Advanced STEM simulation

This tutorial shows how to make an optimal STEM simulation using advanced features of STEM_CELL. It is preferable to have a recent version of the code >2.3.6.0.

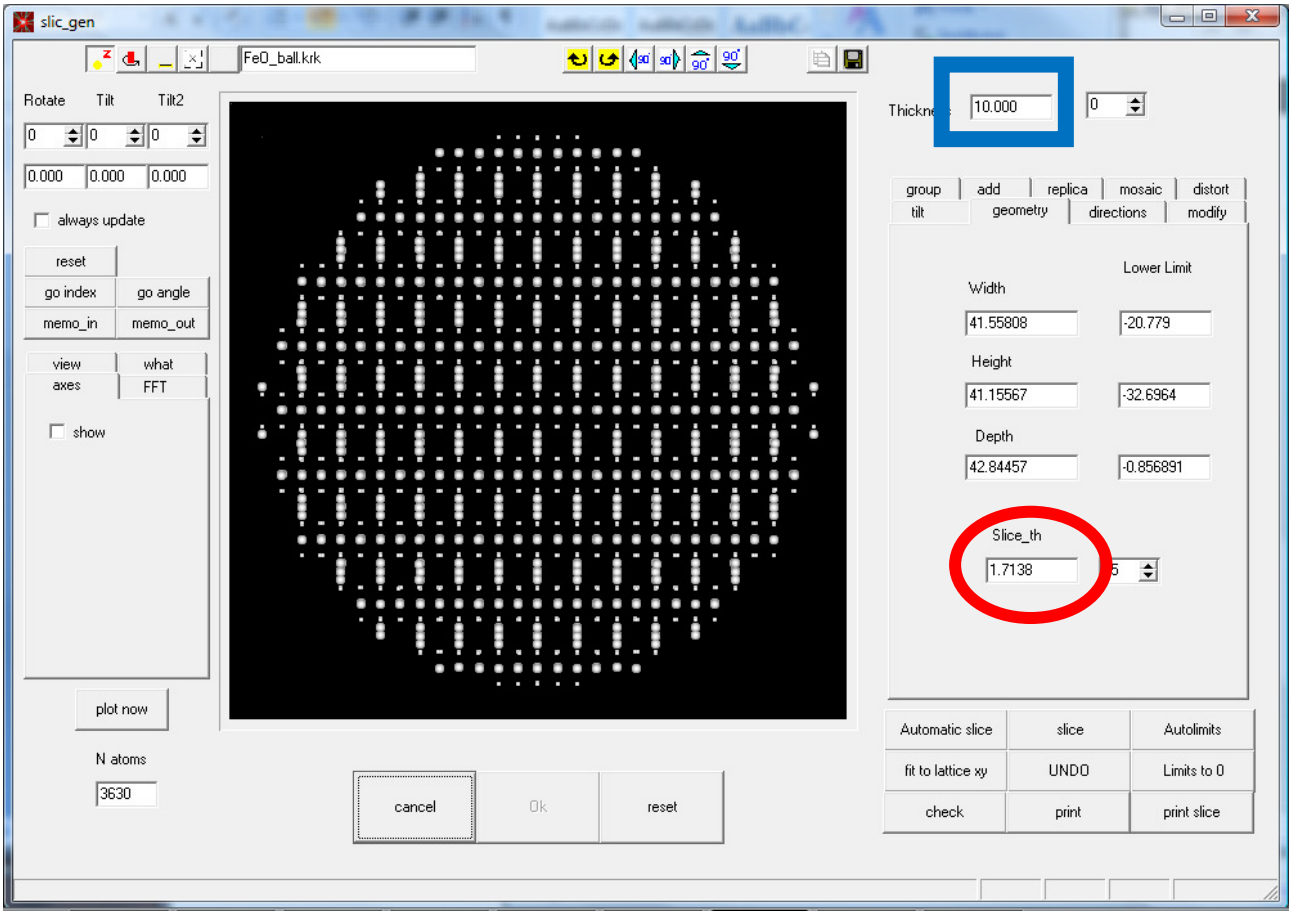
This procedure applies in particular to simulation based on Kirkland *autostem*.

I 'll suppose you already have a 3D supercell available so I'll just load it from HD as a .krk file.

