

MultiSIMNRA Guide

Ver. 0.6

MultiSIMNRA is a computer code designed to control multiple instances of the SIMNRA program, providing a smooth experience of data analysis of multiple ion beam techniques measured at the same sample. MultiSIMNRA counts with computational algorithms to help the user find the sample description that best fit the spectra of the different measurements of the sample.

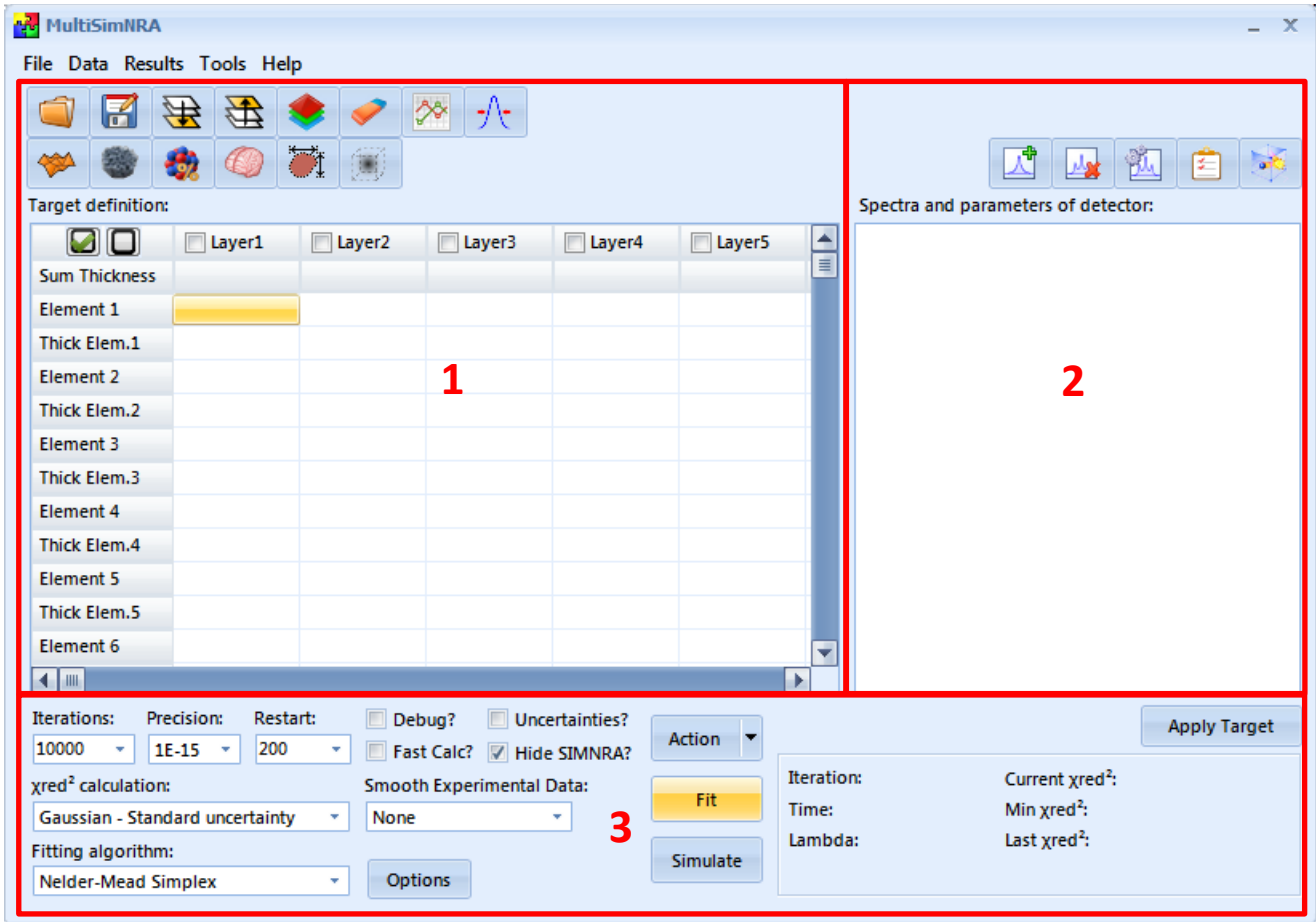
Being capable of dealing with a large number of variables, MultiSIMNRA can be useful in the determination of depth profiles of multi-layered sample, even for single spectra analysis, improving and extending the SIMNRA fitting capabilities.

MultiSIMNRA needs administrator rights to work properly, especially on Windows Vista and superior due User Account Control (UAC). This solution was used to avoid "erratic" operation when calling SIMNRA OLE server using a standard user account type. At the current version, MultiSIMNRA only use network access to check updates (automatically only after 30 days without check). In future version will be implemented network communication to allow cluster computing.

For SIMNRA 6 users, MultiSIMNRA access data of simulated spectra reading SIMNRA exported files of spectrum data. It is a disk intensive task. For SIMNRA 7 users, MultiSIMNRA receive spectra data using OLE automation, in a faster and clean process.

SIMNRA 6 users should use .nra format files and SIMNRA 7 user should use .xnra format. The spectra files need to be prepared before. MultiSIMNRA only include SIMNRA files or import RUMP .rbs format in batch mode to transform in SIMNRA files.

