QSTEM online user Manual

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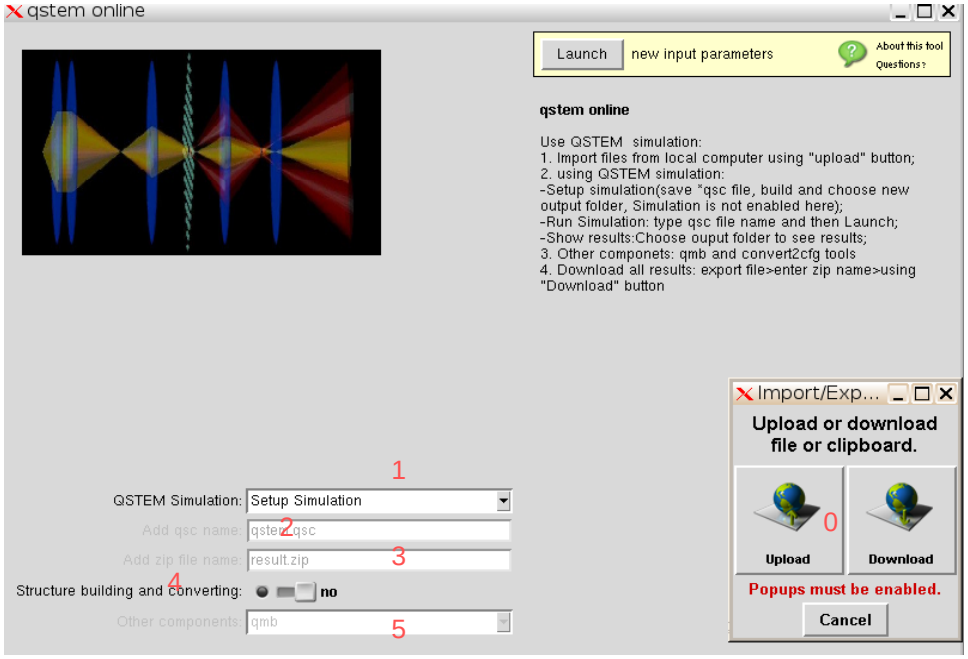
QSTEM Graphical interface Components

Network for Computational Nanotechnology (NCN)

0. Loader: upload/download file from/to local computer;
1. QSTEM simulation, including: Setup simulation, Run simulation, Show results, focal series reconstruction, export results;
2. Enter qsc configuration file name you saved when setting up simulation;
3. Enter zip file name you want to save as;
4. Choose to use Structure building and converting tools;
5. Other components, including: qmb model builder and convert2cfg;



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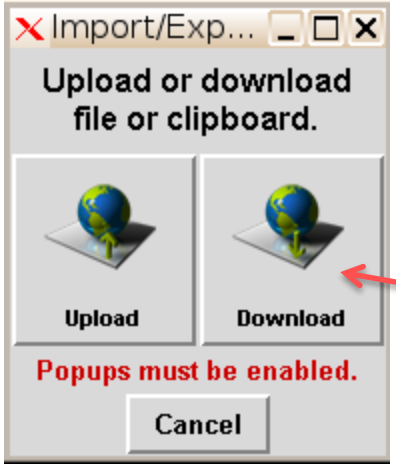
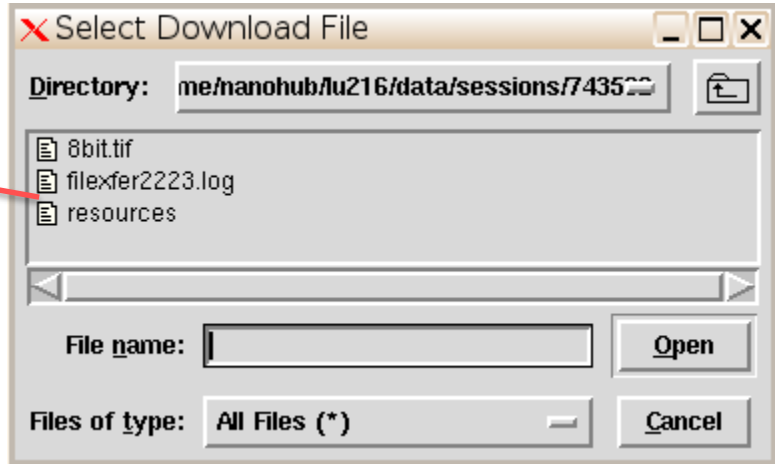
Loader: upload/download

