MULTEM image simulation software

Worksheet for EMAT workshop

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1 Introduction

MULTEM is a software for performing transmission electron microscopy image simulations, developed at EMAT [Lobato and Van Dyck, 2015, Lobato et al., 2016]. This worksheet was designed for the computer practical of the EMAT workshop 2017. It explains the features of MULTEM through a series of practical examples. This tutorial will run through the user interface of MULTEM step by step. As we go along, you will run some examples, to experience hands on what the effect of the different parameters is.

1.1 Running the program

For this workshop, the MULTEM software has been put onto the computers already. For your own use after this workshop, the MULTEM software can found at the following link: `https://github.com/Ivanlh20/MULTEM`.

Installation

Login to the computers using the login and password given in the computer room.
Go to the H: drive on your computer.
Copy the folder MULTEM to the desktop. This folder contains all specimen files you will need in this tutorial, and the software.
Open the folder and double click on the executable multem.exe

1.2 Theory

An introduction to the theory of electron microscopy can be found in [De Graef, 2003]. Furthermore, we recommend [Kirkland, 2010], a book specifically about transmission electron microscopy simulations.

2 User interface

The user interface of MULTEM consists of 4 separate screens: General settings, Specimen, Experiment and Microscope settings. Initially, some default settings will be entered. When you walk through these screens, one by one, the information required to set up your image simulation can be changed in an intuitive order. When you hover over a parameter in any of these windows, an information box appears. The same explanation for the parameter is also shown at the lower left bottom of the interface. This can also be seen in figure 1. After running through all separate screens, you can start the simulation with the green start button. The image simulation can be stopped with the red stop button. The result of your simulation will appear in a new window. All the results can be saved as tif images or as binary format file by right clicking on the image. Parameters can be saved by clicking on the save icon at the top left in the MULTEM user interface. You can also load a saved set of parameters.

Furthermore, you can always return to the default values of MULTEM by clicking on the circular arrow.
In this tutorial, we will walk you through some possibilities that MULTEM has to offer for (S)TEM image simulations. You may notice that some options are disabled. These options will become available in future releases of the MULTEM program.
Throughout this tutorial, all exercises will start from the default values.

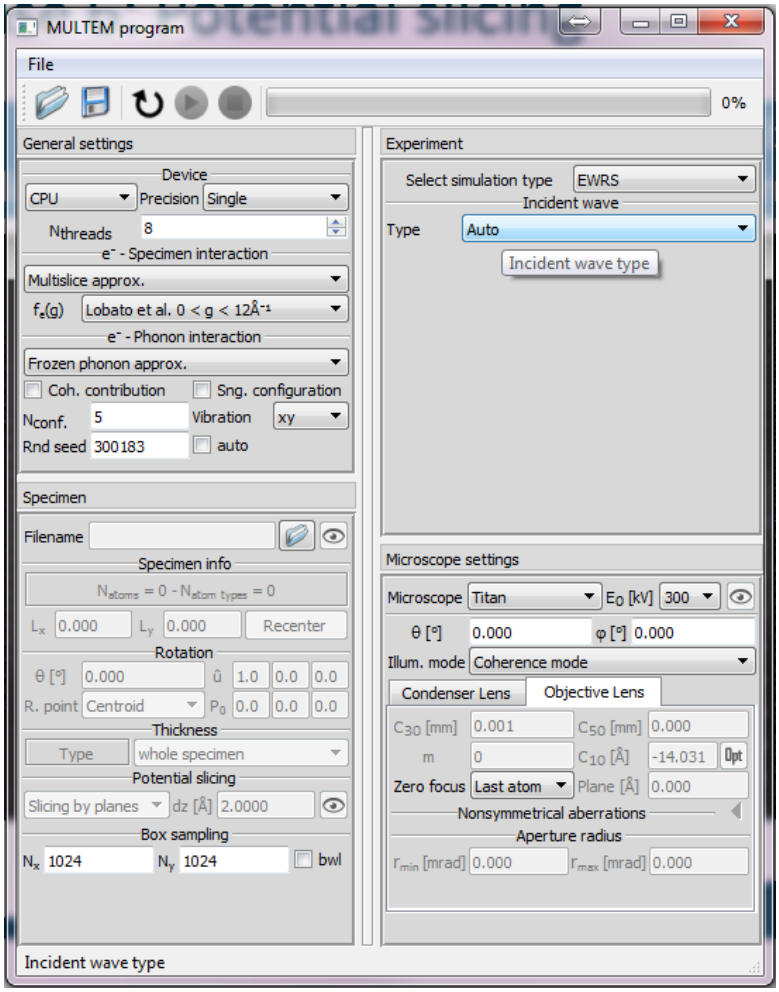

Figure 1: MULTEM user interface, divided into 4 screens: General settings, Specimen, Experiment and Microscope settings. When you hover with your mouse over a parameter, the explanation is shown in a box and at the bottom left, as is shown here for the incident wave type in the Experiment screen.