Let's recall that to load a .krk you just need to do

File-> OpenSample

You can also take alook at the supercell (SC) in Sample->slice_gen



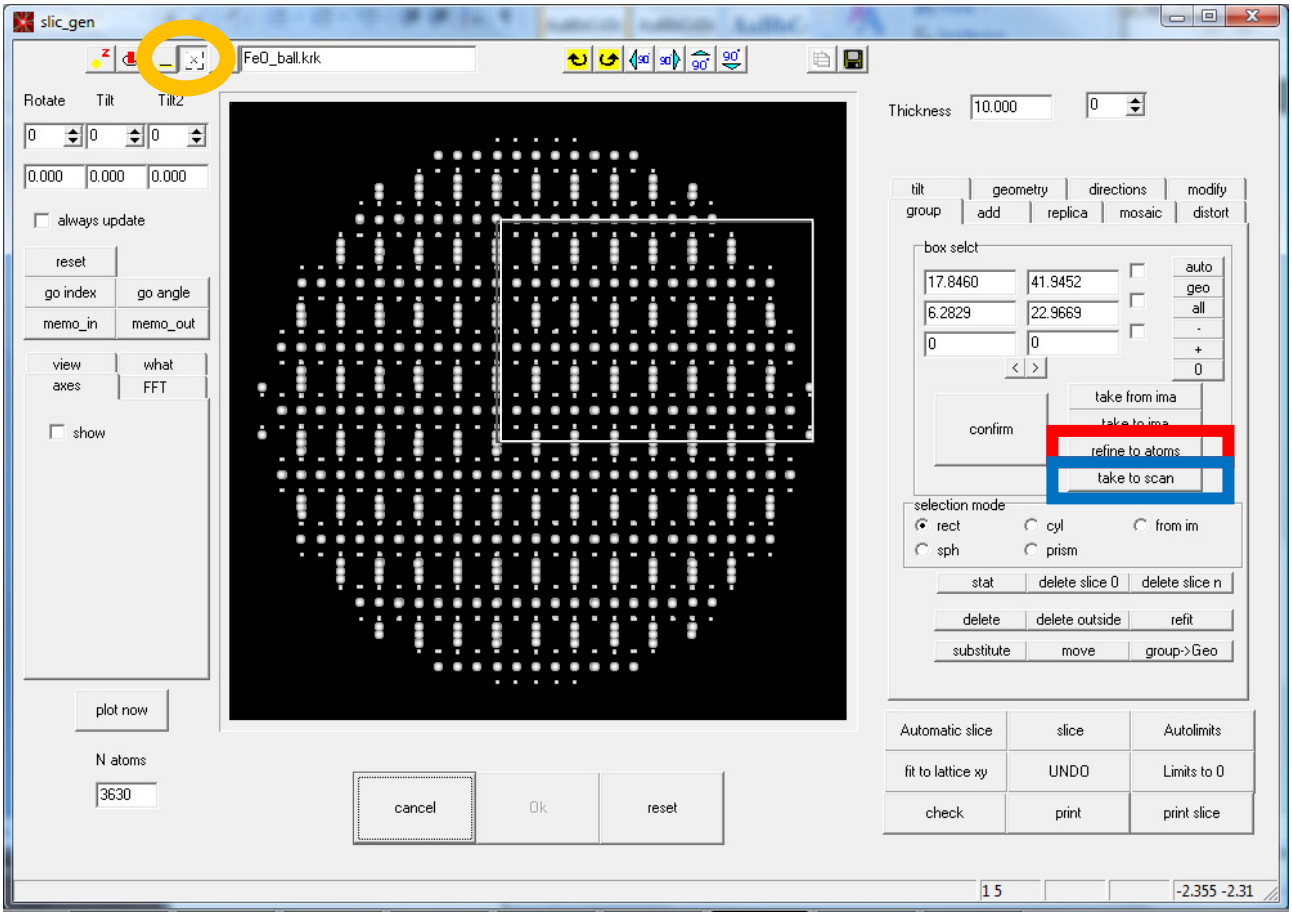
In this example I have used a Fe2O3 ball.

