803.000000	26.345006	0.000000
15	1804.000000	19.756846	0.000000
16	1805.000000	15.915519	0.000000
17	1806.000000	12.011785	0.000000
18	1807.000000	6.889559	0.000000
19	1808.000000	4.039940	0.000000
20	1809.000000	2.896744	0.000000
21	1810.000000	2.340699	0.000000

- Unsurprising, the plots are the same, because on thin sample, rarely, if ever, the Vavilov Distribution never went to the asymptotic Gaussian Distribution.

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**Note:** The research materials are the same of the LabView ERYA program.

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- Excel 2007 file documentation: <https://www.codeproject.com/Articles/208075/How-to-read-and-write-xlsx-Excel-file-Part-I> ; <https://www.codeproject.com/Articles/210014/How-to-read-and-write-xlsx-Excel-file-Part-II>

**Note:** All C# and MatLab code was ported to C++, while the Excel file internal structures are implemented using the native wxWidgets classes for XML and ZIP streams.