2.1 General settings

We start out with the general settings. The program automatically detects whether or not your computer has a GPU. If no GPUs are detected, it will automatically choose CPU and detect the correct number of threads. You can choose between single and double precision. Usually, single precision is enough. Note that switching to double precision will increase the simulation time. This effect is usually small for modern 64-bit CPU, but simulation time can double for GPU.
In this screen, we also describe the electron-specimen interaction. You can choose between multislice approximation, phase object approximation and weak phase object approximation. The next drop down menu, allows you to select the parameterisation of the electron scattering factor you want to use.

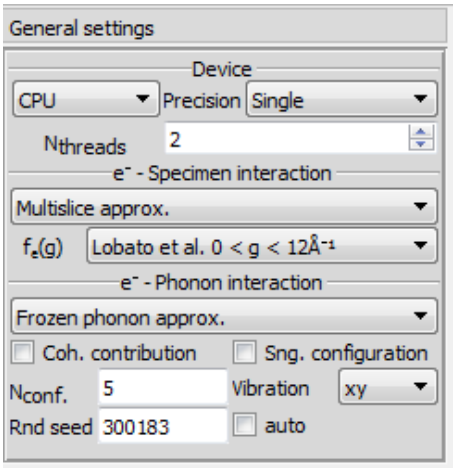

Figure 2: The first screen of the MULTEM user interface allows the user to implement some general settings concerning the computer and the type of image simulation.

Set-up for exercise 1: Electron specimen interaction

↻ Set default values

- Specimen
  - o Load specimen\Cu001_electron_specimen_interaction.txt

Exercise 1: Electron specimen interaction

▶ Run the image simulation for the multislice approximation (default).

Leave the image you obtained open. Change the electron specimen interaction to the weak phase object approximation.

▶ Run the simulation.

Leave the image you obtained open again. Change the electron specimen interaction to the phase object approximation.

▶ Run the simulation. Compare the images. Can you explain the difference between them? Also look at the phase: check the box for Show Coherent wave in the image window, and select Phase instead of Module.

Finally we select the way the electron-phonon interaction is approximated: frozen phonon approximation or still atom approximation. The default will be set to the frozen phonon approximation with 5 configurations.

When you select frozen phonon, you can indicate whether or not you want to calculate the coherent contribution - which for a crystal is the Bragg scattering. Furthermore, you can indicate the number of phonon configurations you want to use in your calculations. If you want to look at the individual configurations, instead of the average of different configurations, you can indicate this by checking the box for Sng. configuration. You can also choose the direction of the vibration, which is set default to xy, which is most commonly used. Be careful to choose vibrations along the z direction, since the slicing scheme will then change for each phonon configuration. Finally, you can enter a number in the box Rnd seed. This offers you the possibility to reproduce the same set of "random" configurations. If you just check the auto box, the software will work fine.

Set-up for exercise 2: Electron phonon interaction

↻ Set default values

- General settings
  - o Change the electron phonon interaction to the still atom approximation
- Specimen
  - o Load specimen\Ag001_electron_phonon_interaction.txt

Exercise 2: Electron phonon interaction

▶ Run the image simulation for the still atom approximation.

Leave the image you obtained open. Change the electron phonon interaction to the frozen phonon approximation. Change the number of configurations to 1.

▶ Run the simulation. Compare the images. Do you understand the difference?

Leave the image you obtained open. Change the number of configurations to 5.

▶ Run the simulation.

Leave the image you obtained open. Change the number of configurations to 20.

▶ Run the simulation. Compare all images obtained with the frozen phonon approximation. Do you understand the improvement?

2.2 Specimen

In this window, you can load a text file containing all information about your specimen. The file should have a specific format. The first row contains information about the simulation box size along x and y direction and the slice thickness. The subsequent rows contain information of each atom of the specimen.

