Tutorial on Monte Carlo methods in XRF analysis

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Outline

- An introduction to XMI-MSIM
- Examples
- Quantification using iterative Monte Carlo simulations
- Using XMI-MSIM

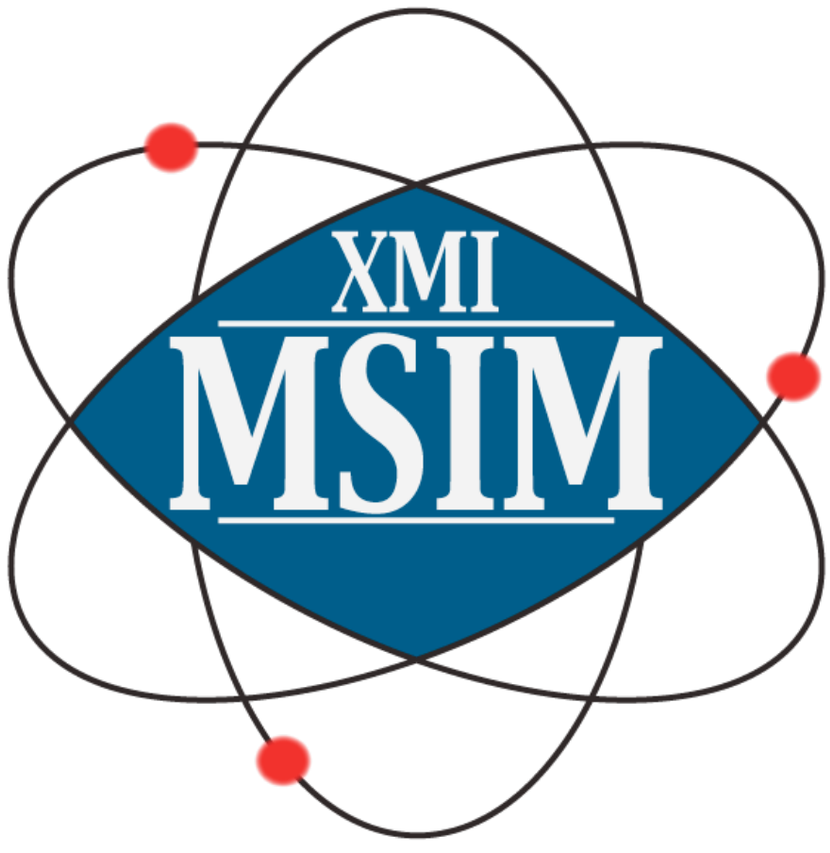
An introduction to XMI-MSIM

XMI-MSIM

- Based on *msim*, developed by Laszlo Vincze
- Fortran 77 and C
- Command-line only
- Advanced variance reduction techniques
- Impressive execution speed due to tables with inverse cumulative distribution data
- 4 publications between 1993-1999

XMI-MSIM

- Collaboration between Ghent University and ESRF
- Goal: rewrite *msim* from scratch and create plug-in for PyMca → Quantification!
- First commit: August 16, 2010
- Development hosted on Github
- GPLv3 license



XMI-MSIM: major additions

1. Simulation of XRF M-lines
2. Cascade effect
3. Detector escape peaks
4. Detector pulse pile-up simulation
5. Collimator support
6. Graphical user interface

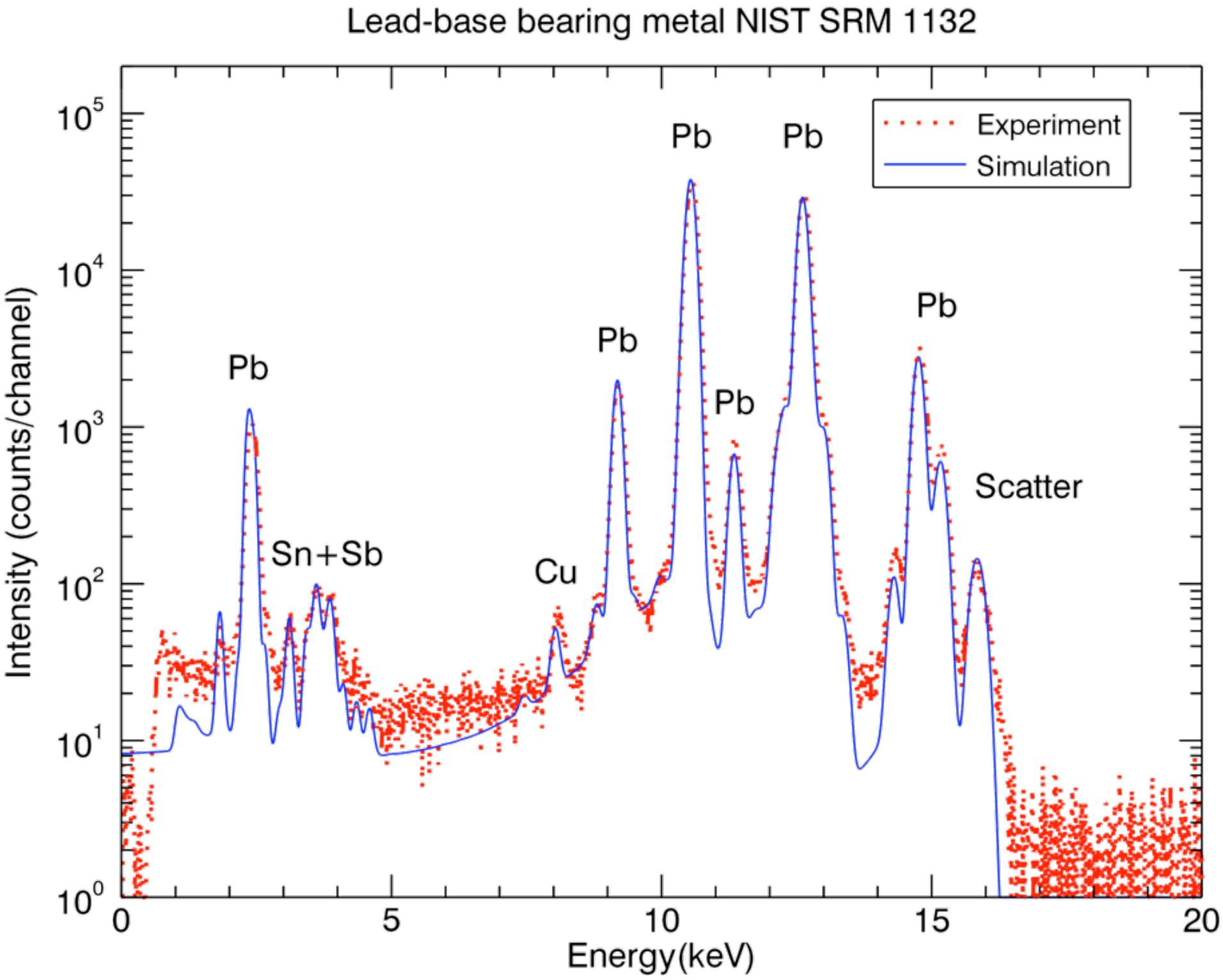
XMI-MSIM: dependencies

- Written in Fortran 2003 and C
- OpenMP
- xraylib
- hdf5
- libxml2
- libxslt
- GNU Scientific Library (GSL)
- FGSL
- glib2
- Graphical User Interface: Gtk2 & GtkExtra
- MPI (optional)

XMI-MSIM: supported platforms

- Mac OS X: 64-bit Intel native app bundle (Snow Leopard and later)
- Windows: 32-bit and 64-bit installers available (Windows 7/8 recommended)
- Linux: 64-bit RPM/DEB packages available for CentOS/ScientificLinux/Fedora and Debian/Ubuntu
- Installer size: 2.0 GB HDF5 data file!
- Memory usage: varies between 14 MB and 1.5 GB

Examples



16 keV

1500 s RT

P_{deg} ~ 92 %

10 x 10 μm^2

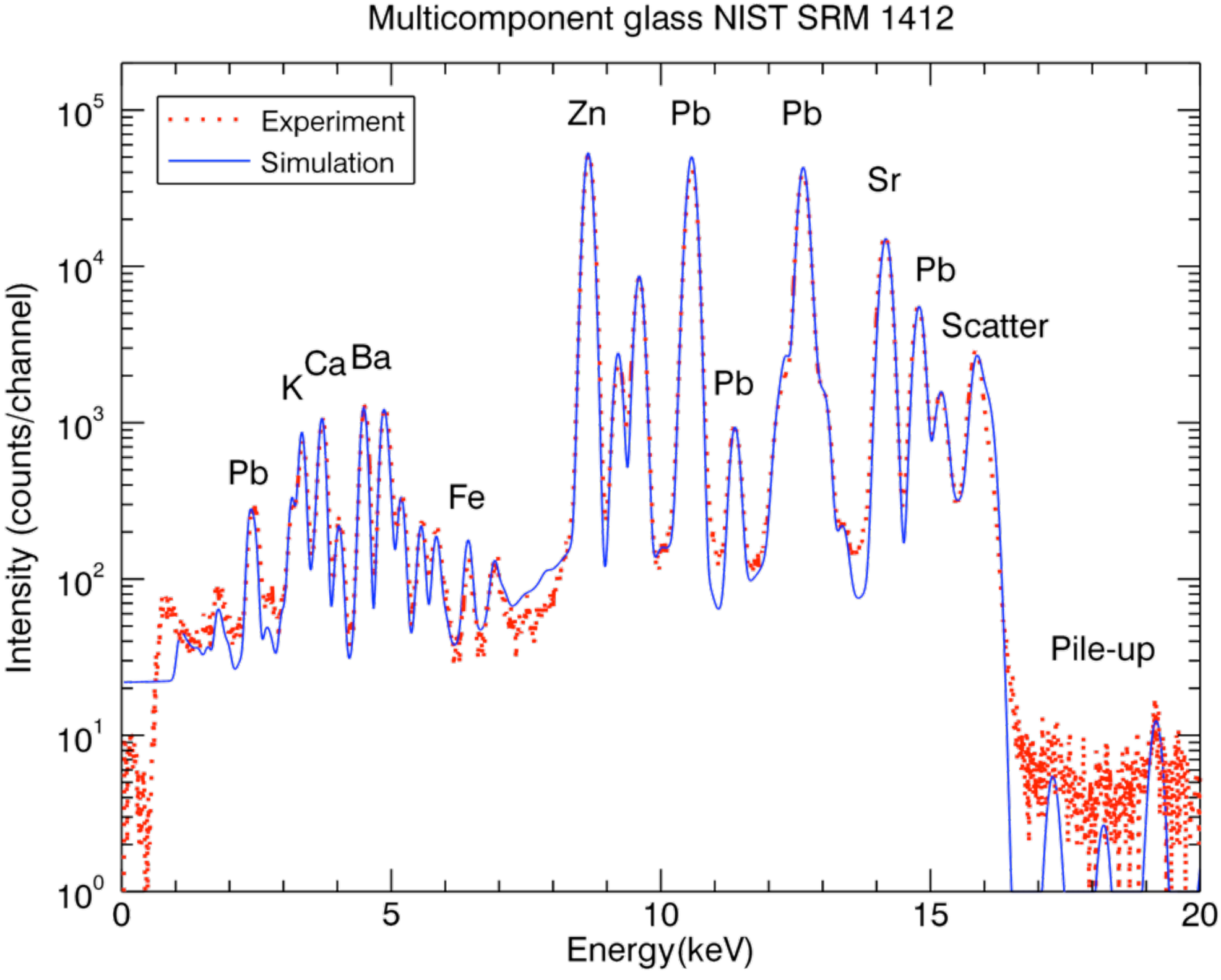
L→M cascade

Lead-base bearing metal NIST SRM 1132: M-lines

Full cascade
No cascade
Radiative cascade
Non-radiative cascade
Experiment

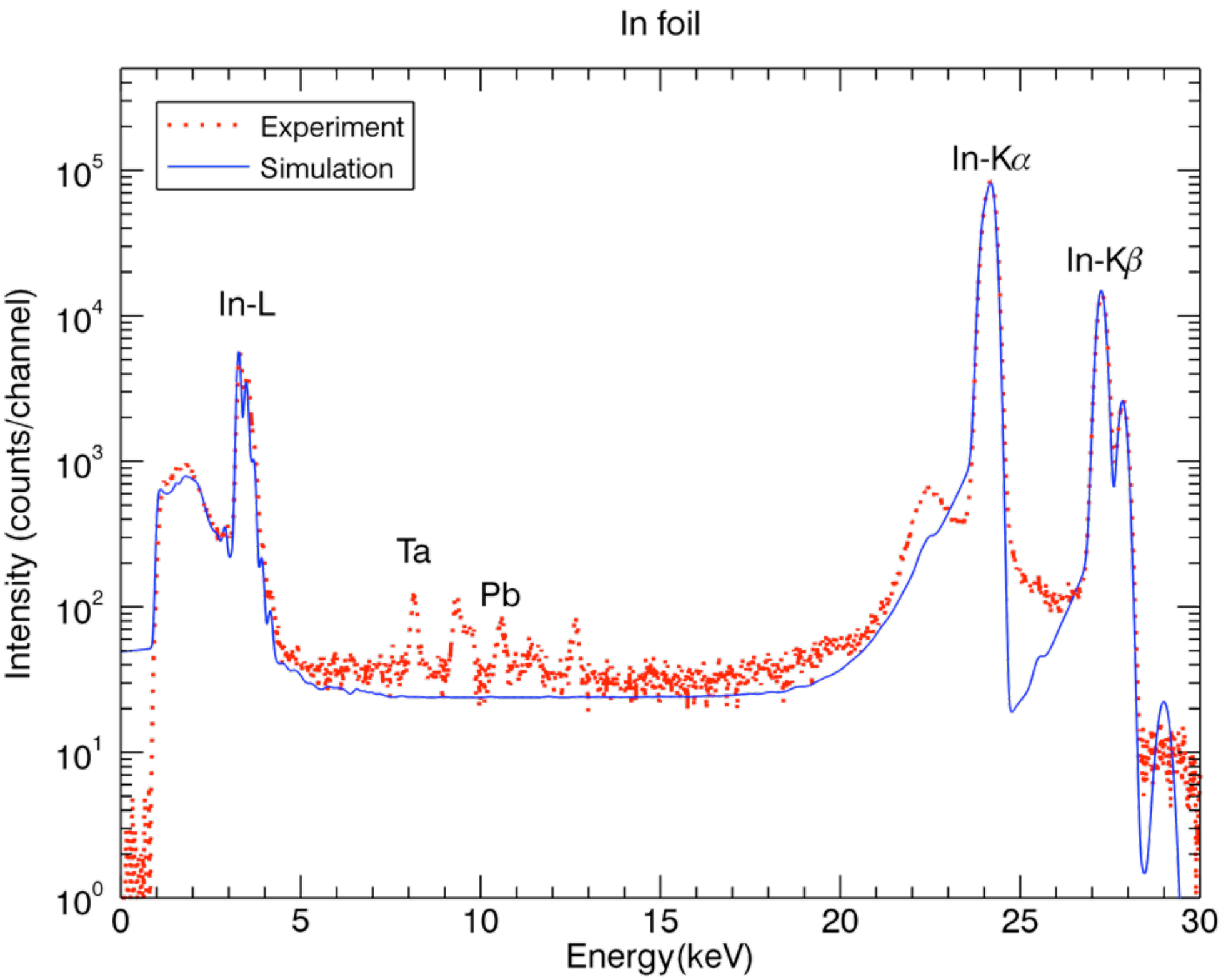
M_5N_{67}
M_5N_3
M_1N_2

Intensity (counts/channel)
10000
1000
100
10
1
1.0
1.5
2.0
2.5
3.0
3.5
Energy(keV)



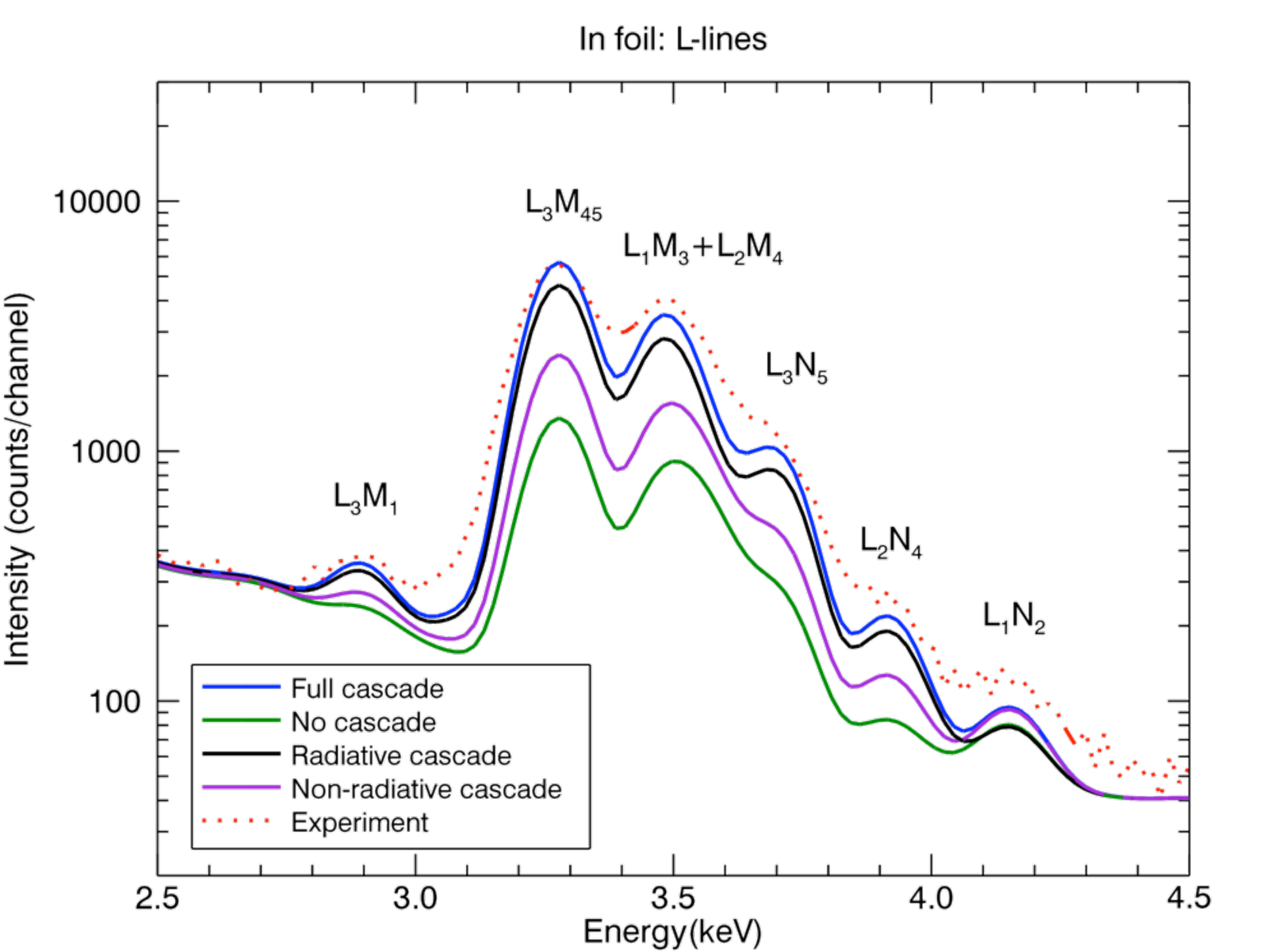
16 keV
1500 s RT
P_{deg} ~ 92 %
60 x 60 μm^2

Gaussian excitation profile

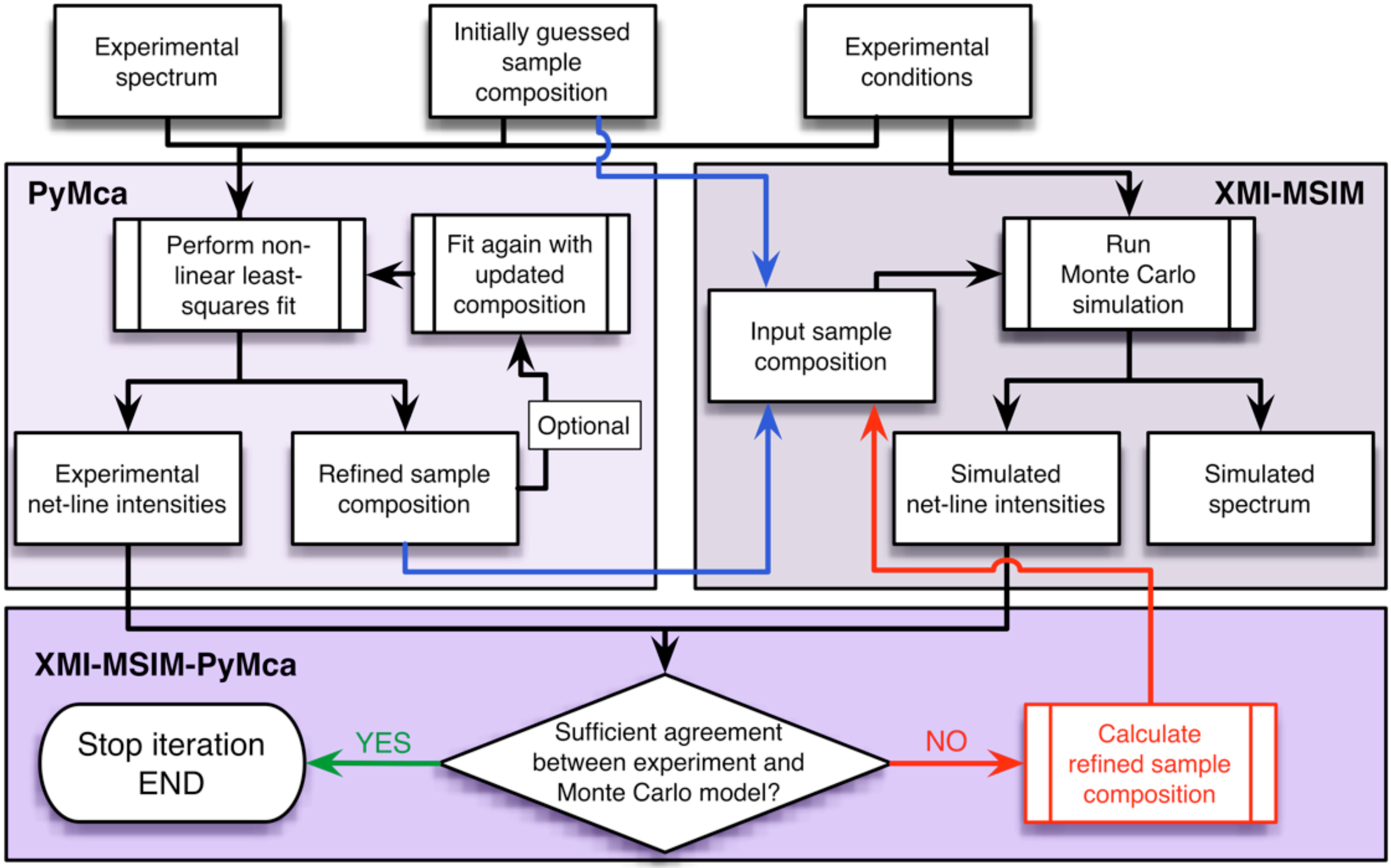


29 keV
1500 s RT
P_{deg} ~ 92 %
10 x 10 μm²

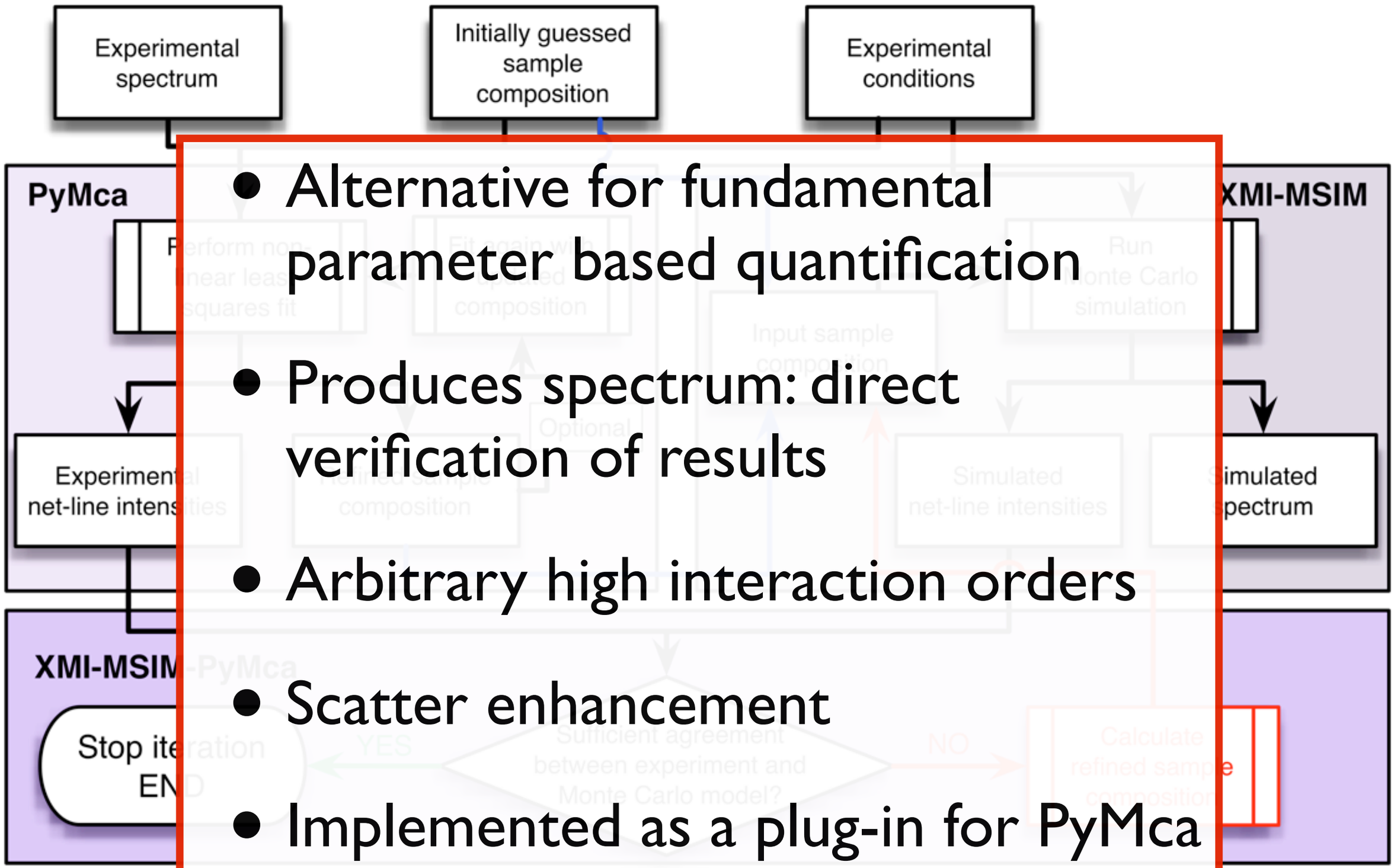
K→L cascade
Compton
escape peak


In foil: L-lines
Intensity (counts/channel)
10000
1000
100
L_3M_{45}
$L_1M_3+L_2M_4$
L_3N_5
L_3M_1
L_2N_4
L_1N_2
Full cascade
No cascade
Radiative cascade
Non-radiative cascade
Experiment
2.5
3.0
3.5
4.0
4.5
Energy(keV)

Quantification using iterative Monte Carlo simulations



XMI-MSIM-PyMca

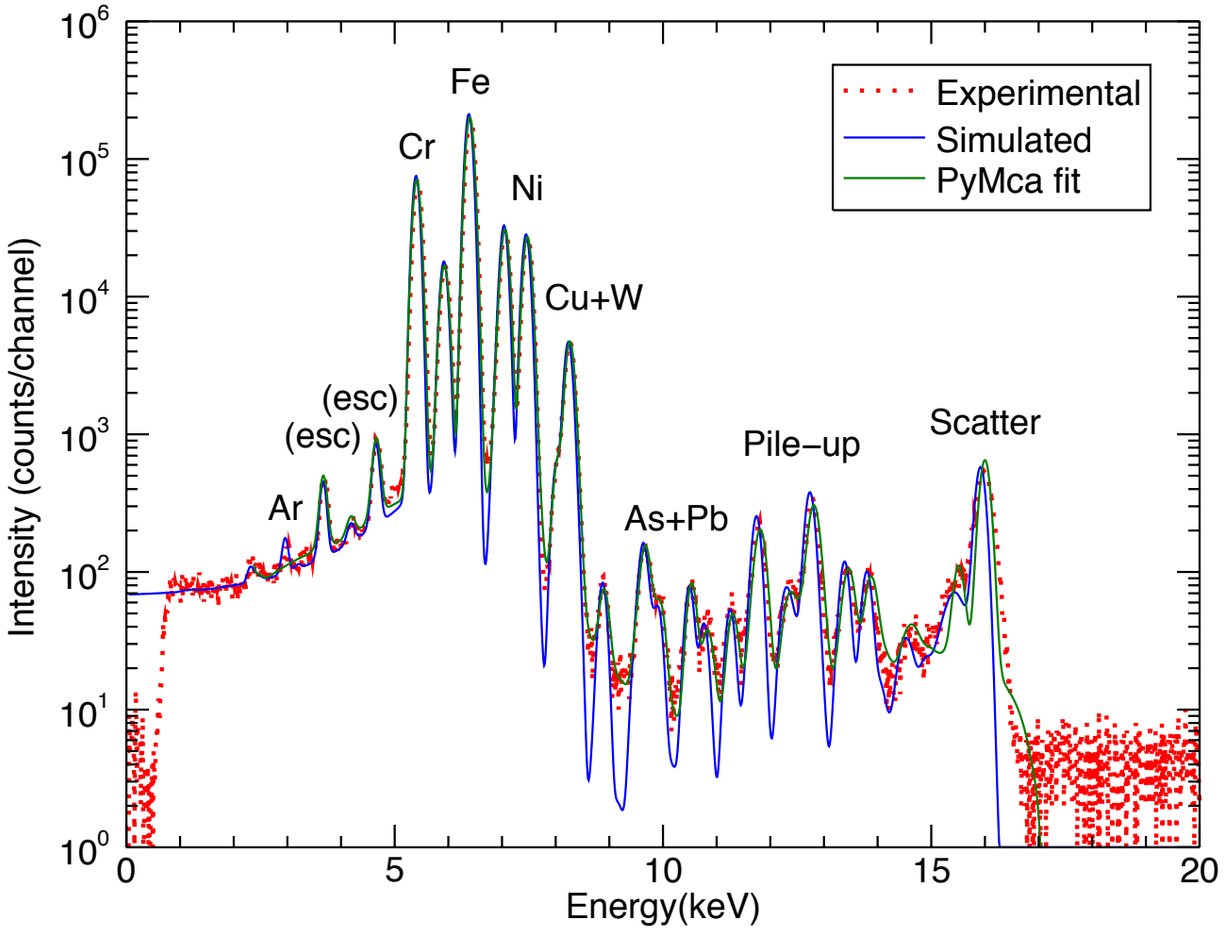


- Alternative for fundamental parameter based quantification
- Produces spectrum: direct verification of results
- Arbitrary high interaction orders
- Scatter enhancement
- Implemented as a plug-in for PyMca

XMI-MSIM-PyMca

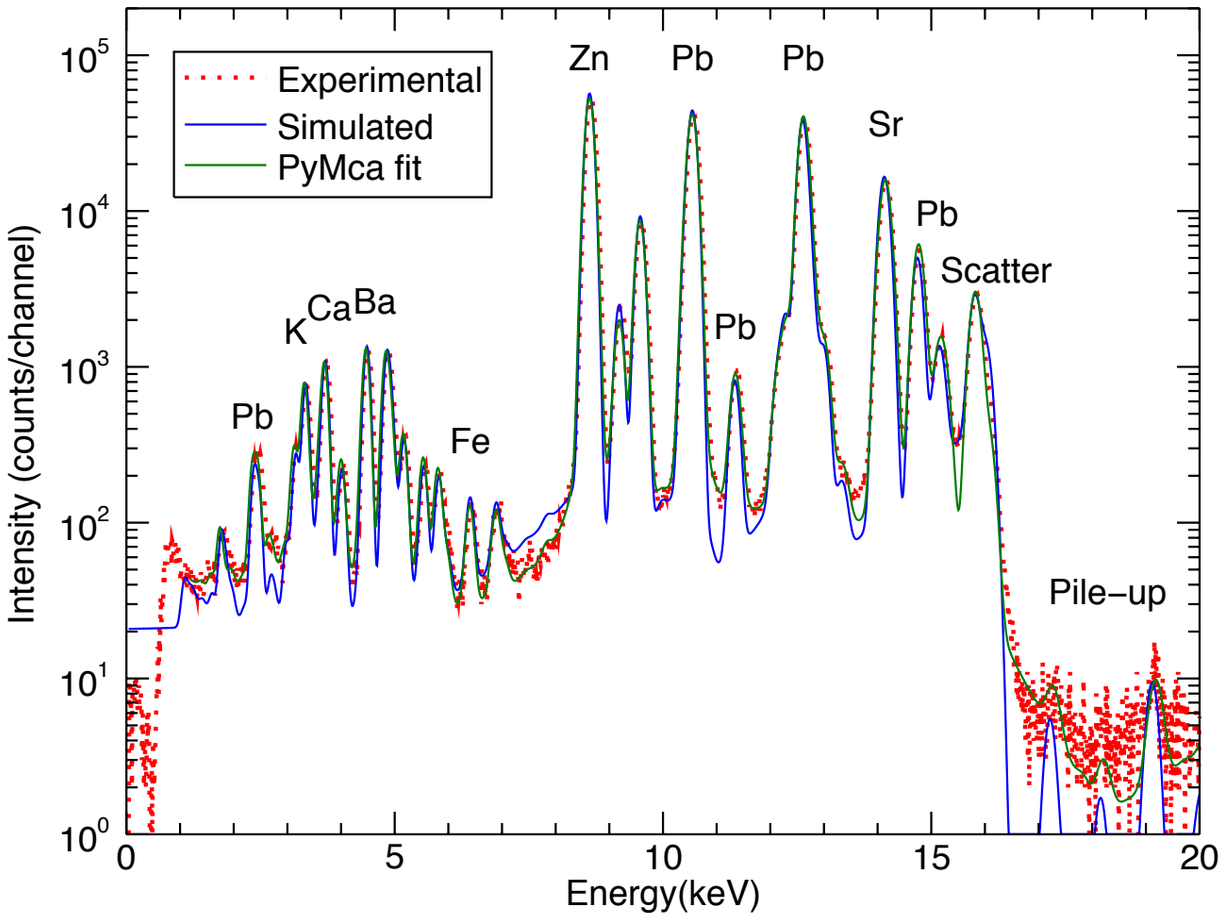
NIST SRM 1155

stainless steel



Element	NIST	XMI-MSIM PyMca
Cr	18.37%	18.37%
Mn	1.62%	1.92%
Fe	64.31%	65.72%
Co	1090 ppm	5325 ppm
Ni	12.35%	12.63%
Cu	1750 ppm	2184 ppm
W*	1100 ppm	1183 ppm
Pb*	10 ppm	75 ppm

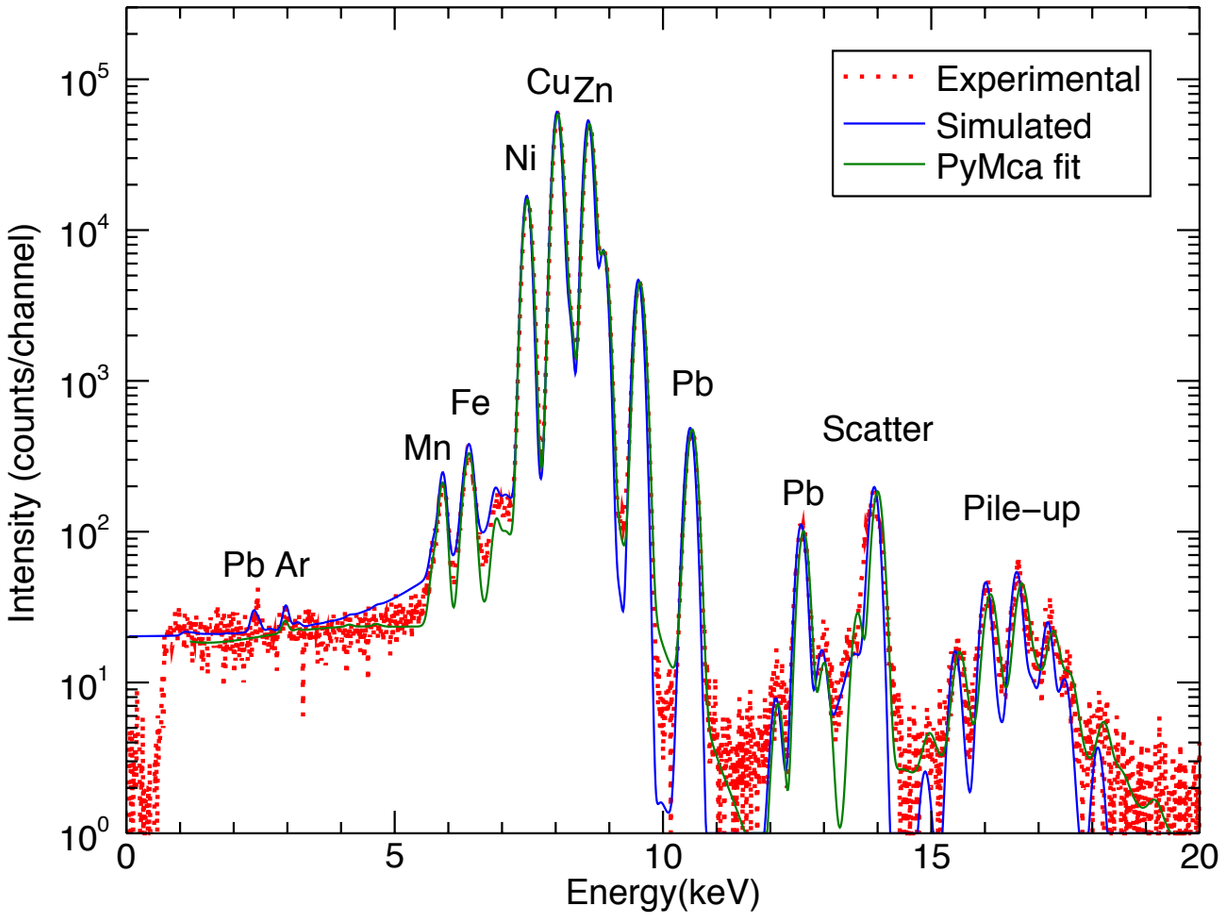
NIST SRM 1412
multicomponent glass



Element	NIST	XMI-MSIM PyMca
O	-	47.61
Si	19.81%	27.83%
K	3.44%	3.26%
Ca	3.24%	3.17%
Fe*	217 ppm	220 ppm
Zn	3.60%	3.63%
Sr	3.85%	3.97%
Cd	3.83%	2.85%
Ba	4.18%	4.27%
Pb	4.08%	3.38%

Goodfellow

Nickel Silver rod



Element	Goodfellow	XMI-MSIM PyMca
Mn	-	0.19%
Fe	-	0.17%
Ni	10.0%	10.12%
Cu	45.0%	46.57%
Zn	43.0%	41.66%
Pb	2.0%	1.29%

Using XMI-MSIM

Outline

1. Launching XMI-MSIM
2. Creating and saving an input-file
3. Starting a simulation
4. Visualizing the results
5. Global preferences
6. Advanced features

Launching XMI-MSIM

- Installation instructions: https://github.com/tschoonj/xmimsim/wiki/Installation-instructions

- Mac OS X: use Finder or Spotlight to locate the App bundle

- Windows: *Start Menu* → *Programs* →*XMI-MSIM*

- Linux: *Start Menu* → *Education* →*XMI-MSIM* or from the command-line: *xmimsim-gui*

New file

New | Open | Save As | Save | Undo | Redo | Cut | Copy | Paste | Batch mode | X-ray sources | Preferences

Input parameters | Simulation controls | Results

General

Outputfile | Save

Number of photons per interval: 10000

Number of photons per discrete line: 100000

Number of interactions per trajectory: 4

Comments

Composition

Number of elements	Elements	Density (g/cm^3)	Thickness (cm)	Reference layer?