Here a couple of check could be necessary

1) Make sure that the correct slice thickness has been set (in case of doubt set a reasonable slice thickness and try an "automatic slice")
2) Set also the overall sample thickness to t>specimen depth. (if this number is larger than 2t the Sc will be repeated in the depth direction

You can use this window also to select the region to be scanned.

To do this choose the graphical selection tool and select approximatively the region you wqnt to scan. Reember that this tool works ONLY it the visualization angle are all to 0 and only if the geometry is correctly set (if not use *refit* button)



In the group TAB you should see the real position of the selection area.

In some cases it can be convenient to make the selection and the scanning exactly on atomic column.

This can be performed by simply pressing “refine to atoms” this works if the selection edges are already quite close to some atomic columns.

In any case to transfer this selection to the scanning option press *“take to scan”*

HINT: if refit the cell the geometry of the SC will be just the minimal that accomadates all atoms. Usually this is not a choice compliant with periodic conditions at boundaries. If you know what the SC geometry should be you can adjust manually the dimension in the geometry TAB and then confirm it with SLICE. If you want a guess you can give a try to “Fit to lattice xy” that tries to fit the lateral periodicity based on your rough guess.

When done press slice and close.

ERROR MESSAGES:

When pressing *slice* the program performs a few check on the structure.

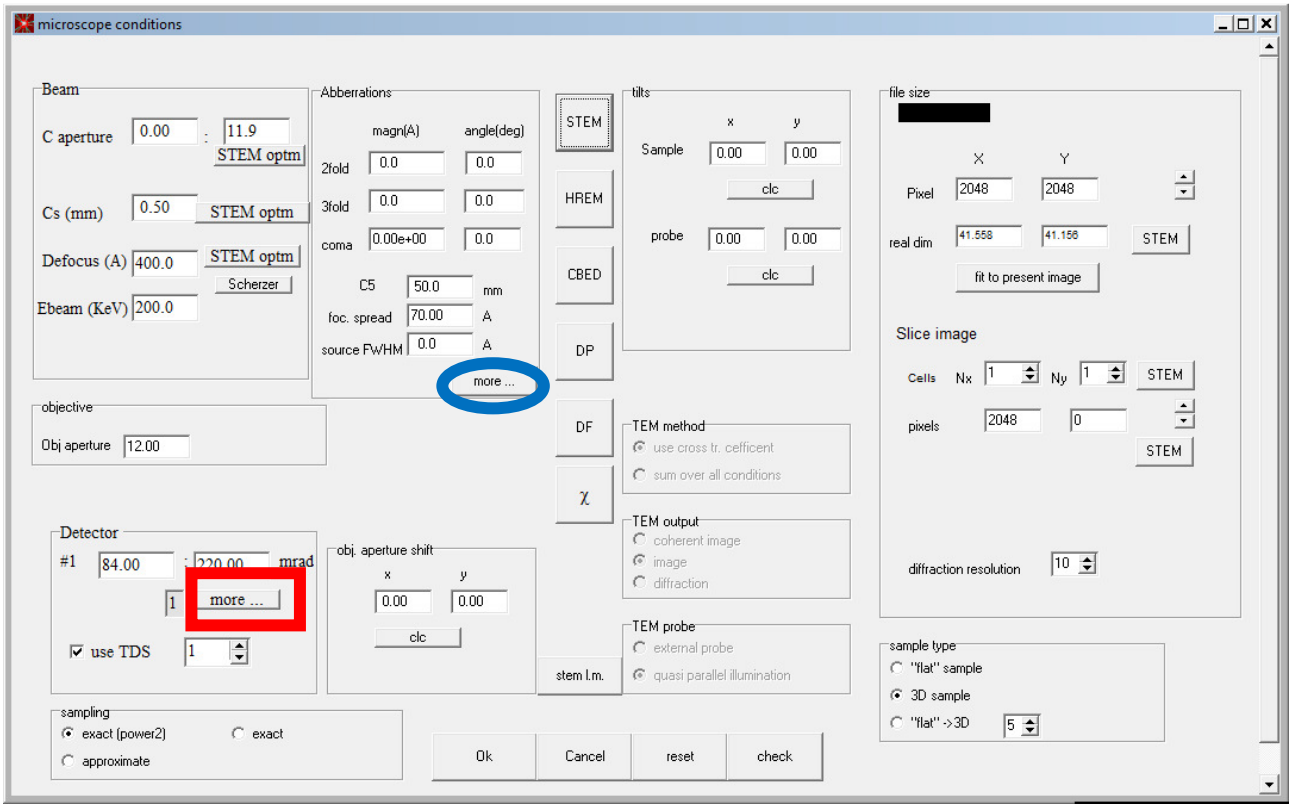
Possible warning are

- If the program warns you that one slice has 0 atoms this is not a crucial problem but it could be advisable to change the slicing setting.
- If the Debye Waller are not set this is notified If you are unsure on the values you can go to the Modify TAB and in the DW area select “use internal”.

Simulation Parameters

It is time now to choose simulation parameters

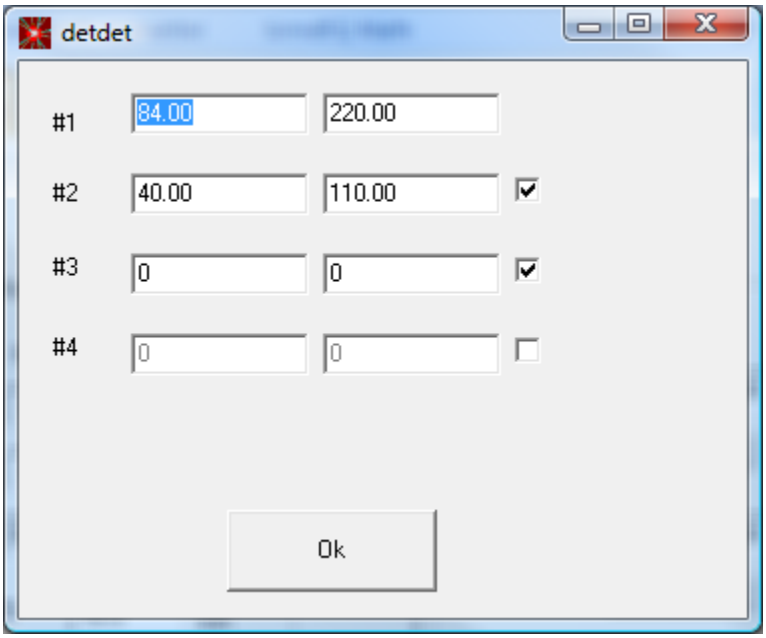
Parameters->Beam det



Select parameters on the left like converegence and aberrations. If you need to choose more aberration use the more button.

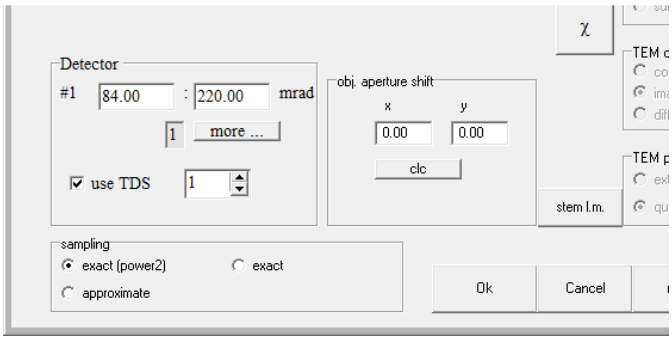
Select also the detector.

In the recent version it is possible to select also to select more (up to 4) detector : make sure that the first is the one with larger outer angle. The first detector setting is directly visible , the other can be chosen by pressing more (here in red).



When all parameters are set press STEM and the sampling parameters will be set.

NOTE presently the number of pixel is forced to a power of 2 but with next version it will e possible to remove this constraint by choosing sampling “exact” instead of “exact (power of 2)”



The number of RUN in TDS should be set to at least 10 for quantitative images but can be reduced for more qualitative analysis.