The first column specifies the type of atom (Z number).

The next three columns specify the coordinates of the atom. Note that the x-y coordinates should be positive.

In column 5, you can specify the root mean square displacement, which is related to the Debye-Waller factor (DWF) by the following formula $rms = \sqrt{\frac{DWF}{8\pi^2}}$.

The entry in column 6 specifies the occupancy.

In column 7, you can enter a number which can indicate different regions of the specimen. You can for example use different numbers to indicate atoms in the crystal and atoms in an amorphous region.

Finally, column 8 allows you to indicate the charge of the atom.

The columns should be saved in a text file, such as the example shown in table 1. You can produce the coordinates using other software such as CrystalMaker or construct them manually. When loading a file in MULTEM, you should make sure that the orientation of your specimen is along the z direction. If you want to study the incident wave, and thus omit the specimen, you can do this by selecting the incident wave in real space (IWRS) option in the simulation type item. Note that any specimen you may have already loaded will then be omitted from the user interface.

10	10	2	0	0	0	0	0
79	0	0	0	0.085	1	0	0
79	2.039	2.039	0	0.085	1	0	0
79	4.078	0	0	0.085	1	0	0
79	0	4.078	0	0.085	1	0	0
79	4.078	4.078	0	0.085	1	0	0
79	0	2.039	2.039	0.085	1	0	0
79	2.039	0	2.039	0.085	1	0	0
79	4.078	2.039	2.039	0.085	1	0	0
79	2.039	4.078	2.039	0.085	1	0	0
79	0	0	4.078	0.085	1	0	0
79	2.039	2.039	4.078	0.085	1	0	0
79	4.078	0	4.078	0.085	1	0	0
79	0	4.078	4.078	0.085	1	0	0
79	4.078	4.078	4.078	0.085	1	0	0

Table 1: Example of a text file containing the sample info to load into MULTEM.

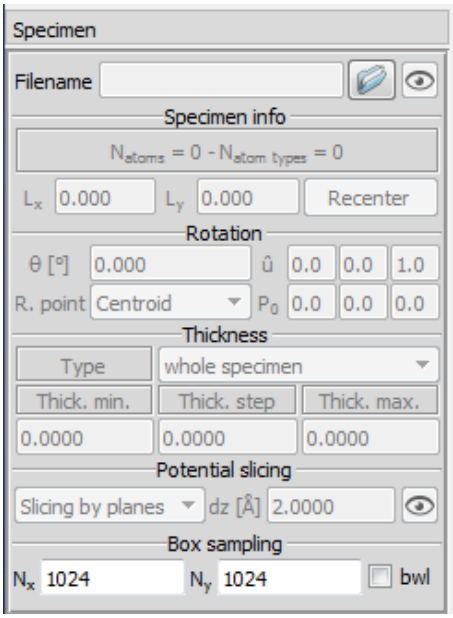

Figure 3: The second screen of the MULTEM user interface allows the user to load all information about the specimen, increase the size of the simulation box, rotate the specimen, and determine the thickness, potential slicing and x-y sampling. The first line contains information about the simulation box size and slice thickness.

After loading the text file, the software will tell you the number of atoms N_{atoms} and the number of atomic types $N_{atomic\ types}$ in the specimen. Furthermore, the size of the simulation box, described by L_x and L_y, is automatically detected. This simulation box size should be such that there is periodicity in the x and y direction. However, if your purpose is to simulate a nanocrystal or nanoparticle, this periodicity is absent. In this case, you should change the size of the simulation box to add a sufficient amount of vacuum, and then push recenter to center your nanocrystal/nanoparticle in the box. This action fulfills the condition of the discrete Fourier transform. Note that the minimally required amount of vacuum increases with the specimen thickness.

Set-up for exercise 3: Adding vacuum

↻ Set default values

Specimen

- o Load specimen\Au001_adding_vacuum.txt
- o Set $L_x = 50\mathring{A}$ and $L_y = 50\mathring{A}$

Exercise 3: Adding vacuum

After loading the specimen, MULTEM indicated that the size of the simulation box is $L_x = 32.6240\mathring{A}$ and $L_y = 32.6240\mathring{A}$. In the set-up, you have added vacuum by increasing the size of the simulation box. In this way you perform a simulation for an isolated nanocrystal.