Top | Add | Up | Edit | Down | Remove | Bottom

Geometry

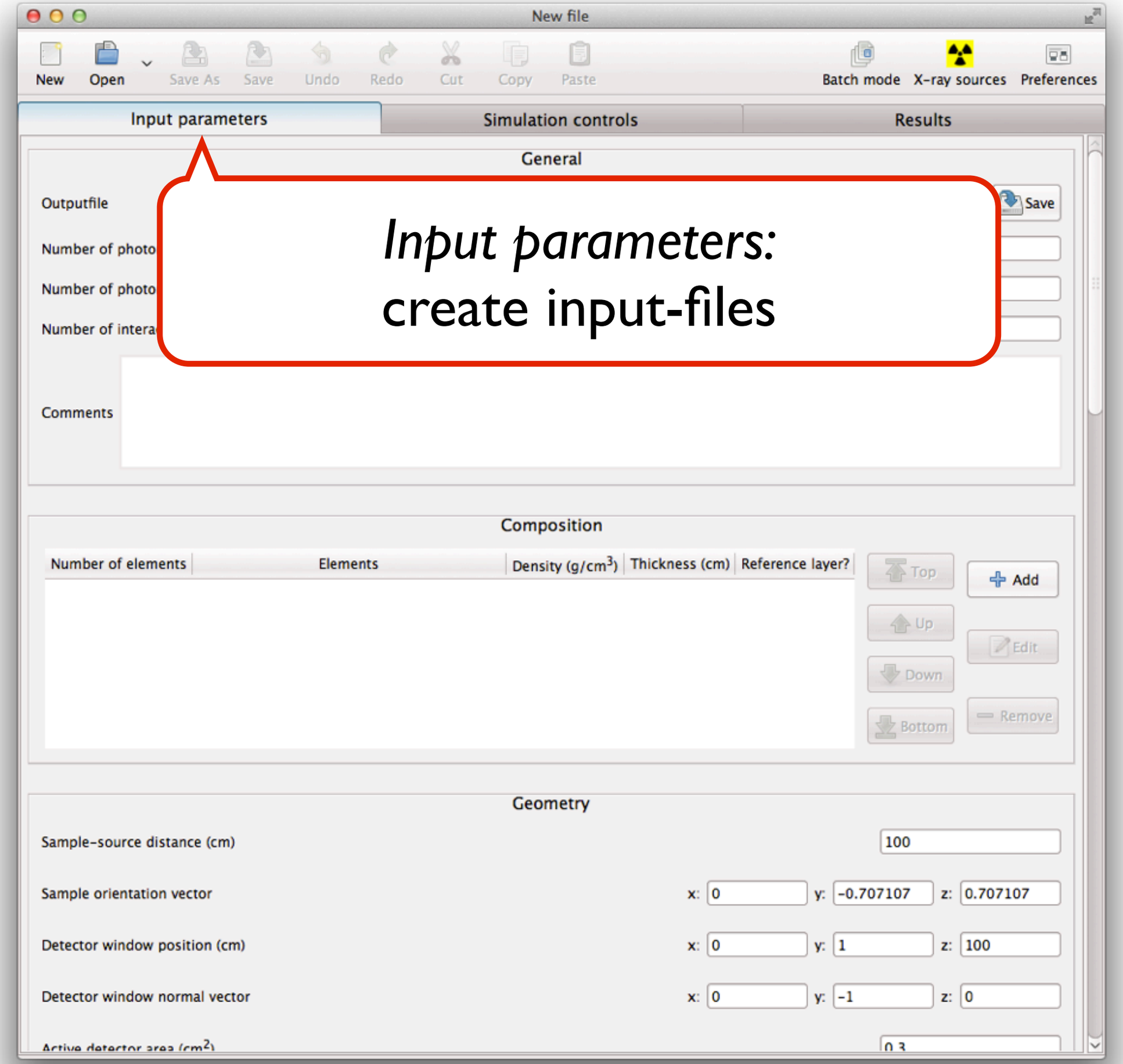
Sample-source distance (cm): 100

Sample orientation vector: x: 0 y: -0.707107 z: 0.707107

Detector window position (cm): x: 0 y: 1 z: 100

Detector window normal vector: x: 0 y: -1 z: 0

Active detector area (cm^2): 0.3


New file
New
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X-ray sources
Preferences
Input parameters
Simulation controls
Results
General
Outputfile
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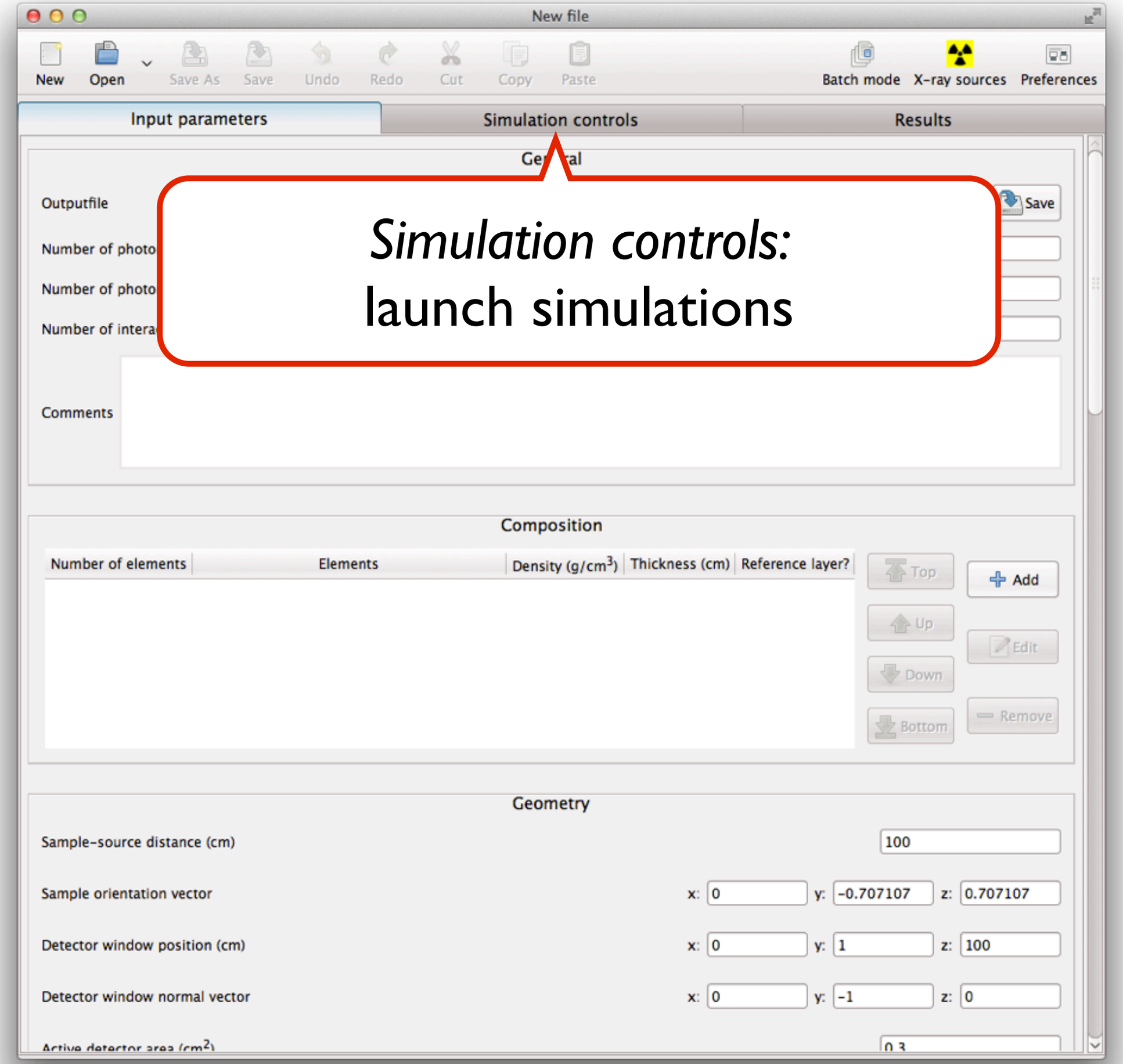
Comments
Input parameters:
create input-files
Composition
Number of elements
Elements
Density (g/cm3)
Thickness (cm)
Reference layer?
Top
Add
Up
Edit
Down
Remove
Bottom
Geometry
Sample-source distance (cm)
100
Sample orientation vector
x: 0
y: -0.707107
z: 0.707107
Detector window position (cm)
x: 0
y: 1
z: 100
Detector window normal vector
x: 0
y: -1
z: 0
Active detector area (cm2)
0.3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Simulation controls
Results
Outputfile
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Comments
Simulation controls:
launch simulations
Composition
Number of elements
Elements
Density (g/cm3)
Thickness (cm)
Reference layer?
Top
Add
Up
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Down
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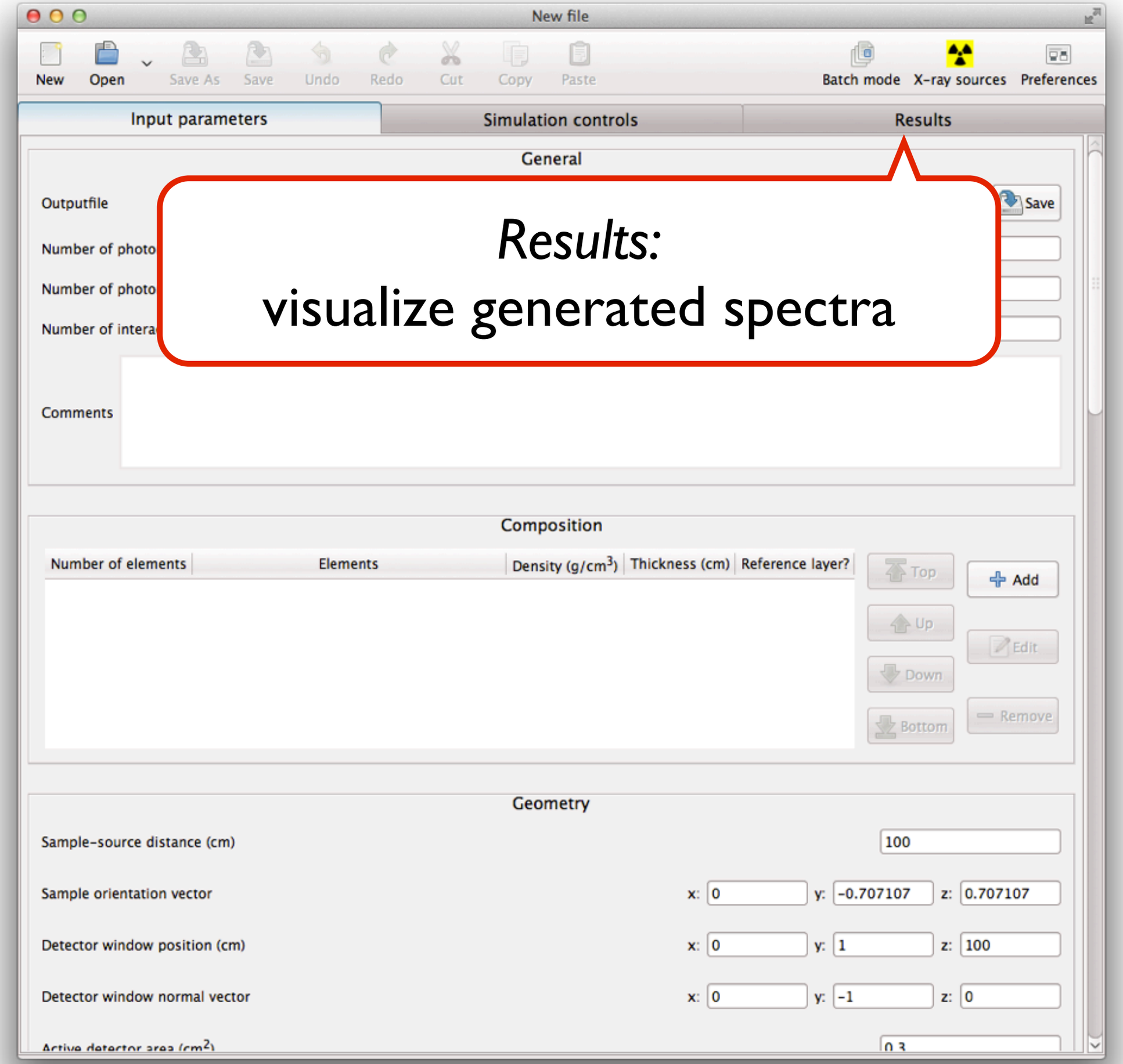
Bottom
Geometry
Sample-source distance (cm)
100
Sample orientation vector
x: 0
y: -0.707107
z: 0.707107
Detector window position (cm)
x: 0
y: 1
z: 100
Detector window normal vector
x: 0
y: -1
z: 0
Active detector area (cm2)
0.3


New file
New
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Input parameters
Simulation controls
Results
General
Outputfile
Save
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Comments
Results:
visualize generated spectra
Composition
Number of elements
Elements
Density (g/cm3)
Thickness (cm)
Reference layer?
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Edit
Down
Remove
Bottom
Geometry
Sample-source distance (cm)
100
Sample orientation vector
x: 0
y: -0.707107
z: 0.707107
Detector window position (cm)
x: 0
y: 1
z: 100
Detector window normal vector
x: 0
y: -1
z: 0
Active detector area (cm2)
0.3

Creating and saving an input-file

General parameters

General parameters

Name of the outputfile:
File extension: XMSO

General parameters

Number of photons
that will be simulated

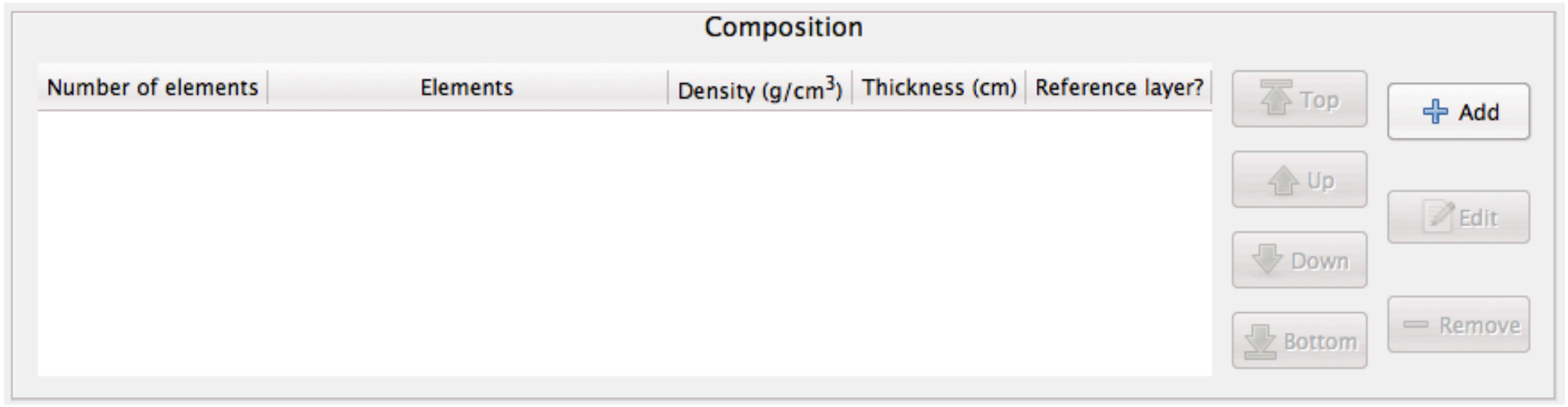
General parameters

Maximum number of interactions per photon trajectory

General parameters

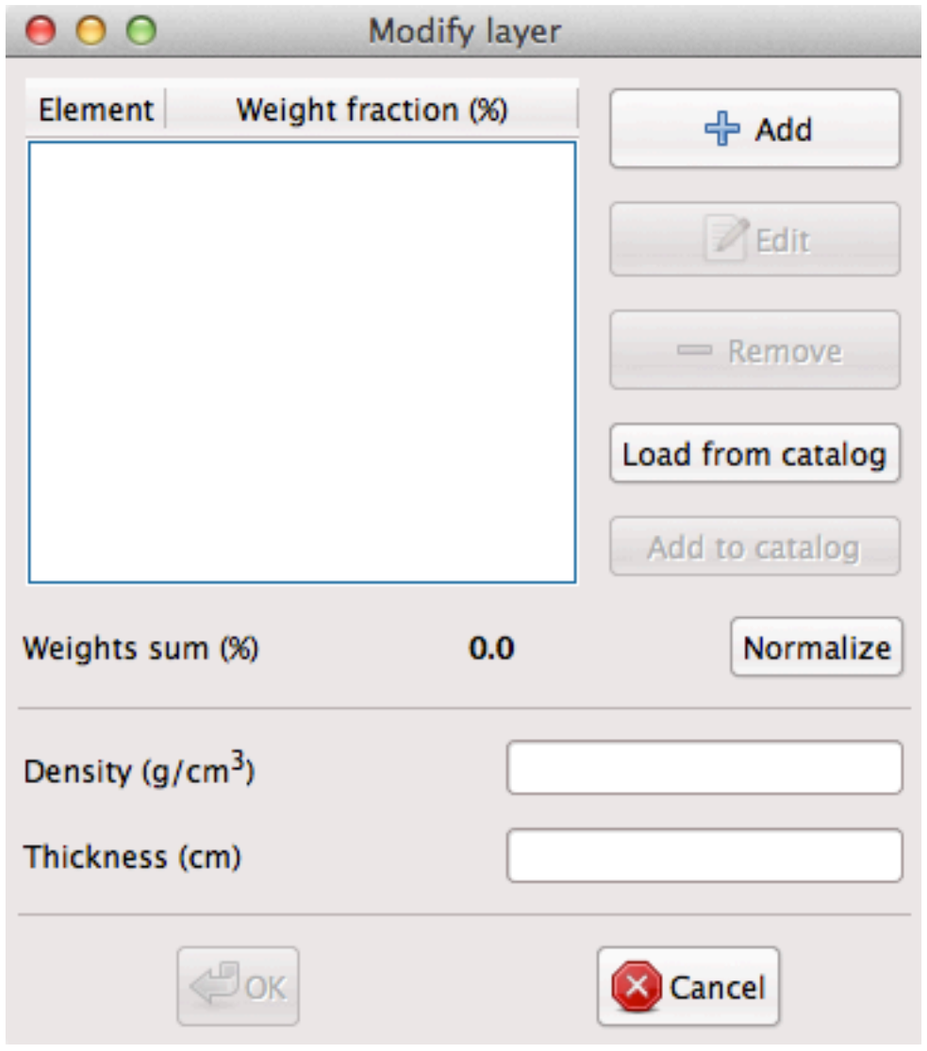
Comments section

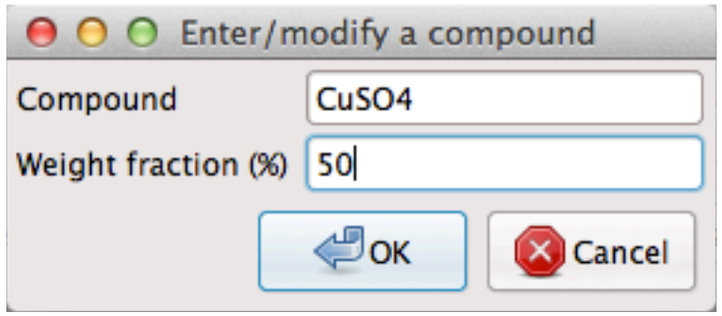
Sample composition

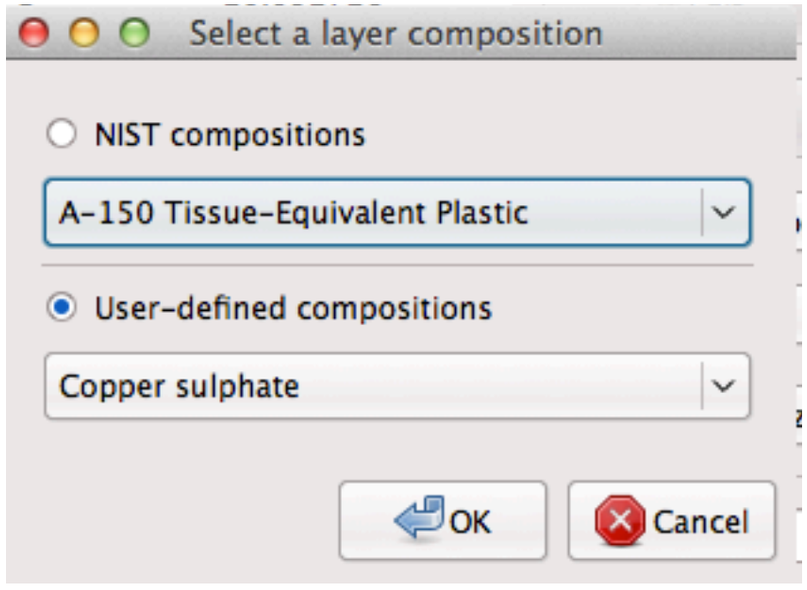


- Each layer defined by a composition, density and thickness along sample normal vector
- Add, Edit and Remove layers
- Ordering is *very* important: according to distance from the source. First layer is closest!
- Reference layer corresponds to *Sample-source distance*

Add or modify a layer

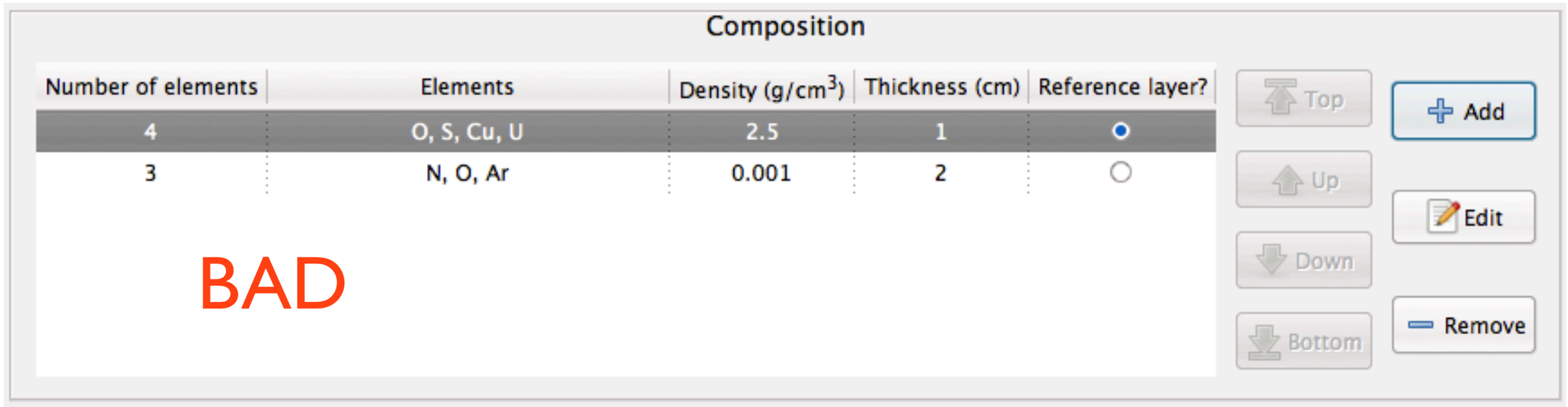


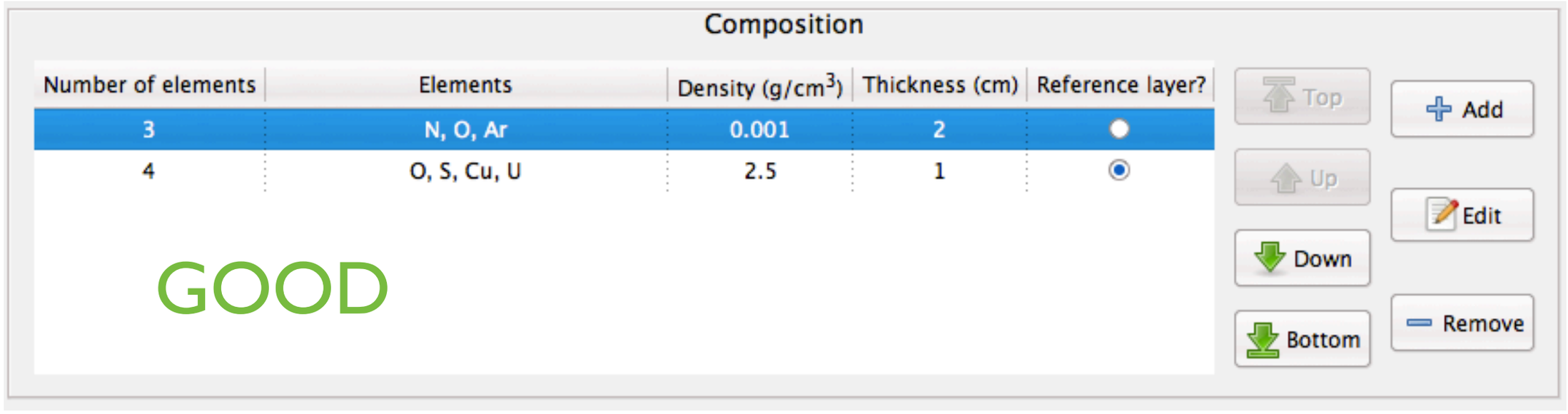




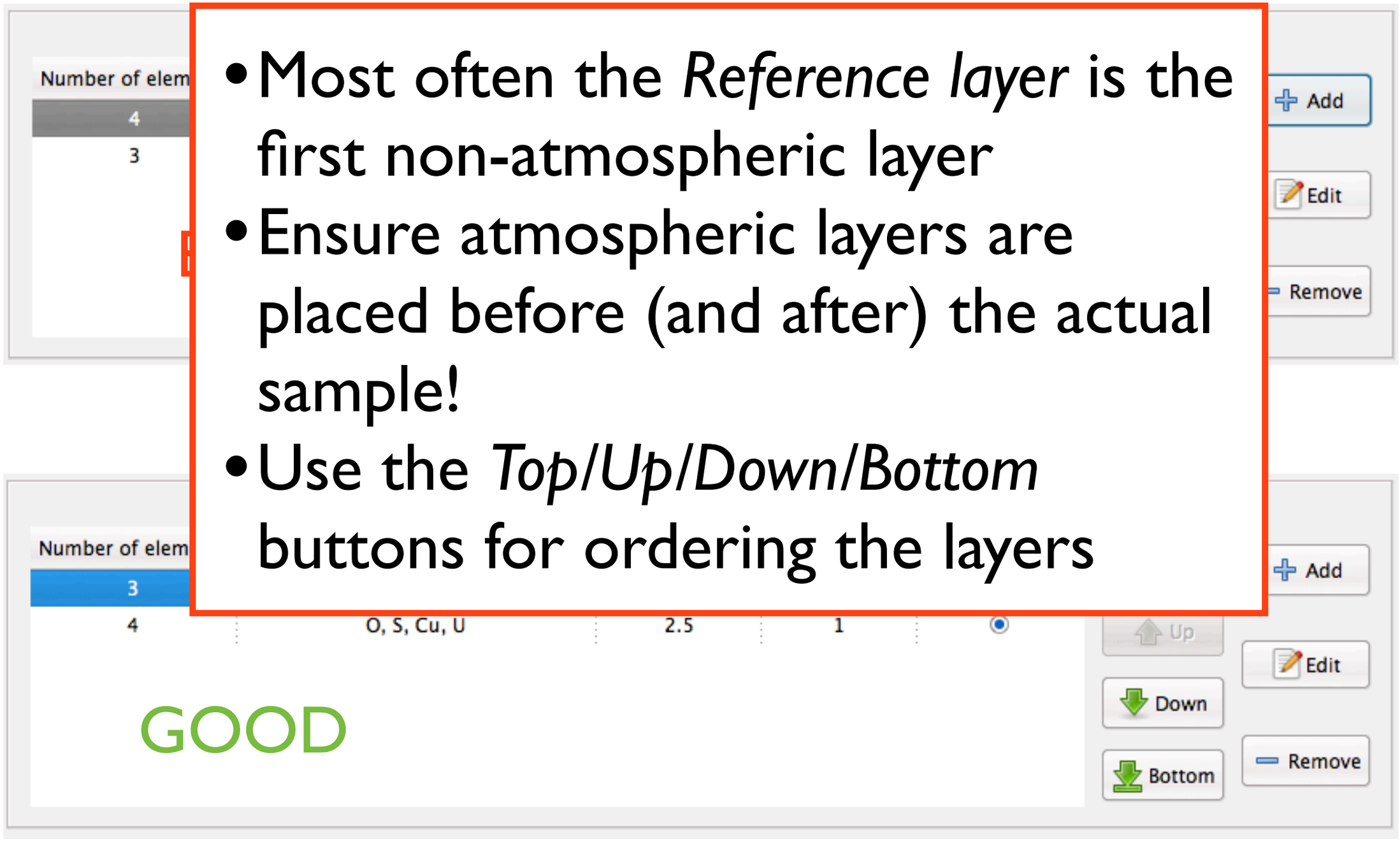
Includes density!

Ordering the layers



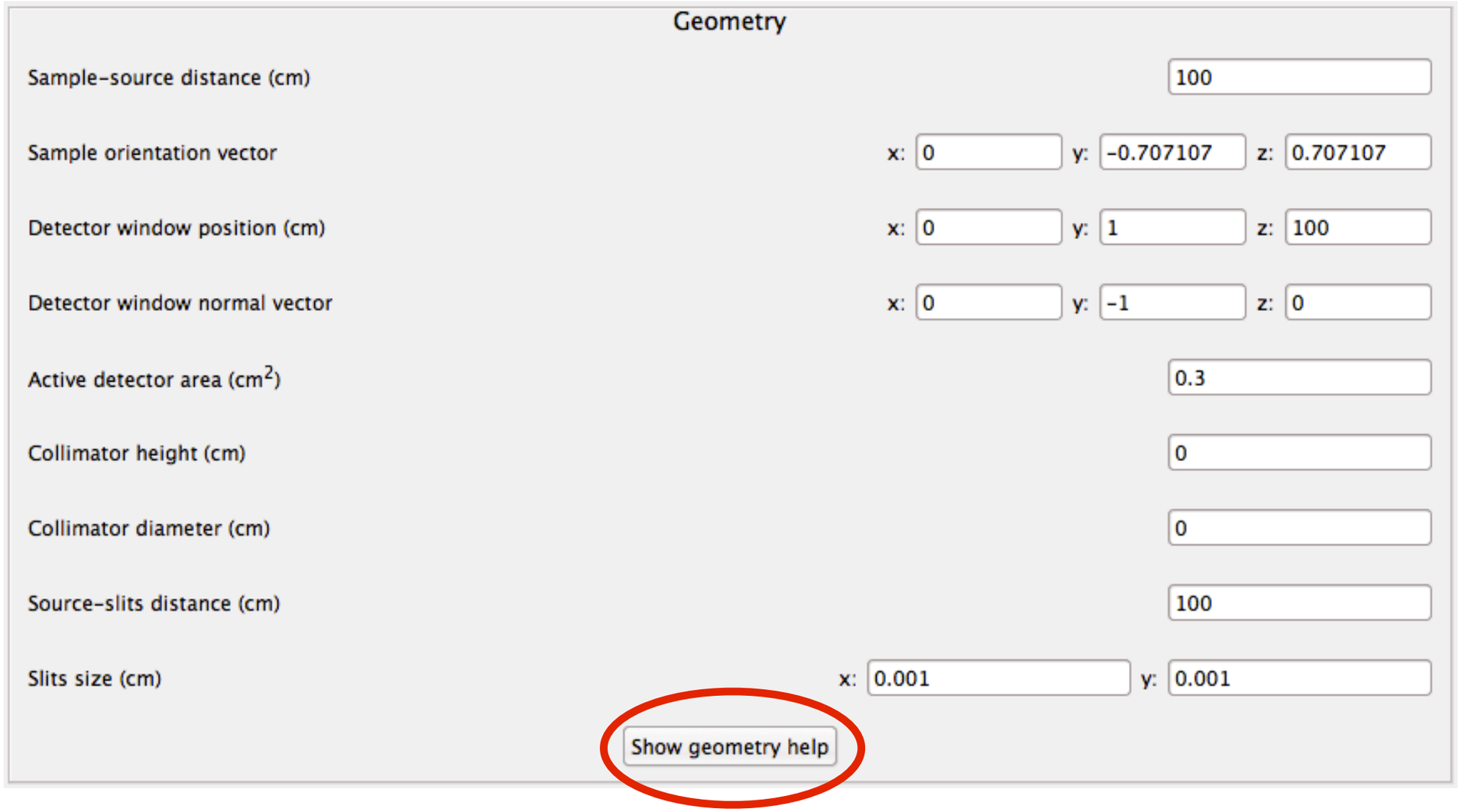


Ordering the layers

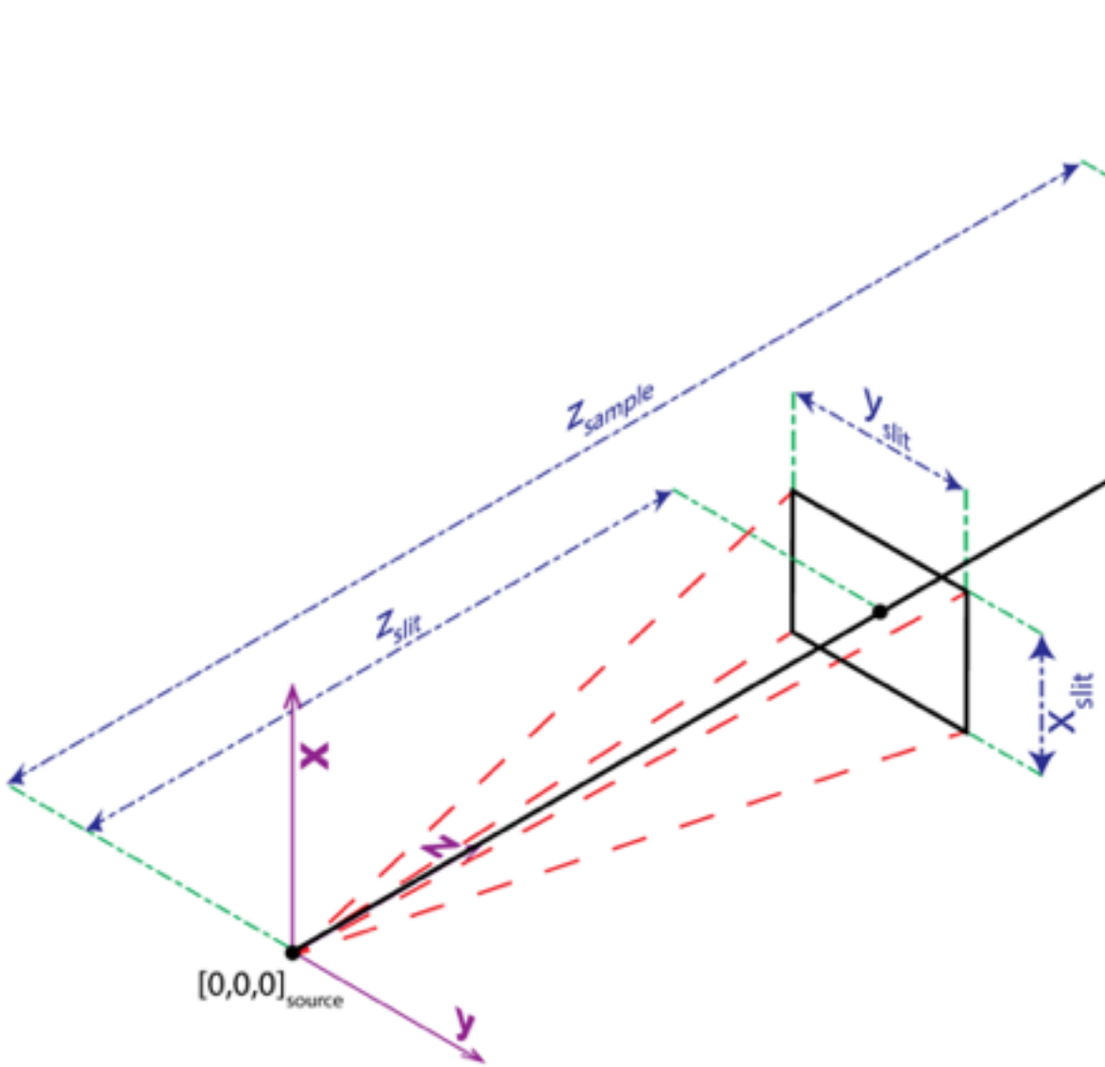


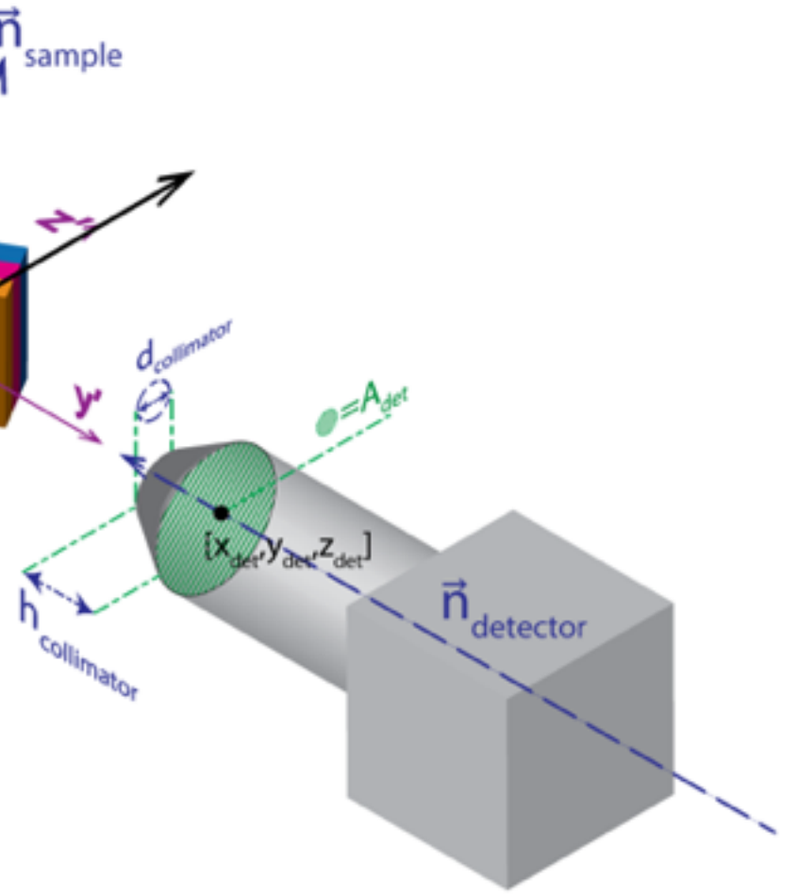
- Most often the *Reference layer* is the first non-atmospheric layer
- Ensure atmospheric layers are placed before (and after) the actual sample!
- Use the *Top/Up/Down/Bottom* buttons for ordering the layers