Upload: upload files from local computer

Download: Download files to local computer





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Setup simulation

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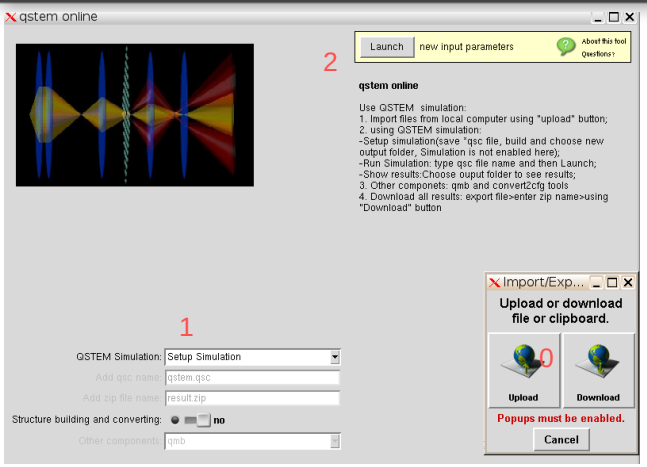
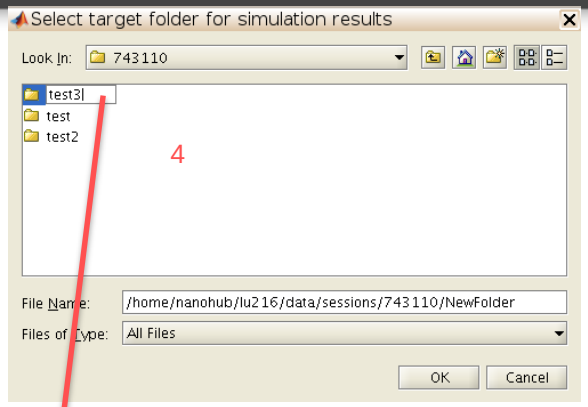
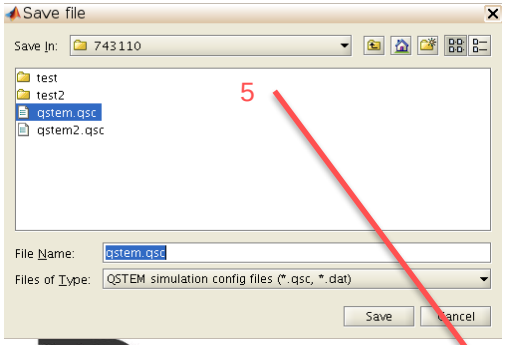
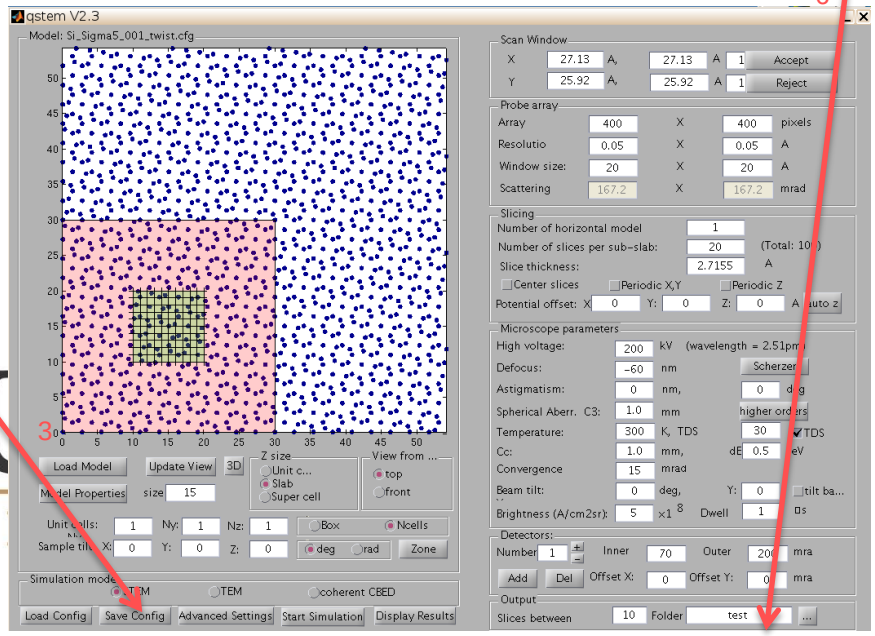