▶ Run the image simulation. Do you notice anything out of the ordinary? E.g. near the edge of the simulated image?

Leave the image window open. Now push the recenter button.

▶ Run the simulation again and compare your result.

The specimen can also be rotated. MULTEM allows you to describe rotation angle, rotation vector and rotation point. The latter can be chosen as the centroid, or entered manually. This option is especially useful for simulating nanocrystals or nanoparticles that are rotated with respect to the beam direction.

However, you should not use rotation to change the orientation of a periodic crystal. The rotated simulation box will be periodically repeated. This causes the thickness to vary throughout the crystal. The result therefore is not the periodic crystal in a different zone axis orientation. To load a different zone axis orientation, you should load another input file, obtained for example by rotating a supercell in a program such as CrystalMaker, and then cutting this specimen perpendicular to the required zone axis.

Set-up for exercise 4: Rotation

↻ Set default values

- Specimen
  - o Load specimen\Pt001_rotation.txt
  - o Set the rotation angle $\theta = 45°$

Exercise 4: Rotation

▶ Run the image simulation. Is the result what you would have expected?

Leave the image open for comparison. Now add vacuum (set $L_x = 70\mathring{A}$ and $L_y = 70\mathring{A}$ and push the recenter button), in order to create a rotated **nano**crystal.

▶ Run the image simulation. Compare the images.

The next part of this screen is the thickness. When simulating a nanocrystal or nanoparticle, we will simply use whole specimen. However, when simulating a crystal, the periodicity allows you to calculate different thicknesses in one calculation. This can be obtained by choosing by thickness in

the drop down menu. Once you have selected this option, three more boxes will appear. Through these boxes you can determine the minimum thickness, step thickness, and the maximum thickness. MULTEM will automatically round the numbers you enter to the position of the nearest atomic layer. Note that increasing the number of thicknesses you want to obtain as an output from the simulation, will increase the needed memory and will therefore decrease the speed of the simulation.

Set-up for exercise 5: Simulate crystal by thickness

↻ Set default values

- Specimen
  - o Load specimen\Au001_thickness.txt
  - o Select by thickness instead of whole specimen
  - o Set Thick. step equal to 4.078 $\mathring{A}$.

Exercise 5: Simulate crystal by thickness

▶ Run the image simulation. Use the sliding bar at the top of the image window to look at the images for different thicknesses. What effect do you see?

A very important part of this second screen, which will only be activated when you chose the multislice approximation in the first window, is the potential slicing. An interesting feature of MULTEM is that it has an option to determine the slices automatically using the option Slicing by planes. You can also determine the slicing yourself, by changing the drop down menu to slicing by dz or subslicing by dz. In a future release, you will also be able to slice automatically. This will be particularly interesting if you have a simulation box with two different distances between your atomic planes, such as is for example the case in a diamond structures. Also in a future version, MULTEM will offer a visualisation of the chosen slicing when you click on the currently disabled eye shaped icon.

Set-up for exercise 6: Potential slicing

↻ Set default values

- Specimen
  - o Load specimen\Au_nanoparticle_slicing.txt
  - o Add vacuum to the simulation box (set $L_x = L_y = 70\mathring{A}$) and push the recenter button
  - o Choose slicing by dz and leave the slice thickness at 2 $\mathring{A}$

Exercise 6: Potential slicing

▶ Run the image simulation.

Leave the image open for comparison. Now change to a slice thickness of 20 $\mathring{A}$.
▶ Run the simulation. Can you explain the difference?

Change the potential slicing to slicing by planes.
▶ Run the simulation. What happens for this nanoparticle?

The last part of this specimen screen is the box sampling. MULTEM will round the number of sampling points you enter for N_x and N_y to the nearest number that is computationally efficient. Checking the bwl box will limit the bandwith of the matrices involved in the multislice calculation. This means that high frequencies are cut off in Fourier space, such that they are not overlapping with themselves when they are periodically repeated. This avoids aliasing.
Furthermore, note that the number of sample points should be increased if the size of the simulation box is increased. A rule of thumb is to keep $L_j/N_j \approx 0.05\mathring{A}$ for j=x,y, in order to correctly sample the potential.

Set-up for exercise 7: Sampling

↻ Set default values

- Specimen
  - Load specimen\GaAs001_sampling.txt
  - Change the sampling to N_x=128 and N_y=128

Exercise 7: Sampling

▶ Run the simulation and zoom in on an atomic column by scrolling with your mouse while hovering over the image.