Geometry



- The coordinate system is right-handed Cartesian
- The z-axis is aligned with the beam direction and points from the source towards the sample.
- The y-axis defines, along with the z-axis, the horizontal plane
- The x-axis emerges out from the plane formed by the y- and z-axes

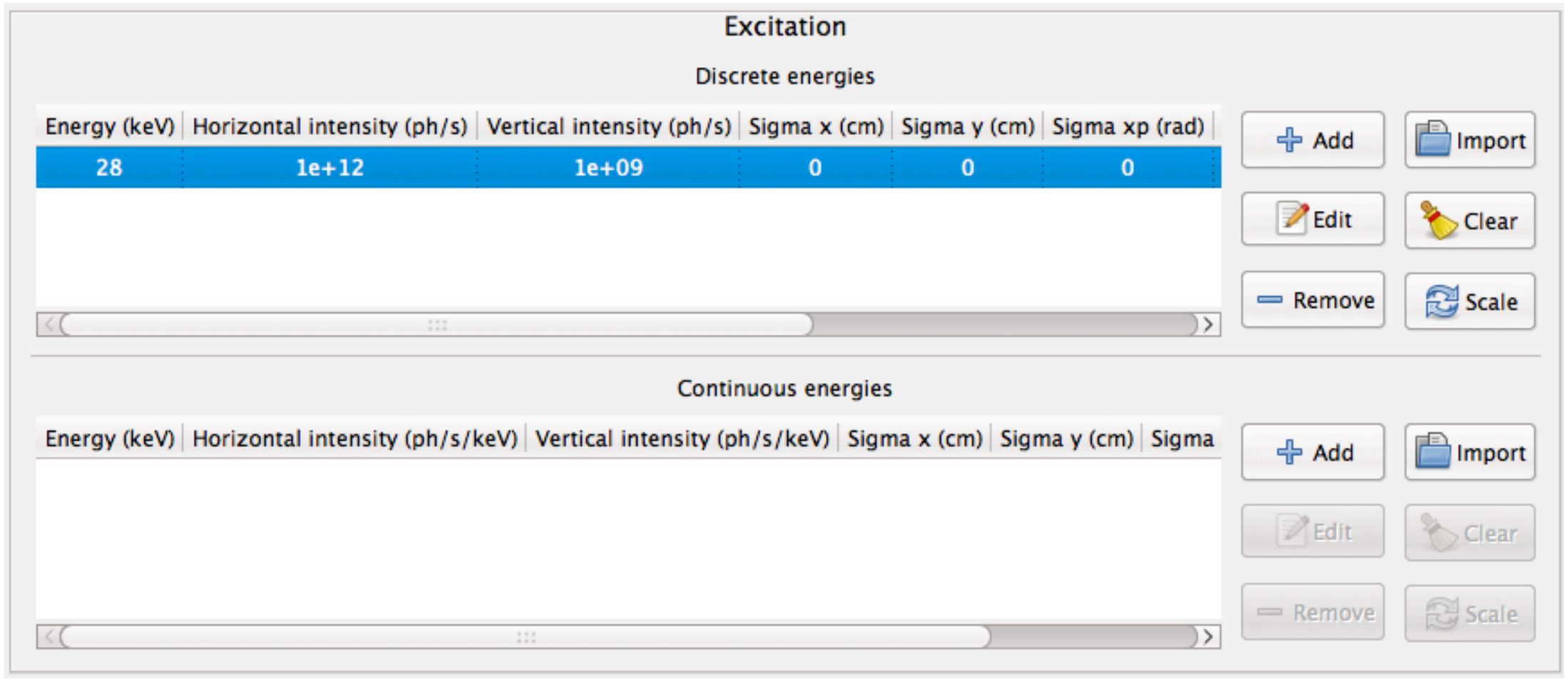




Hover mouse over image or over the entries

By Jan Garrevoet

Excitation spectrum

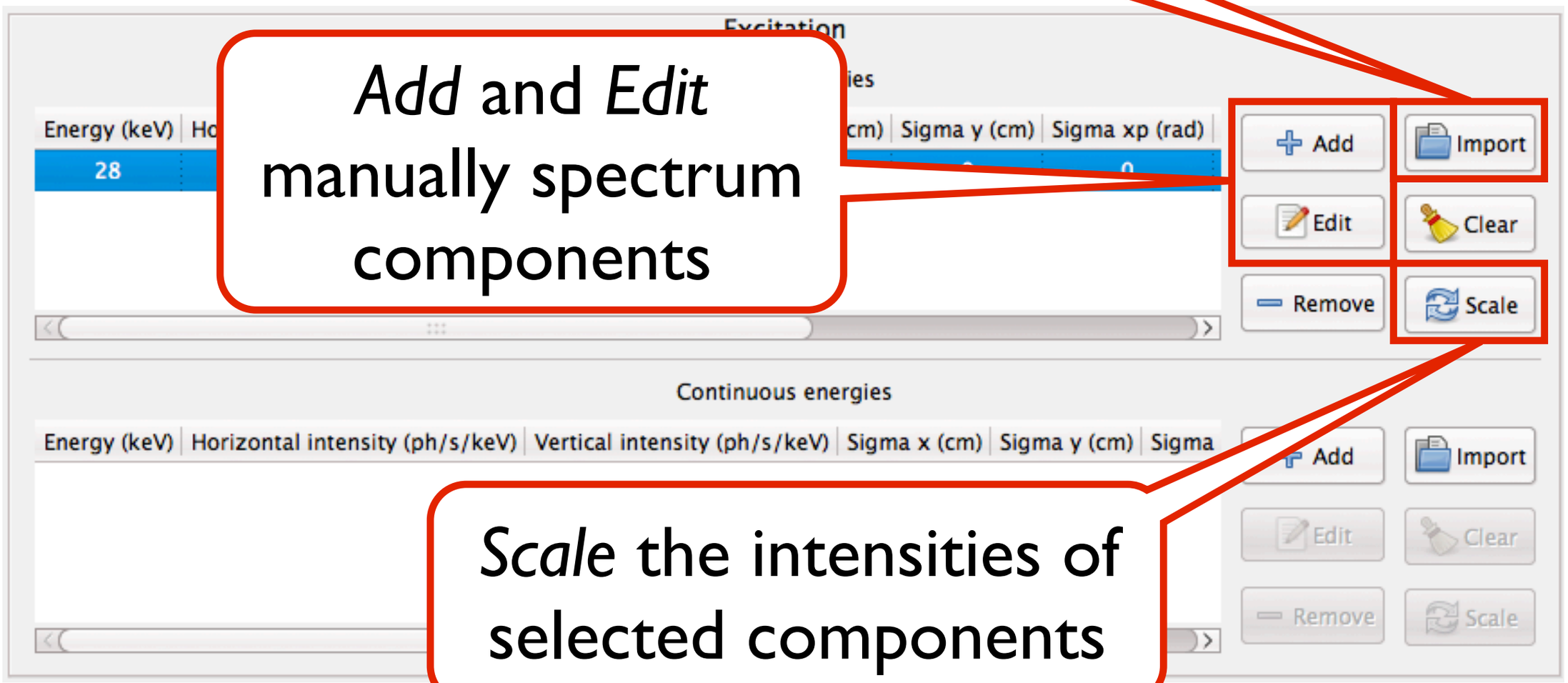


- Discrete energy components (line intensities): photons/s
- Continuous energy components (intensity densities): photons/s/keV

Ex ctrum

Import from ASCII file:
2, 3 or 7 columns!

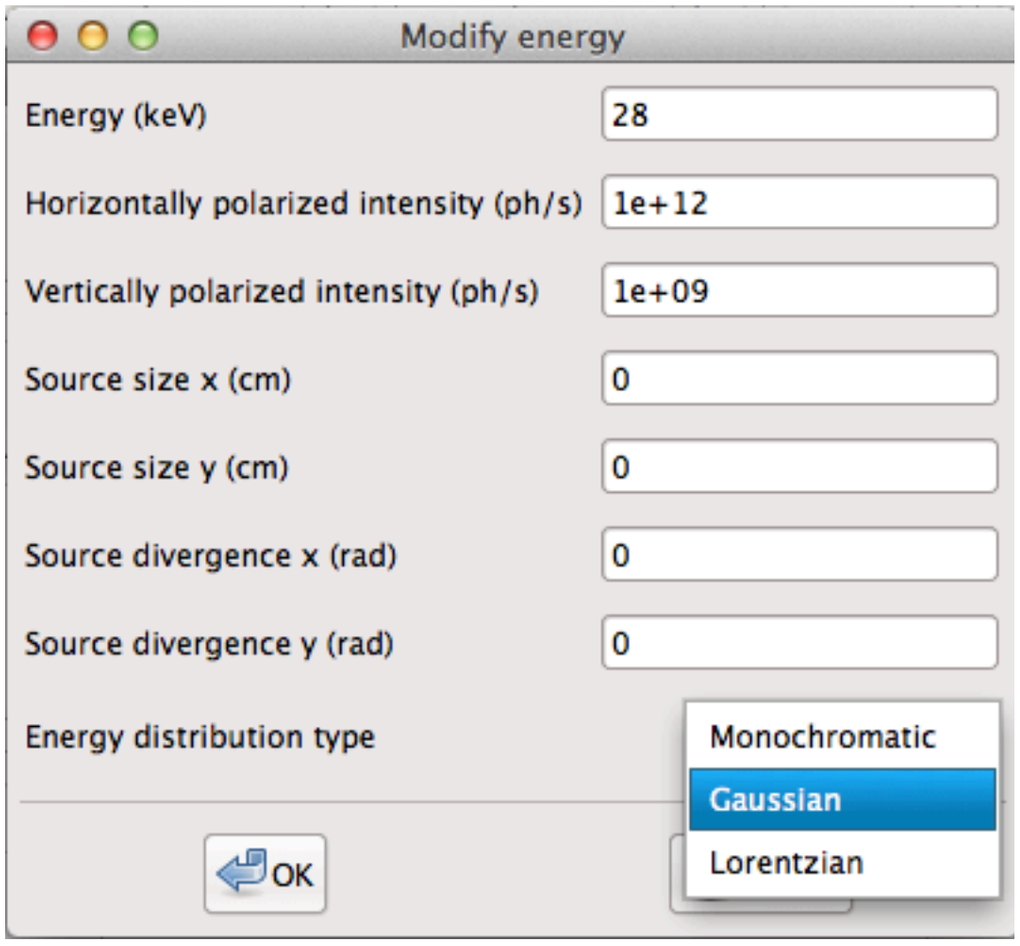
Add and *Edit*
manually spectrum
components



Scale the intensities of
selected components

- Discrete energy components (line intensities): photons/s
- Continuous energy components (intensity densities): photons/s/keV

Manually adding or editing a spectrum component



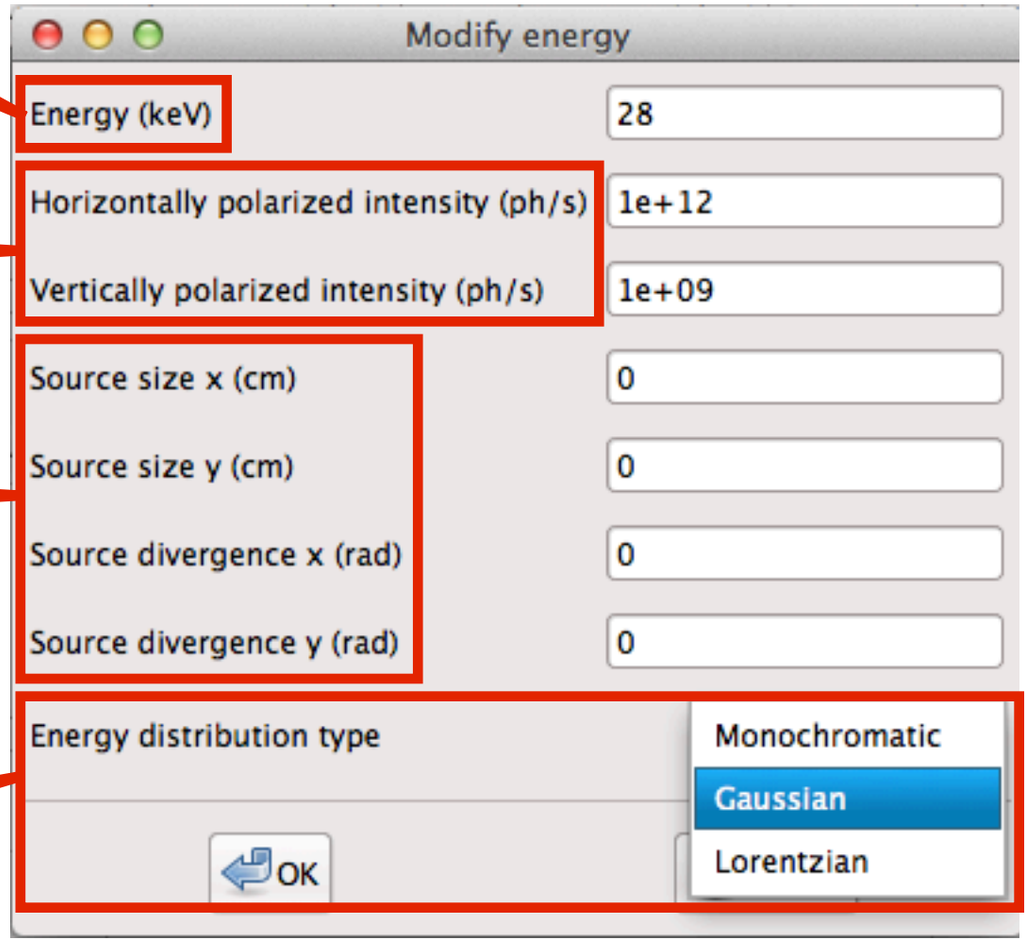
Manually adding or editing a spectrum component

Energy of the component

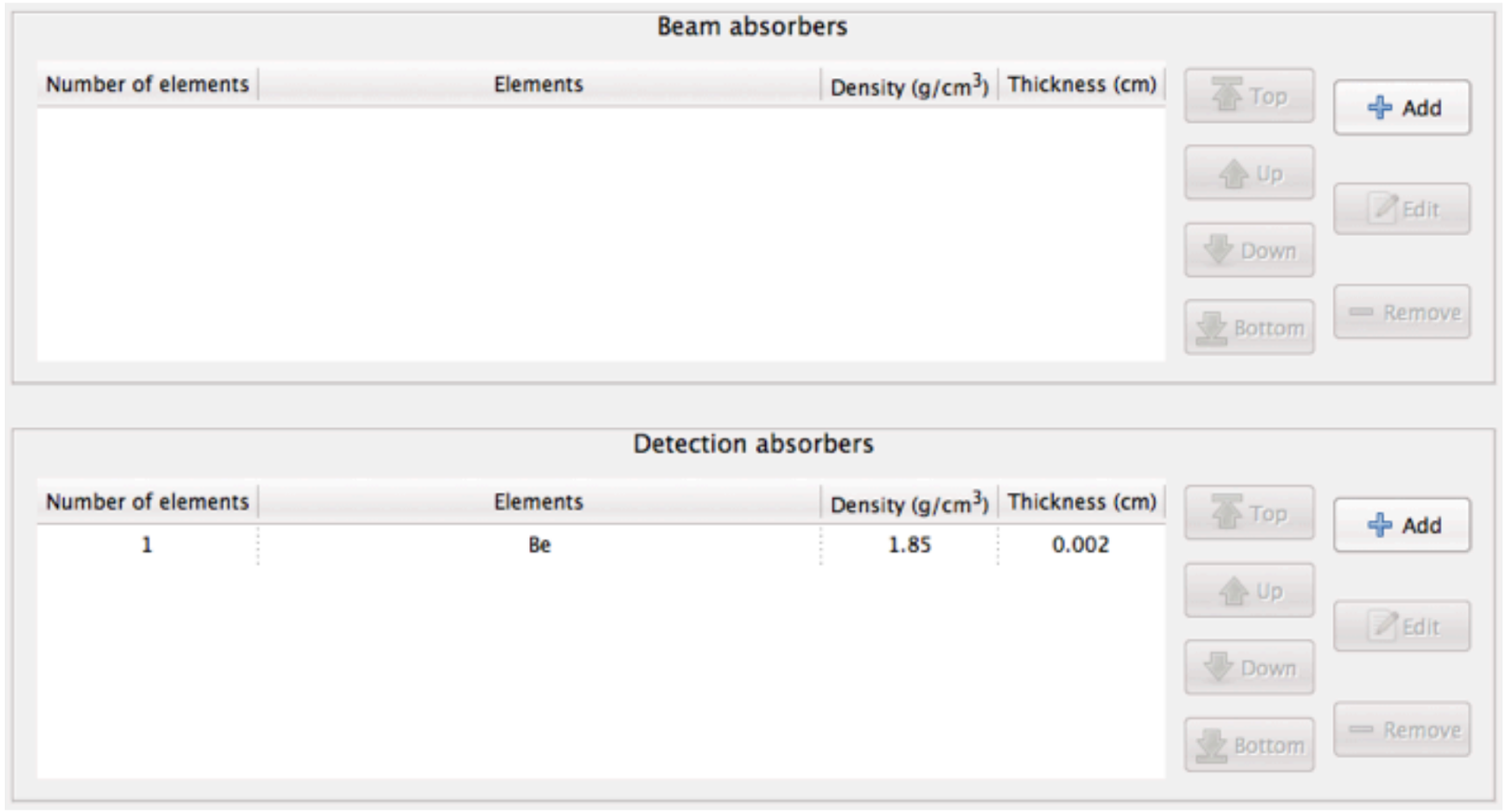
Intensity according to degree of polarization: if equal then unpolarized

Source sizes and divergence: advanced sources with Gaussian distributions

Energy distribution type: monochromatic, Gaussian and Lorentzian distributions (discrete only)



Absorbers: excitation and detector channel



1. Beam absorbers: exciting radiation
2. Detection absorbers: X-ray fluorescence!

Detector parameters

Detector settings

Detector type	Si(Li)
Number of spectrum channels	2048
Detector gain (keV/channel)	0.02
Detector zero (keV)	0
Detector Fano factor	0.12
Detector electronic noise (keV)	0.1
Live time (s)	1
Pulse width (s)	1e-05

Number of elements	Elements	Density (g/cm^3)	Thickness (cm)
1	Si	2.33	0.5

Top
Up
Down
Bottom
Add
Edit
Remove

Dete ameters

Selects detector response function

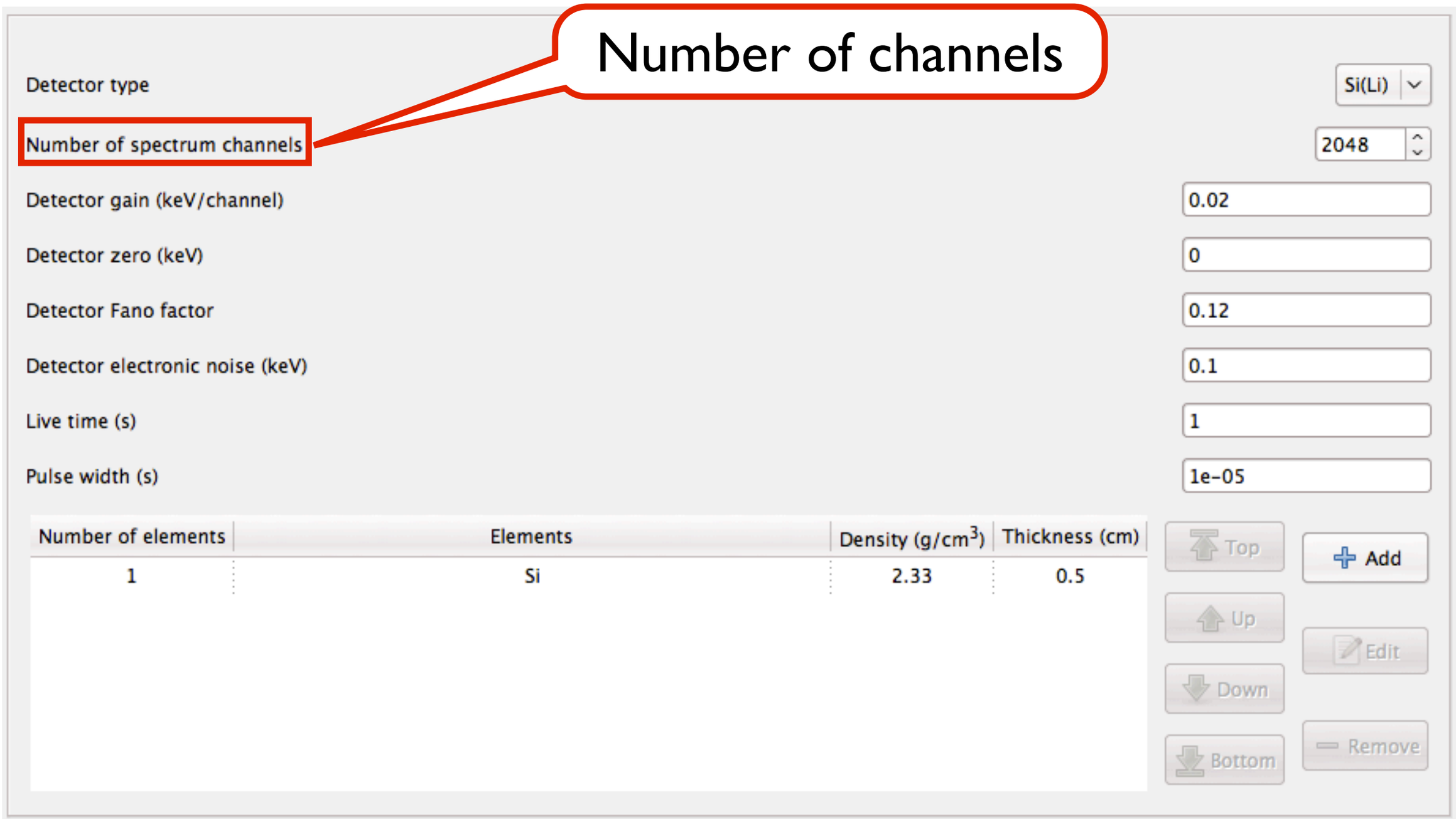
Detector settings

Detector type	Si(Li)
Number of spectrum channels	2048
Detector gain (keV/channel)	0.02
Detector zero (keV)	0
Detector Fano factor	0.12
Detector electronic noise (keV)	0.1
Live time (s)	1
Pulse width (s)	1e-05

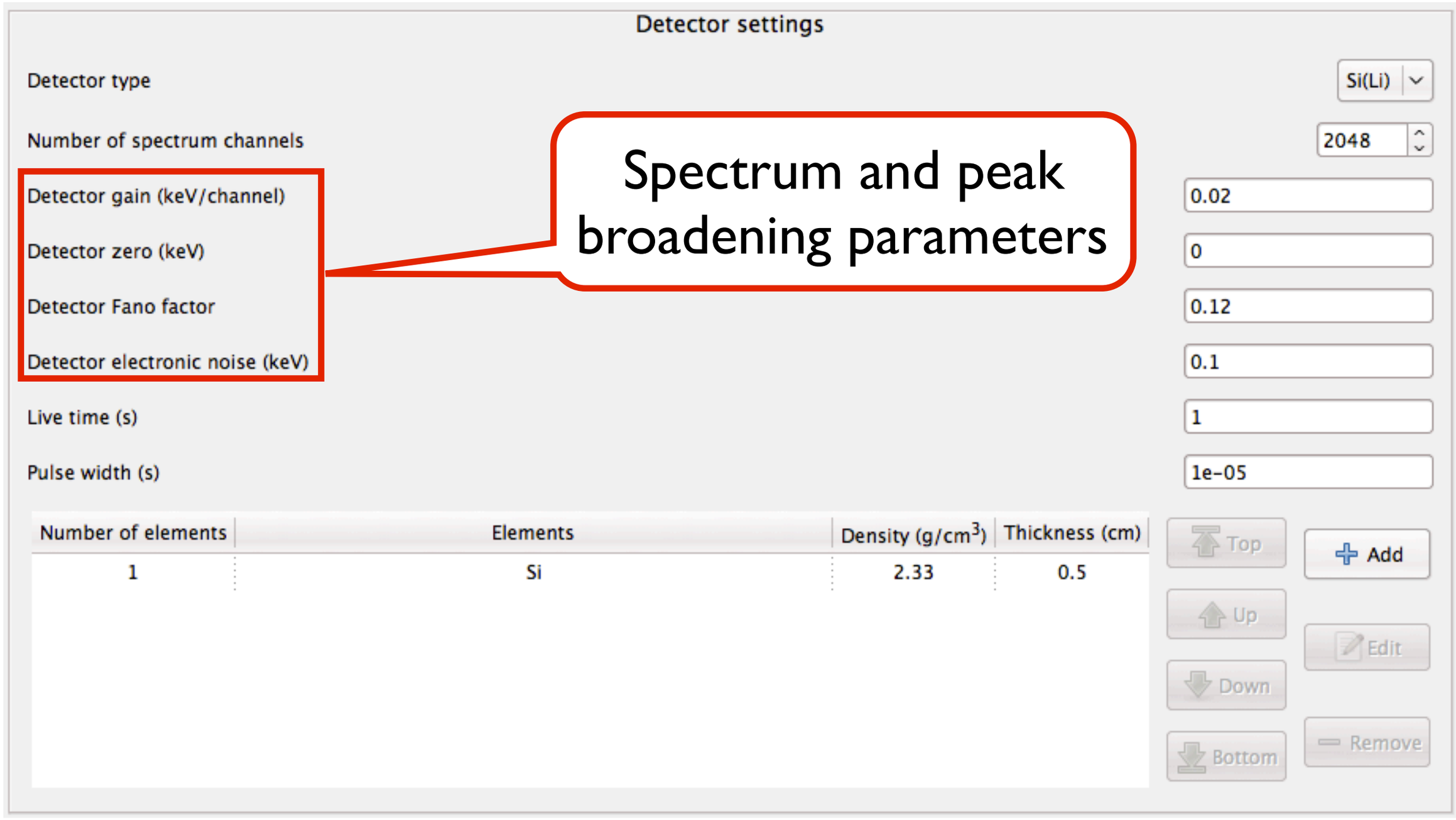
Number of elements	Elements	Density (g/cm^3)	Thickness (cm)
1	Si	2.33	0.5