1 - Main window:



The main window is formed by three blocks of definitions: Target (1), Setup (2) and Fit Algorithms (3).

TIP: press [Alt] and click on the spectra icon in the list of loaded spectra to open the corresponding SIMNRA file in SIMNRA.

1.1 - Target layers:

	Layer1	Layer2	Layer3	Layer4	Layer5
Sum Thickness	42.9329452	467.247205	78.0757303	198.165105	1612.85490
Element 1	H	H	H	H	H
Thick Elem.1	1.25400609	70.7009698	11.2912263	17.5958837	120.081410
Element 2	C	C	C	C	C
Thick Elem.2	14.6509893	13.0707204	6.44591761	171.473931	1422.36959
Element 3	O	O	O	O	O
Thick Elem.3	19.2500522	44.1719132	26.1290744	9.09529006	70.4038980
Element 4	Al	Al	Al		
Thick Elem.4	4.26583998	212.191285	22.9455054		
Element 5	Ti	Ti	Ti		
Thick Elem.5	3.35403401	98.5673422	8.77176364		
Element 6	Ta	Ta	Ta		

The target table accepts only valid elements as input with two letters. All check-boxes defines if the parameter of target will be included as a fitting parameter. PS.: A popup menu is activated with right click on any layer in the target table. Tools for layer handling are presented.

Slice layer
Scale layer
Insert layer
Copy layer
Paste layer
Remove layer
Simulate layer

Slice layer: equally slice the selected layer in a defined number.

Scale layer: multiply selected layer thickness by a factor.

Insert layer: insert a blank layer before selected layer

Copy layer: copy layer selection to clipboard

Paste layer: paste a layer from clipboard

Remove layer: remove selected layer

Simulate layer: plot the contribution of an individual layer to the total simulated spectra

1.2 - Target definition toolbar

	Load MultiSIMNRA project.
	Save MultiSIMNRA project.
	Load .tar (SIMNRA 6) or .xtarget (SIMNRA 7) files with target definition (layers and roughness).
	Save .tar (SIMNRA 6) or .xtarget (SIMNRA 7) files with target definition (layers and roughness).
	Organize target, ordering elements by name.
	Clear project definition (both target and setup).
	Show graph of current depth profile.
	Execute ResolNRA to calculate depth resolution of enabled spectra and build graph of minimum depth resolution for each element. (SIMNRA 7)
	Open window to set roughness of layers and substrate. Also enables to include roughness to be fitted.
	Open window to set porosity of layers. Also enables to include porosity to be fitted. (SIMNRA 7)
	Open window to set isotopic composition rules. Also enables isotopic composition to be fitted. (SIMNRA 7)
	Open window to set constraints of fitting parameters.
	Open a window to set limits to fitting parameters. When using Differential Evolution or Evolutionary Annealing-Simplex algorithms these limits are used as ranges for the searching limits for the parameters.
	Select concentration parameters to fit. Select an element by name or all with an empty input.
	Unselect concentration parameters to fit. Unselect an element by name or all with an empty input.

1.2.1 - Roughness

Fit?	<input type="checkbox"/> Layer1	<input type="checkbox"/> Layer2	<input type="checkbox"/> Layer3	<input type="checkbox"/> Layer4	<input type="checkbox"/> Layer5		
Has Layer Roughness:	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
Layer Roughness	0	0	0	0	0		
Minimum	0	0	0	0	0		
Maximum	0	0	0	0	0		

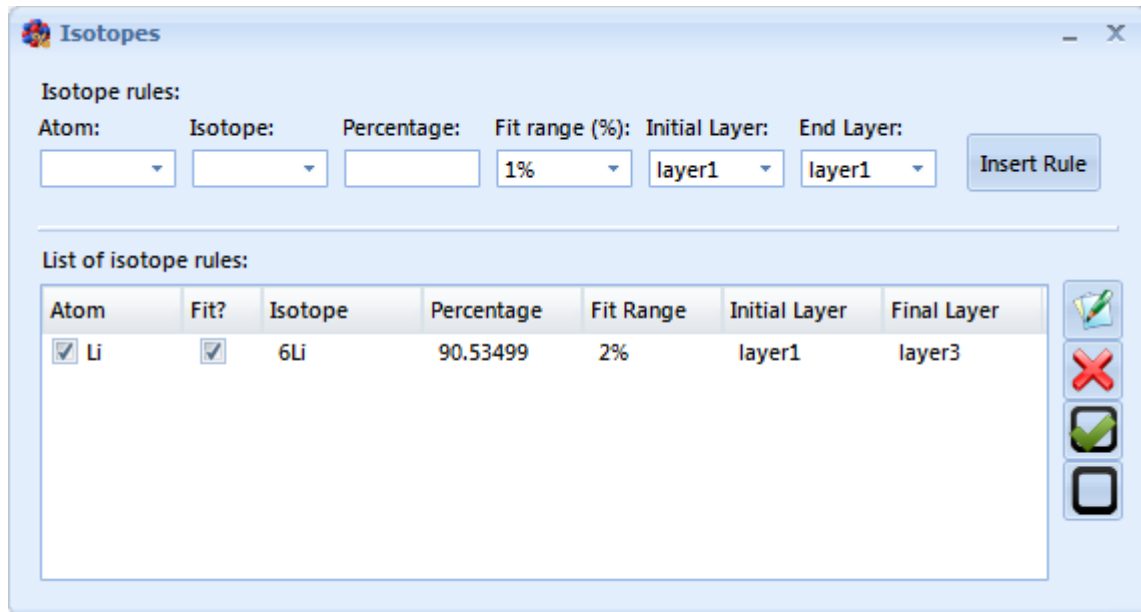
In this window it is possible to define roughness of layers and substrate, select which parameter to fit and the range limits for the parameters during fitting.