When ready press OK

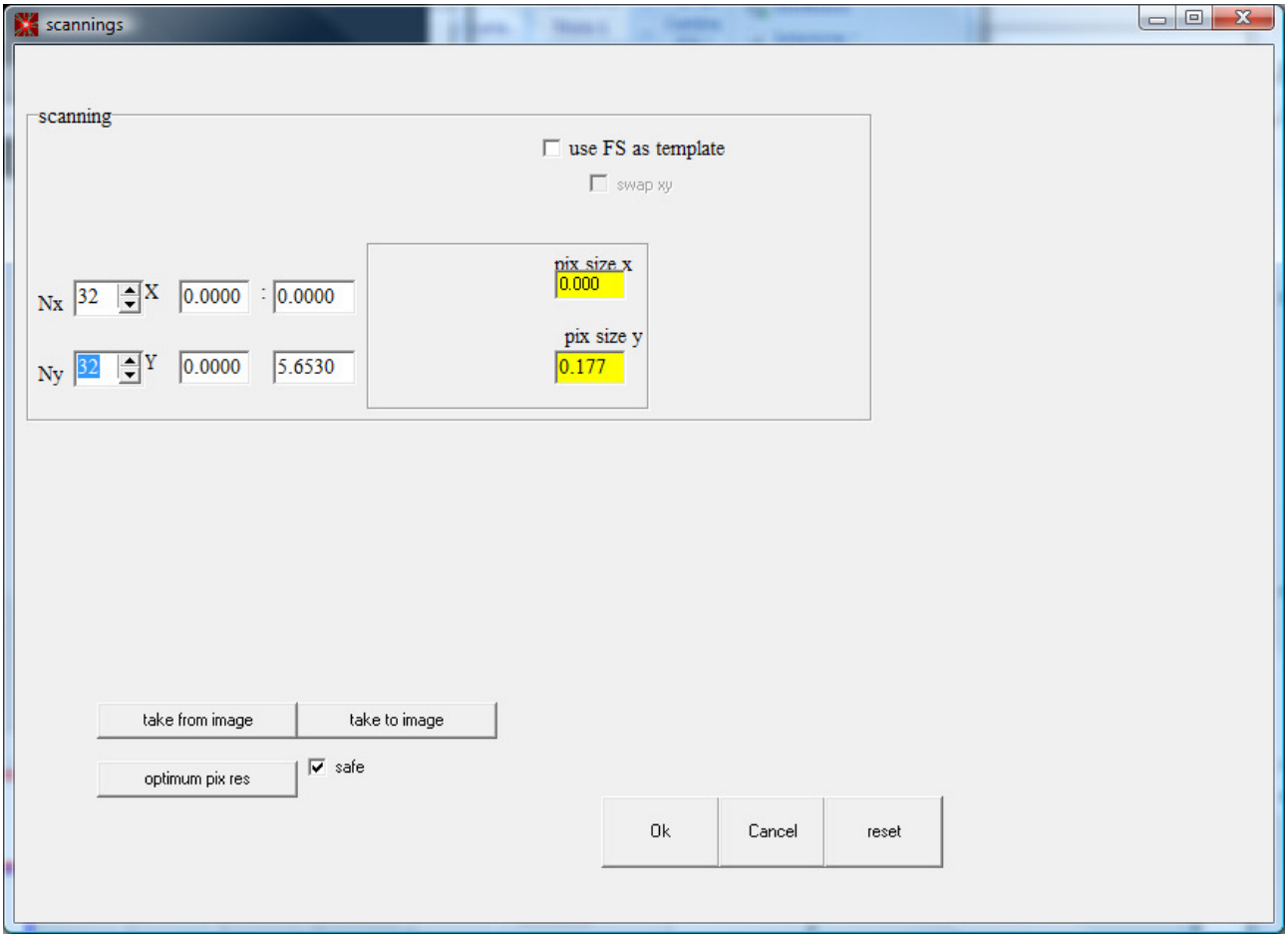
The selection of the outer detection angle is very important in determining the actual sampling For qualitative simulation it can be usefull to limit the outer detection angle(typically <150 mrad) in order to reduce the computation time at the cost of some precision.