Top
Up
Down
Bottom
Add
Edit
Remove

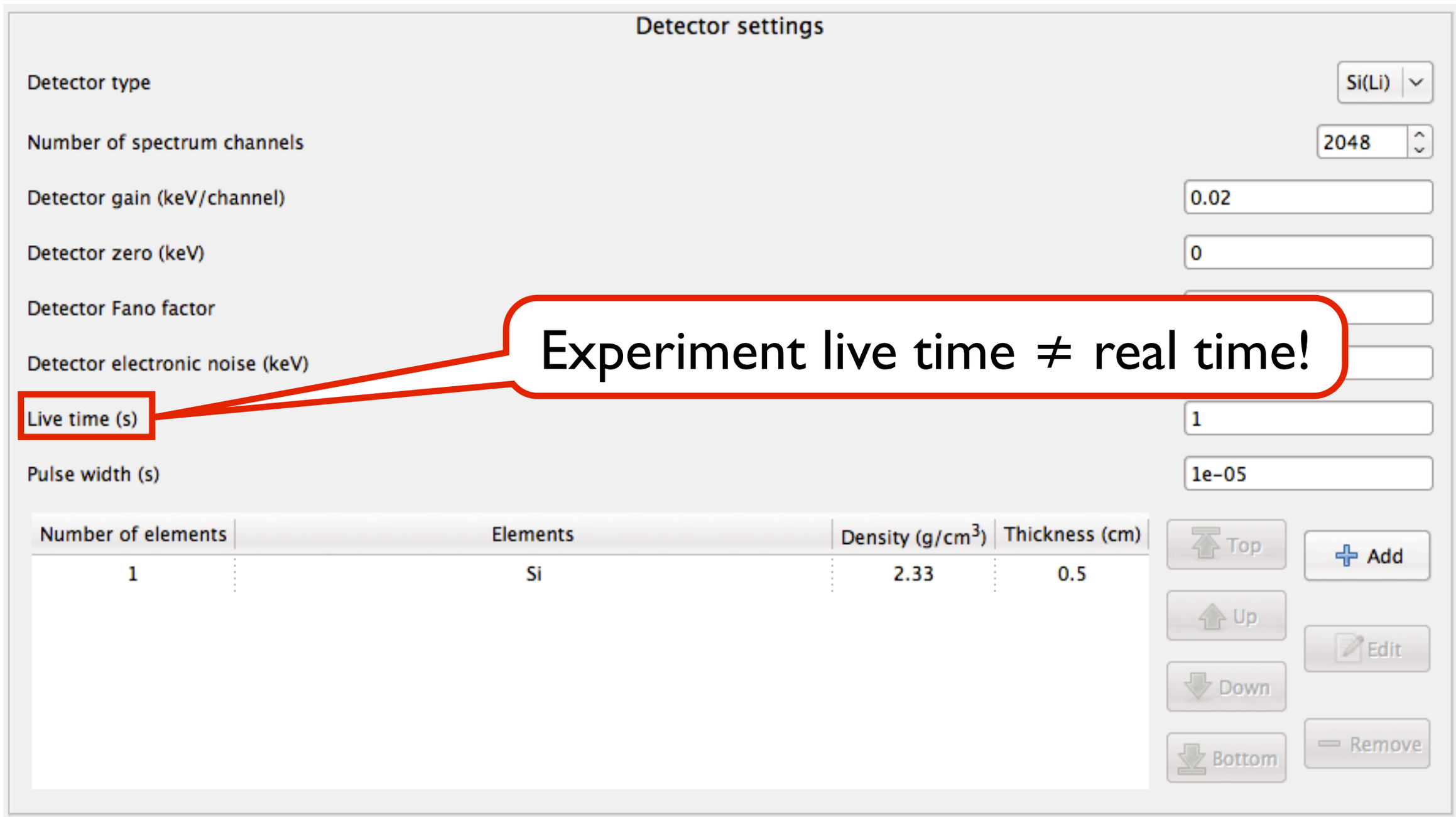
Detector parameters



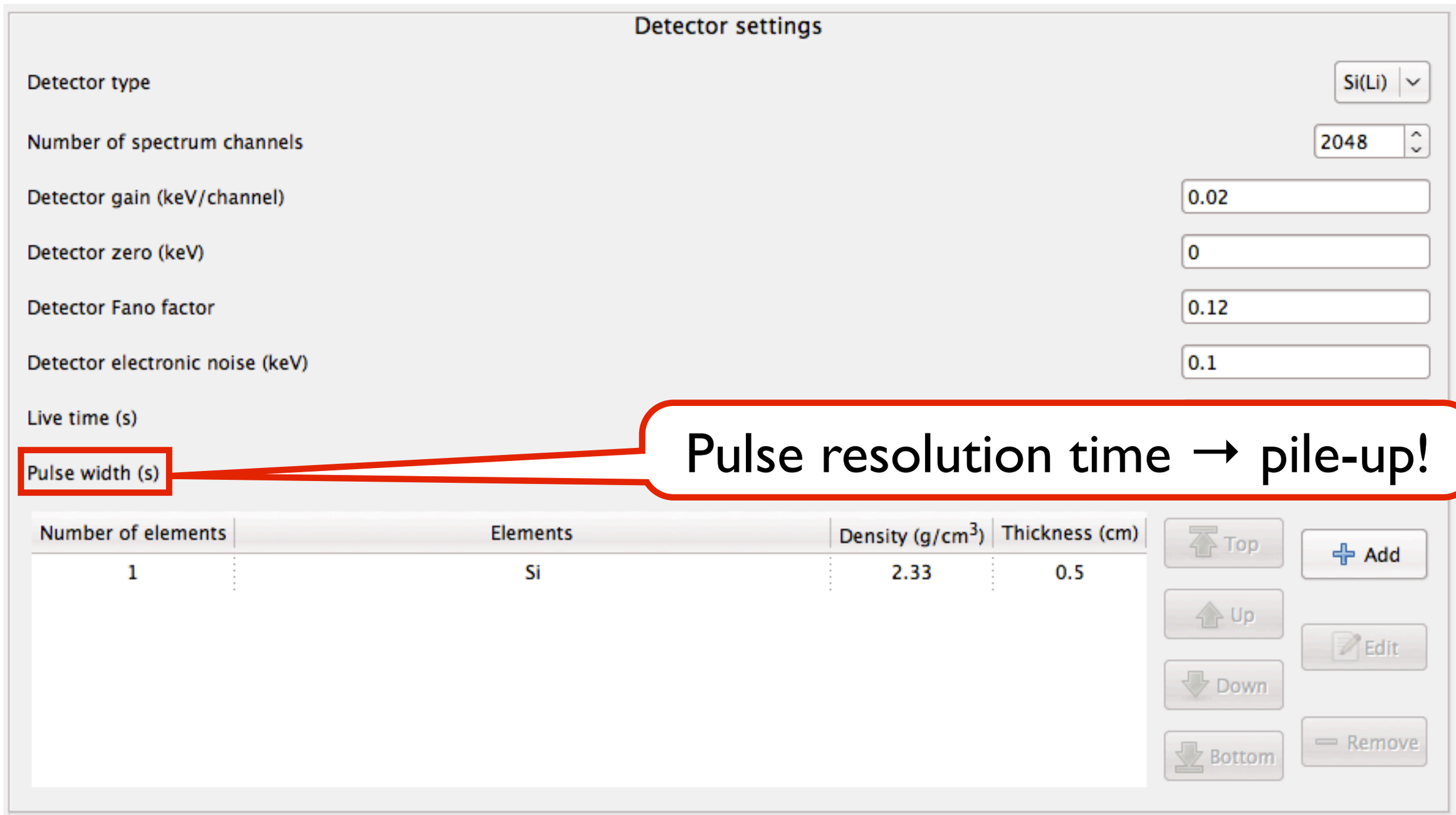
Detector parameters



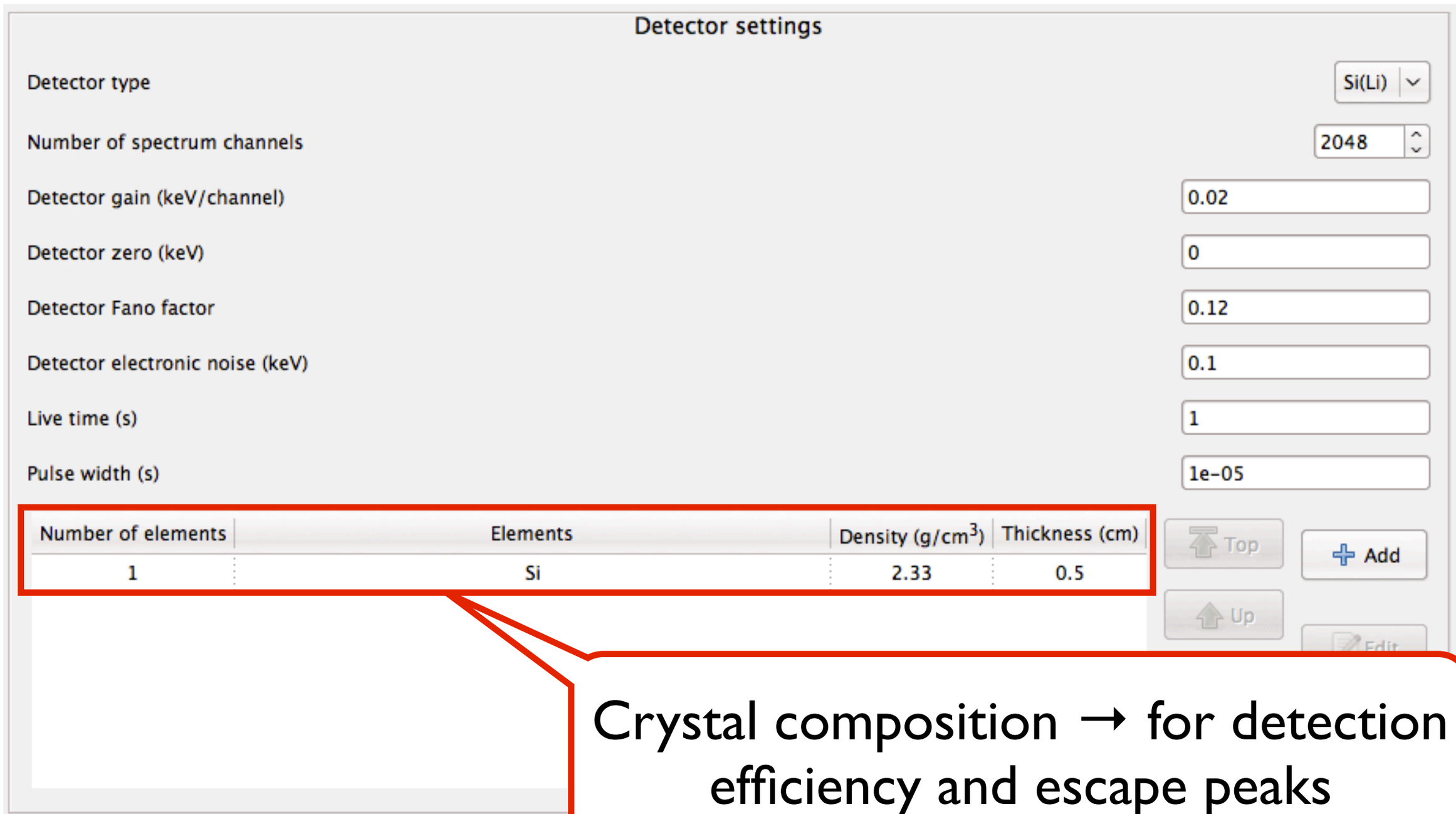
Detector parameters



Detector parameters



Detector parameters

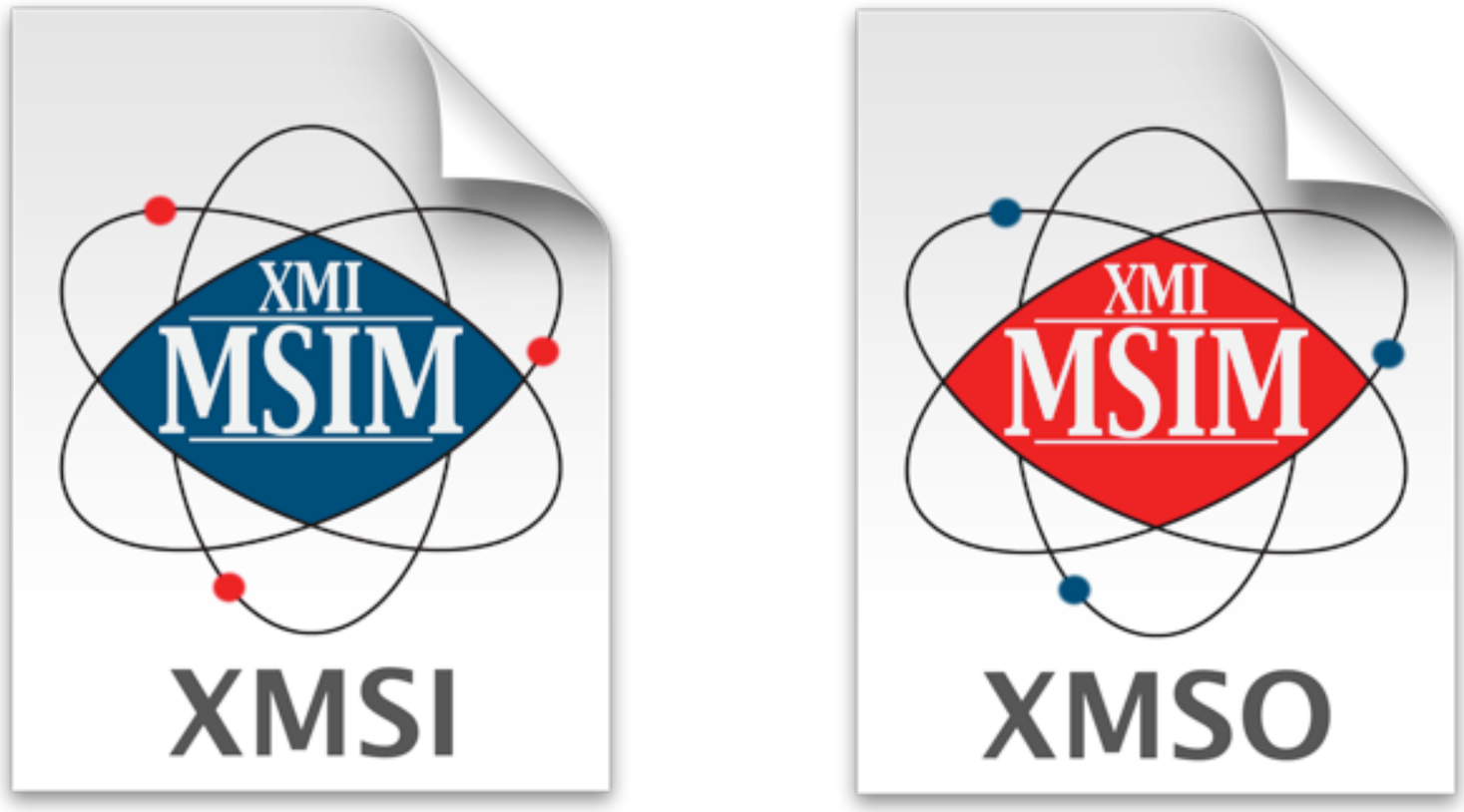


Saving an input-file

- Only possible when acceptable values of all parameters have been introduced
- Use menubar or toolbar *Save* and *Save As* buttons
- XMSI file extension

Saving an input file

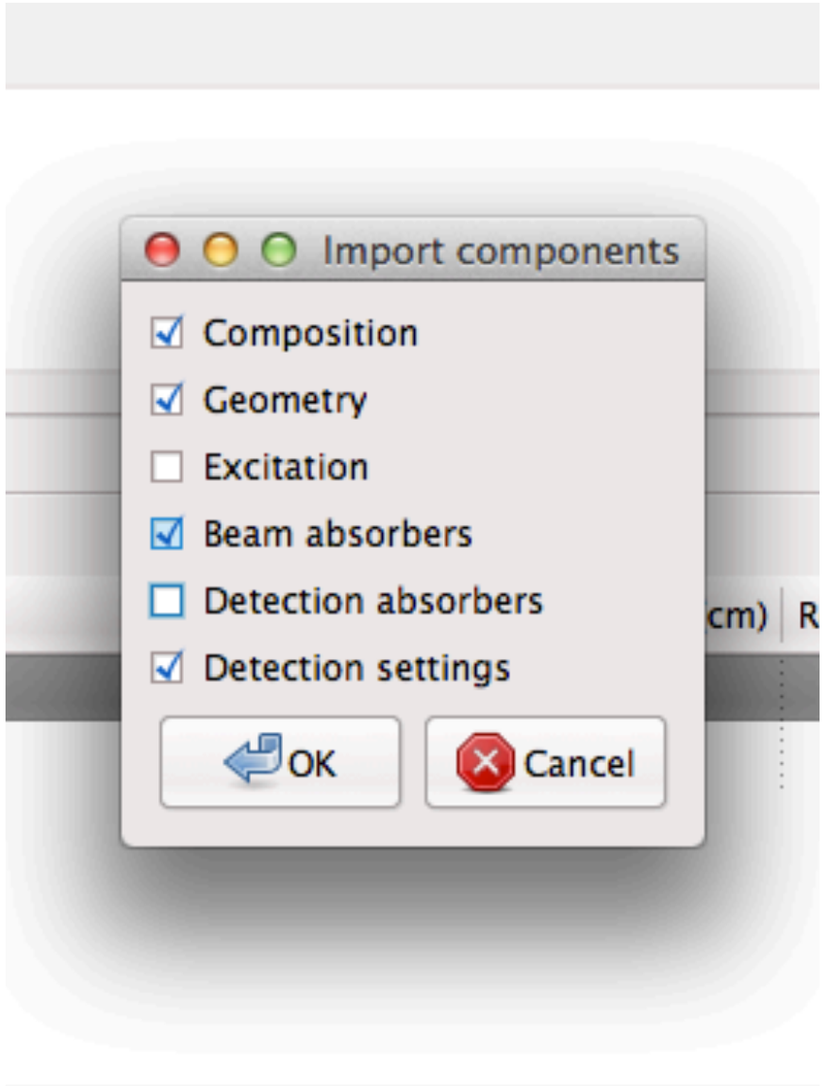
- all
- s



Input-file Output-file

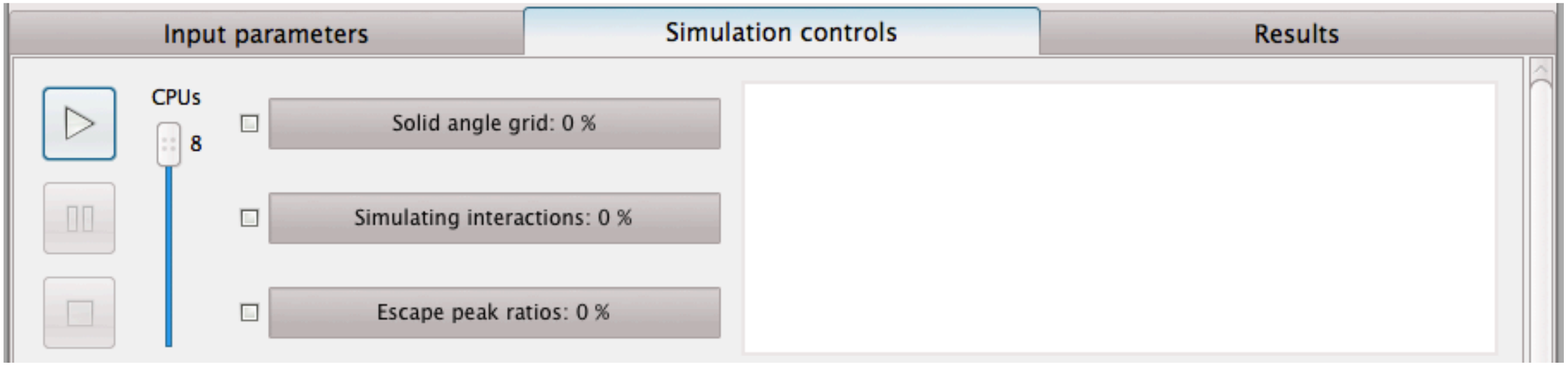
Import from XMSI and XMSO files

- In menubar: *File*→*Import*
- Select the desired components



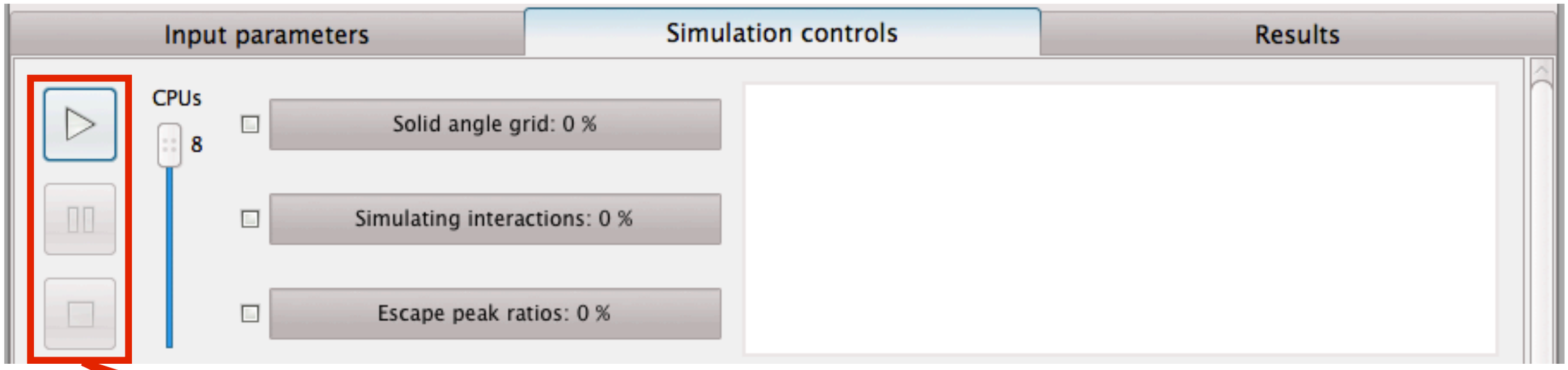
Starting a simulation

Control panel



- Input-file has to be loaded in *Input parameters!*
- Either just created (and saved) or loaded from filesystem

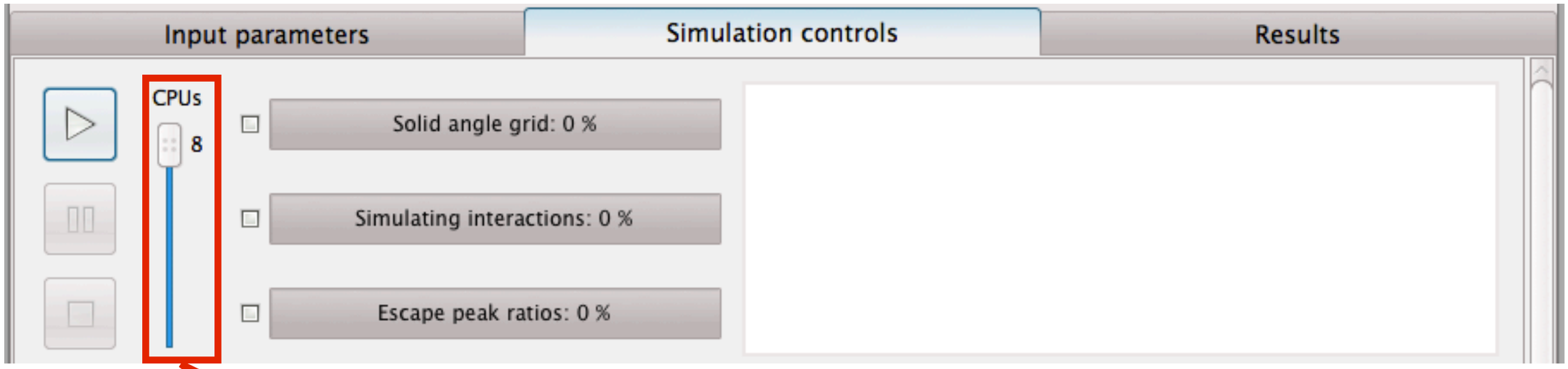
Control panel



Play → Start/Resume simulation
Pause → Suspend simulation
Stop → Terminate simulation

- Input-file has to be loaded in *Input parameters!*
- Either just created (and saved) or loaded from filesystem

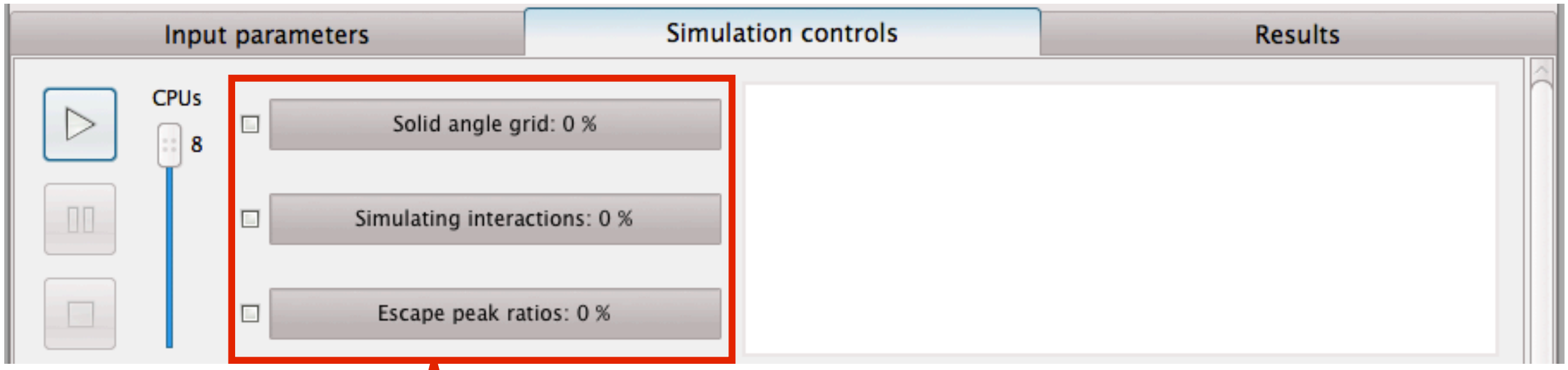
Control panel



CPUs: sets the number of threads that will be used during the simulation. Default is to use the number of available *logical* CPUs

- Input-file has to be loaded in *Input parameters!*
- Either just created (and saved) or loaded from filesystem

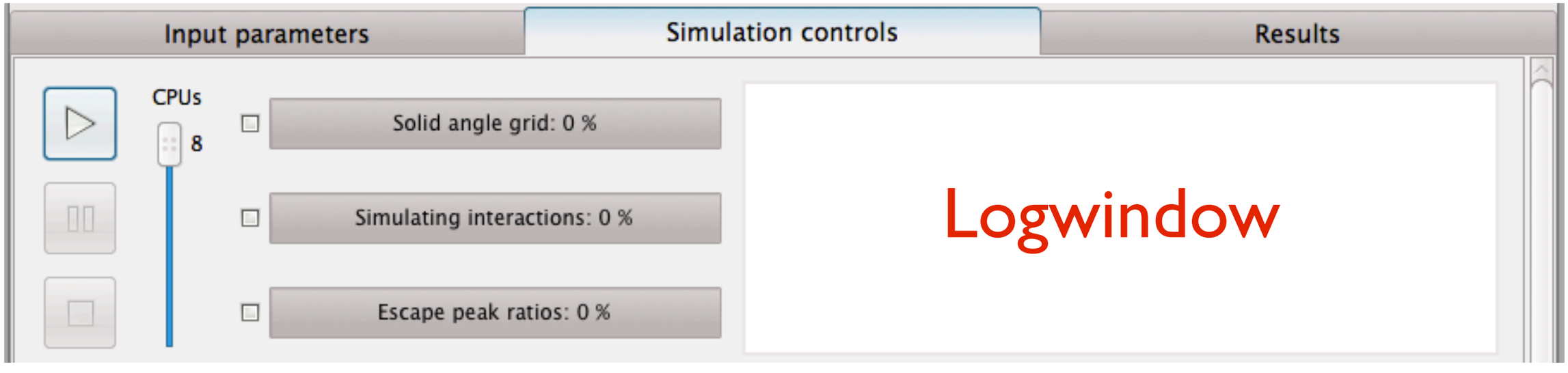
Control panel



Three progressbars allow to estimate how much longer a simulation will take. First and third bar will often not be used → *Loaded from file*

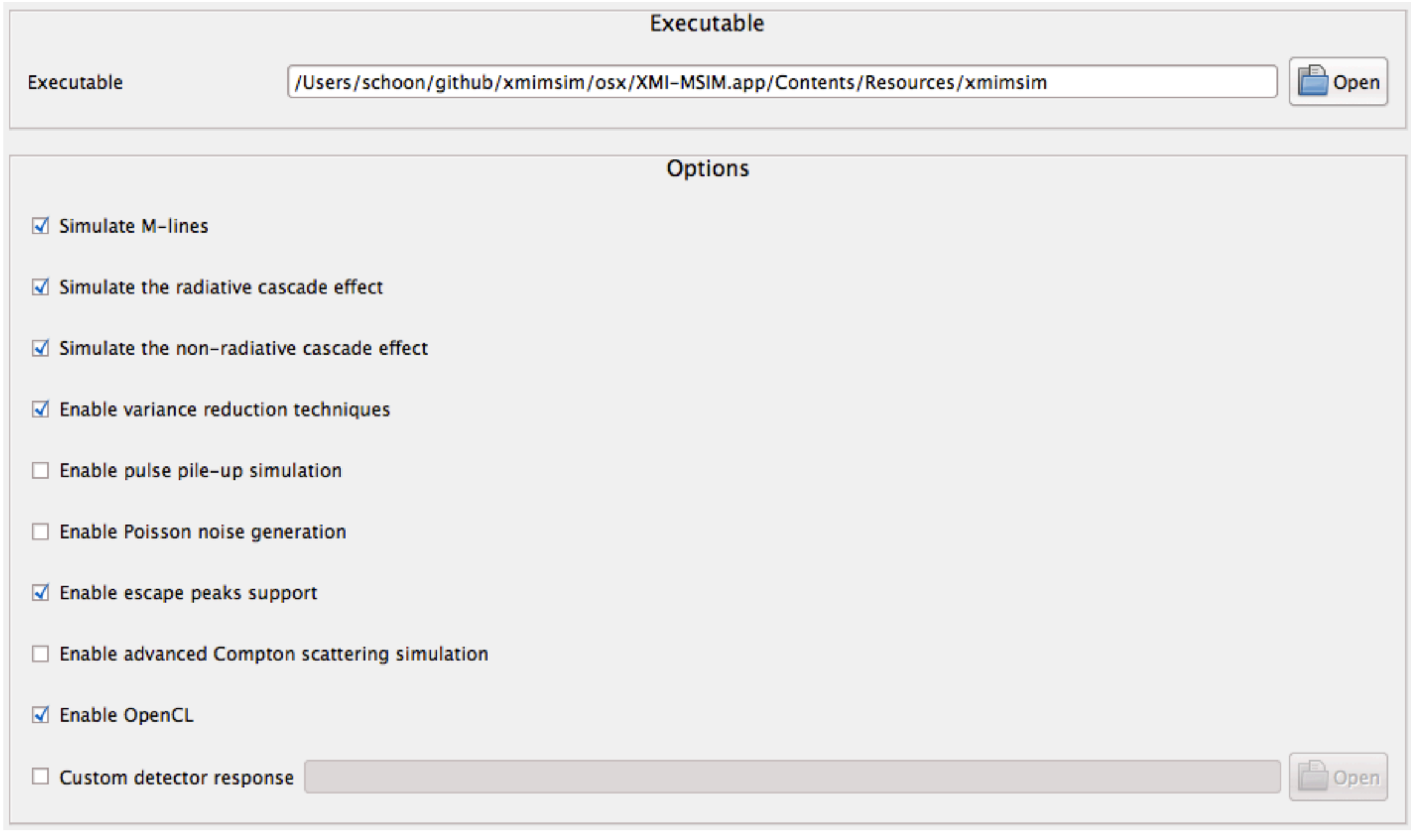
- Input-file has to be loaded in *Input parameters!*
- Either just created (and saved) or loaded from filesystem

Control panel



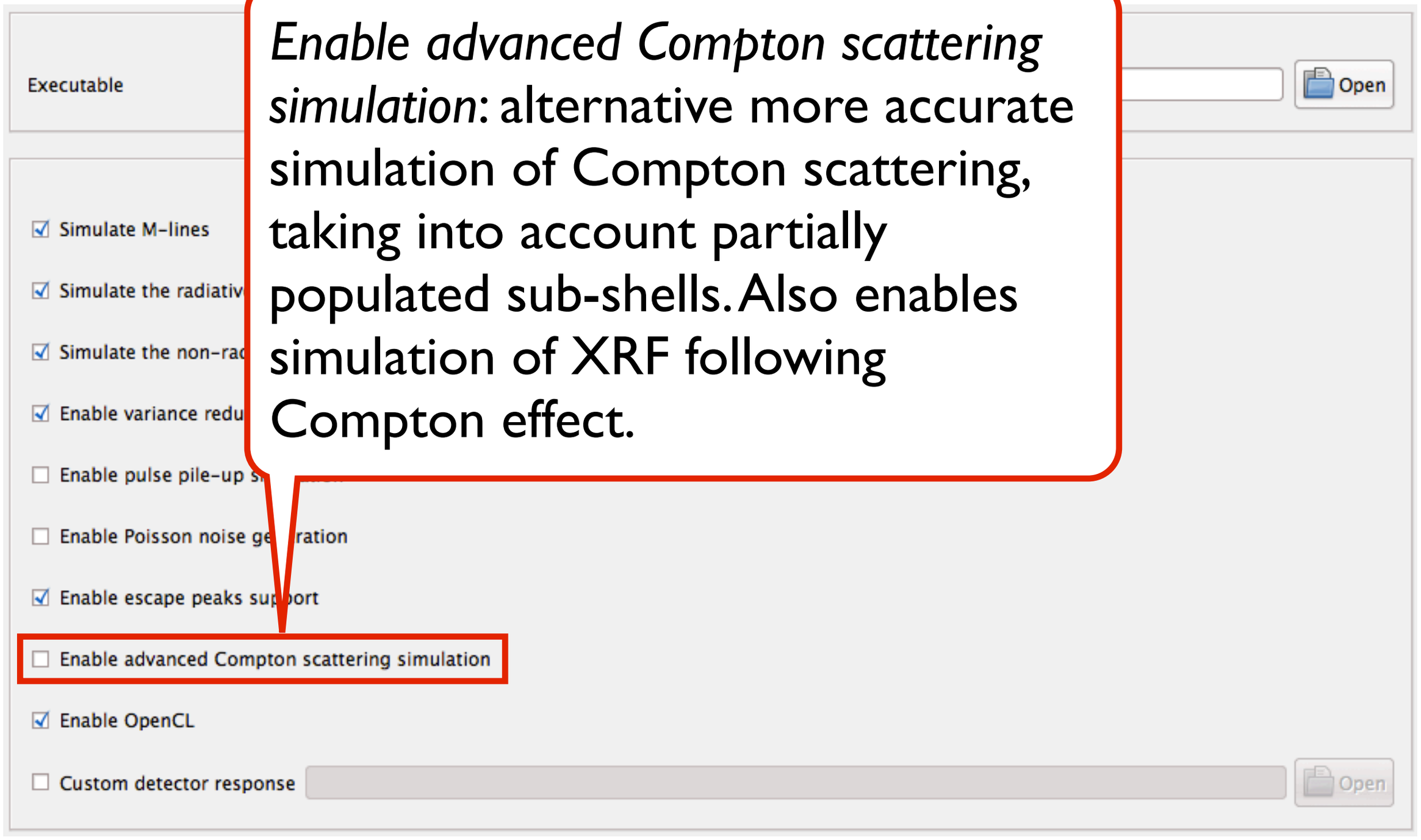
- Input-file has to be loaded in *Input parameters!*
- Either just created (and saved) or loaded from filesystem

Simulation options

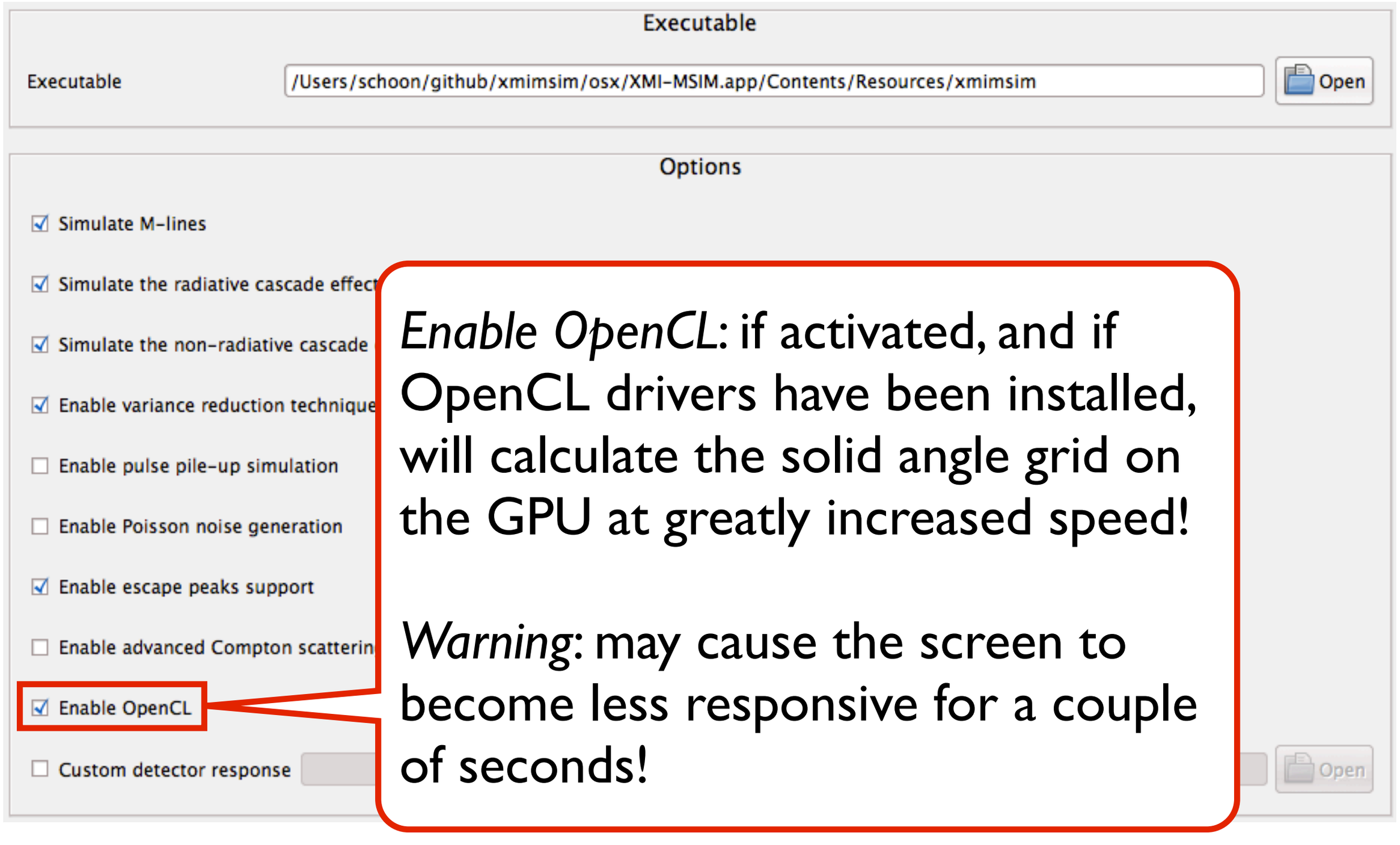


Simulation options

Enable advanced Compton scattering simulation: alternative more accurate simulation of Compton scattering, taking into account partially populated sub-shells. Also enables simulation of XRF following Compton effect.



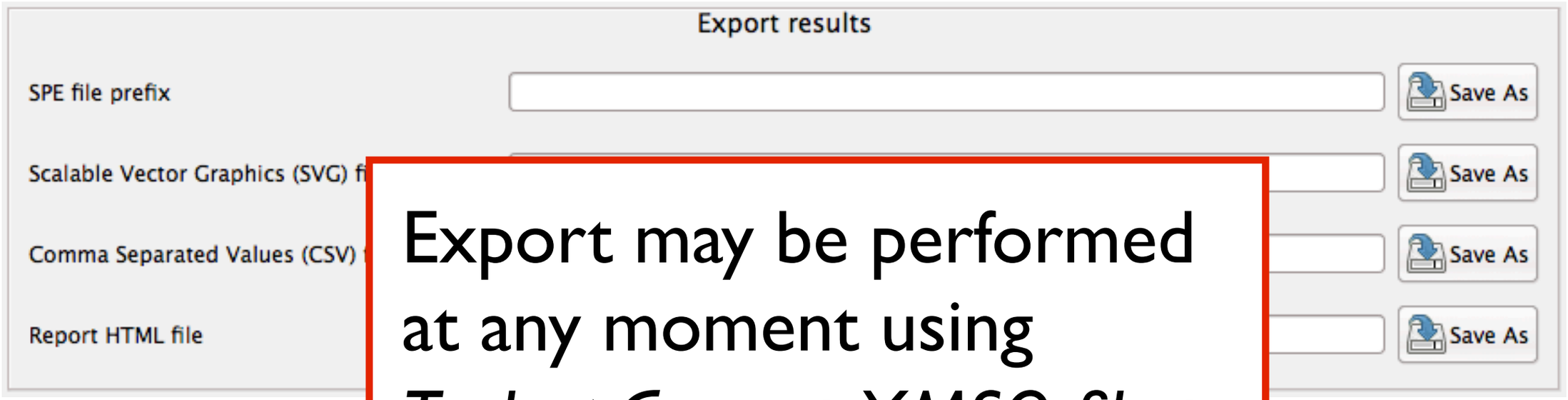
Simulation options



Export results

- XMSO: always
- *SPE file prefix*: suitable for PyMca and AXIL
- *Scalable Vector Graphics (SVG) file*: plot of spectra
- *Comma Separated Values (CSV) file*: contains spectra for increasing number of interactions (Excel)
- *Report HTML file*: standalone interactive overview of the results