1.2.2 - Porosity

Fit Porosity Fraction?	<input type="checkbox"/> Layer1	<input type="checkbox"/> Layer2	<input type="checkbox"/> Layer3	<input type="checkbox"/> Layer4	<input type="checkbox"/> Layer5
Fit Pore diameter?	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Has Layer Porosity?	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Layer Porosity Fraction	0	0	0	0	0
Minimum fraction	0	0	0	0	0
Maximum fraction	0	0	0	0	0
Layer Pore diameter	0	0	0	0	0
Minimum diameter	0	0	0	0	0
Maximum diameter	0	0	0	0	0

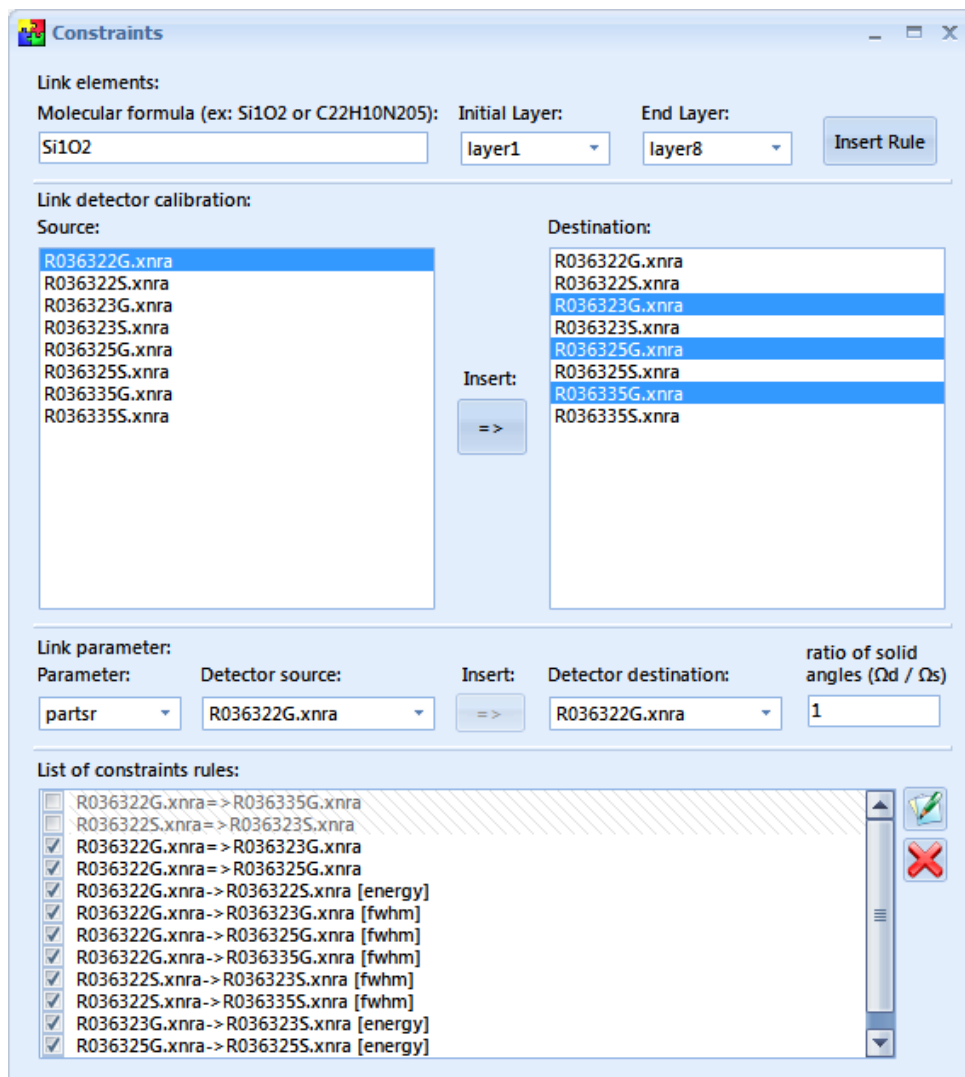
In this window it is possible to define porosity of layers, select which parameter to fit and the range limits for the parameters during fitting.

1.2.3 - Isotopes



In this window it is possible to define roughness of layers and substrate, to select which parameter to fit and the range limits for the parameters during fitting.