Leave the image open. Change the sampling back to 1024.
▶ Run the simulation and zoom in.

2.3 Experiment

In the experiment screen, the type of TEM experiment is selected and described. Possible simulation types currently provided in MULTEM are the following:

- Scanning transmission electron microscopy (STEM)
- Imaging scanning transmission electron microscopy (ISTEM)
- Convergent beam electron diffraction (CBED)
- Convergent beam electron imaging (CBEI)
- Electron diffraction (ED)
- High resolution transmission electron microscopy (HRTEM)
- Precession electron diffraction (PED)
- Hollow cone TEM (HCTEM)
- Exit wave in Fourier space (EWFS)
- Exit wave in real space (EWRS)
- STEM electron energy loss spectroscopy (STEM_EELS)
- Energy filtered TEM (EFTEM)
- Incident wave in real space (IWRS)

- Projected potential in real space (PPRS)
- Transmission function in real space (TFRS)

Whichever of these simulation types you choose, there is always an Auto option, which represents the most commonly used incident wave.

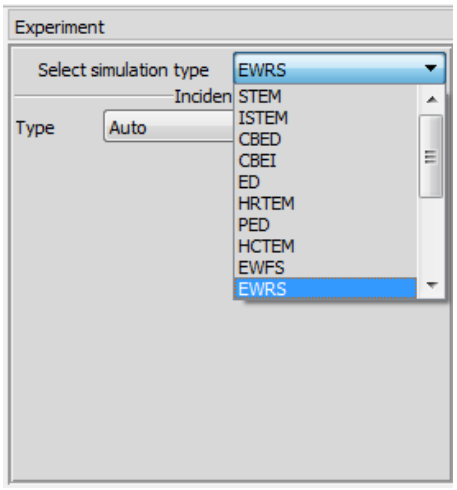

Figure 4: The third screen of the MULTEM user interface allows the user to select the type of TEM experiment, and provide details about the experiment set-up.

We will discuss the features of HRTEM, ED, STEM and EFTEM. The other simulation types fall outside the scope of this tutorial.

The HRTEM option is fairly straightforward. You can select the incident wave, with choices between auto, plane wave or user define. The latter will require you to load a binary file with a complex matrix describing the incident wave.

Set-up for exercise 8: High resolution transmission electron microscopy

↻ Set default values

- Specimen
  - Load specimen\Si001_HRTEM.txt
  - Select by thickness instead of whole specimen
  - Set Thick. step equal to 5.4307 $\mathring{A}$.
- Experiment
  - Select HRTEM

Exercise 8: High resolution transmission electron microscopy

▶ Run the image simulation. Scroll through the images for different thicknesses.

Also the ED option is fairly straightforward. You can select the incident wave, with choices between auto, plane wave or user define. The latter will require you to load a binary file with a complex matrix describing the incident wave.

Set-up for exercise 9: Electron diffraction

↻ Set default values

- Specimen
  - o Load specimen\Si001_ED.txt
  - o Select by thickness instead of whole specimen
  - o Set Thick. step equal to 5.4307 $\AA$.
- Experiment
  - o Select ED

Exercise 9: Electron diffraction

▶ Run the image simulation. Scroll through the images for different thicknesses.

When using the STEM option, not only the incident wave can be given as input, but some input about the scanning pattern and the detectors is required as well. You can choose between a line scan or an area scan. An input field allows you to define the number of scan points N_{scans}. The drop down menu selects the scanning direction: max, L_x or L_y, where the first option will select the largest out of L_x and L_y. Next to this drop down menu, you see a check box for pbc. Checking this means you want to exclude the last scan point from your simulation box. This option is particularly interesting in case of a periodic crystal, since in that case the last point is the same as the first point of the simulation box. To fully describe the scanning pattern, you need to indicate the starting and ending point of the scan. This can be done by entering the x and y positions in $\AA$. In a future version of MULTEM you will be able to select this area on a figure by clicking on the button next to the input fields, which is currently still disabled.
MULTEM allows you to simulate using one or multiple detectors. You can enter the inner and outer angle (in mrad) for each detector by changing the number of the detector N_{det} using the drop down menu. Furthermore you can choose whether your detector is ideal or if you want to upload a matrix with your custom detector. MULTEM provides a visualisation of your detector(s).
Note that you need to input a large crystal, and then afterwards select a small area to scan. Starting with such a large crystal is necessary for three reasons: to avoid self-interaction of the probe, to ensure periodicity since different phonon configurations break periodicity over small areas, and to self contain the probe which broadens with the thickness when traveling through the specimen. In the resulting image, you can replicate the simulated scanned area, since it is periodic. You replicate by changing the numbers Rep. x and Rep. y at the lower left bottom of the image window which opens after you finished your simulation.