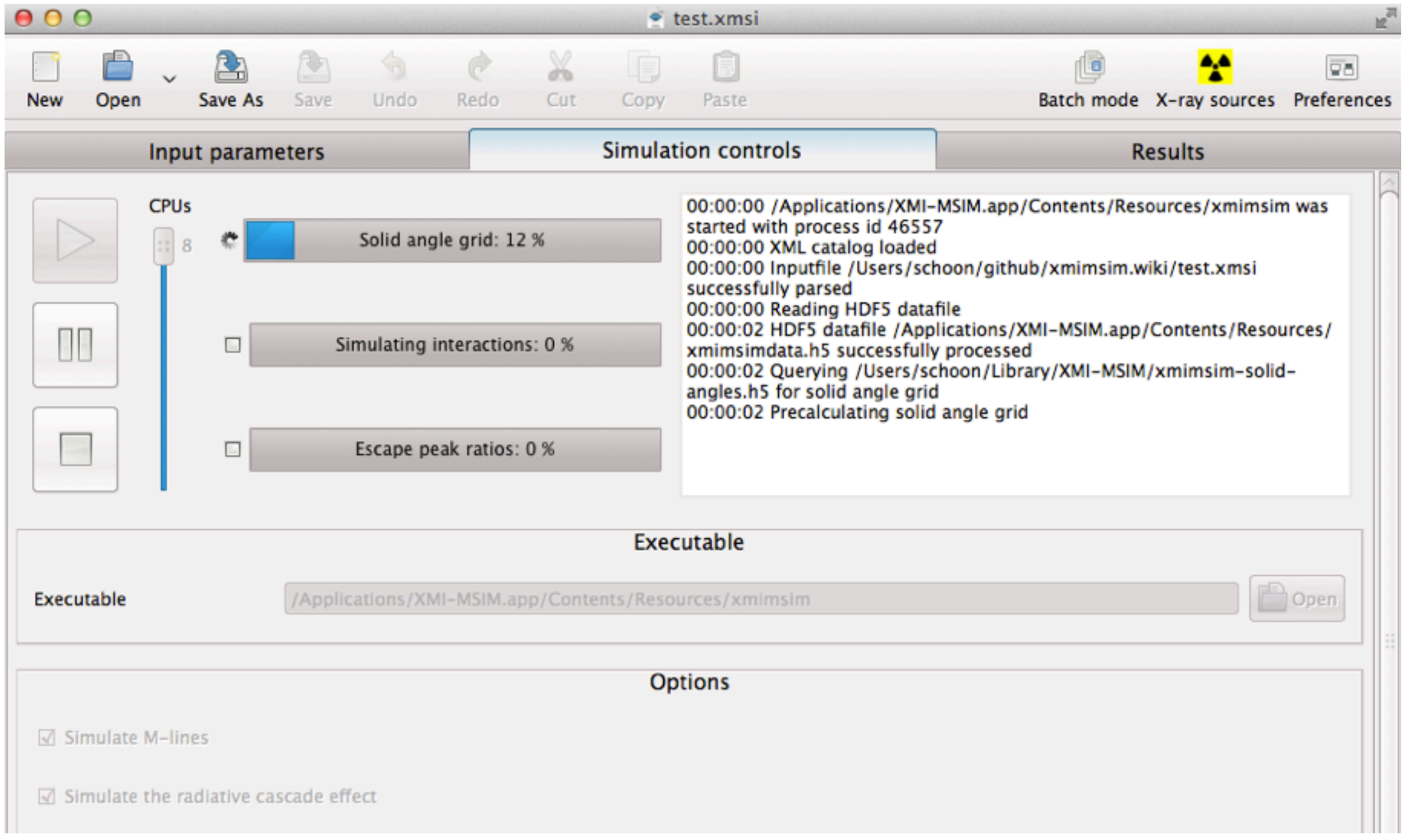
Export results



Export may be performed at any moment using *Tools → Convert XMSO file to*

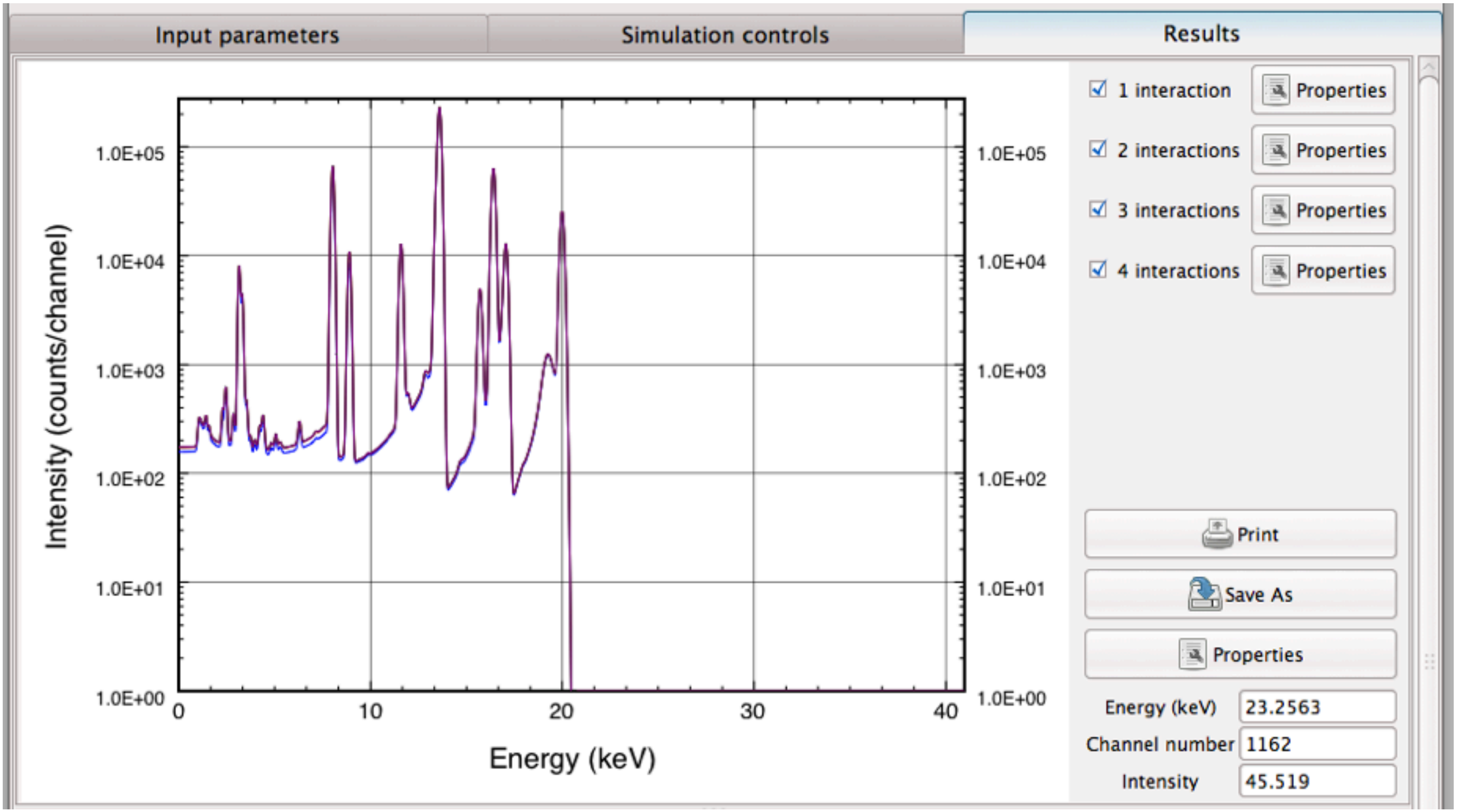
- XMSO: always
- *SPE file prefix*: suitable for PyMca and AXIL
- *Scalable Vector Graphics (SVG) file*: plot of spectra
- *Comma Separated Values (CSV) file*: contains spectra for increasing number of interactions (Excel)
- *Report HTML file*: standalone interactive overview of the results

During a simulation

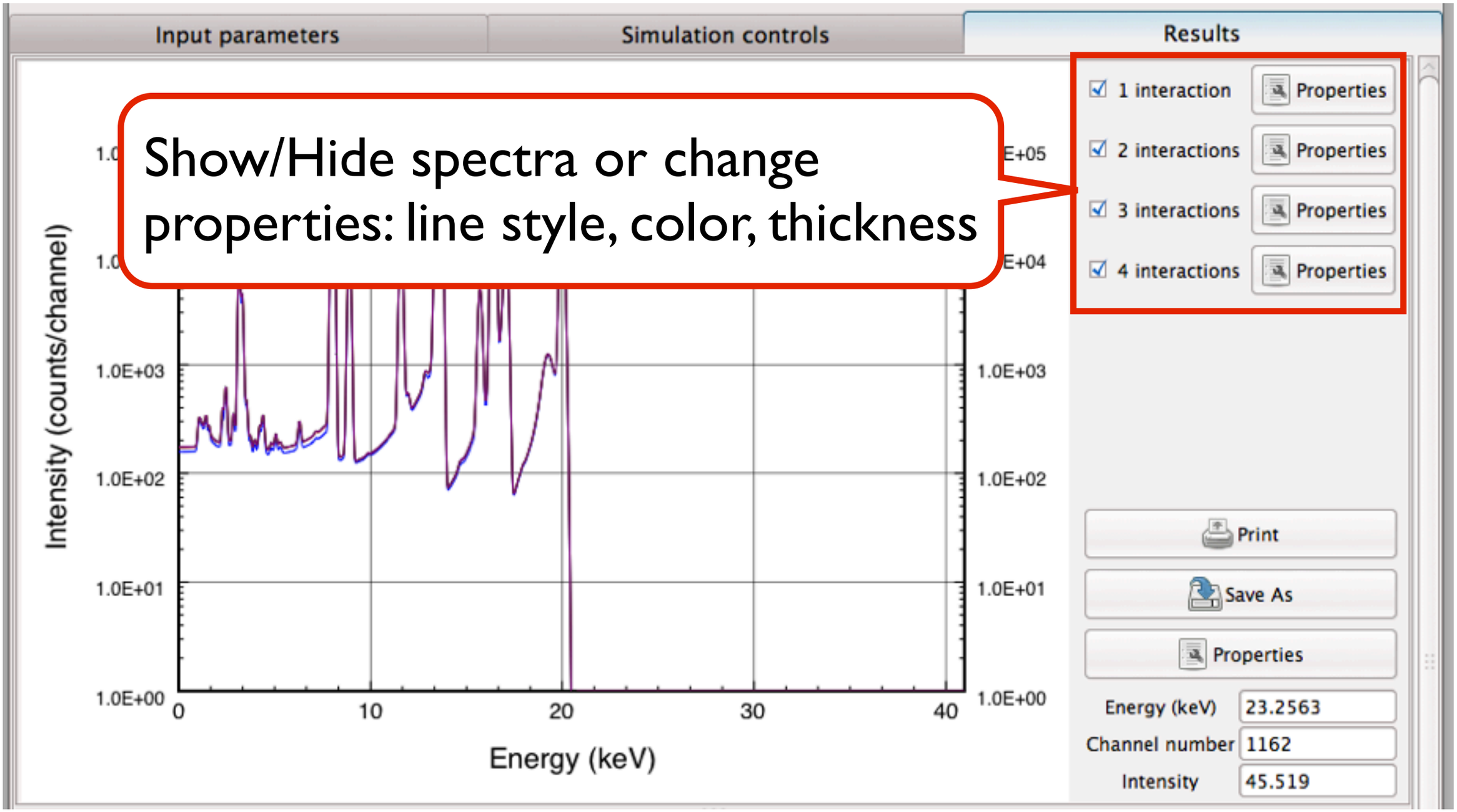


Visualizing the results

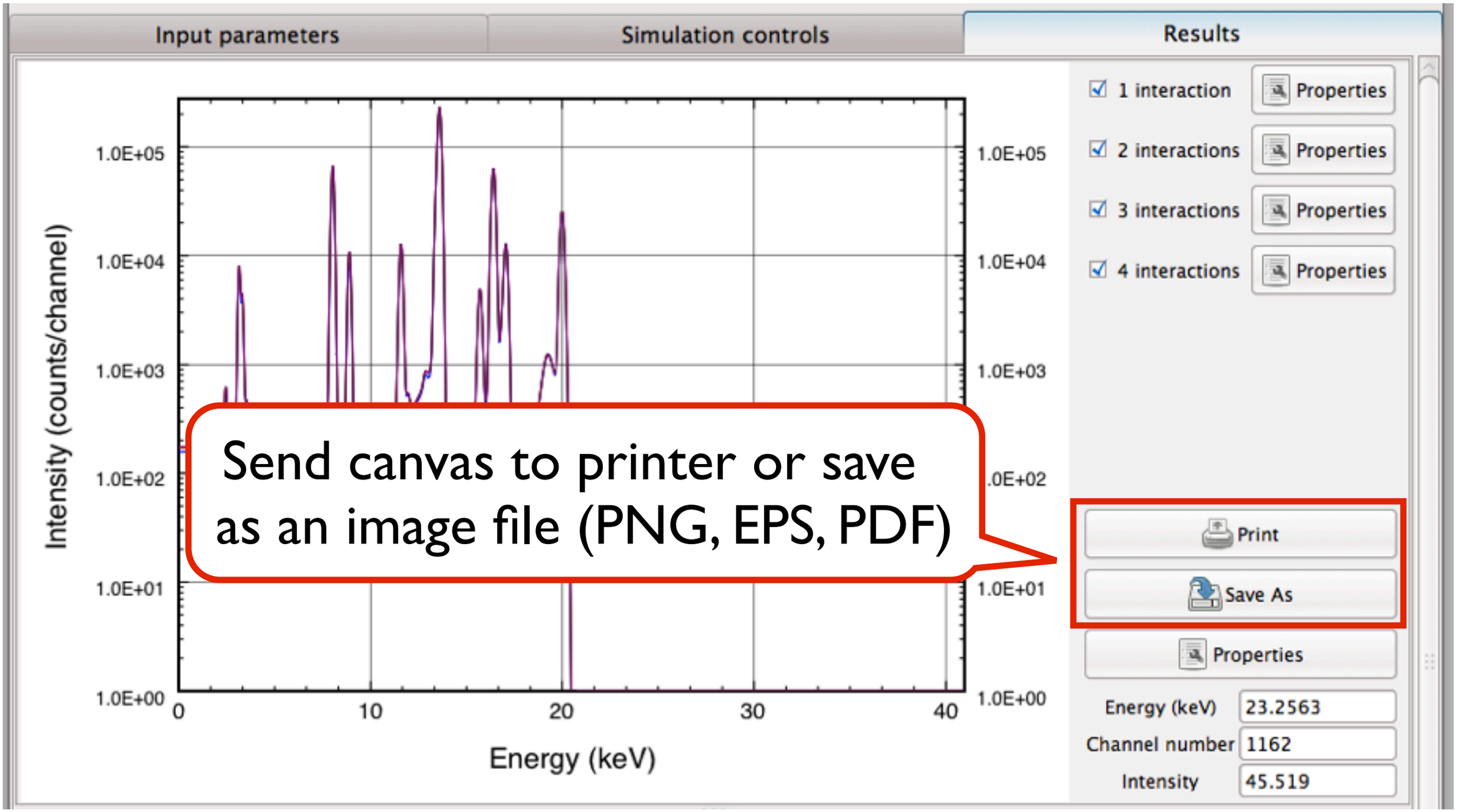
Plot canvas


Input parameters
Simulation controls
Results
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
Intensity (counts/channel)
0
10
20
30
40
Energy (keV)
Print
Save As
Properties
Energy (keV) 23.2563
Channel number 1162
Intensity 45.519

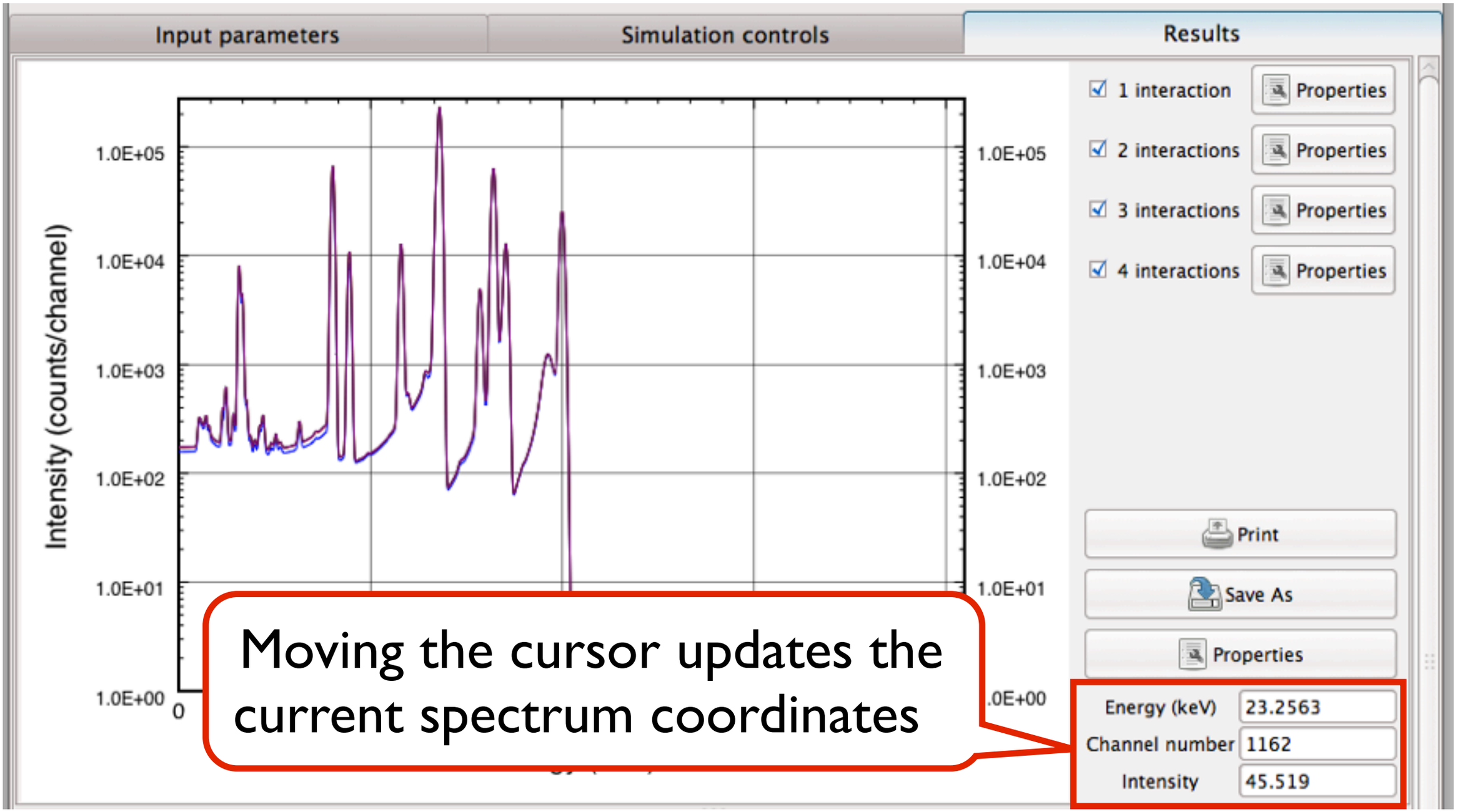
Plot canvas


Input parameters
Simulation controls
Results
Show/Hide spectra or change properties: line style, color, thickness
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
Intensity (counts/channel)
1.0E+03
1.0E+02
1.0E+01
1.0E+00
0
10
20
30
40
Energy (keV)
Print
Save As
Properties
Energy (keV) 23.2563
Channel number 1162
Intensity 45.519

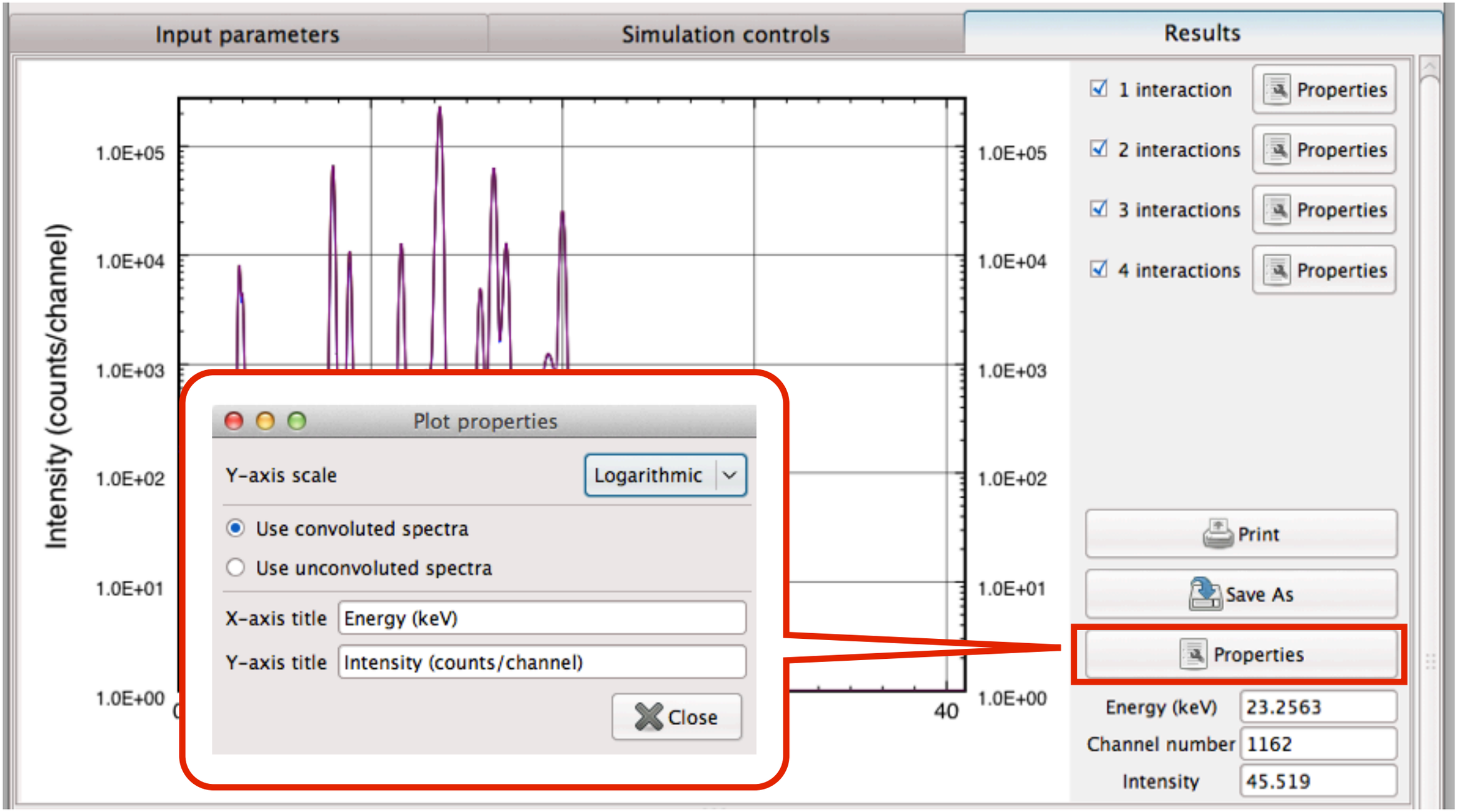
Plot canvas


Input parameters
Simulation controls
Results
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
Intensity (counts/channel)
0
10
20
30
40
Energy (keV)
Send canvas to printer or save as an image file (PNG, EPS, PDF)
Print
Save As
Properties
Energy (keV) 23.2563
Channel number 1162
Intensity 45.519

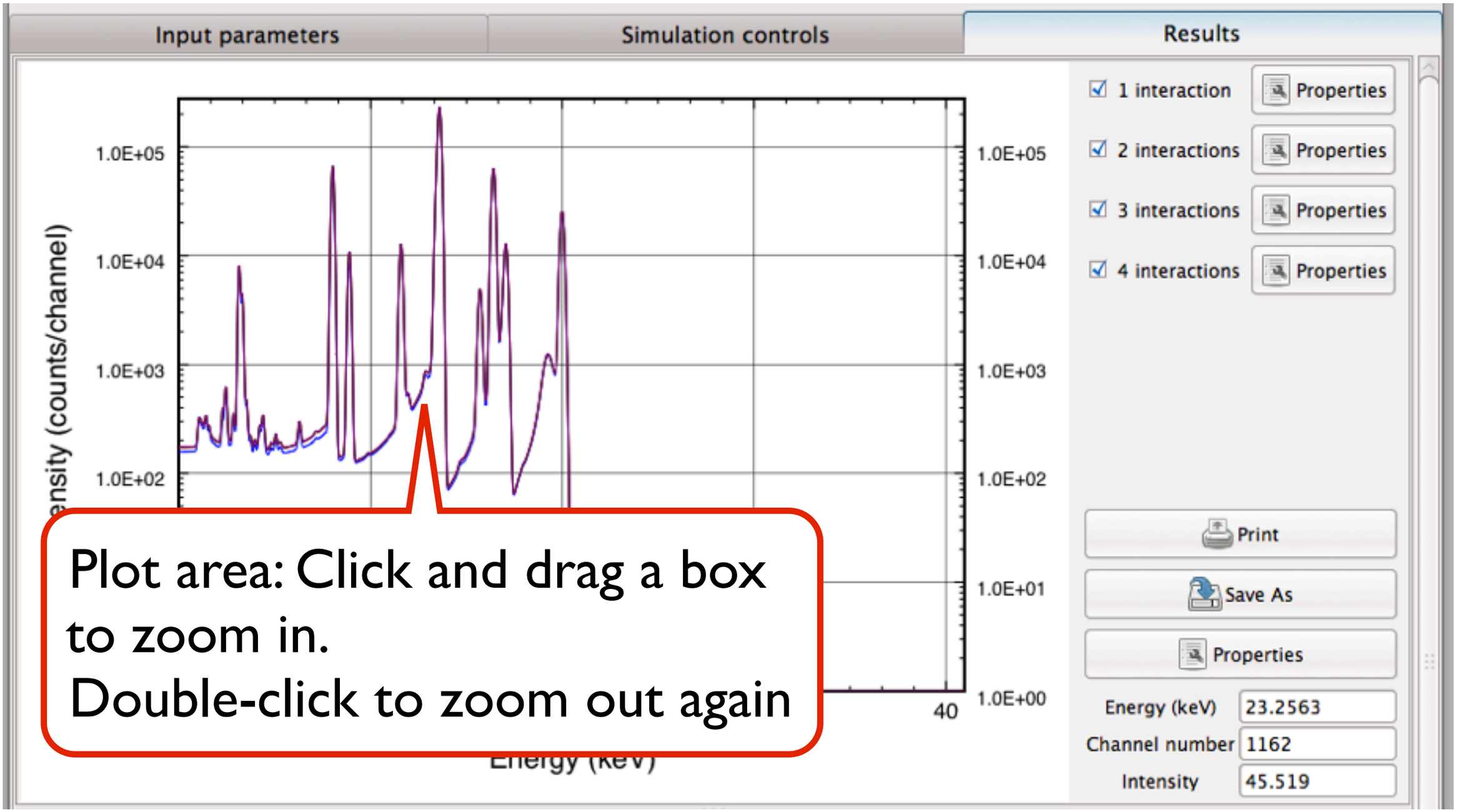
Plot canvas


Input parameters
Simulation controls
Results
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
0
Intensity (counts/channel)
Print
Save As
Properties
Energy (keV) 23.2563
Channel number 1162
Intensity 45.519
Moving the cursor updates the current spectrum coordinates

Plot canvas


Input parameters
Simulation controls
Results
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
Intensity (counts/channel)
40
Plot properties
Y-axis scale
Logarithmic
Use convoluted spectra
Use unconvoluted spectra
X-axis title
Energy (keV)
Y-axis title
Intensity (counts/channel)
Close
Print
Save As
Properties
Energy (keV)
23.2563
Channel number
1162
Intensity
45.519

Plot canvas


Input parameters
Simulation controls
Results
1 interaction
Properties
2 interactions
Properties
3 interactions
Properties
4 interactions
Properties
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
40
Energy (keV)
Print
Save As
Properties
Energy (keV) 23.2563
Channel number 1162
Intensity 45.519
Plot area: Click and drag a box to zoom in.
Double-click to zoom out again

Net-line intensities

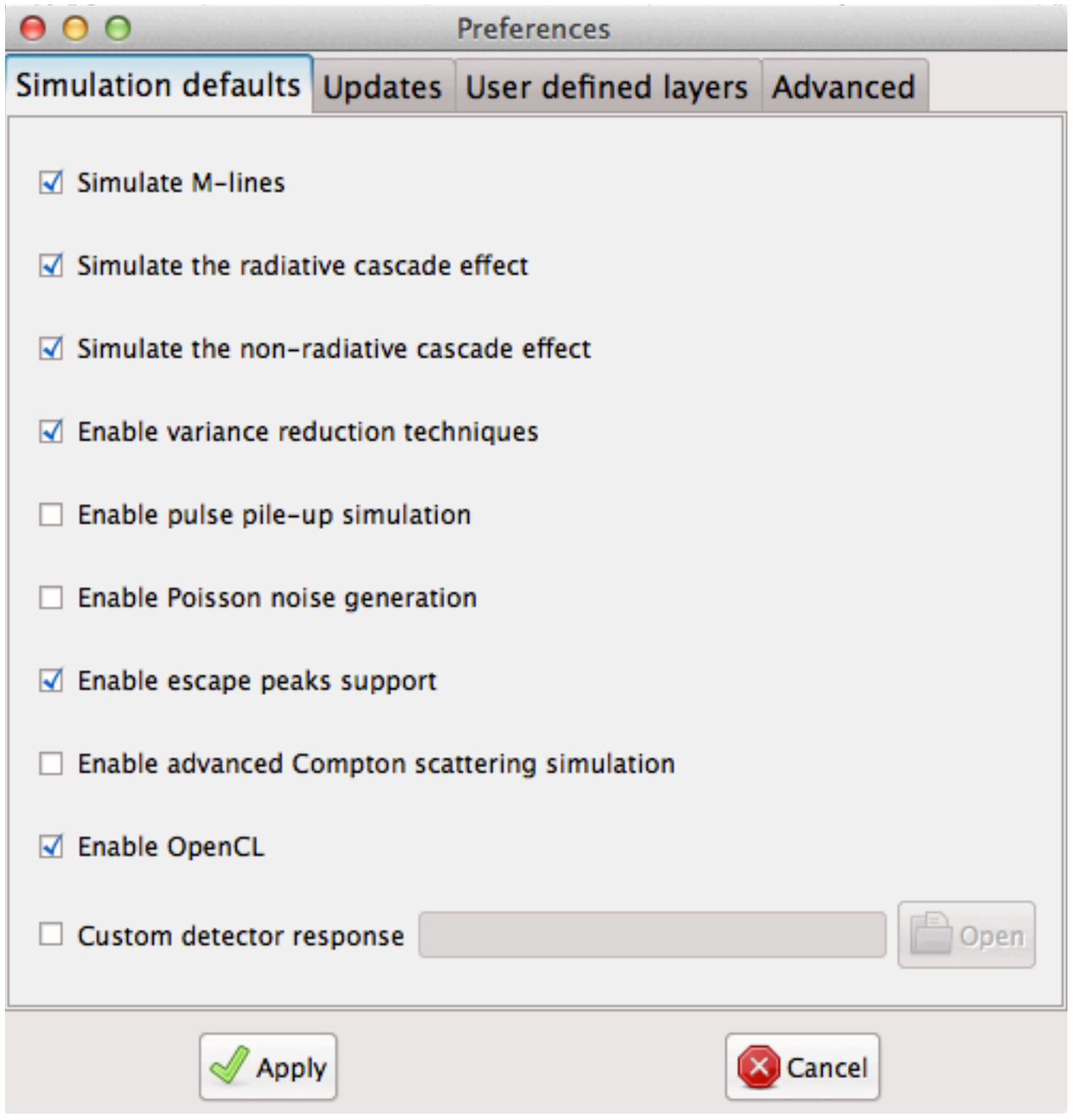
Element	XRF line	Energy	Show line	# Interactions	Intensity
S	all		☑	all	1489.28
Ar	all		☐	all	401.863
Cu	all		▬	all	748394
	KL2	8.0279	☐	all	216933
	KL3	8.0478	☑	all	424951
	KM2	8.9053	☐	all	35990.6
	KM3	8.9053	☐	all	70519.5
	L1M2	1.0225	☐	all	0.025663
	L1M3	1.0225	☐	all	0.047226
	L1M4	1.0945	☐	all	0.000218
	L1M5	1.0945	☐	all	0.000323

- Show and hide lines on plot canvas: individual or per element
- XRF net-line intensity per element, per line and per interaction!

Global preferences

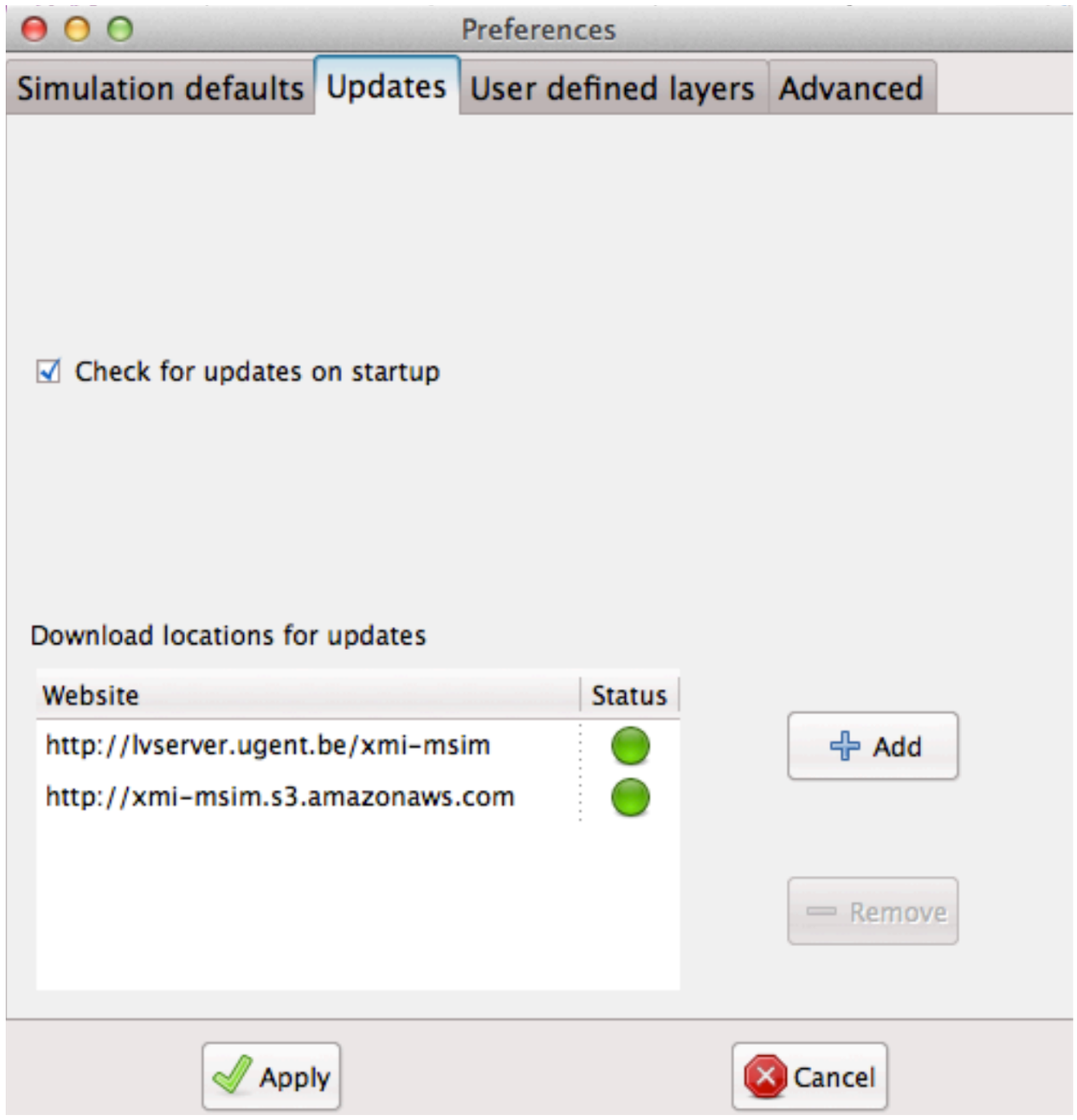
Simulation defaults

Determines the default settings in *Simulation controls*.
Requires a restart of XMI-MSIM before becoming active



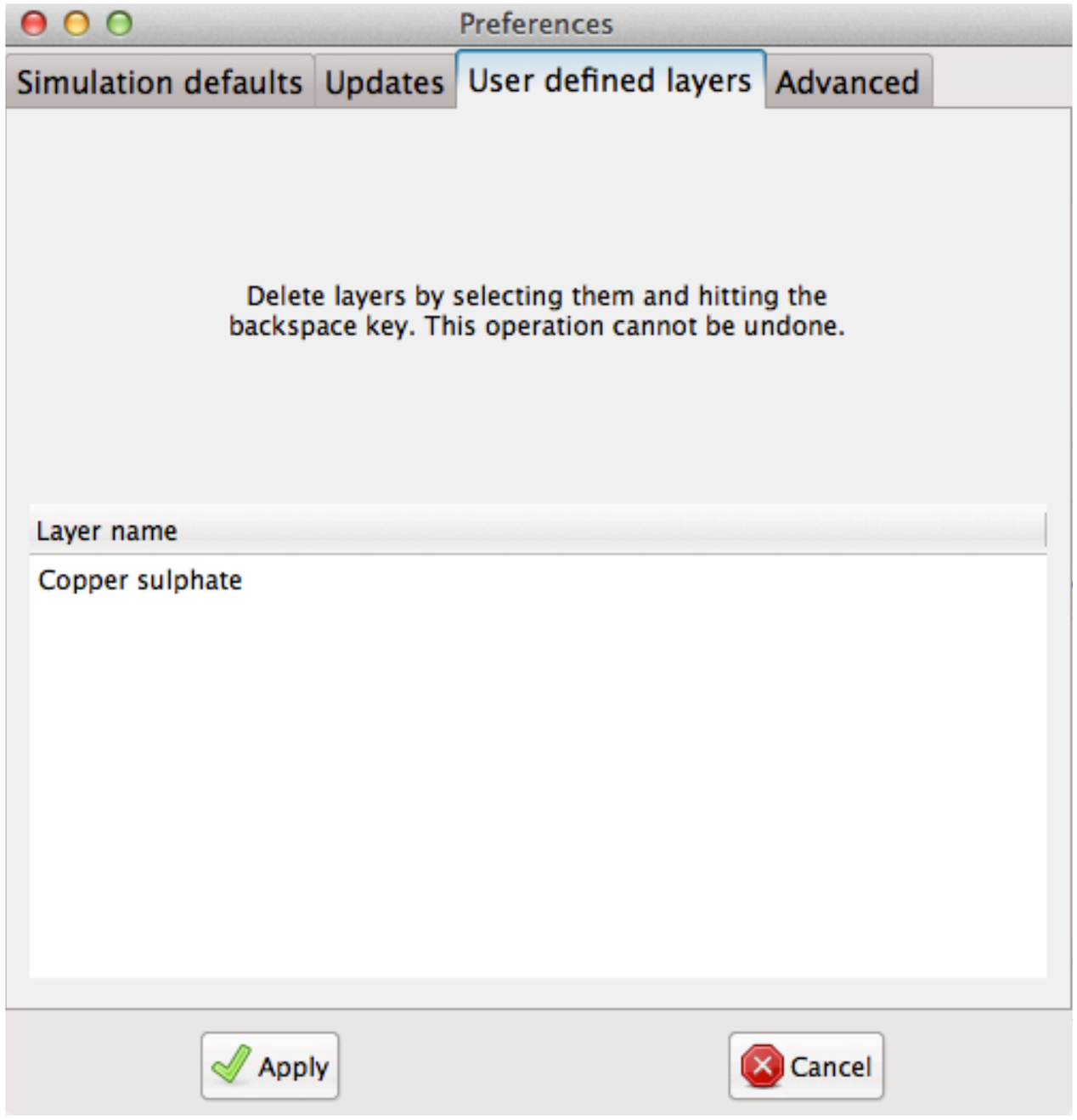
Automatic updates

- Enable/disable checking for updates on startup.
- Download locations should be left untouched.
- Optional feature