Steps for setting up simulation:

0. upload cfg file from local computer;
1. Choose setup simulation;
2. Press Launch;
3. Load cfg model





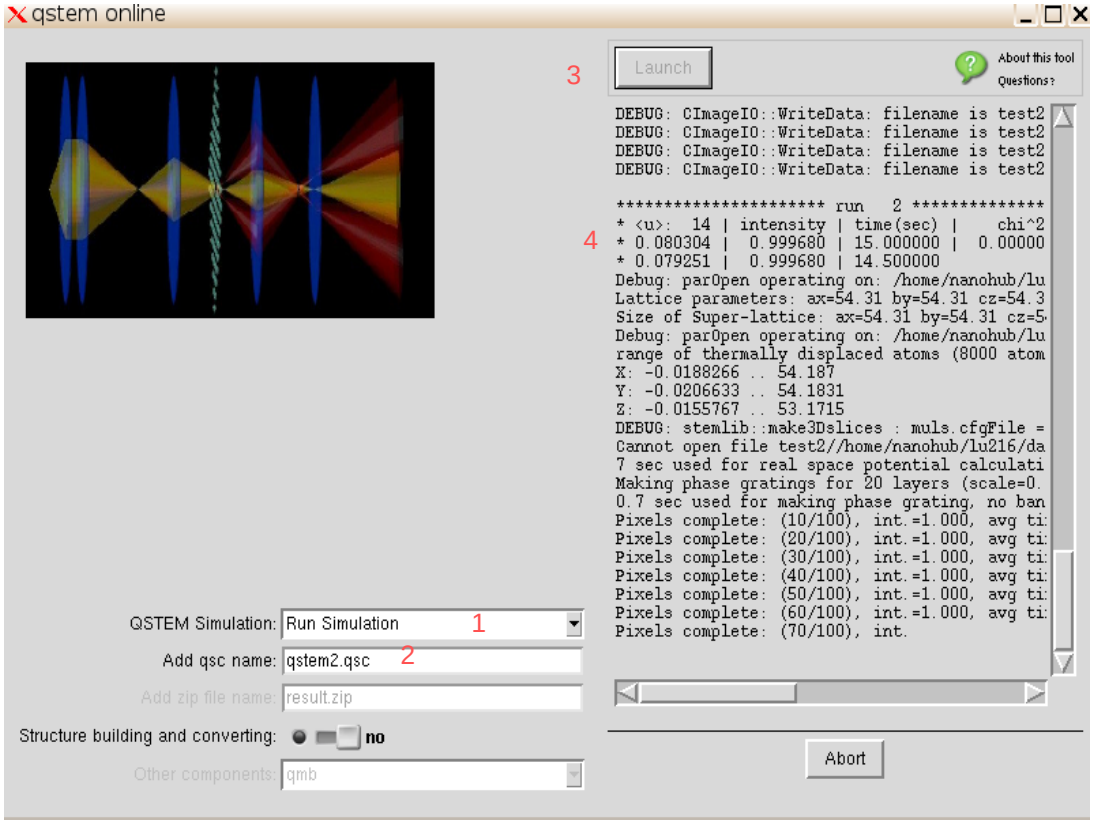


4.Create and select a new folder for results for each simulation;
5. Save a new qsc file for each simulation;
6. Close this page(simulation is not enabled through this page).