SCANNING

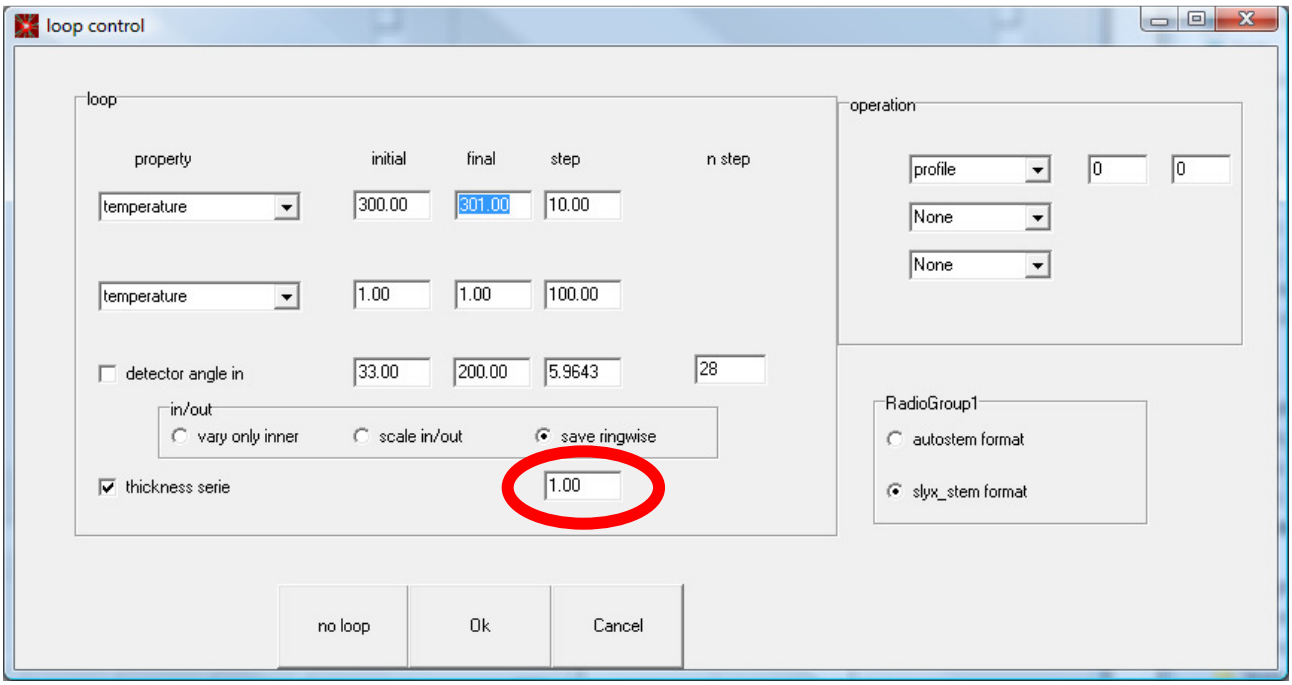
If you have already selected the scanning region previously you can read it here in this screen , conversely if you know where to scan you can select it manually or use the procedure in appendix involving linear image simulation.

When ready you can select the optimal number of pixel in the scan with the command “optimum pix res”. This command adjustes your N of pixels according to the expected resolution and

More option on this will be available in future versions.



LOOP



This windows permits to specify how to plan more simulation for example to obtain a defocus series but in principle any parameter can be scanned. This feature is so far tested only for TEM I' cannot guarantee for STEM.

Meanwhile you can use the thickness series feature to obtain multiple output of your stem images at different thicknesses. 1 means only the final results.