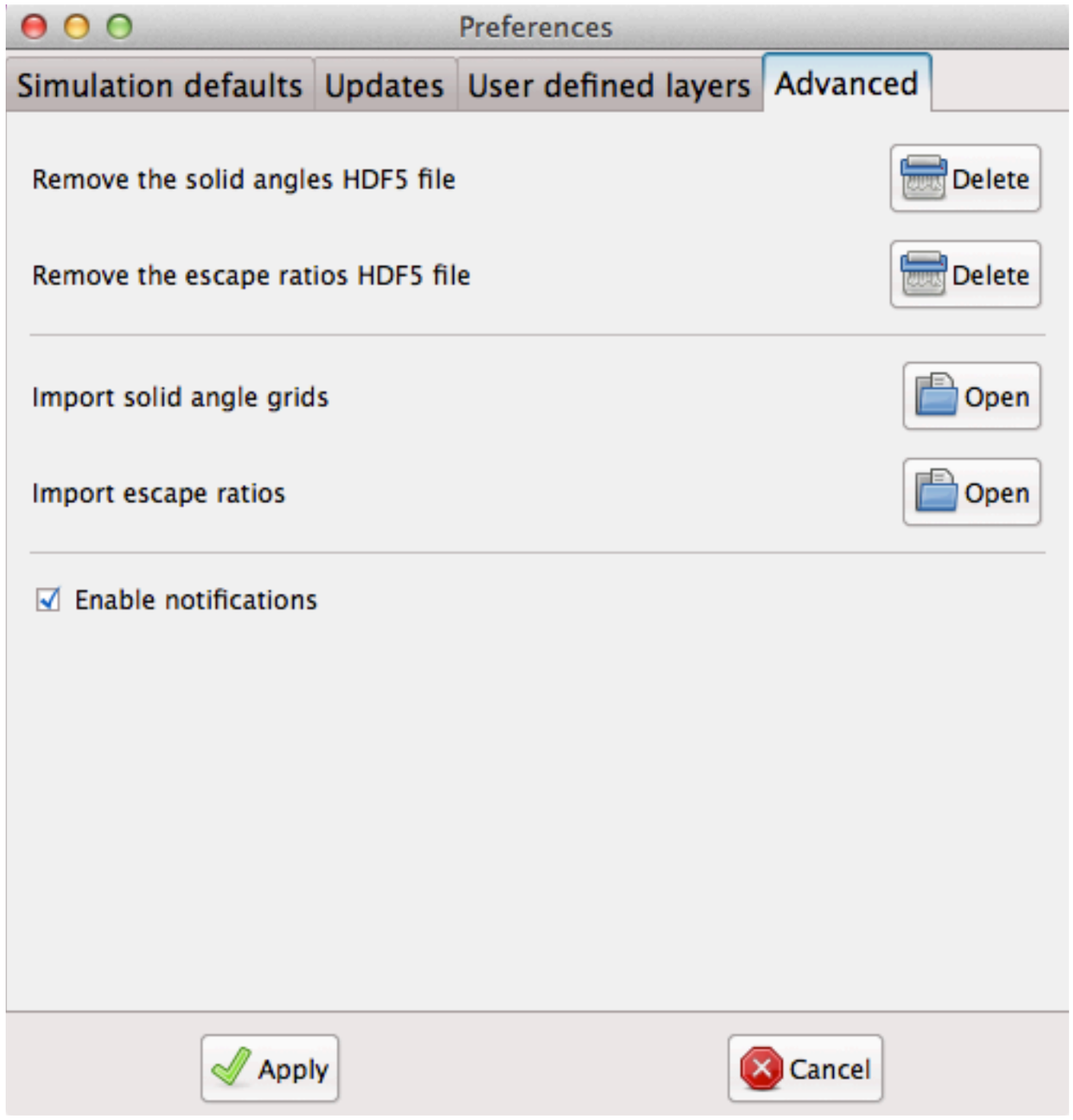
User defined layers

- Delete layers defined in the *Modify layer* dialog

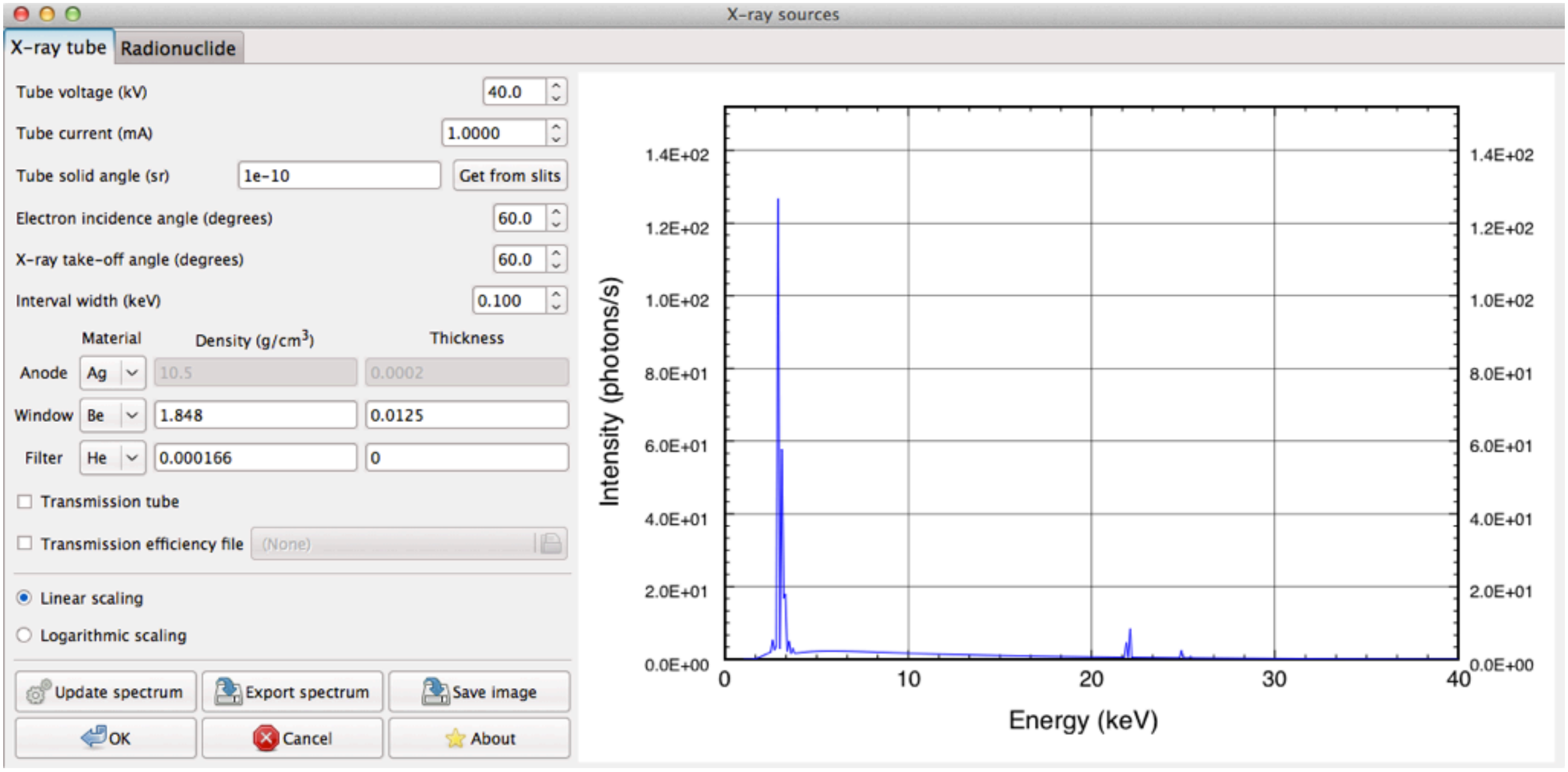


Advanced preferences

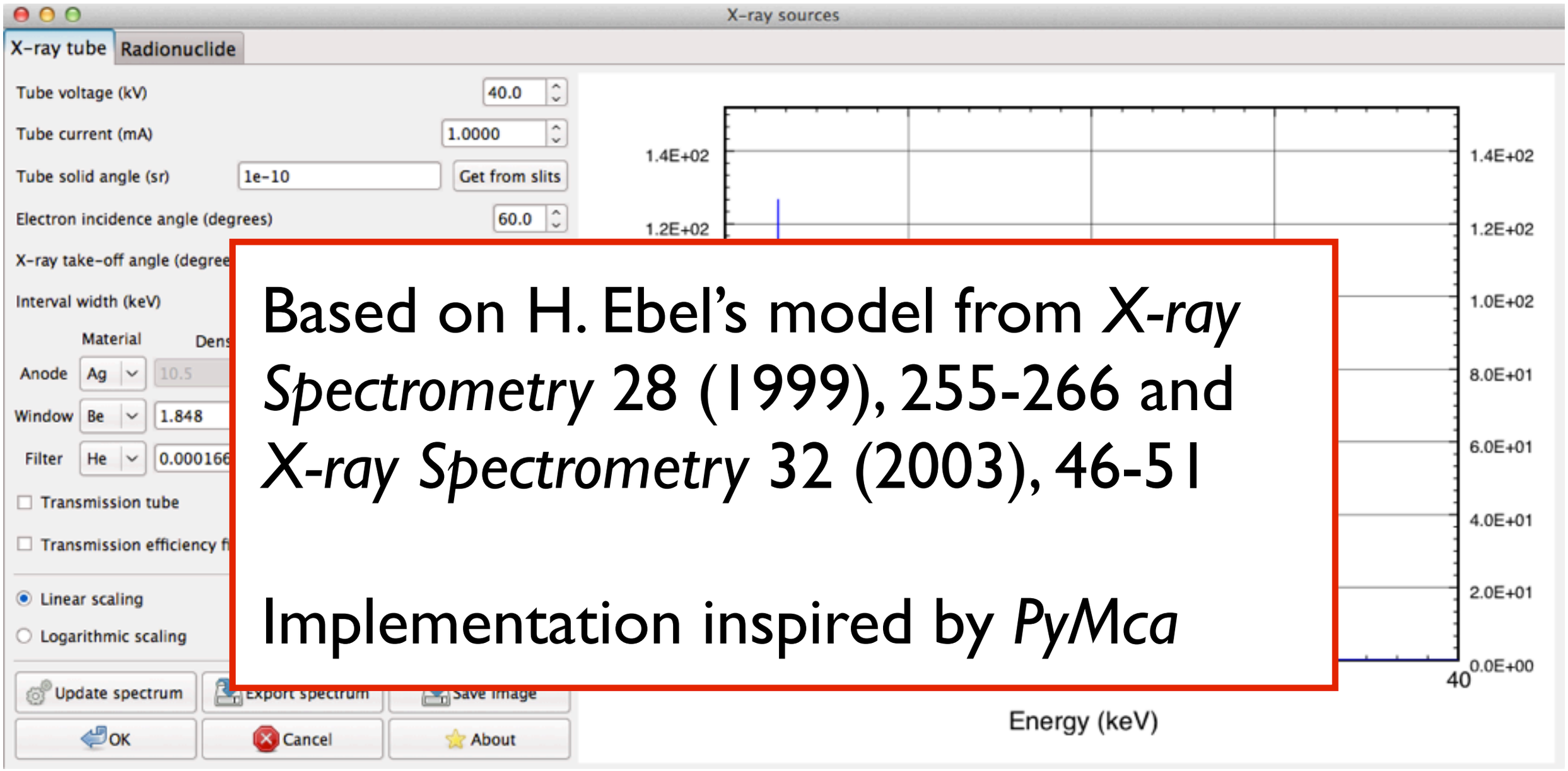
- Remove HDF5 files: when doing a complete uninstall
- Import from other HDF5 files: saves time
- Notification support (optional)



Advanced features



X-ray tube spectrum generator

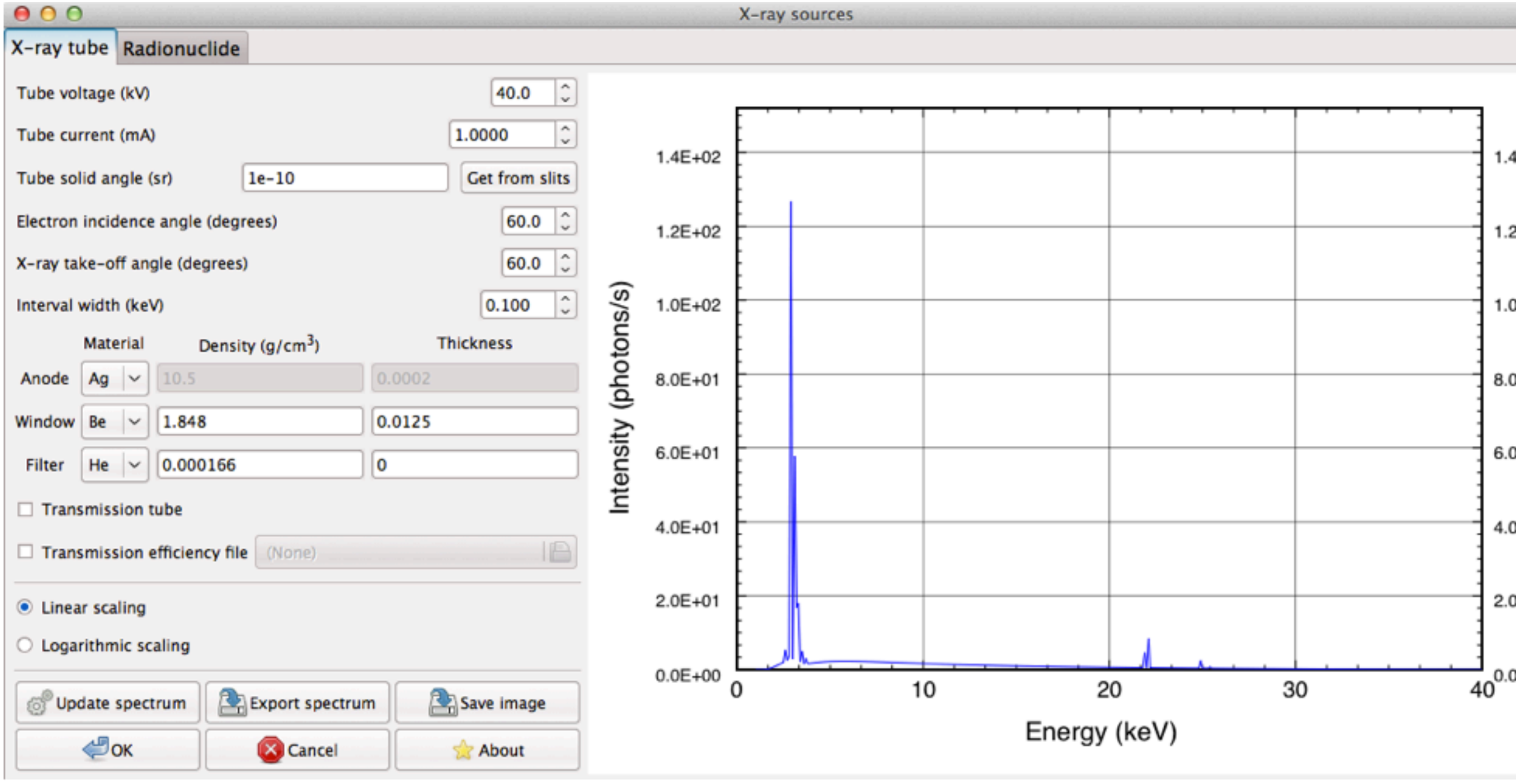


Based on H. Ebel's model from *X-ray Spectrometry* 28 (1999), 255-266 and *X-ray Spectrometry* 32 (2003), 46-51

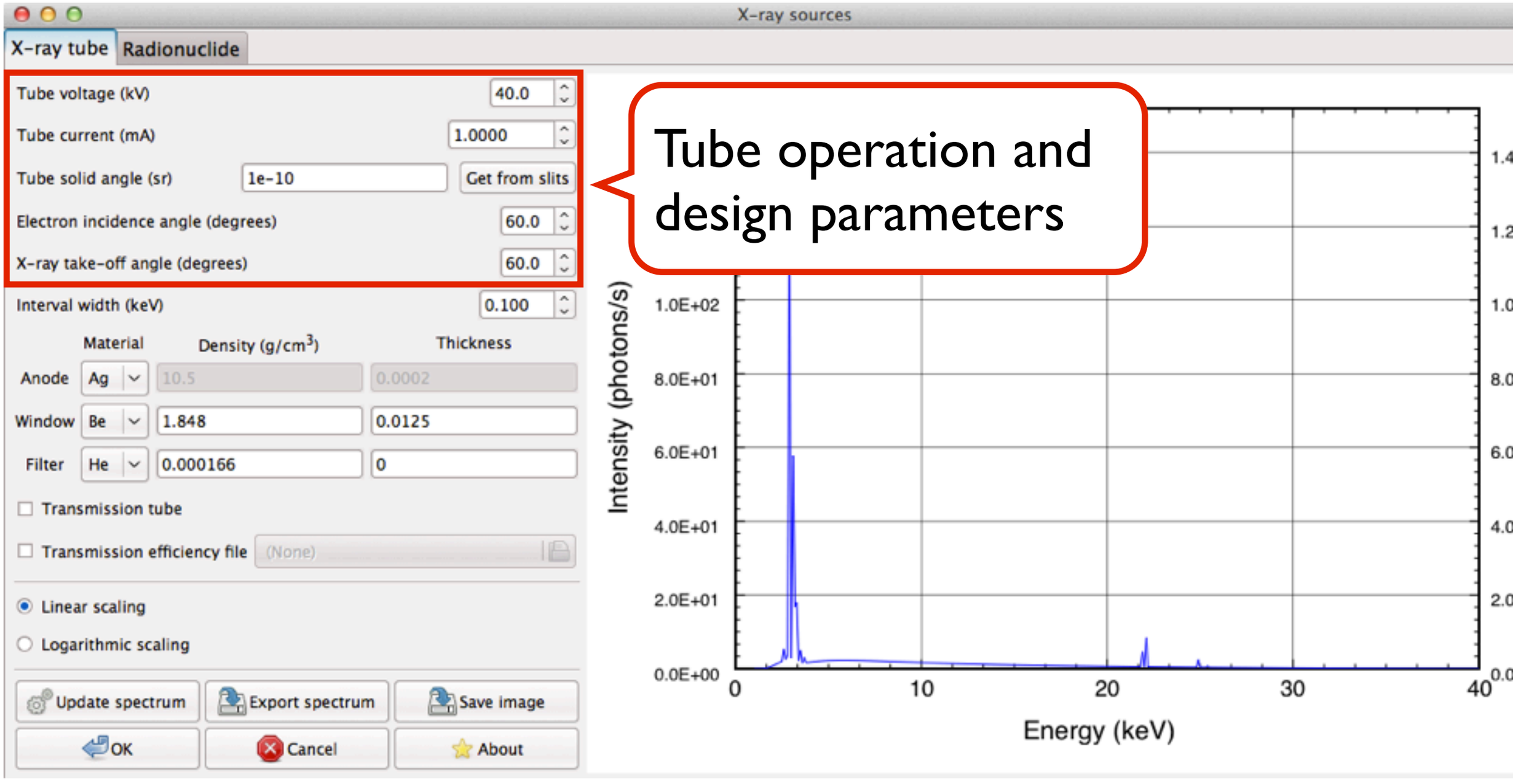
Implementation inspired by *PyMca*

X-ray tube spectrum generator

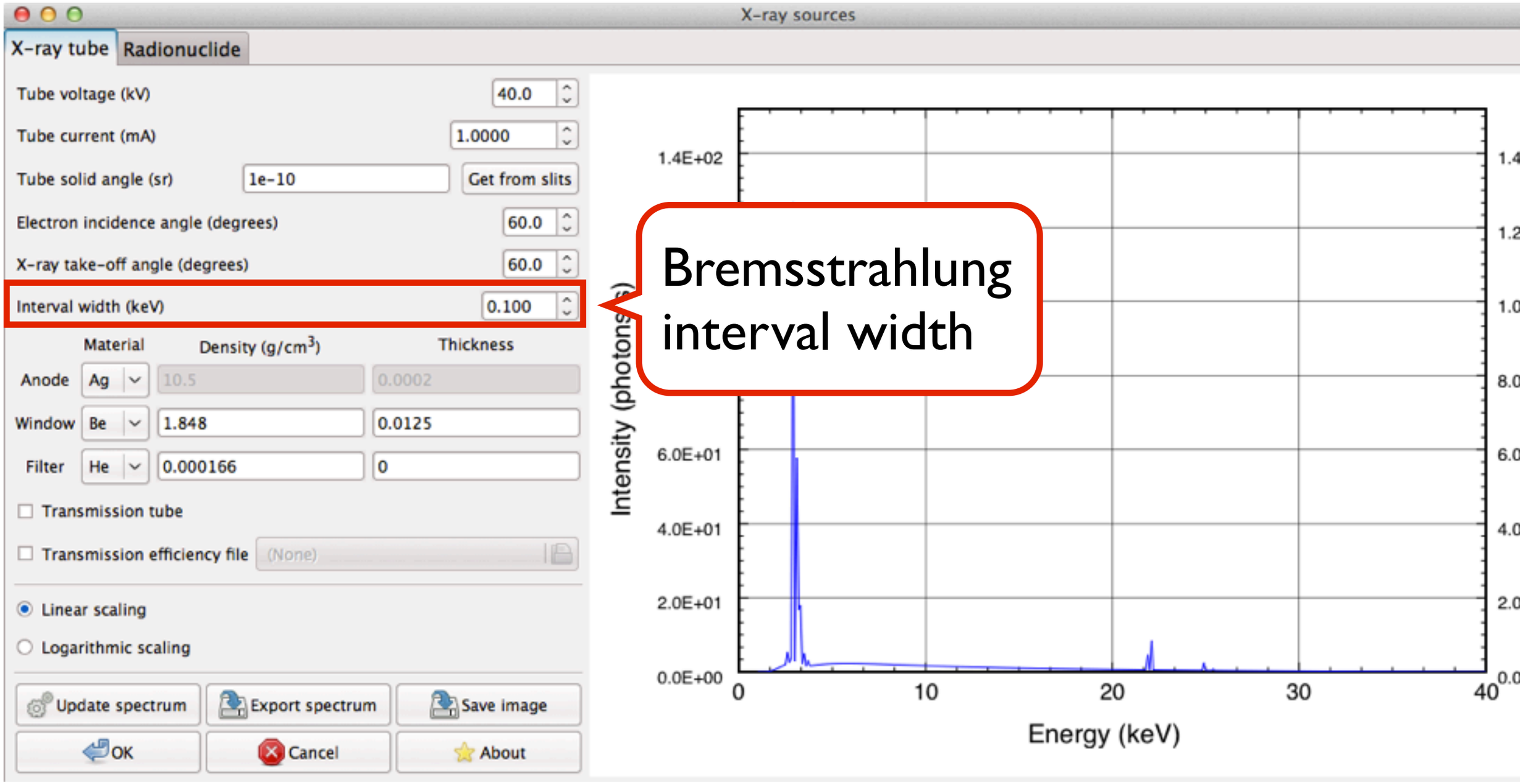
X-ray tube
spectrum generator



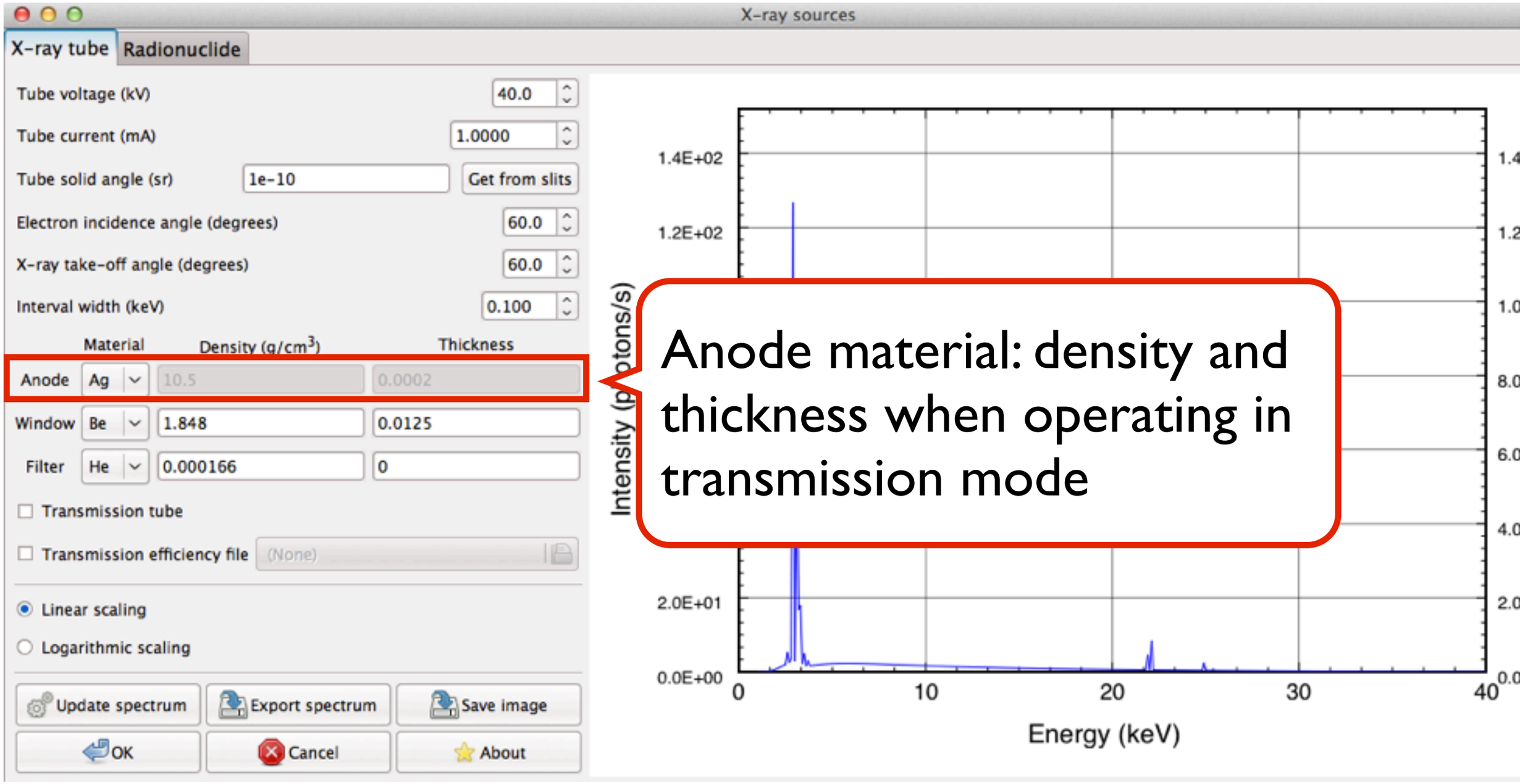
X-ray tube spectrum generator



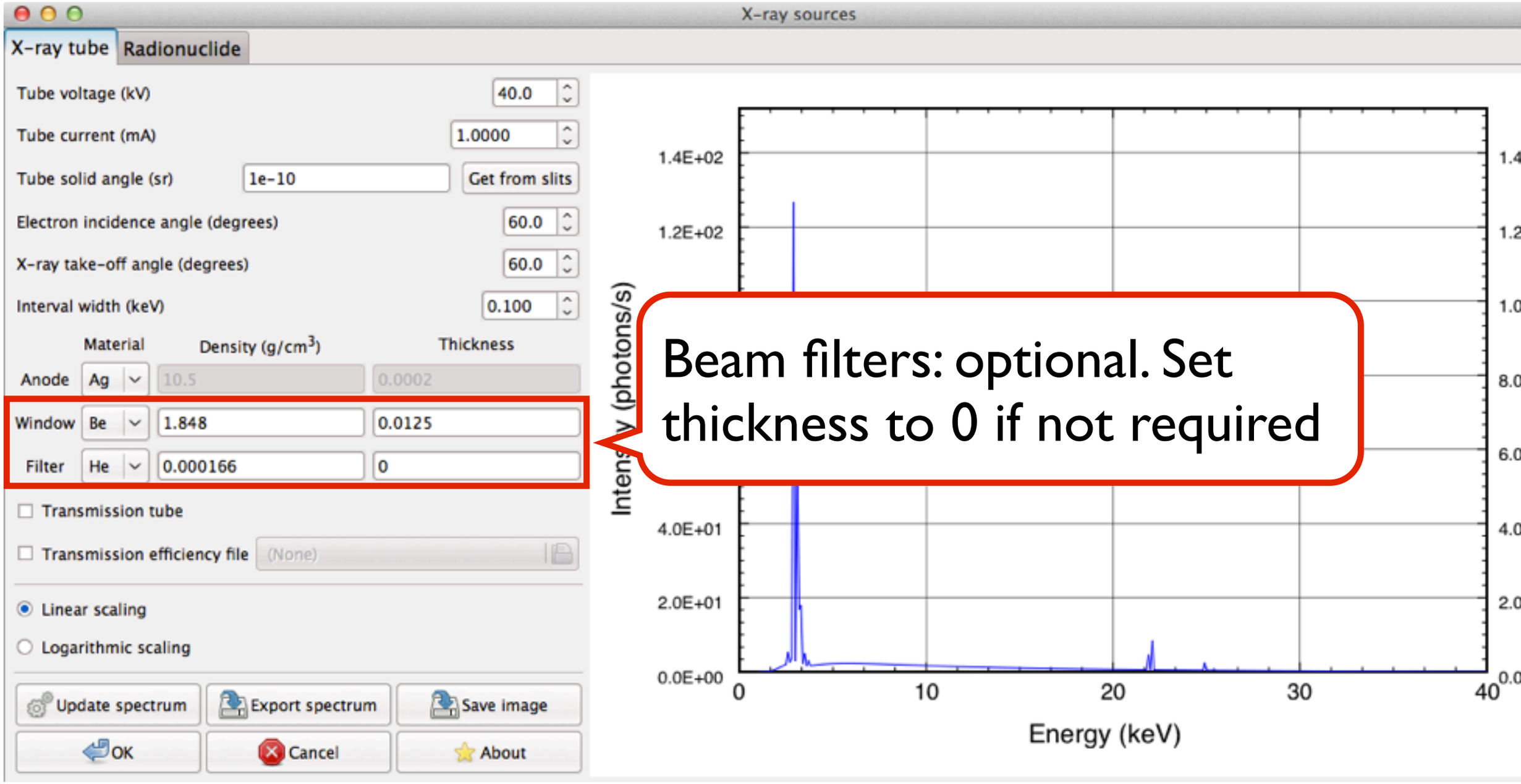
X-ray tube spectrum generator



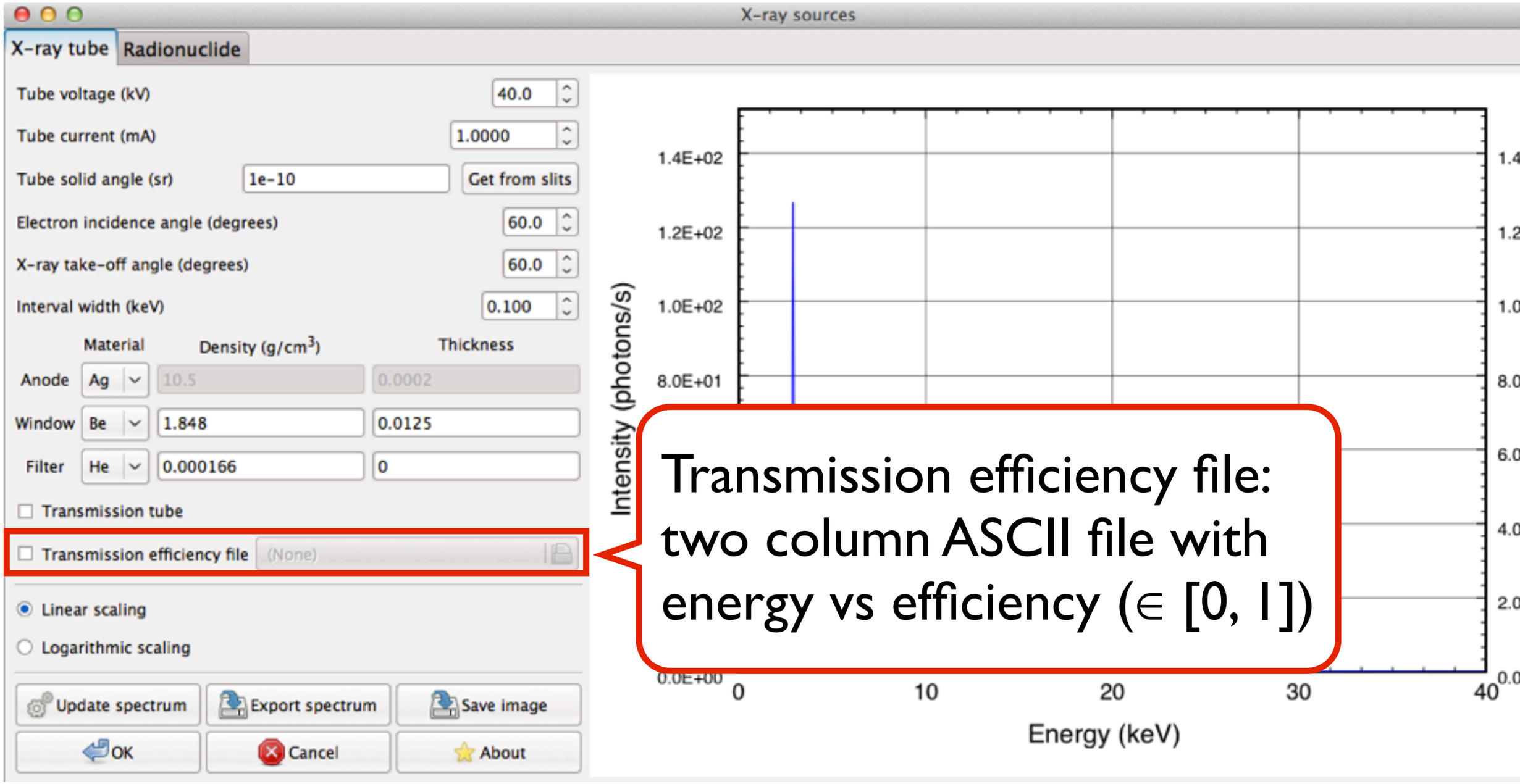
X-ray tube spectrum generator



X-ray tube spectrum generator

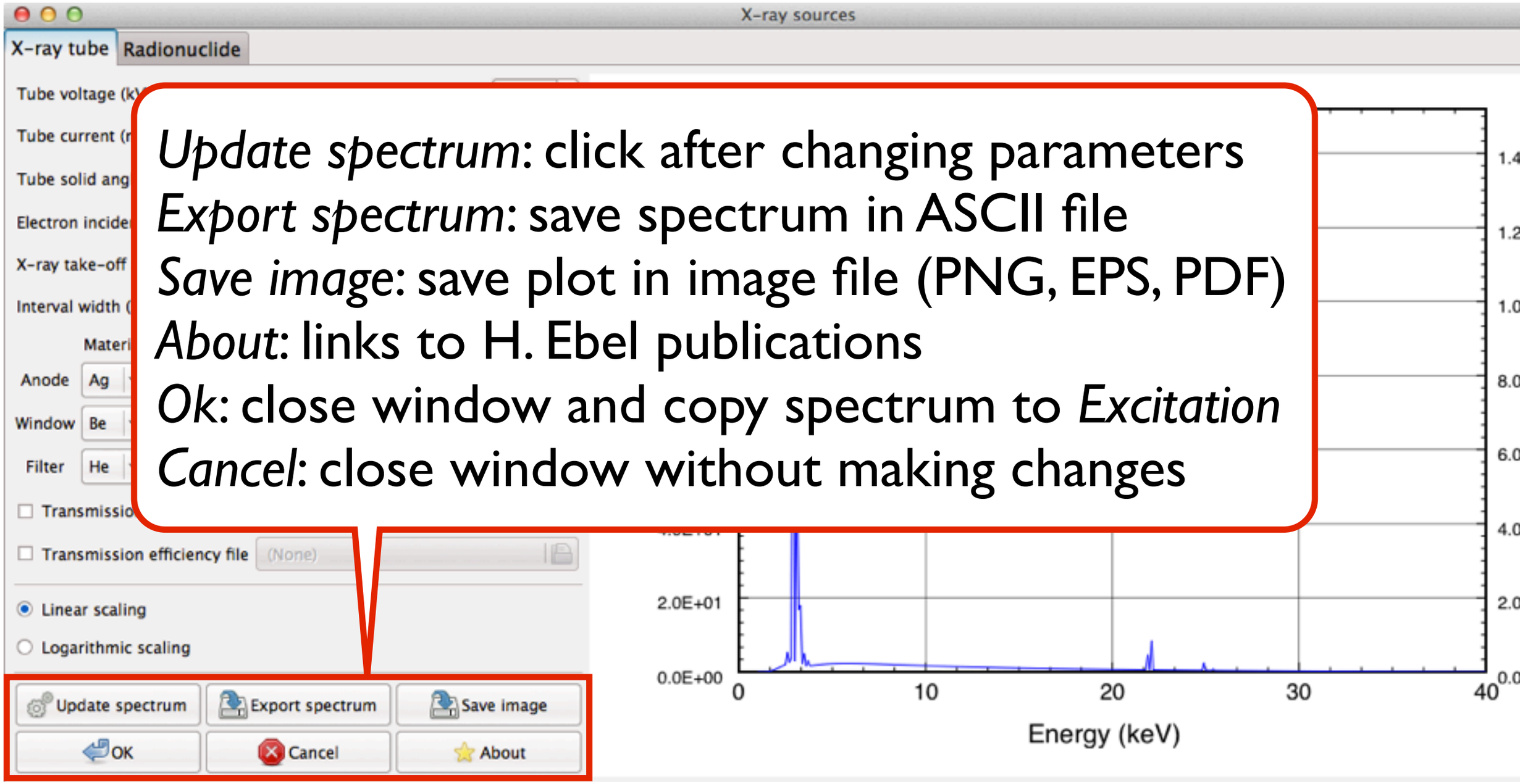


X-ray tube
spectrum generator

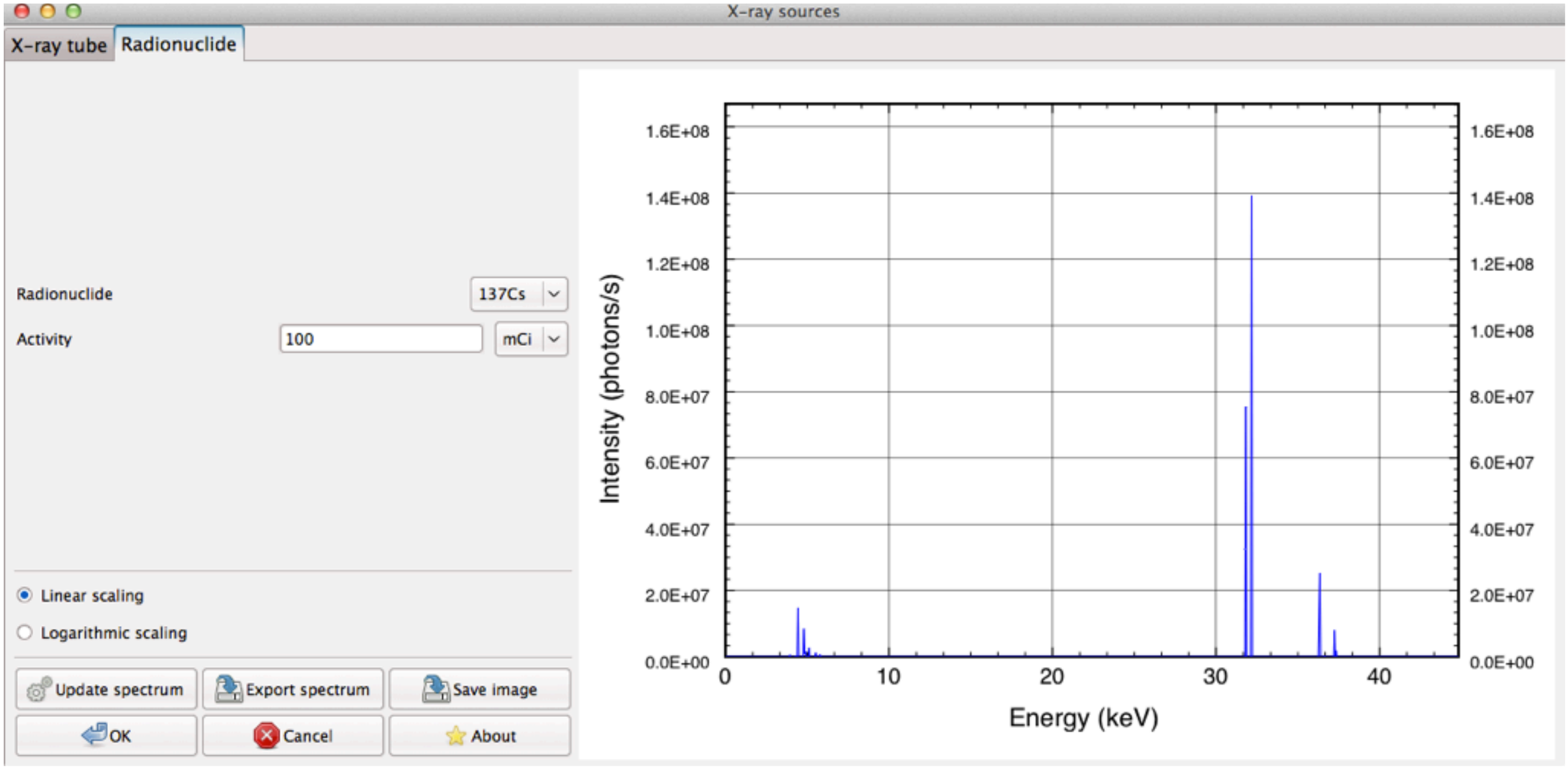


Transmission efficiency file: two column ASCII file with energy vs efficiency ($\in [0, 1]$)