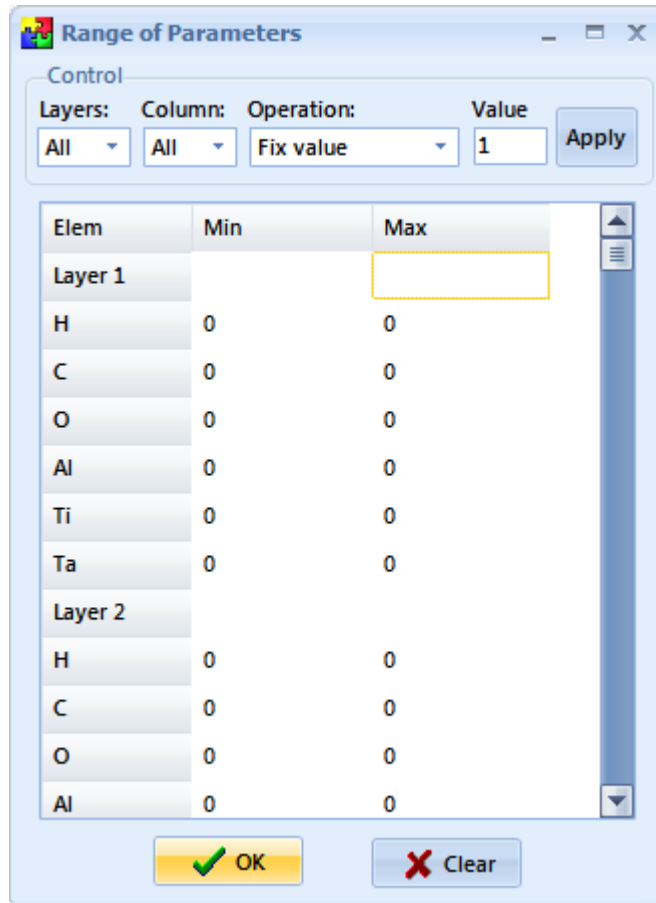
1.2.4 - Constraints



In this window it is possible to define constraints for element proportion for layers and substrate (simulating chemical formulas), energy calibration, and other parameters (e.g. beam energy, part*sr, detector resolution, beam spread and detector dead-layer). Check box indicates if the created constraints are active.

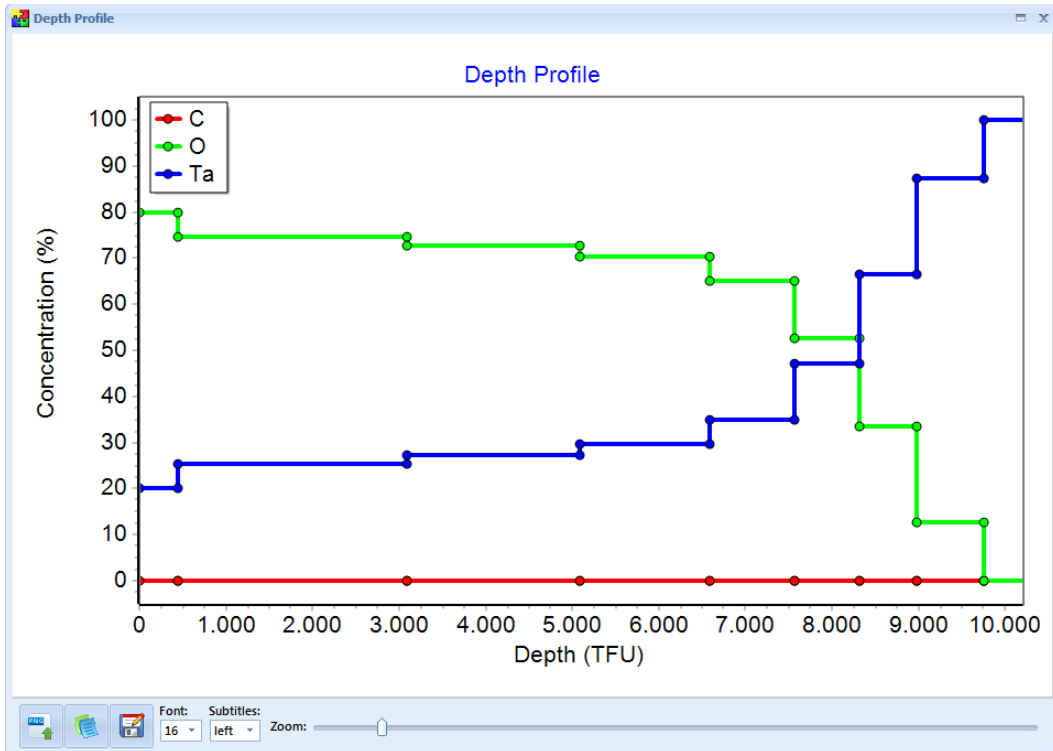
PS.: To insert element proportion for SiO_2 it is necessary insert text Si1O2 in the rule.