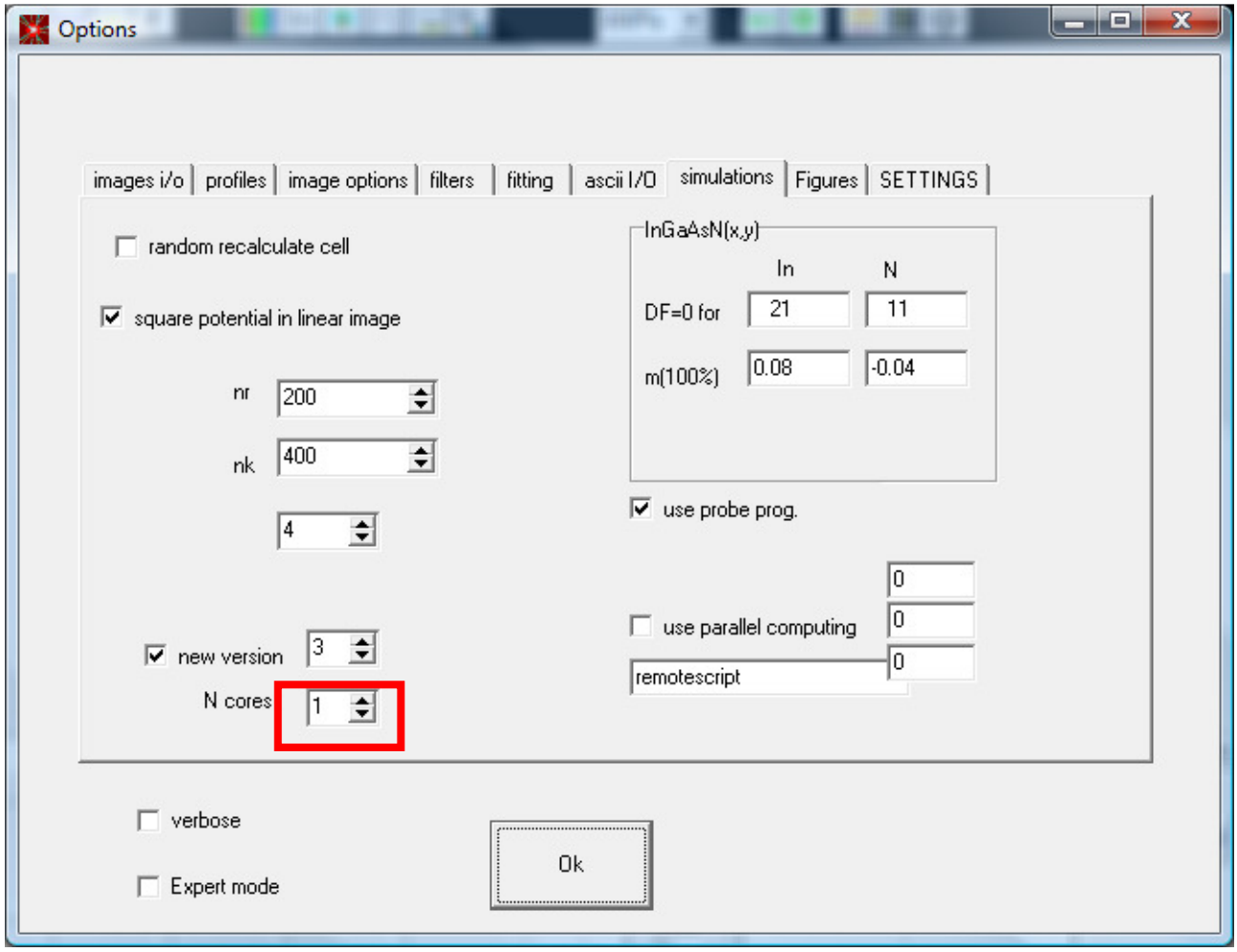
Select the highlighted value to indicate how many intermediate thickness you want to sample in your output. If you have selected multiple detector and multiple thickness the two option are combined and Ndet x Nthick output will be given.

Whereas multiple detector could be also selected from here this functionality is under test for autoslice and will be available in future versions.

Actual RUN

You can optionally decide how many treads are to be sued for your simulation. This should not exceed the number of cores of your PC.

Extra->Option simulation TAB



When ready press

Press SIM_Driver-> STEM->Autostem

The first output will be automatically loaded. If other output are to be read tehse can be opened by File->OenImageT32 selecting the appropriate file. All output are named detectedxxxxxxx.tif

Where xxx are substituted by some number.

Smart postprocessing

It is clever not scan the whole SC if this is just the repetition of a basic unit cell at least I one direction.

So when you select the scanning area choose a single unit cell (use fit to atom to be very precise at border.

Generally the kirkland code adds a border to the image so at best you should first remove it . Here is the procedure :
1) select you unit cell STEM image
2) press Edit->selec_all(no bord)
3) cut using the scissor button
Now you are ready for a replica

"Tool->Transform-> replicate image"

This will replicate the image as many times as necessary.