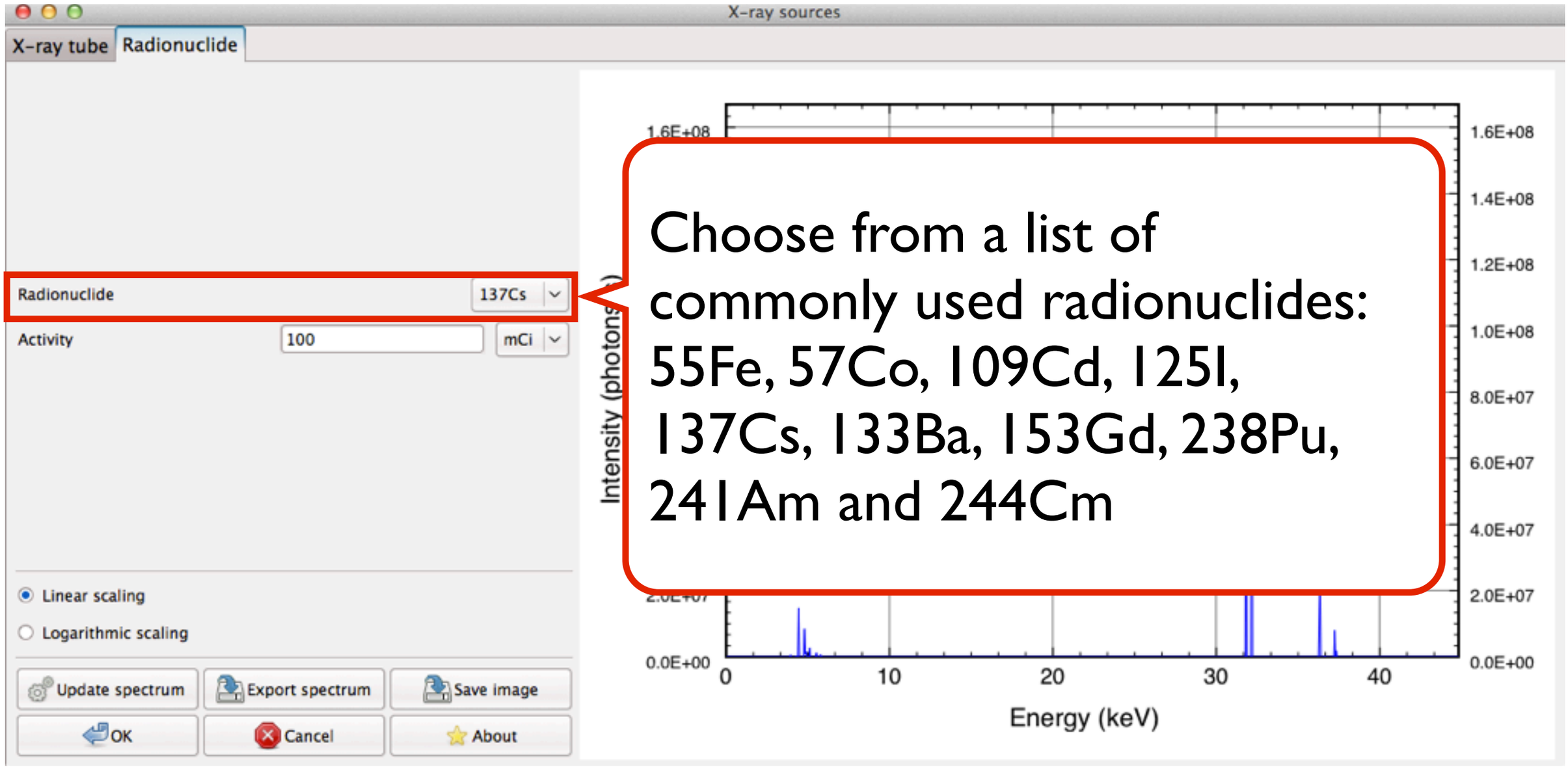
X-ray tube
spectrum generator



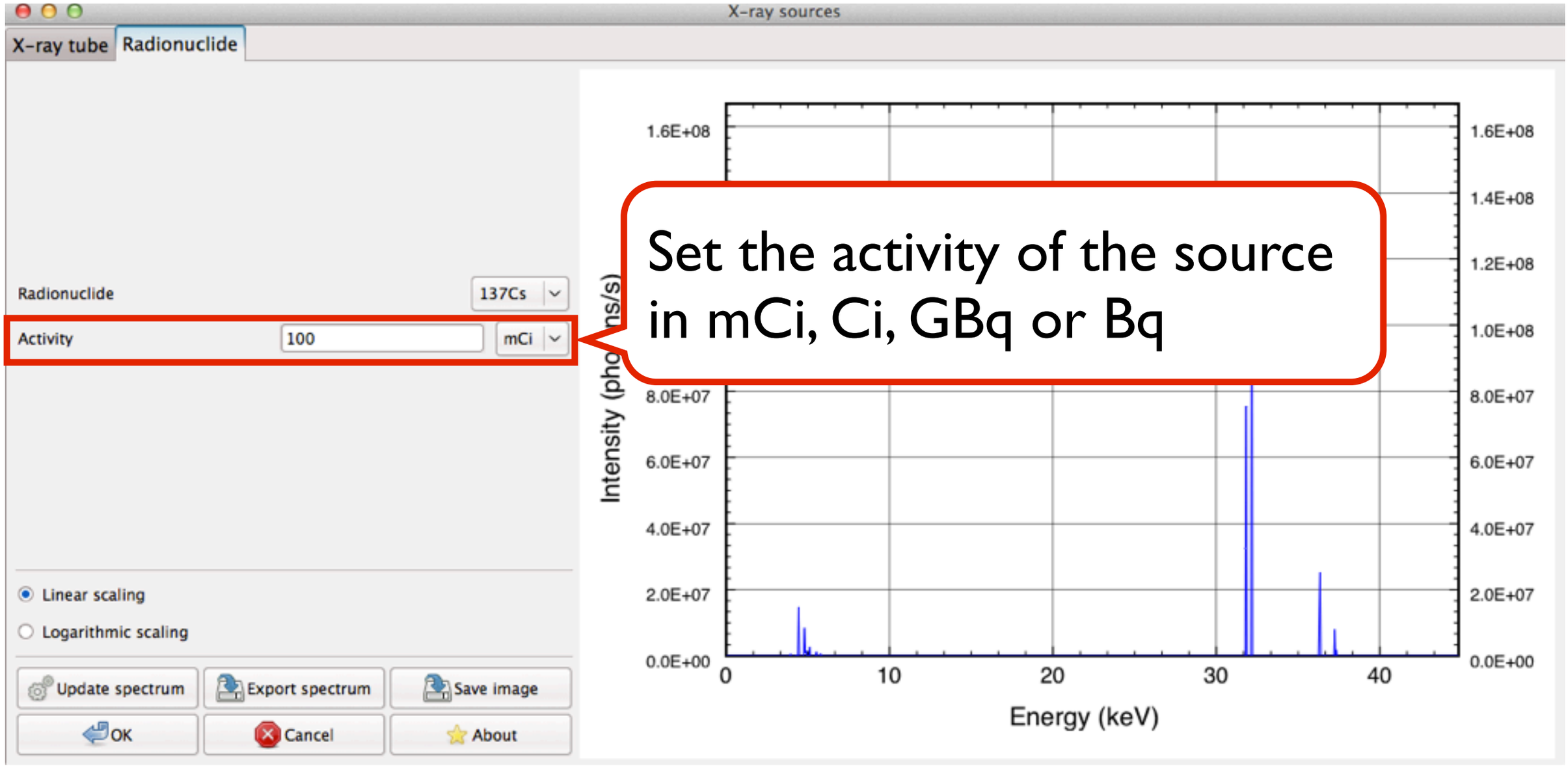
Update spectrum: click after changing parameters
Export spectrum: save spectrum in ASCII file
Save image: save plot in image file (PNG, EPS, PDF)
About: links to H. Ebel publications
Ok: close window and copy spectrum to *Excitation*
Cancel: close window without making changes



Radionuclides



Radionuclides



Radionuclides

Batch mode

Click toolbar button or go to menubar:

Tools→Batch mode

Behavior determined by file-selection dialog

1. Simulate a batch of unrelated input-files
2. Create a batch based on one input-file by varying one or two parameters

Input parameters | Simulation controls | Results

General

Outputfile

Number of photo

Number of photo

Number of intera

Comments

Number of elen

Geometry

Sample-source distance (cm) 100

Select one or more files

Recently Used

Places
- Search
- Recently Used
- /
- schoon
- Desktop
- File System
- ChangE3

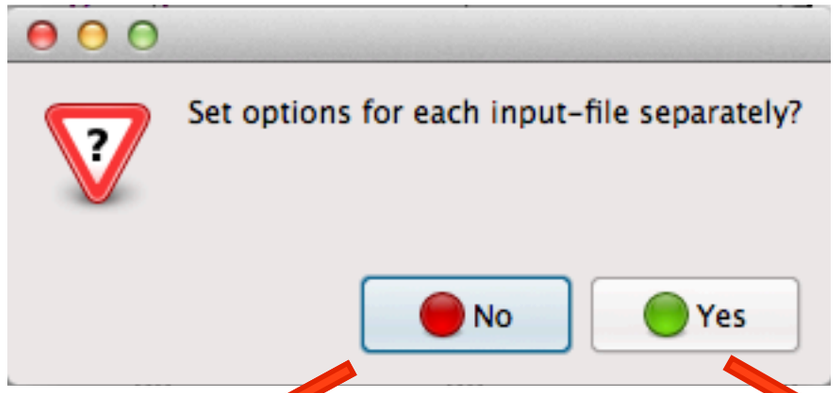
Name	Size	Modified
GBW07105_scaledflux.xmsi	11.9 kB	01/15/14
GBW07105.xmsi	11.2 kB	01/14/14
GBW07105_109Cd_nolorentz.xmsi	10.4 kB	01/14/14
GBW07105_55Fe_nolorentz.xmsi	5.9 kB	01/14/14
GBW07105_scaledflux_nolorentz.xmsi	11.1 kB	01/14/14

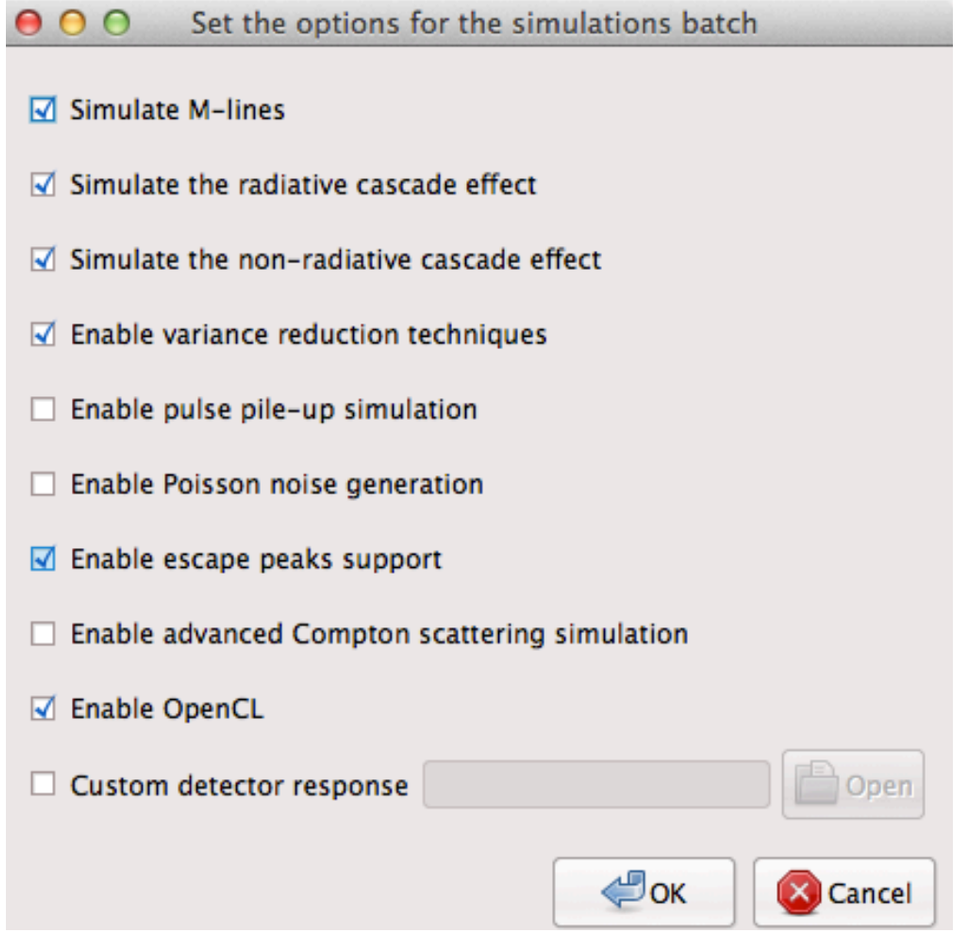
XMI-MSIM inputfiles

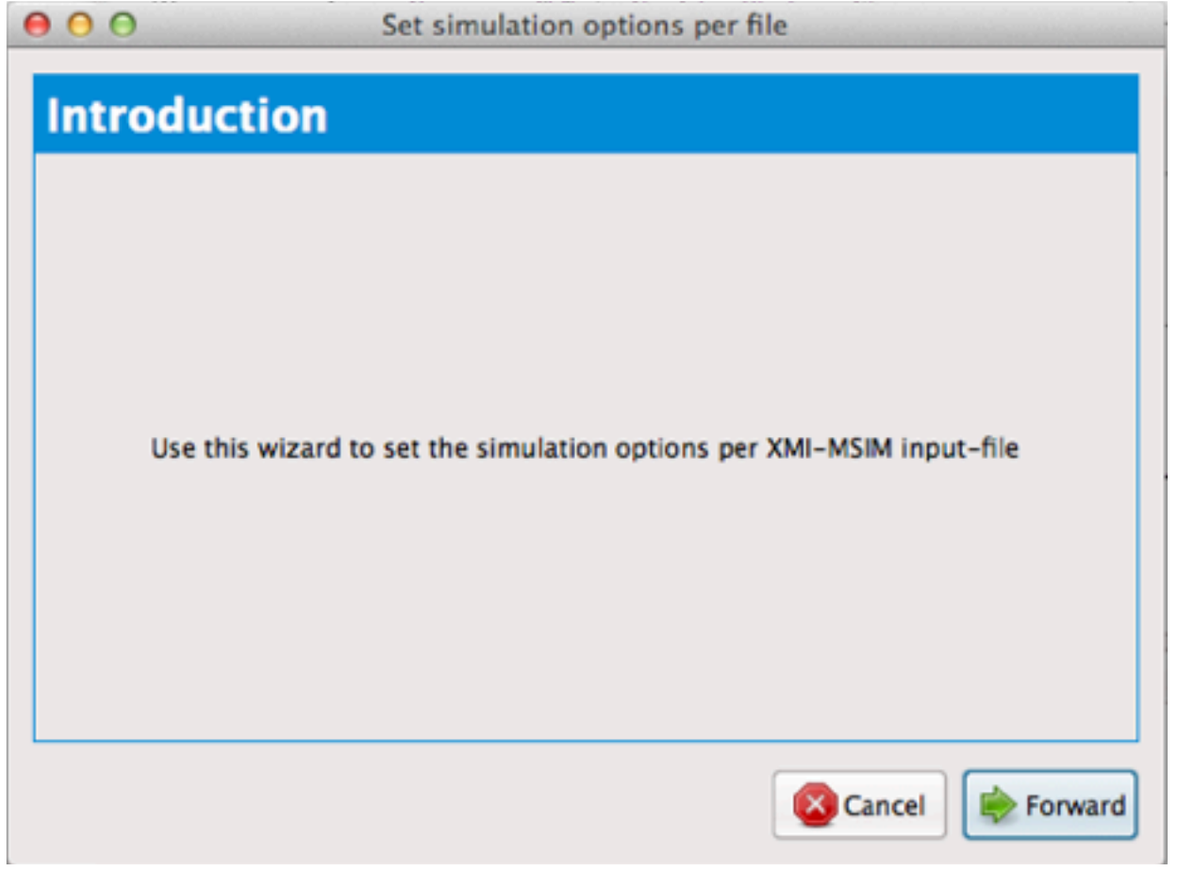
If one file is selected then a batch of files will be created based on this file with one variable parameter. Selecting multiple files will result in all these files being executed.

Cancel | Open

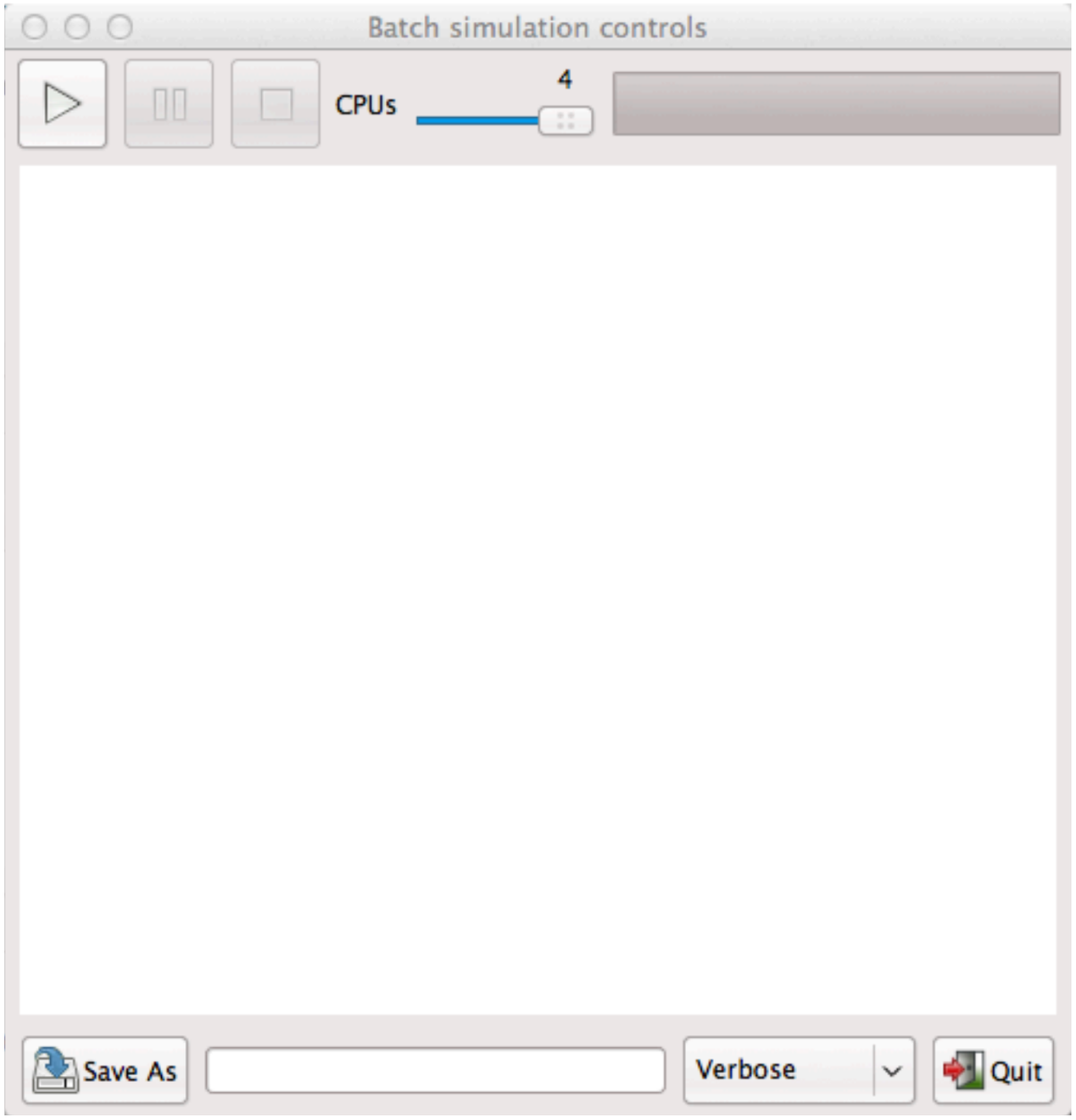
Batch mode I: simulation options





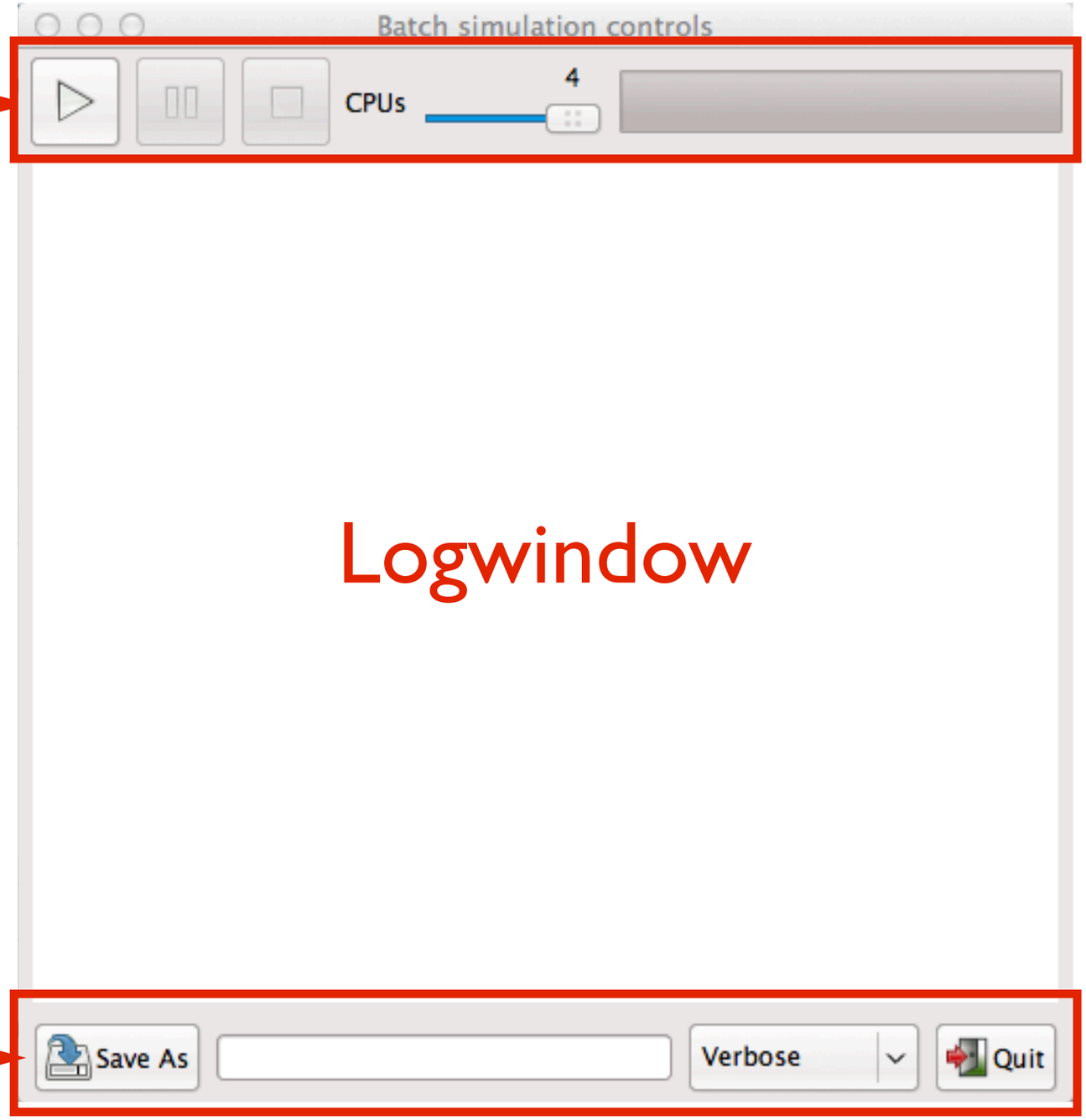


Batch mode I: running the batch



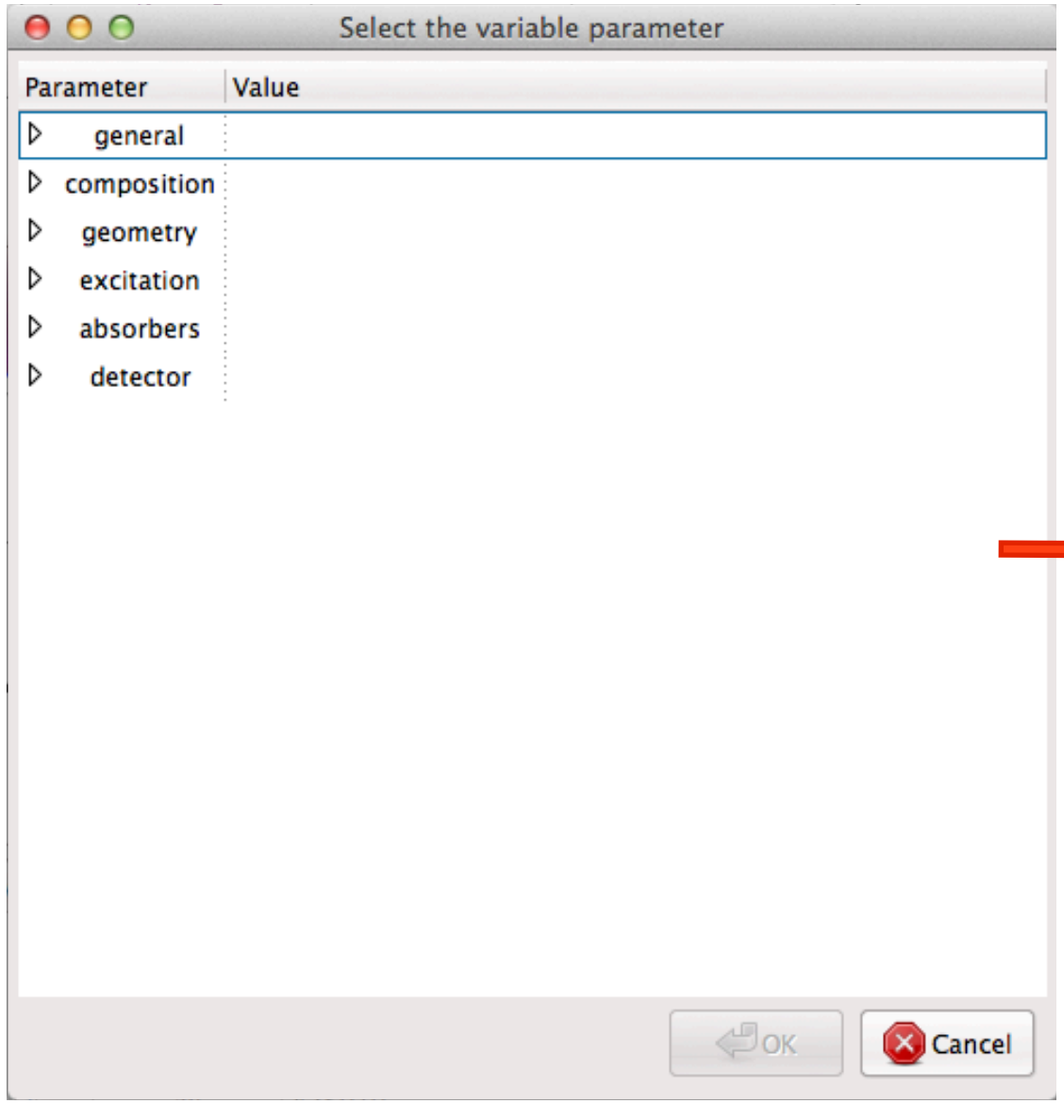
Batch mode I: running the batch

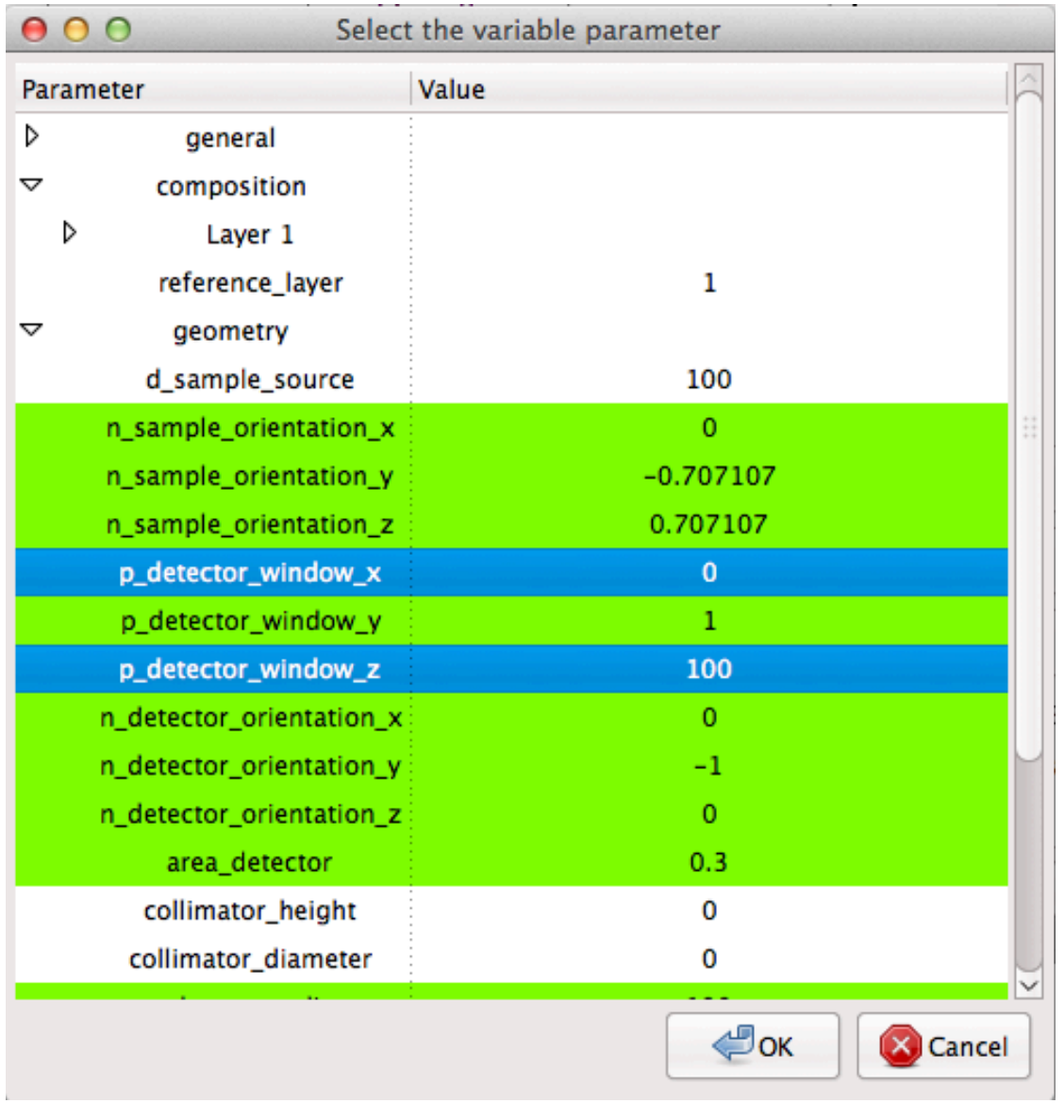
Simulation controls: set the number of *logical* CPUs, *Start*, *Pause* and *Stop*



Set verbosity level and direct output to a logfile

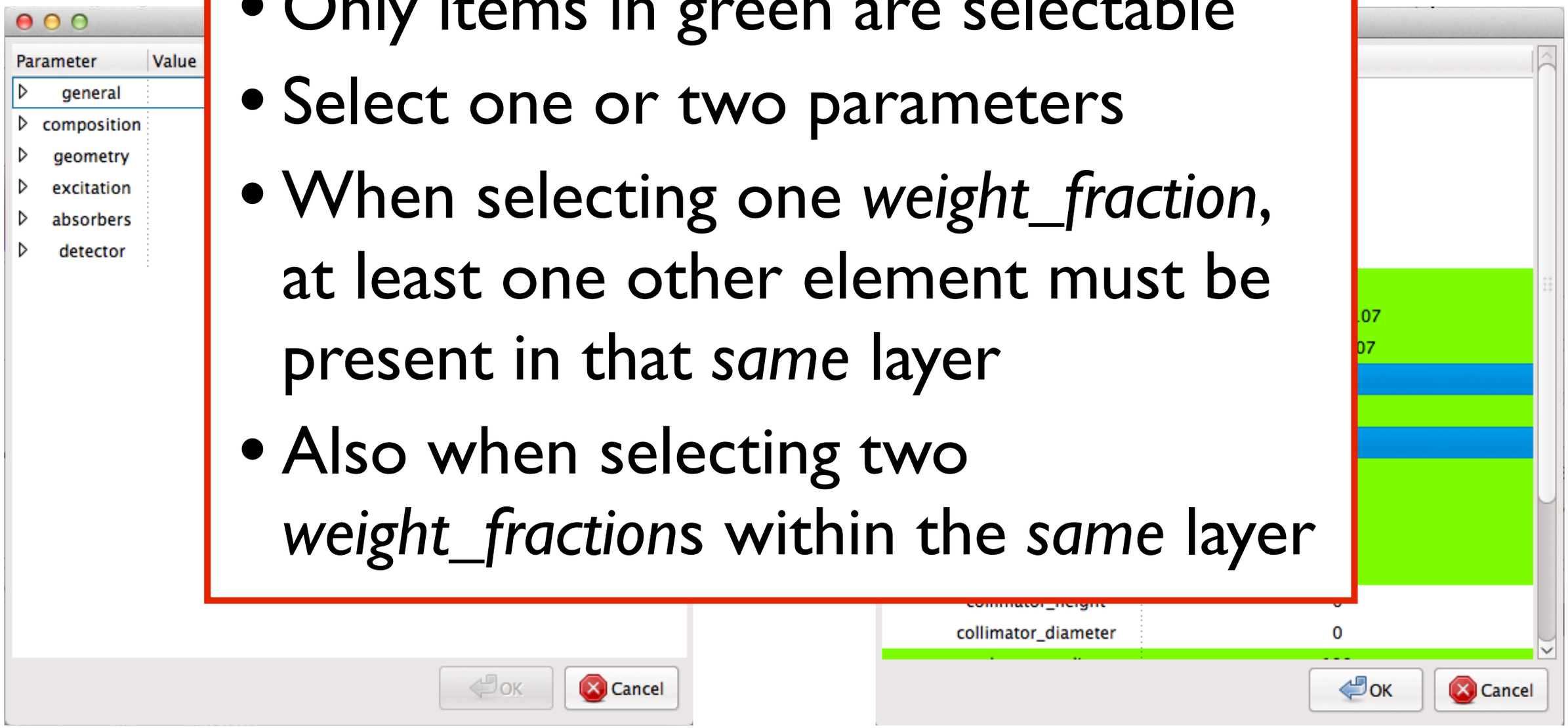
Batch mode 2:
select the variable parameters