1.2.5 - Range of parameters



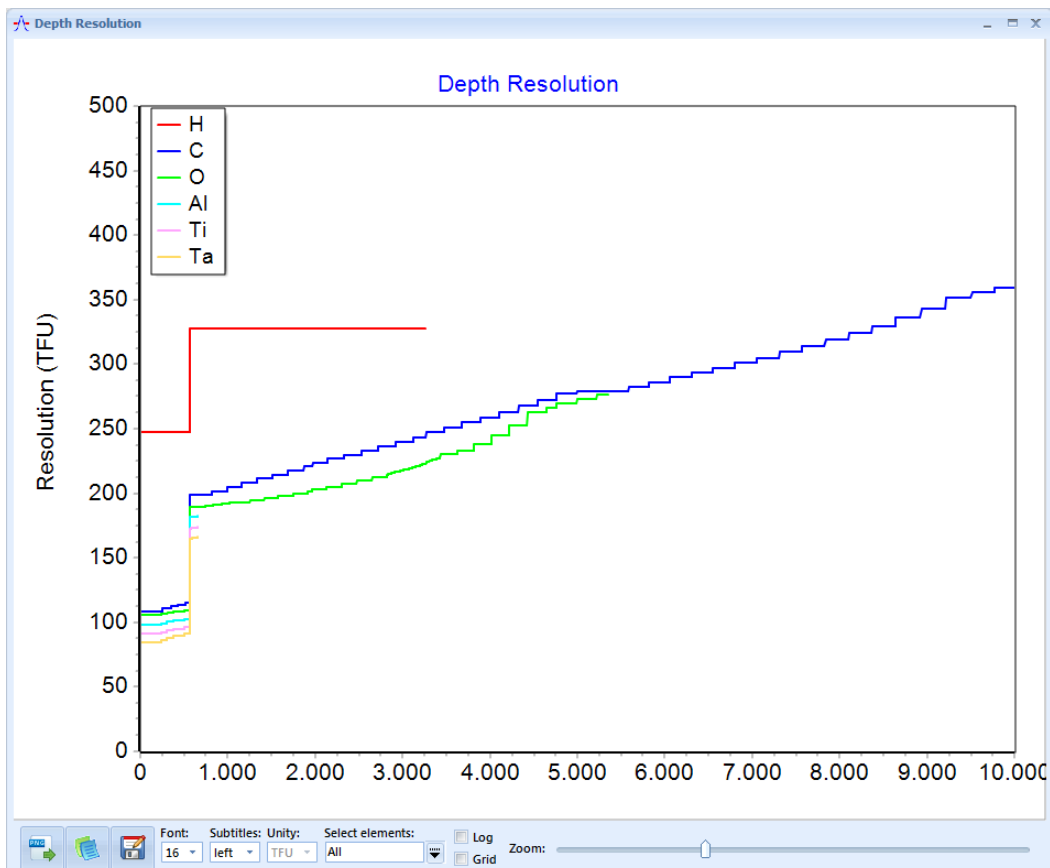
With this window is possible to set the range limits for each parameter of target layers which are selected to fit.

1.2.6 - Depth profile








Show a graph of current depth profile. PgDn, PgUp, Home and arrows are used for navigation and Ctrl+X and Ctrl+Y to set range limits. In the bottom bar has controls of the font size, legend position, export image and data.

1.2.7 - Depth resolution



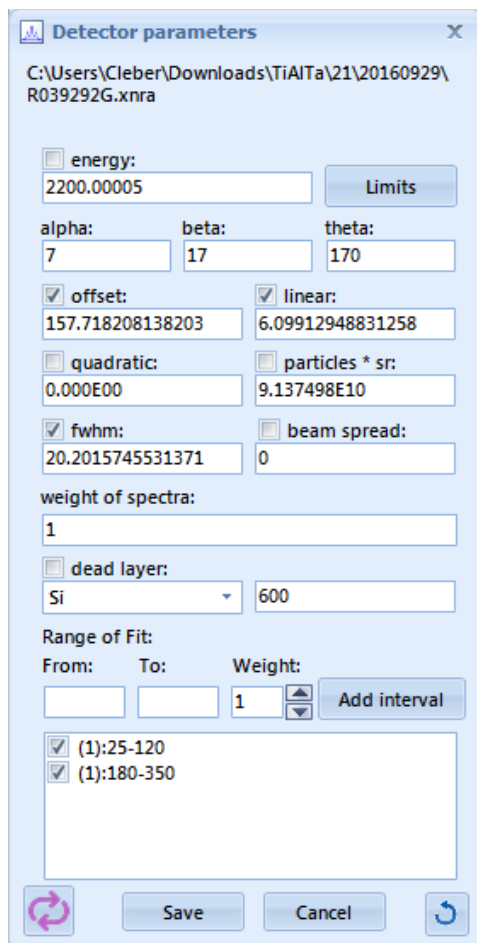
Show a graph of minimum depth profile resolution for each element calculated by ResolNRA program for all spectra selected. Right Button open a dialogue box to define plot range. PgDn, PgUp, Home and arrows are used for navigation. In the bottom bar has controls of the font size, legend position, export image and data.

2 – Setup

	Include .nra (SIMNRA 6) or .xnra (SIMNRA 7) Simnra files (the files must be completely configured, including reactions that will be used).
	Remove selected spectra from the list
	Edit detector – Use to configure parameters of experimental setup of selected file
	Select or deselect fitting parameters for all spectra
	Batch operations on parameters, limits and ranges of all or selected spectra

TIP: press [Alt] and click on the spectra icon in the list of loaded spectra to open the corresponding SIMNRA file in SIMNRA.

2.1 - Edit detector



Detector parameters

C:\Users\Cleber\Downloads\TiAlTa\21\20160929\R039292G.xnra

energy: 2200.00005 Limits

alpha: 7 beta: 17 theta: 170

offset: 157.718208138203 linear: 6.09912948831258

quadratic: 0.000E00 particles * sr: 9.137498E10

fwhm: 20.2015745531371 beam spread: 0

weight of spectra: 1

dead layer: Si 600

Range of Fit:

From: To: Weight: 1 Add interval

(1):25-120
 (1):180-350



Refresh Save Cancel Refresh

This window can be accessed by a double click on the spectra icon in the list of loaded spectra or clicking in then button Edit detector to edit data of selected spectra. In this window parameters of

experimental setup are defined. It is possible to select which parameters will be fitted by checking the check-boxes and define their limit range by clicking in the button Limits.