Set-up for exercise 10: Scanning transmission electron microscopy

↻ Set default values

- Specimen
  - o Load specimen\SrTiO3001_STEM.txt
  - o Change the sampling to N_x=512 and N_y=512
- Experiment
  - o Select STEM

- Set the number of scan points N_{scans}=5
- Define the area to scan: $X_0 = 11.7150\mathring{A}$, $X_e = 15.6200\mathring{A}$, $Y_0 = 11.7150\mathring{A}$, and $Y_e = 15.6200\mathring{A}$.

Exercise 10: Scanning transmission electron microscopy

Run the image simulation.

Replicate the image by changing Rep. x and Rep. y at the lower left bottom of the image window to 3. Center the image by double clicking on it.
Leave the image open. Now change the number of scan points to 20.
Run the simulation. Replicate the image by changing Rep. x and Rep. y at the lower left bottom of the image window to 3. Center the image by double clicking on it. What difference do you see?

Add a second detector with inner angle 0 mrad and outer angle 20 mrad. Set the number of scan points N_{scans}=10.
Run the simulation. Look at the images obtained by both detectors. Scroll through the images for different detectors using the sliding bar at the top of the image window.

The EFTEM option requires the type of incident wave, and some information about the Energy Loss. You can select the element you are interested in, using a drop down menu, as well as the energy for that element. You can indicate the angle in mrad that determines the size of the objective aperture, the mixed dynamic object spectrum (MDOS) selection rule and the approximation: single channelling, mixed channelling or double channelling.

Set-up for exercise 11: Energy filtered transmission electron microscopy

Set default values

- Specimen
  - Load specimen\SrTiO3001_EFTEM.txt
  - Change the sampling to N_x=512 and N_y=512
- Experiment
  - Select EFTEM
  - Select Element to Sr
  - Change Energy edge to 1940
  - Select double channelling approximation.

Exercise 11: Energy filtered transmission electron microscopy

Run the image simulation.

Leave the image open. Now change Element and Energy edge to O and 532, respectively.
Run the simulation. What difference do you see?

2.4 Microscope settings

In this final screen of the MULTEM user interface, you can set up the microscope parameters. You can choose the acceleration voltage. Note that in the forward scattering approximation, image simulations for low acceleration voltages are less accurate.

Set-up for exercise 12: Acceleration voltage

↻ Set default values

- Experiment
  - o Select IWRS
- Microscope settings
  - o Set $E_0 = 80$ kV

Exercise 12: Acceleration voltage

▶ Run the simulation for $E_0 = 80$ kV.

Leave the image open. Change the acceleration voltage to 300 kV.
▶ Run the simulation and compare.

Furthermore, you can indicate the orientation of the incident beam using spherical coordinates θ and φ. You can also choose you illumination mode: coherence mode, partial coherence mode, or incoherent numerical integration. The default setting of the illumination mode changes depending on the selected simulation type.

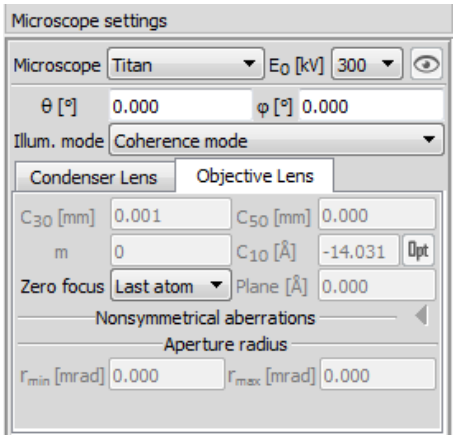

Figure 5: The last screen of the MULTEM user interface allows to describe the settings of the microscope, such as acceleration voltage, orientation of the incident beam, illumination mode, and different types of aberrations for the objective and/or condenser lens.