Batch mode 2:
select the variable parameters

- Only items in green are selectable
- Select one or two parameters
- When selecting one *weight_fraction*, at least one other element must be present in that *same* layer
- Also when selecting two *weight_fractions* within the *same* layer



Batch mode 2:
set the simulation options

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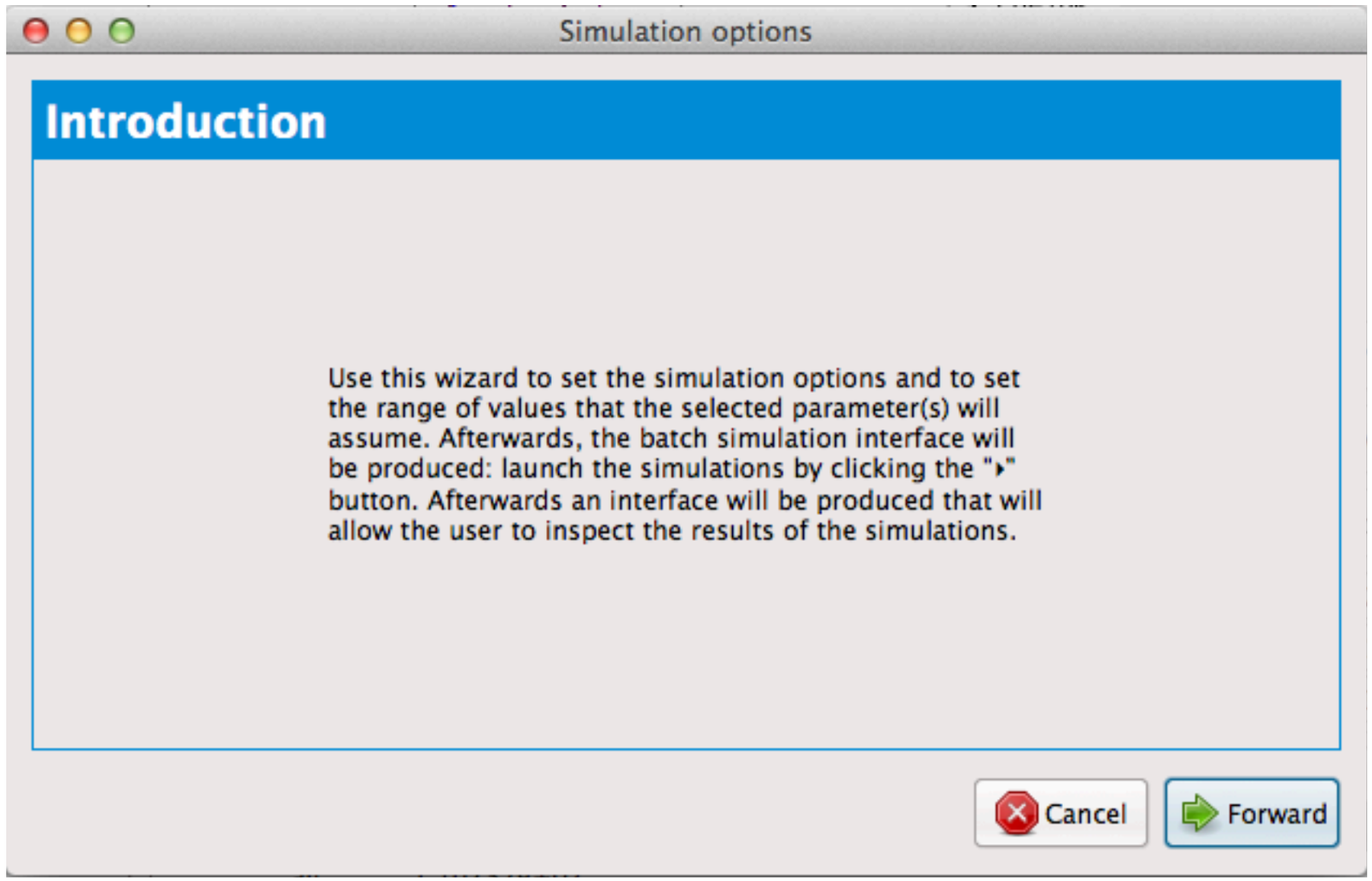
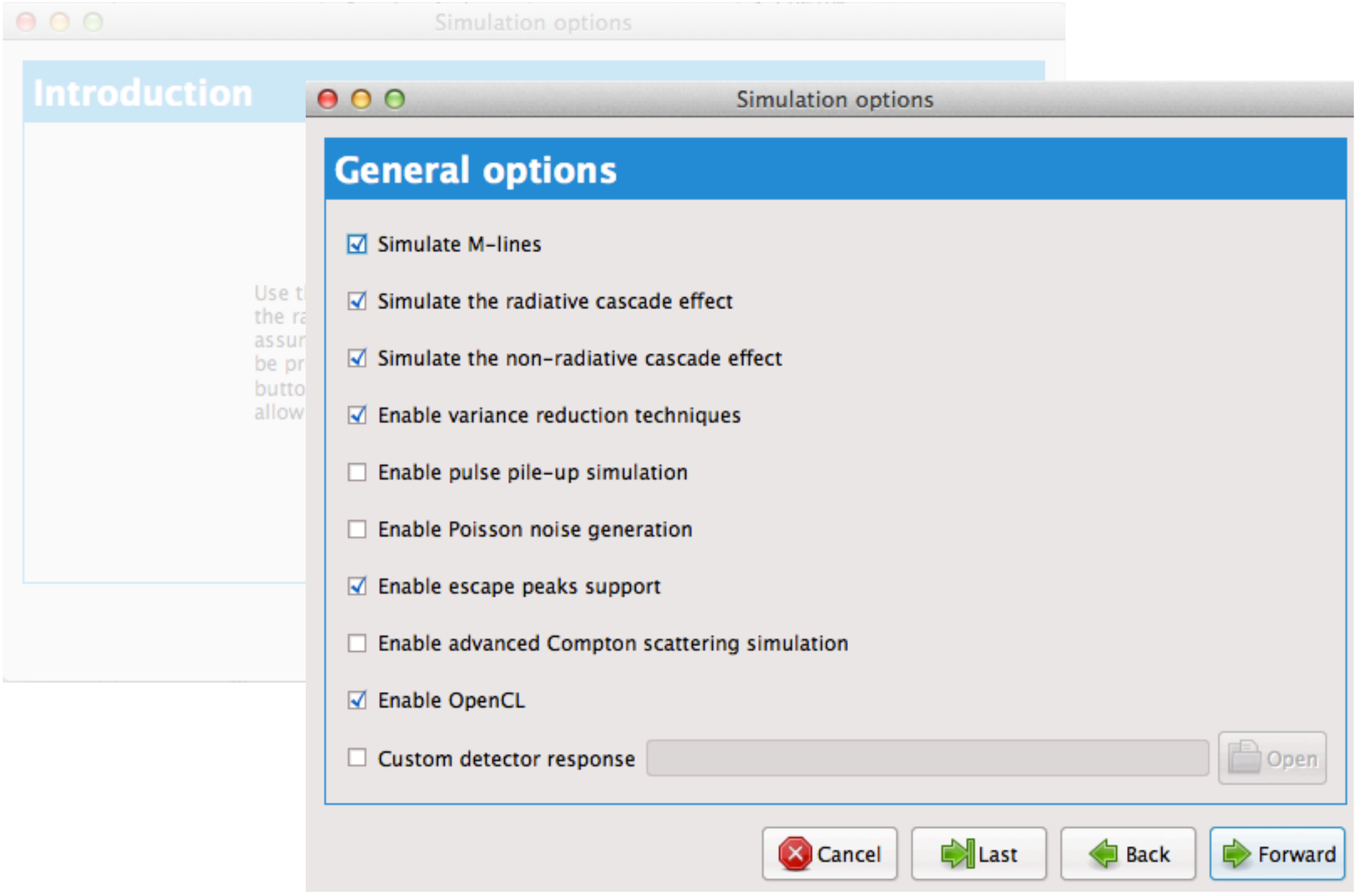
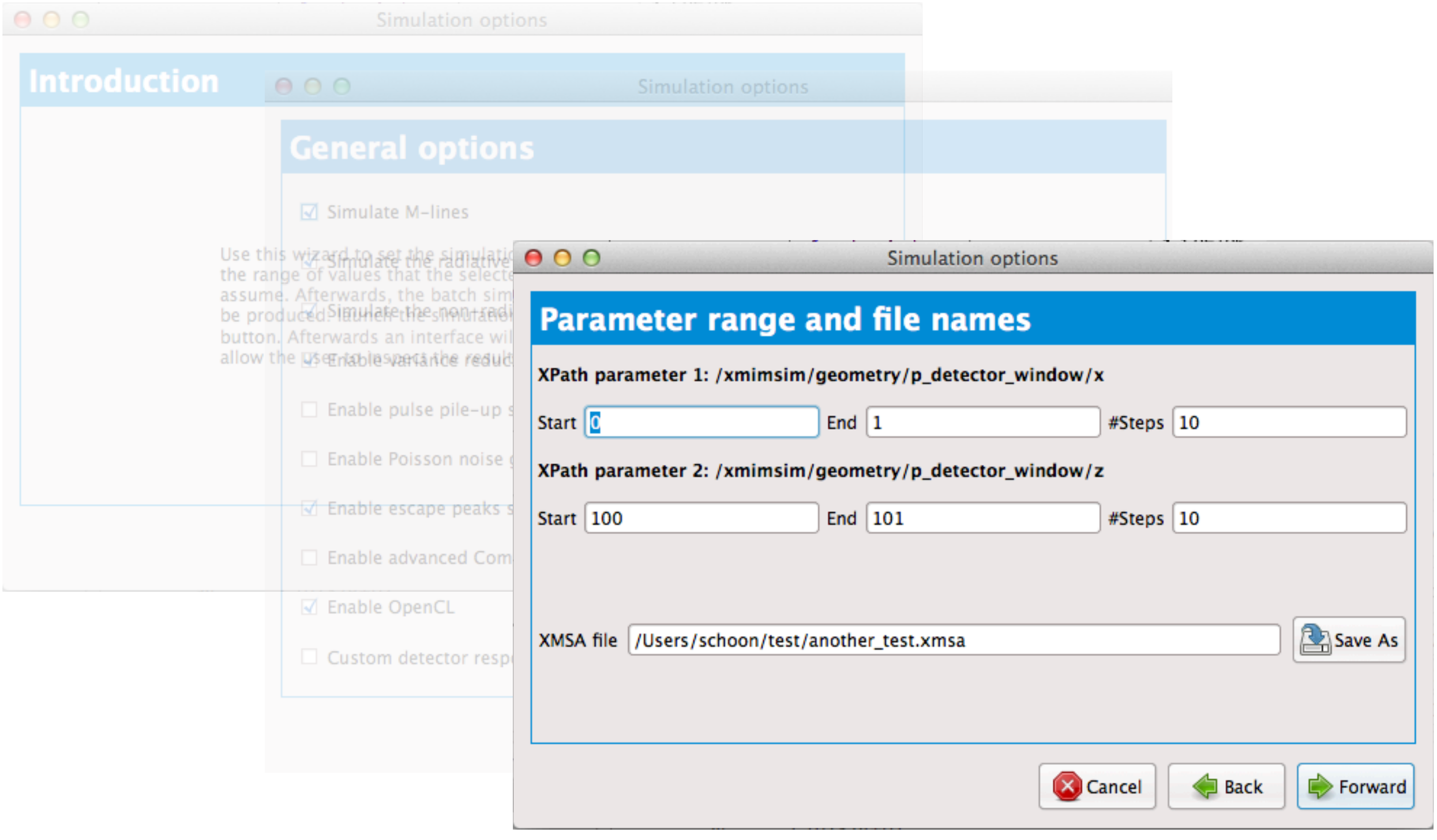
set the simulation options



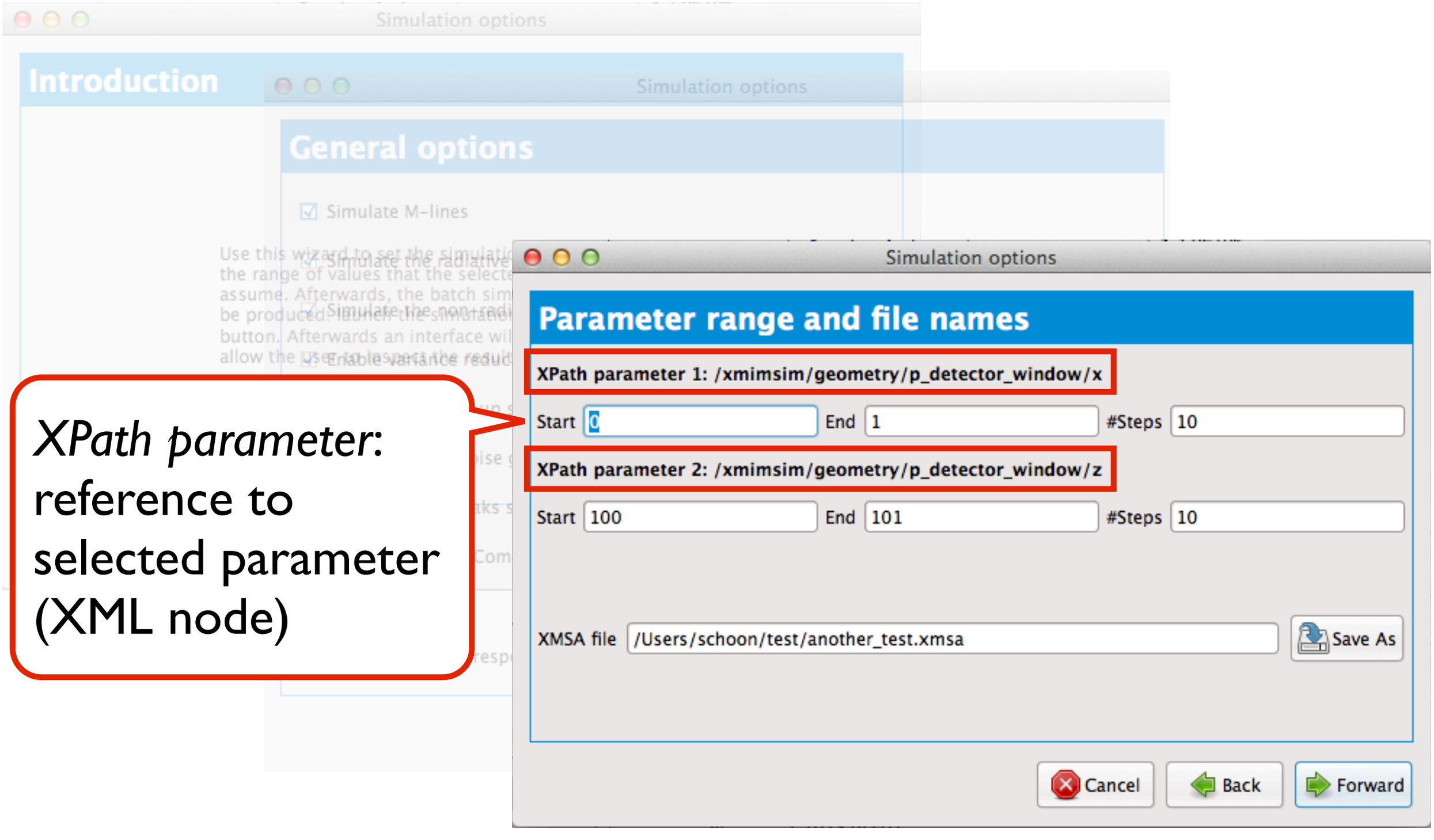
Batch mode 2:
set the simulation options



Batch mode 2:
set the simulation options



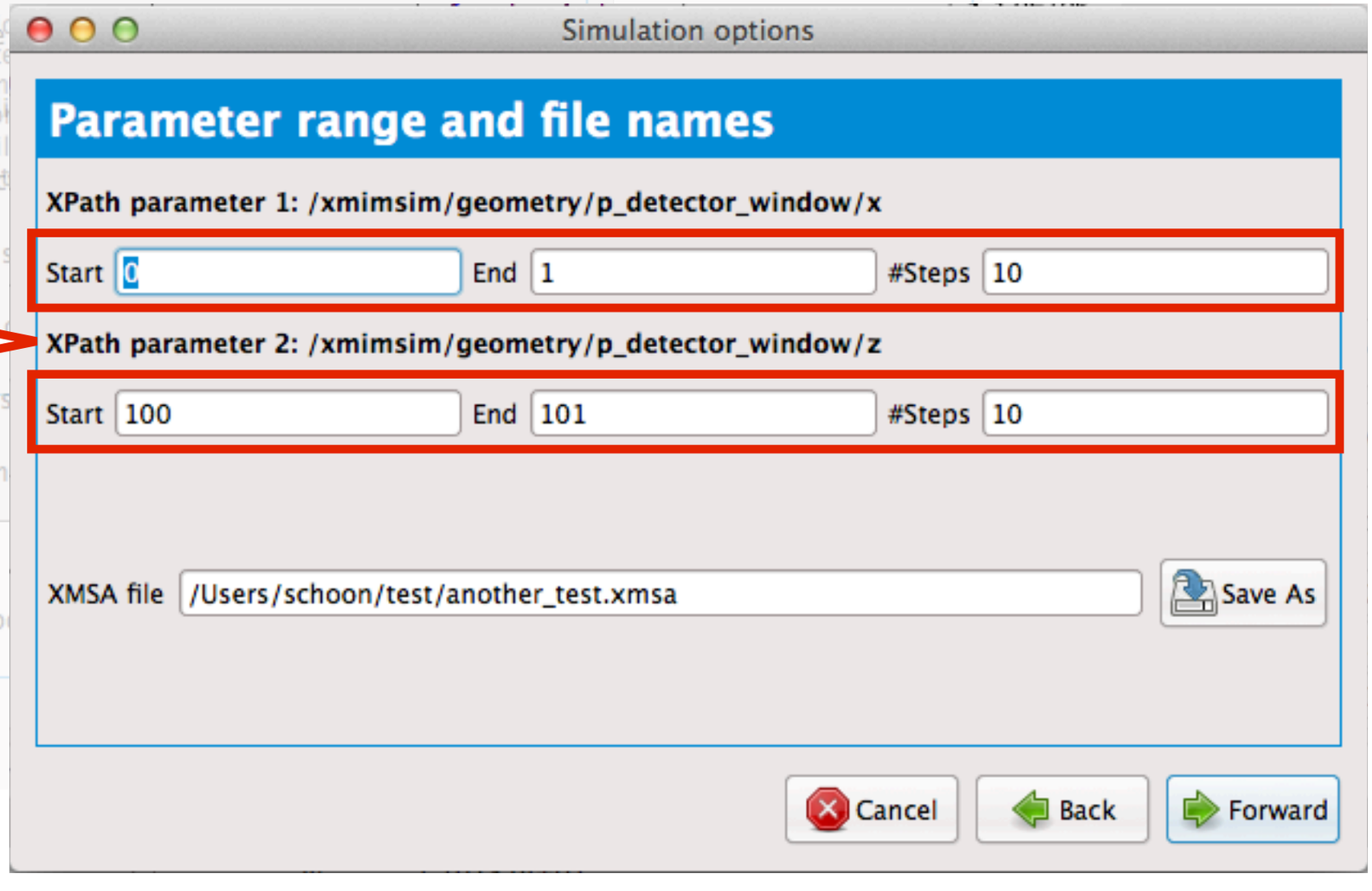
Batch mode 2: set the simulation options



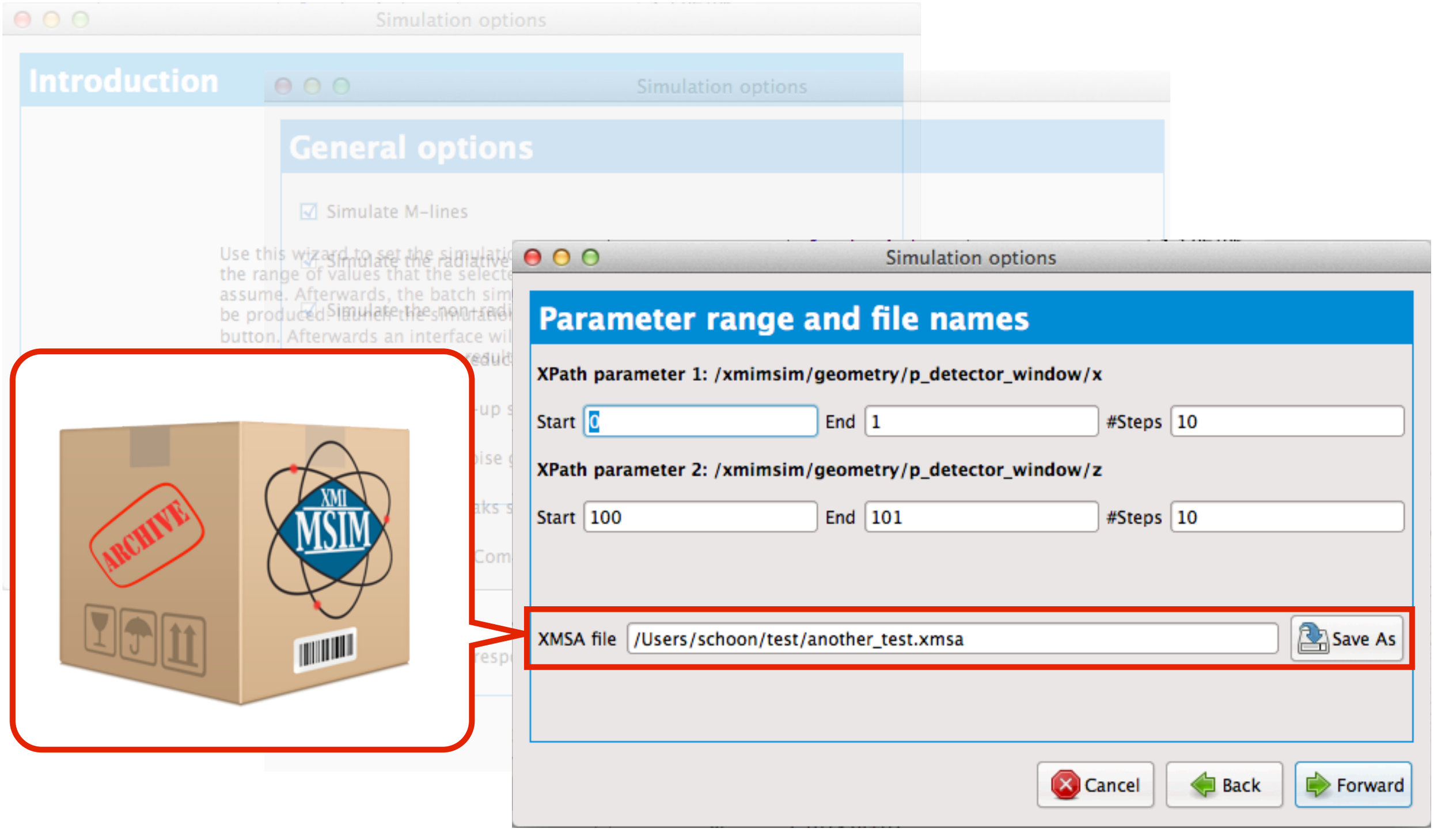
XPath parameter: reference to selected parameter (XML node)

Batch mode 2:
set the simulation options

Define range from *Start* to *Stop* using *#Steps*.

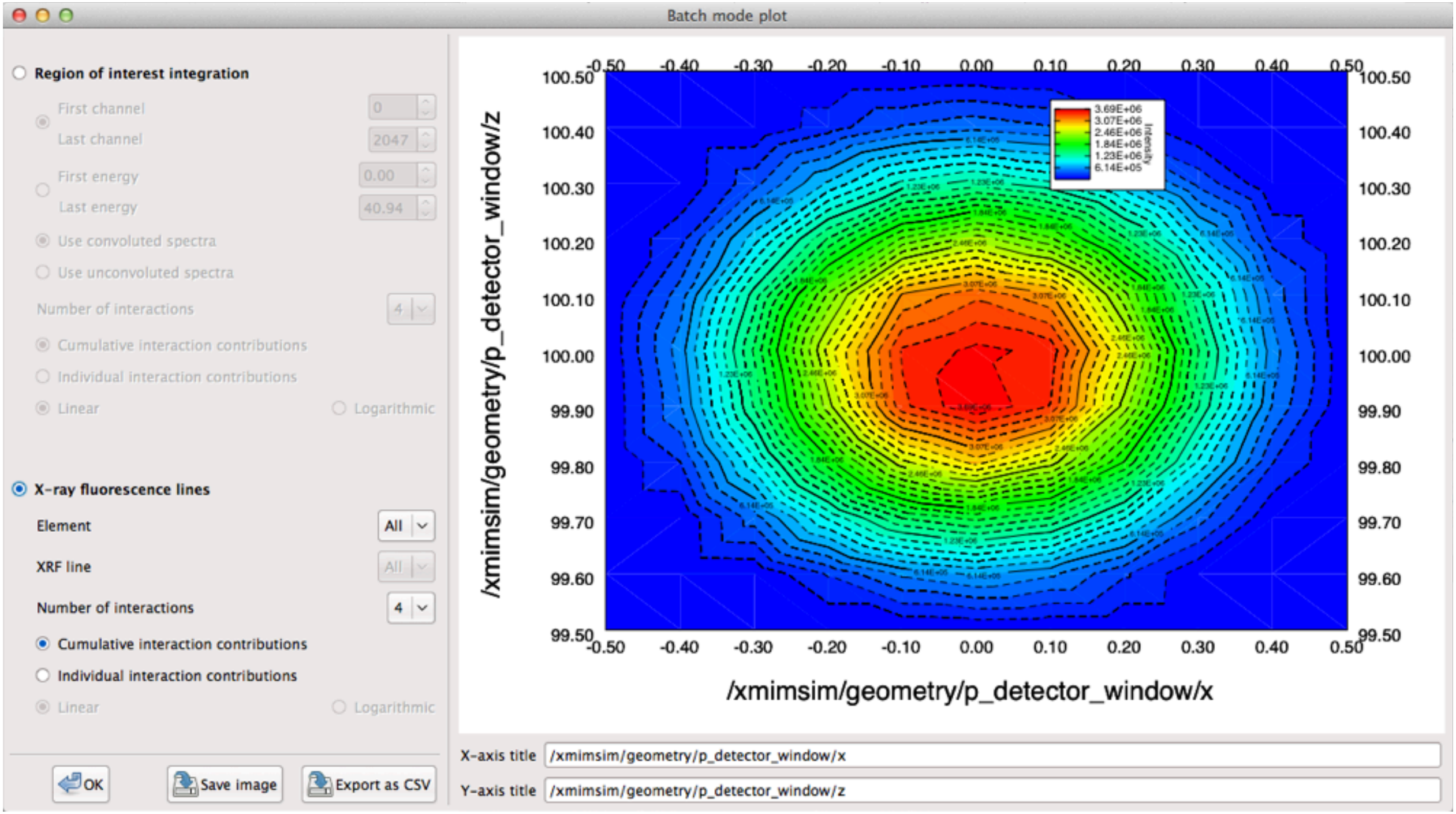


Batch mode 2:
set the simulation options

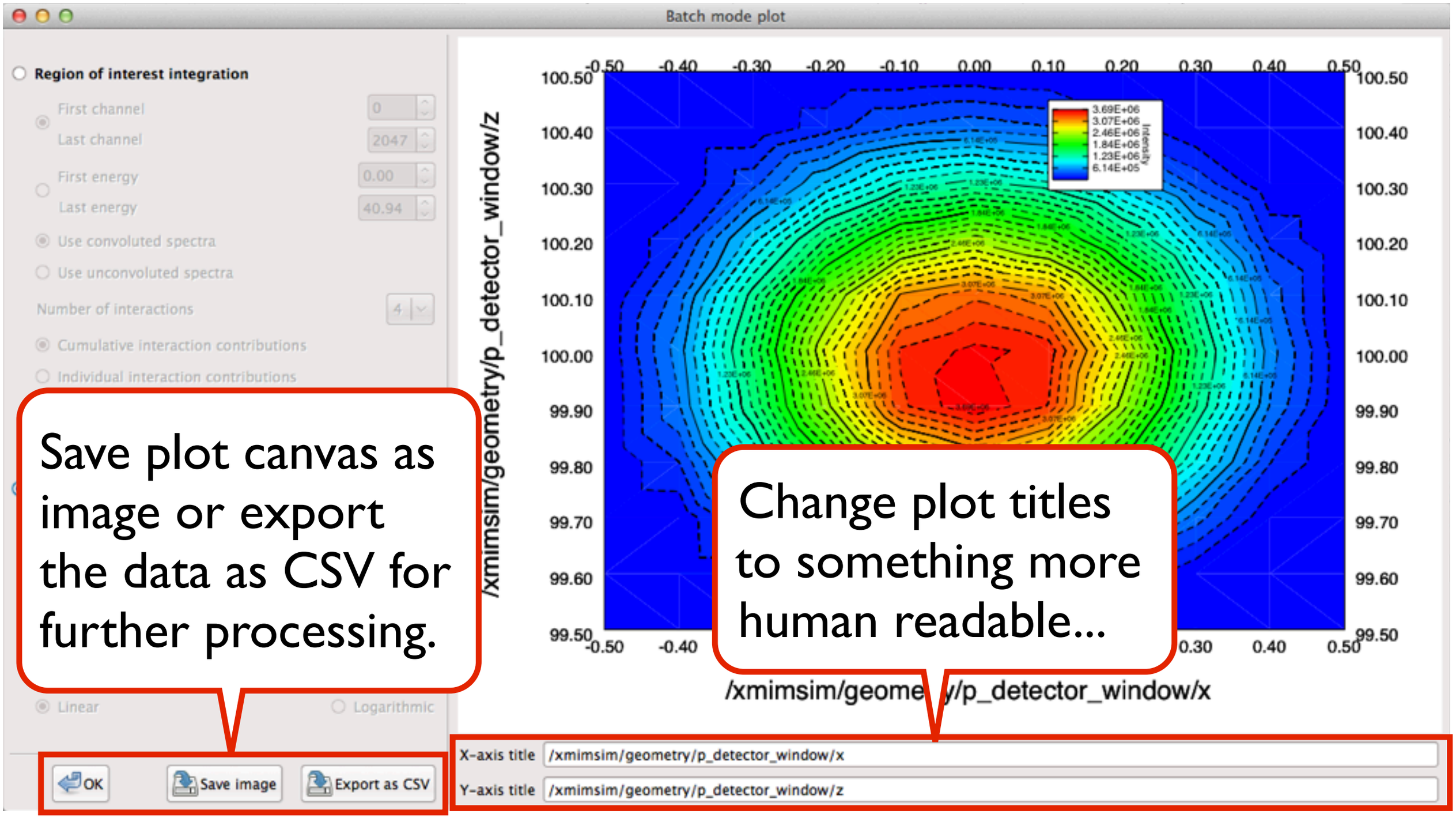


Batch mode 2: confirm and simulate

And wait...



- Region of interest integration: use channel or energy ranges.
- X-ray fluorescence lines: select element or specific lines
- Choose number of interactions: individual or cumulative
- Updates after every modification



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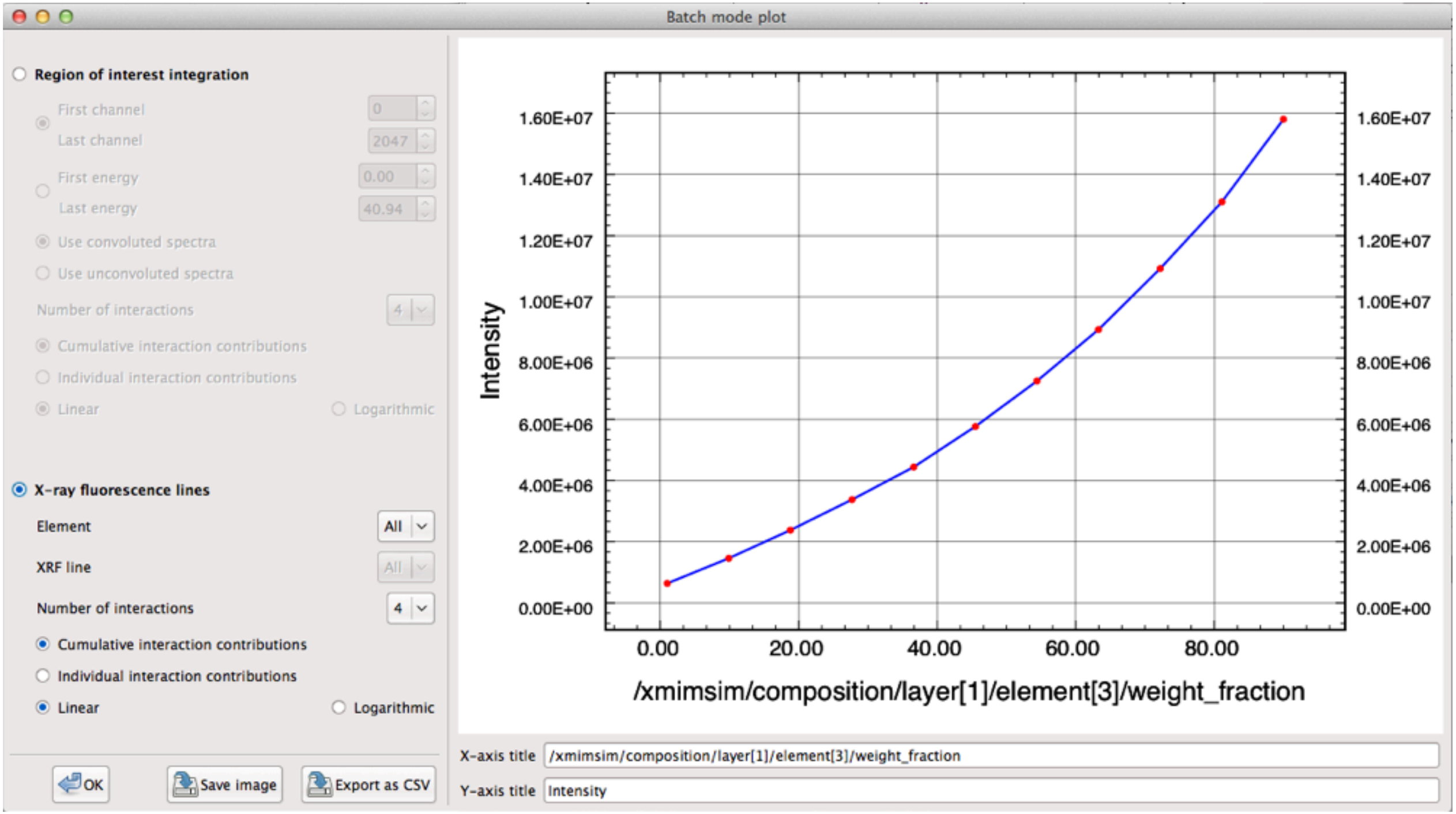

Batch mode 2: one variable parameter

File manipulation with XPath and XSLT

- XMSI, XMSO and XMSA are XML files
- Conversion to SPE, SVG, HTML, CSV performed with XSL transformations: easy to write customized variants
- Modify and create new files using an XML parser/writer in your favorite language...
- Example script available in manual (Perl)

Generate XRMC input-files

- Use: *Tools* → *Convert XMSO file to XRMC*
- Especially useful when a proper simulation of the collimator is required
- Requires installation of XRMC with its bindings to XMI-MSIM!

Command-line tools

- *xmimsim*: actual simulation executable (use *xmimsim-cli.exe* on Windows)
- *xmimsim-pymca*: PyMca's quantification plug-in
- *xmimsim-db*: generates *xmimsimdata.h5*
- *xmimsim-harvester*: seed collecting daemon (UNIX)
- *xmso2xmsi, xmso2spe, xmso2csv, xmso2htm, xmso2svg*: command-line equivalents of GUI's "Convert XMSO to" functions

Including XMI-MSIM in your own application

- Link against *libxmimsim*
- Many functions exported through interfaces in C and Fortran 2003: headers and modules
- Example: *XRMC* uses *XMI-MSIM*'s detector response function and X-ray tube spectrum generator

Custom detector response functions

- To be used when the builtin functions fail at properly describing your detector response functions
- Create a dynamically loadable module (plug-in) that exports the function:
  xmi_detector_convolute_all_custom
- Use the XMI-MSIM API to minimize work
- Works well in C/C++ and Fortran
- Detailed instructions in manual!

- Based on the manual at https://github.com/tschoonj/xmimsim/wiki

- Access from XMI-MSIM: *Help* → *Visit XMI-MSIM User guide*

- Also available as pdf

- Send me bug-reports and feature requests

Exercise 1
three-layer system

1. Air
   - Composition: 78 % N2, 21 % O2, 1% Ar
   - Thickness: 5 cm
   - Density: 0.001205 g/cm^3
2. CaSO4 → reference layer!
   - Thickness: 500 µm
   - Density: 2.96 g/cm^3
3. Gold
   - Thickness: 50 µm
   - Density: 19.3 g/cm^3

Simulate 1 million photons

Disable escape peaks!!!

Afterwards: exchange layers 2 and 3 and simulate again!

Exercise II
batch mode: one parameter

- Start Batch mode
- Select the file from the previous exercise
- Composition → Layer 2 → Element (third one) → weight_fraction
- Parameter variation between 0 and 100 in 10 steps

Disable escape peaks!!!

Exercise III collimator

- Add collimator to existing file

  1. Height: 1 cm
  2. Diameter: 0.2 cm

- Move collimator to y = 2 cm
- Simulate and compare results with first exercise

Disable escape peaks!!!

Exercise IV
batch mode: two parameters

- Start Batch mode
- Select the file from the previous exercise

Disable escape peaks!!!

- Geometry → p_detector_window_x AND p_detector_window_z
- Parameter I variation between -1 and 1 in 5 steps
- Parameter II variation between 99 and 101 in 5 steps