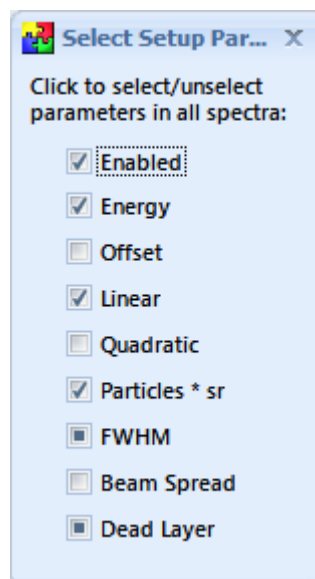
Here it is possible to define the weight of the spectra in the χ^2 calculation (this can be used to inform to MultiSIMNRA that one spectra is more important than other) and different regions of interest for the fit, also with different weights to χ^2 calculation (At least one range must to be defined. Multiple regions can be defined. Overlaps are allowed and different weights can be given to privilege some regions of the spectra). The algorithm compute ranges as defined by user during fitting process however, during calculation of uncertainties, the program remove weights and overlaps of intervals and calculates the standard χ^2 .

PS: double-click to edit an interval. One click and pressing delete, removes the selected range.

	Reload configuration from file (except range).
	Change spectra file location

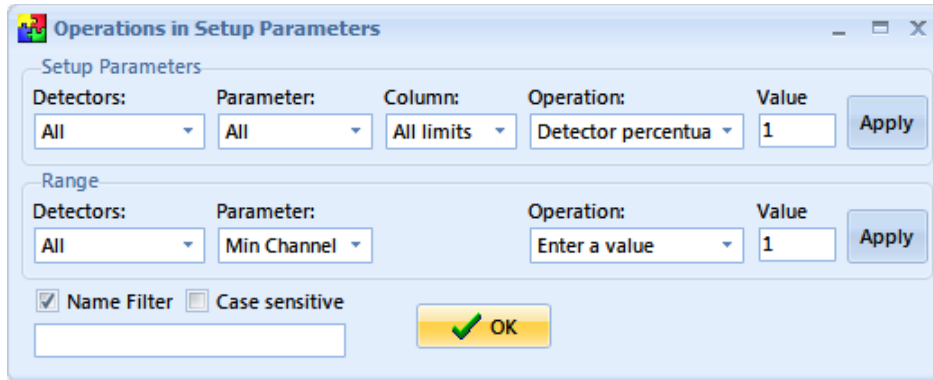
PS.: If any change is made manually in the SIMNRA file, it is ignored by MultiSIMNRA. If you want to incorporate such changes, the Reload button must to be used to refresh the setup parameters.

2.2 - Select setup parameters



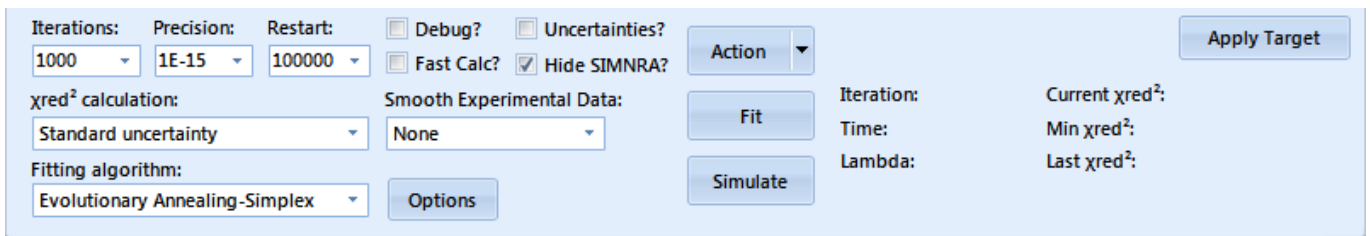
This window shows which setup parameters are selected to fit and can change the state of this in all spectra. It is a fast way to select and deselect parameters to fit.

2.3 – Batch operations in setup parameters



This window enables batch operations in setup parameters, operating in the parameter value or in it limits. This tool can change the minimum and maximum channel of ROI of all spectra.