Next, you enter information about the condenser lens and/or the objective lens. Depending on the selected simulation type (STEM, HRTEM, ...), some parameters will be blanked.
In HRTEM, the relevant lens for imaging is the objective lens. You can indicate the third order spherical aberration C_{30}, fifth order spherical aberration C_{50}, vortex momentum m, and the defocus C_{10}. For the defocus, a button opt exists to put the defocus equal to the optimal Scherzer defocus.
You can choose the reference for the defocus. Possible options are putting the zero defocus at the first atom, at half thickness, at the last atom or at a user defined plane, to be entered in the box next to

the drop down menu for zero focus. Furthermore, you can enter a value for the defocus spread, if you have chosen for the partially coherence mode or the incoherent numerical integration.
In STEM, the relevant lens for imaging is the condenser lens. For this lens as well, you can now enter the symmetric aberrations mentioned before for the objective lens in HRTEM. Concerning the reference point for the defocus value, we now have less options, since this lens sits above (before) the specimen. We can therefore choose to focus at the first atom or at a user defined plane.

Set-up for exercise 13: Defocus

↻ Set default values

- Specimen
  - Load specimen\Au_nanoparticle_defocus.txt
  - Change the potential slicing to slicing by dz and leave the slice thickness at 2 $\mathring{A}$

Exercise 13: Defocus

▶ Run the image simulation for zero focus at the last atom (default).

Leave the image open. Change to zero defocus at the first atom in the objective lens tab.
▶ Run the image simulation.

Leave the image open. Change to zero defocus in the middle of the specimen.
▶ Run the image simulation. Compare the images to see the effect of defocus.

Set-up for exercise 14: Spherical aberration

↻ Set default values

- Experiment
  - Select IWRS
- Microscope settings
  - C_{30} = 0.010 mm
  - Optimise the defocus by pushing the Opt button (Scherzer defocus)

Exercise 14: Spherical aberration

▶ Run the image simulation.

Leave the image open. Change the spherical aberration to C_{30} = 0.1 mm.
▶ Run the simulation and compare the images to see the effect of the amount of spherical aberration.

Now optimise the defocus and compare the wave again.
▶ Run the simulation.

Set-up for exercise 15: Two-fold astigmatism

↻ Set default values

- Experiment
  - o Select IWRS
- Microscope settings
  - o Unfold the nonsymmetrical aberrations of the condenser lens and set $C_{12} = 20\mathring{A}$

Exercise 15: Two-fold astigmatism

▶ Run the image simulations. What is the effect on the probe?

Leave the image open. Change the azimuthal angle of two-fold astigmatism to $\phi_{12} = 45°$.
▶ Run the simulation and compare the images.

Set-up for exercise 16: Vortex beam

↻ Set default values

- Experiment
  - o Select IWRS
- Microscope settings
  - o Set the vortex momentum equal to $m = 1$

Exercise 16: Vortex beam

▶ Run the image simulation. What is the effect on the probe?

Leave the image open. Set $m = 2$.
▶ Run the simulation. What is the difference?
Leave the image open. Set $m = 0$.
▶ Run the simulation. What is the difference? Compare all images by looking at Module as well as at the Phase.

Finally, there is the possibility to add an aperture before the lens to limit the incoming beam. The inner and outer radius can be entered in milliradians. Increasing the size of this aperture allows higher angles to be used, and should result in a more focussed probe. However, experimentally the electrons scattered over high angles carry high order aberrations which cause a distortion of the probe.

Set-up for exercise 17: Aperture outer radius

↻ Set default values

- Experiment
  - Select IWRS

Exercise 17: Aperture outer radius

▶ Run the image simulation.

Leave the image open. Change the aperture outer angle from 21 mrad to 7 mrad.
▶ Run the image simulation.

Leave the image open. Change the aperture outer angle to 50 mrad.
▶ Run the image simulation. Which aperture outer radius results in the best probe?

Change the aberrations. Set for example $C_{30} = 0.01$ mm and $C_{12} = 20\mathring{A}$.
▶ Run the simulation again for the different aperture outer angles (7 mrad, 21 mrad, 50 mrad) and compare the images. Which aperture outer radius is now optimal?

Set-up for exercise 18: Aperture inner radius

↻ Set default values

- Experiment
  - Select IWRS
- Microscope settings
  - Set the inner aperture radius equal to 10 mrad

Exercise 18: Aperture inner radius

▶ Run the image simulation. You have now created a Bessel beam. Look at the phase.

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