*** Start simulation/Display results buttons will not work in the QSTEM online. Will be fixed soon***

Network for Computational Nanotechnology (NCN)

1. Choose Run simulation;
2. Enter qsc config file name you saved when setting up simulation;
3. Press Launch;
4. Simulation Processing;



Show Results & Focal Series Reconstruction

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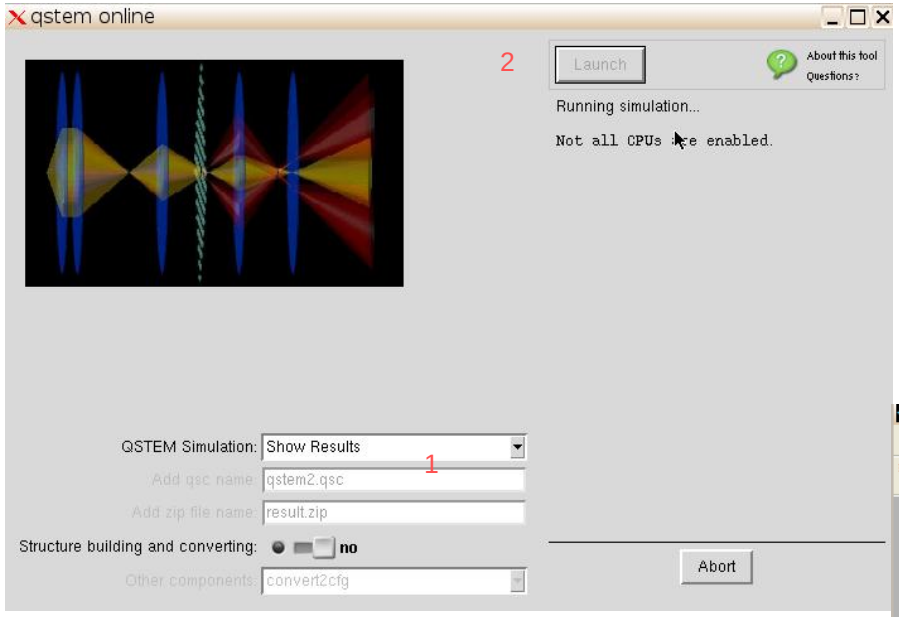
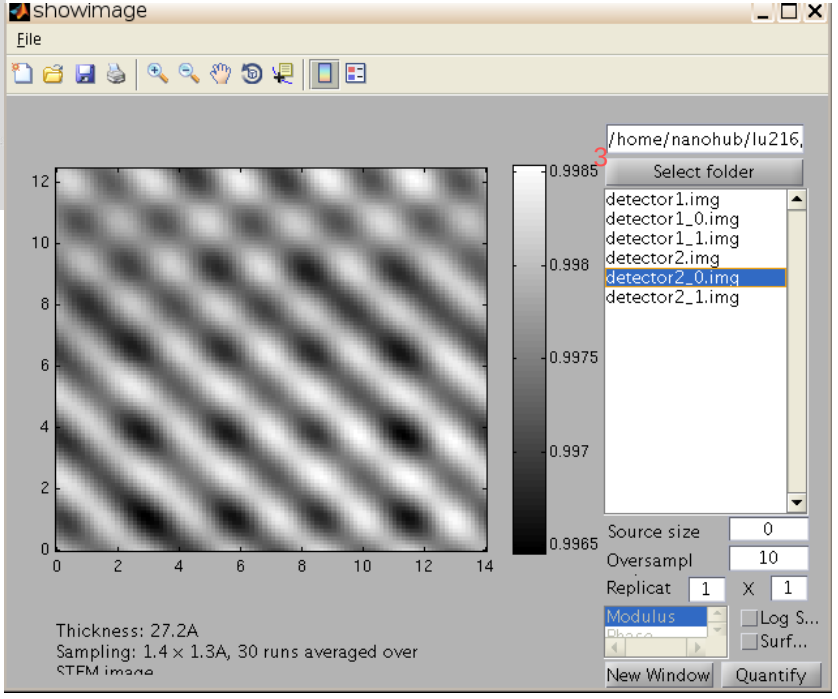