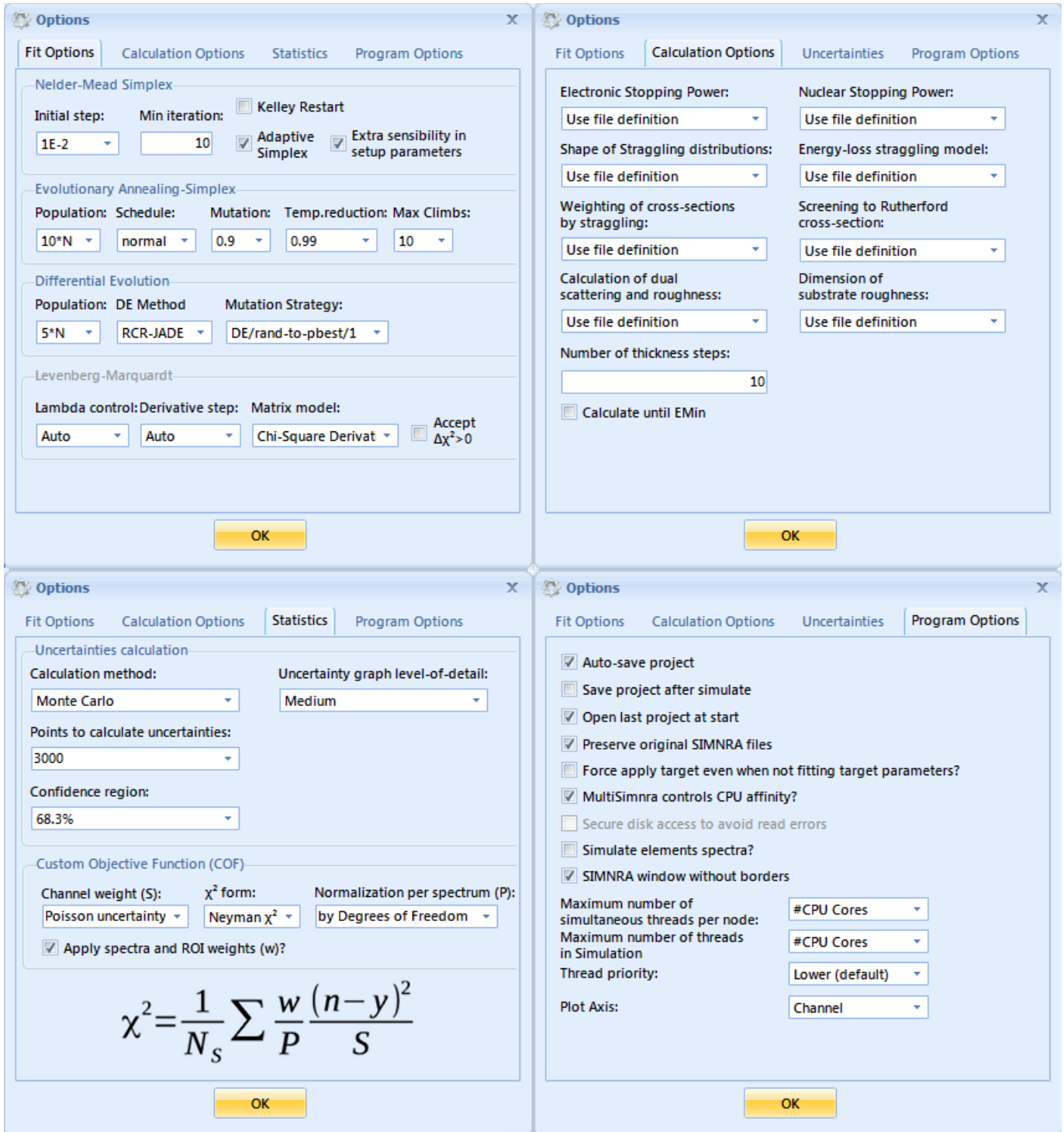
3 – Options of fitting Algorithm



Some options are duplicated in window Results and can be changed during the fit.

- Iteration limit: algorithm stop when complete this number of iterations.
- Precision: algorithm stop when the dispersion of best solutions are smaller than this value
- Restart: If algorithm is stalled in a local minimum, after this number of iterations without finding a better solution, the best solution receive a small perturbation to try overcome the local minimum. Specially implement to enable multiple starts for the Simplex algorithm.
- χ_{red}^2 calculation: Select if χ_{red}^2 is computed using standard uncertainties (square root of counts if higher than 4 and 2 if lesser or equal than 4) or no uncertainties (used for better definition of higher peaks).
- Fitting algorithm: Choose one of four implemented algorithm: Simplex, Evolutionary Annealing Simplex, Differential Evolution or Levenberg-Marquardt.
- Debug: print more information on log file
- Uncertainties?: Estimate uncertainties of fitted parameters by evaluation of χ^2 in the neighborhood of the fitted parameters.
- Hide SimNRA: is an option to hide SimNRA windows for obtain better performance while program run fit procedure. This option can be disabled any time to view the fitting progress.

3.1 – Options



All fit options change parameters in real time or on the next iteration. At now, only changes in Population can eventually produce a crash in some cases due memory reallocation. Calculation options are set only in the initialization. Uncertainties options are set when the uncertainties estimation procedure starts. Program options are selected in real time, except Plot Axis and CPU affinity control.

3.1.1 – Fit Options

Simplex

- Initial Lambda: This value is shared with Levenberg-Marquardt (LM) initial dumping factor (λ). This is also used in Simplex to control the initial step, as fraction of median simplex.

- Min iterations: Used to force a minimum of iterations before converge (works on all algorithms).
- Adaptive Simplex: Use a modified version of Simplex, in principle it is better than original Simplex when fitting a higher number of parameters.

Levenberg-Marquardt

- Lambda Control: The Levenberg-Marquardt algorithm is dependent of a good choose of Lambda for obtained convergence. In Automatic the algorithm chooses the best value for Lambda in each iteration. The other values manually force reduce or increase Lambda value.
- Accept $\Delta\chi^2 > 0$ is an option to Levenberg-Marquardt algorithm try to find alternative path to minimize chi-square and avoid a local minimum.

Evolutionary Annealing-Simplex

- Population: define the population size for the algorithm. A recommended value is 10 times the number of parameters, but the user can use a smaller or a bigger population, to speed up convergence or cover well all space range.
- Schedule and temperature reduction controls the simulated annealing search process.
- Mutation: control the mutation of populations. The crossover of populations is controlled using the downhill simplex pattern.
- Max Climbs: define the max number of uphill steps. Use a value 5 or 10.