Accounting for source size effect

The effect of finite source is to blur experimental feature. In order to account for this you can use

Tool->transform-> Gaussian Blur

Selct the appropriate Gaussian parameters. For our JEOL 2200 uncorrected 1A is necessary whiel corrrected Titan may require about 0.5 A. The exact value can be chosen by inspection

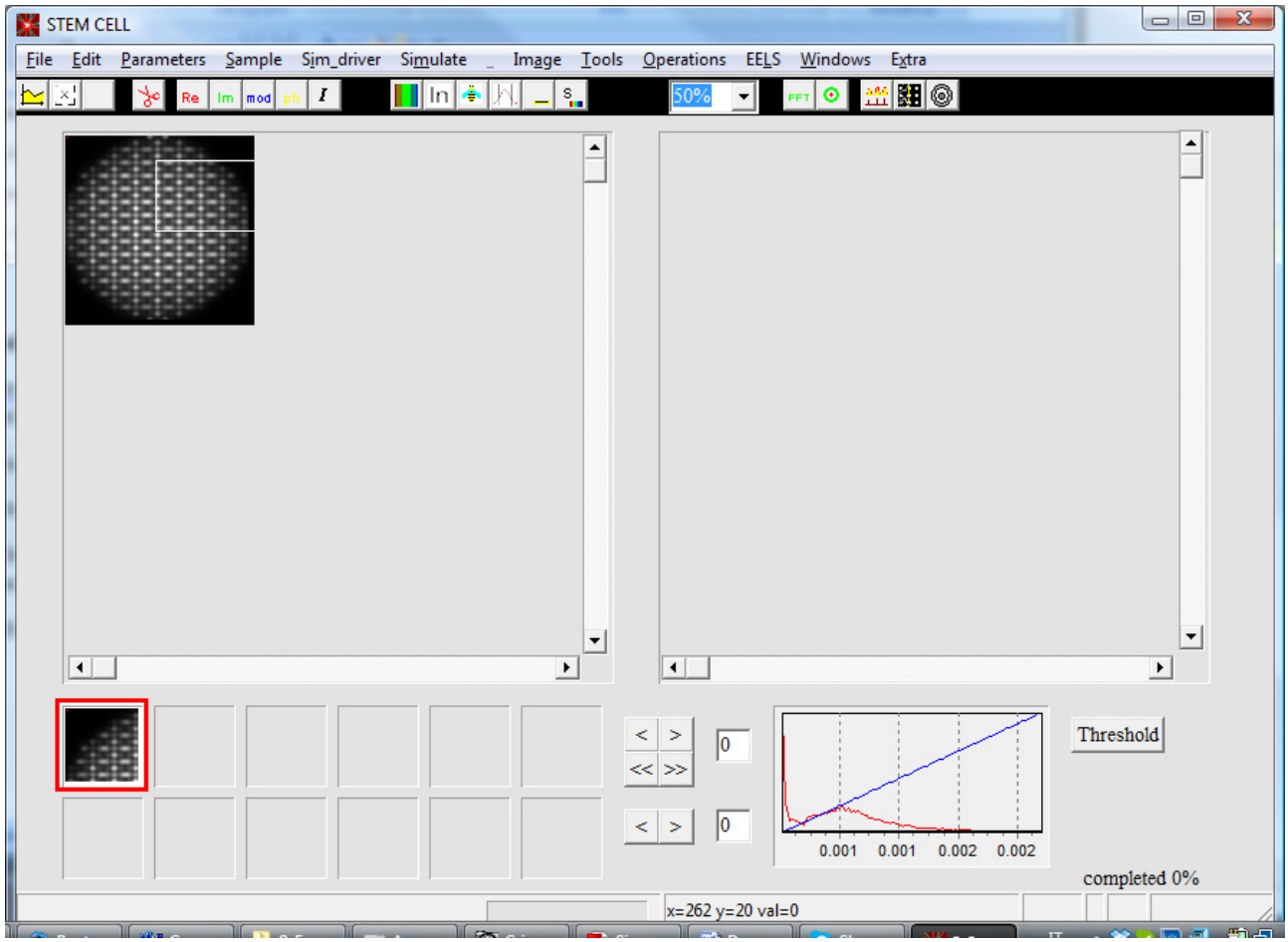
Appendix

An alterative selction of the scanning area can be performed using a linear simulation of the SC.

Make sure tha main parameters have been set and

Use Simulation->Linear Stem-> Linear Image approx

Select by right button drag and drop the rectangle that sets the region to be scanned.



Open the scanning widow now and press “Select form image”