Steps for showing results(similar procedure for focal series reconstruction):

1. Choose Show results;
2. Press Launch;
3. Select folder and img file.



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Export Results

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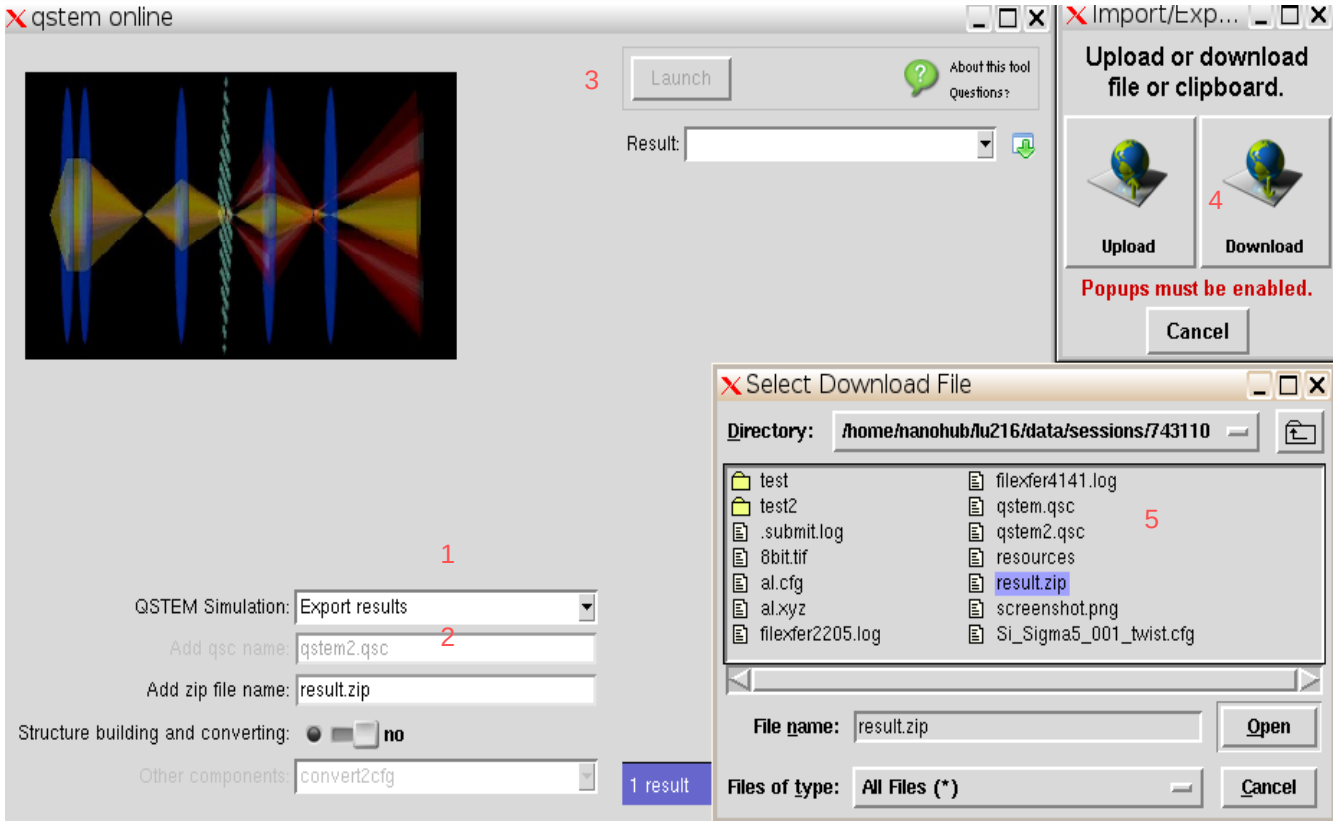
Steps for exporting results:

1. Choose Export results;
2. Enter zip file name you want to save as;
3. Press launch;
4. Press “Download” ;
5. Find the zip file you saved and export to local. (zip file contains all the files including cfg file, folders, img files and other config files)