Adaptive Differential Evolution

- DE Method: There are two options: JADE (an Adaptive Differential Evolution) and RCR-JADE (JADE with Repairing Crossover Rate). Normally, RCR-JADE give better results, but not always.
- Mutation strategy: Two options: DE/current-to-pbest/1 and DE/rand-to-pbest/1. DE/rand-to-pbest/1 has more population diversity. Try to start with DE/rand-to-pbest/1, and if algorithm is unsuccessful to minimize χ^2 , change the strategy.

3.1.2 – Calculation Options

- These options are used to ensure that the same basic physical database or models are applied in all spectra. If different models are necessary, the User Defined option must to be selected and the option must to be changed manually in each spectra. Some controls are disabled for SIMNRA 6 users.

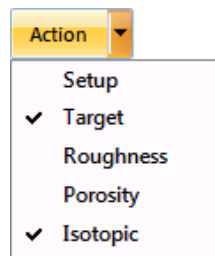
3.1.3 – Uncertainties

- Calculation method: at present version, only a Monte Carlo method is implemented. This consists in randomly generate several new sets of parameters with χ^2 value inside of confidence region selected. With the distribution of new sets, calculate the uncertainty of each parameter.
- Points to calculate uncertainties: Number of new sets accepted by the procedure.
- Confidence region: Select the confidence region used to accept new set of parameters. The recommended value is 68.3%. For others, the procedure will calculate 2σ or 3σ to obtain uncertainty σ for each parameter.

3.1.4 – Program Options

- Auto-save project: when selected, save MultiSIMNRA Project after 15 minutes.
- Save project after simulate: when selected, Save SIMNRA file after click in Simulated button.
- Open last project at start: Remember last project used, and open in the next use of MultiSIMNRA.
- Preserve original SIMNRA files: when selected, all spectra include in MultiSIMNRA project are copied to a new file, preserving the original one.
- MultiSIMNRA controls cpu affinity: when selected, MultiSIMNRA distribute SIMNRA calculation for available cpu cores, forcing this calculation to run only in this cpu core and sum of calculation time minimized. When disable, Windows controls and newer Windows versions do a good job, sometimes faster than the distributed calculation. Distributed calculations have some advantages to not conflict with other programs and in some cases enable processor to use a higher frequency turbo clock, etc. In the current version, the schedule system is not finished.
- Maximum number of simultaneous threads per node: Define the maximum number of SIMNRA calculation at the same time in the schedule. It is essential for a higher number of spectra than cpu cores. The fastest option normally is to use the number of running threads equal of cpu cores or in simple models, use two times the number of cpu cores. Too many threads can produce high concurrency competing for resources.
- Thread priority: Define thread priority for running threads and SIMNRA instances.
- Plot Axis: MultiSIMNRA can plot spectra using channel or energy on the abscissa axis.

3.2 - Action button



The button action select what group of parameters will be included on fit procedure. This not select any parameter, only determine the inclusion of selected parameters in fit process.

Global HotKeys:

- Ctrl + Alt + Win + M → Show Main or Fitting window of active MultiSIMNRA.
- Ctrl + Alt + Win + D → Show Depth Profile window of active MultiSIMNRA
- Ctrl + Alt + Win + U → Show Depth Profile with Uncertainties window of active MultiSIMNRA
- Ctrl + Alt + Win + P → Show Plot window of active MultiSIMNRA
- Ctrl + Alt + Win + R → Show Depth Resolution window of active MultiSIMNRA
- Ctrl + Alt + Win + F → Show Fit Results window of active MultiSIMNRA

Good practices:

- Calibrate energy before trying to fit target.
- Try start the fitting with the smaller number of layers and parameters as possible, to obtain a first approximation. After that, slice the layer or create new ones to improve the model.
- Just after obtaining a good target using the fitting process, insert parameters like calibration and beam energy with restrict range (less than 1%) just for a fine tuning.
- **WHEN INSERTING A NEW ELEMENT IN THE TARGET, IT IS NECESSARY TO CLICK THE APPLY TARGET BUTTON AND THEN OPEN THE SIMNRA FILES AND SELECT THE CROSS-SECTION IN THE REACTION LIST. THIS IS NECESSARY EVEN IN THE CASE OF RUTHERFORD CROSS-SECTIONS.**
- **BE CAREFUL! ELEMENTS WITH NO CROSS-SECTION DEFINED MAY SERVE AS A HIDDEN ELEMENT AND LEAD THE ALGORITHMS TO FIND WRONG RESULTS.**
- If any change is made in the experimental setup of a particular file, IT WILL NOT BE UPLOADED IN THE MULTISIMNRA EXPERIMENTAL SETUP! You must to go to the experimental setup window in the MultiSIMNRA program and click on the refresh button.
- Be careful with the LAMBDA choice in Levenberg-Marquardt! When the code approaches the minimum χ^2 solution, small value of LAMBDA tends to make the algorithm unstable, prevent the convergence.
- It is a good idea when fitting resonances, let the beam energy vary a little bit. Small errors in the machine calibration may prevent the algorithm to converge.
- Just very special cases require different weight to different spectra. Try to keep it as close to one as possible.