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Structure Building and converting

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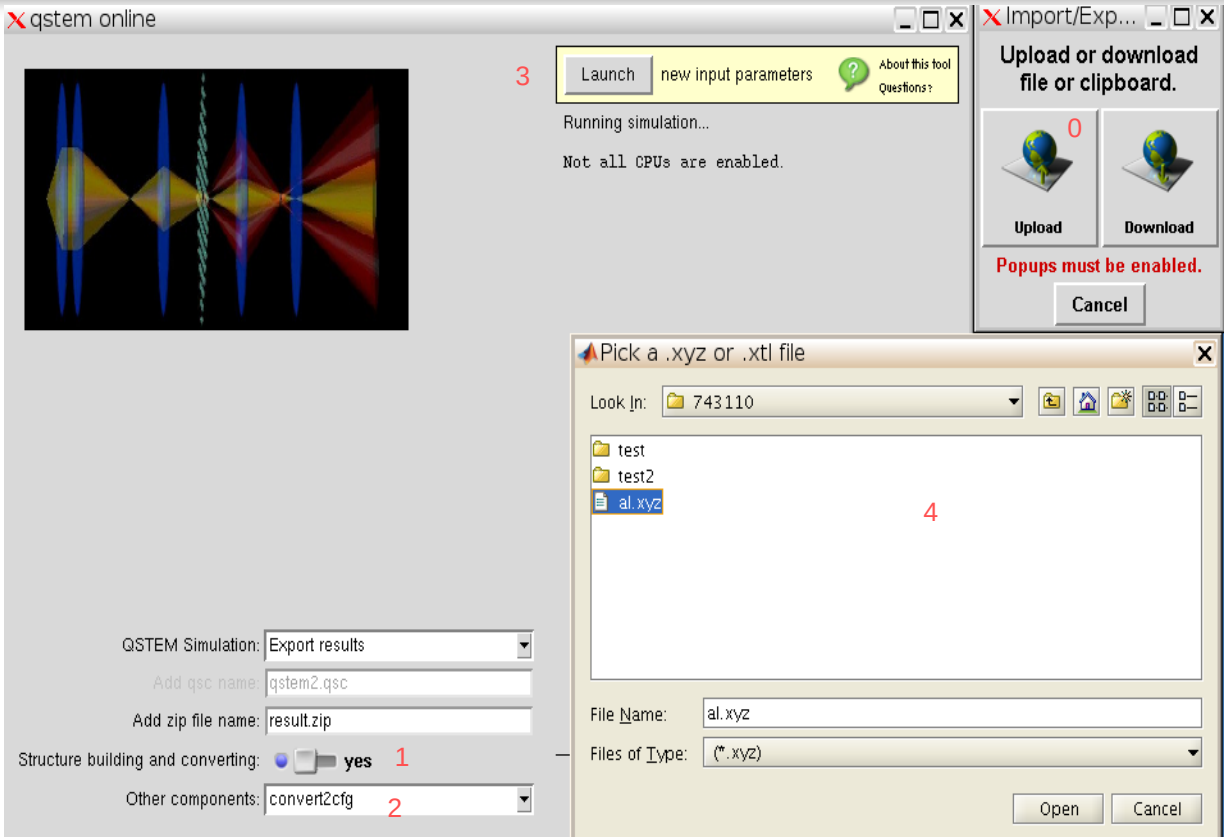
Steps for using file converting:
0. Upload xyz or xtl file using loader
1. Choose “yes” for “Structure building and converting”;
2. Choose “convert2cfg”
3. Press Launch;
4. Choose file you want to convert.



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QMB model builder is not fully functional in this version! We are trying to make it functional in later version.

Reference

- More resources:

QSTEM software introduction: http://qstem.org/

QSTEM group mailing list: https://groups.google.com/forum/#!forum/qstem

QSTEM software at Ulm University: http://elim.physik.uni-ulm.de/?page_id=834

QSTEM source code is hosted on github.com.

- Reference

Christoph Koch, “Determination of Core Structure Periodicity and Density Along Dislocations,” PhD dissertation, Arizona State University (2002)