Using the *DEBUSSY v2.0beta* with the Graphical User Interface: a quick guide

Contents

Introduction

The *DebUsSy Suite* is an open source software package implementing the Debye scattering equation (DSE) for the analysis of powder diffraction pattern from nanocrystalline, defective and/or non-periodic materials.
The *DebUsSy Suite* strategy is of bottom-up type and consists of two main steps, managed respectively by the *CLAUDE* Suite (generating populations of NCs) and the Debussy program (implementing the calculation of DSE and the model parameters optimization against the experimental data).
This quick guide provides a general overview of the multiple tasks that can be performed using the *DebUsSy Suite*, release v2.0 (both *CLAUDE* and Debussy programs), through the Graphical User Interface (*GUI*). The users can directly perform some of these tasks. A **tutorial** is available at **http://debussy.sourceforge.net/debussy/tutorial.html**, including input files, experimental data and detailed instructions.

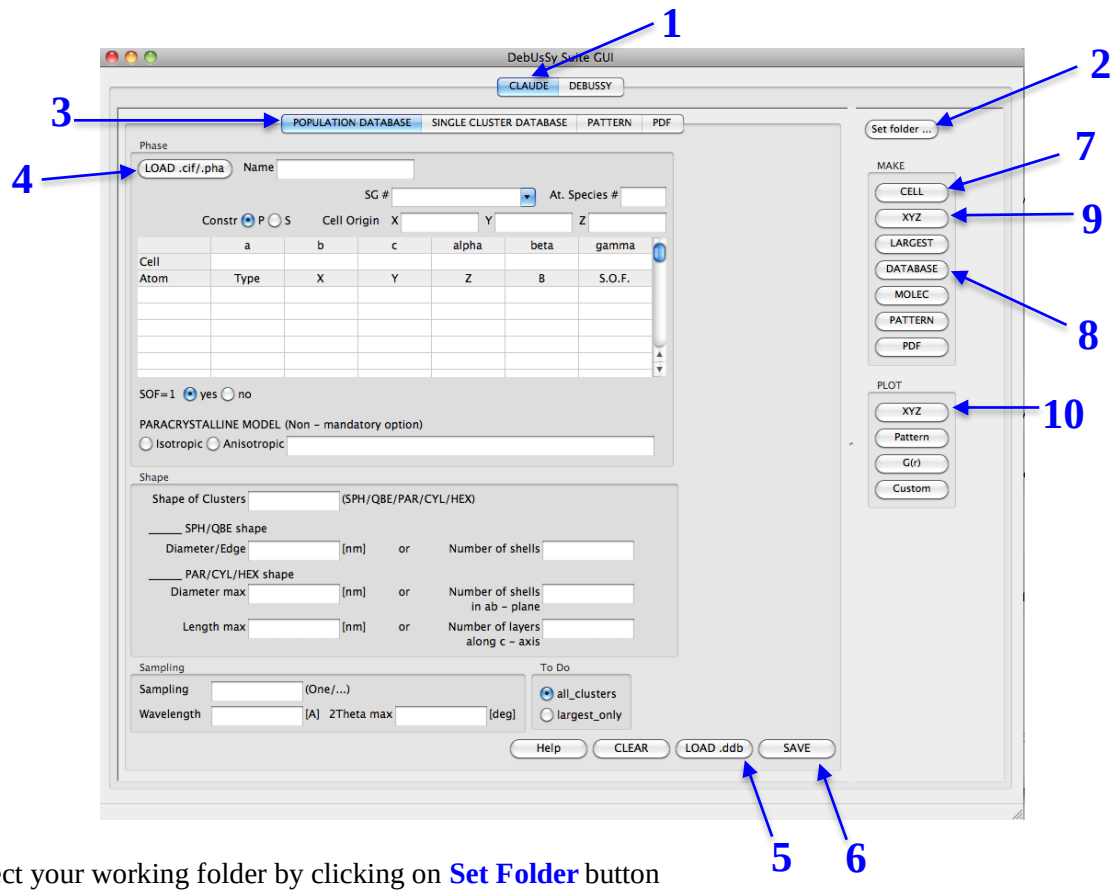
Quick guide for the *CLAUDE_GUI*

The *CLAUDE_GUI* can perform several tasks, which are shortly introduced here, in the following order:

- Building the sampled interatomic distances of a population of NCs.
- Building the sampled interatomic distances for a single cluster.
- Building the sampled interatomic distances starting from a user-defined *.xyz* file.
- Computing a powder pattern from a single cluster (*.smp* file).
- Computing the Pair Distribution Function from a powder diffraction pattern.

All the *CLAUDE_GUI* tasks require selecting the *CLAUDE* tab of the *GUI* (**1**).
All the operations described in each section must be performed in the order indicated by the numbered lists.

Building the sampled interatomic distances of a population of NCs



2) Select your working folder by clicking on **Set Folder** button

3) Select the **POPULATION DATABASE** tab.

4) Upload your *.cif/.pha* file by clicking on **LOAD .cif/.pha** button and select the right file. The *.cif* file is automatically converted in the *.pha* file that is displayed in the *GUI* window. Edit this *.pha* file for re-organizing the number/type of atomic species, according to the specificity of your structure, if necessary. Otherwise all the atoms with the same atomic symbol will be grouped in a single atomic species.

5) Fill the **POPULATION DATABASE** tab or load an already existent *.ddb* file using **LOAD .ddb** button.

6) **SAVE** the *.ddb* file.

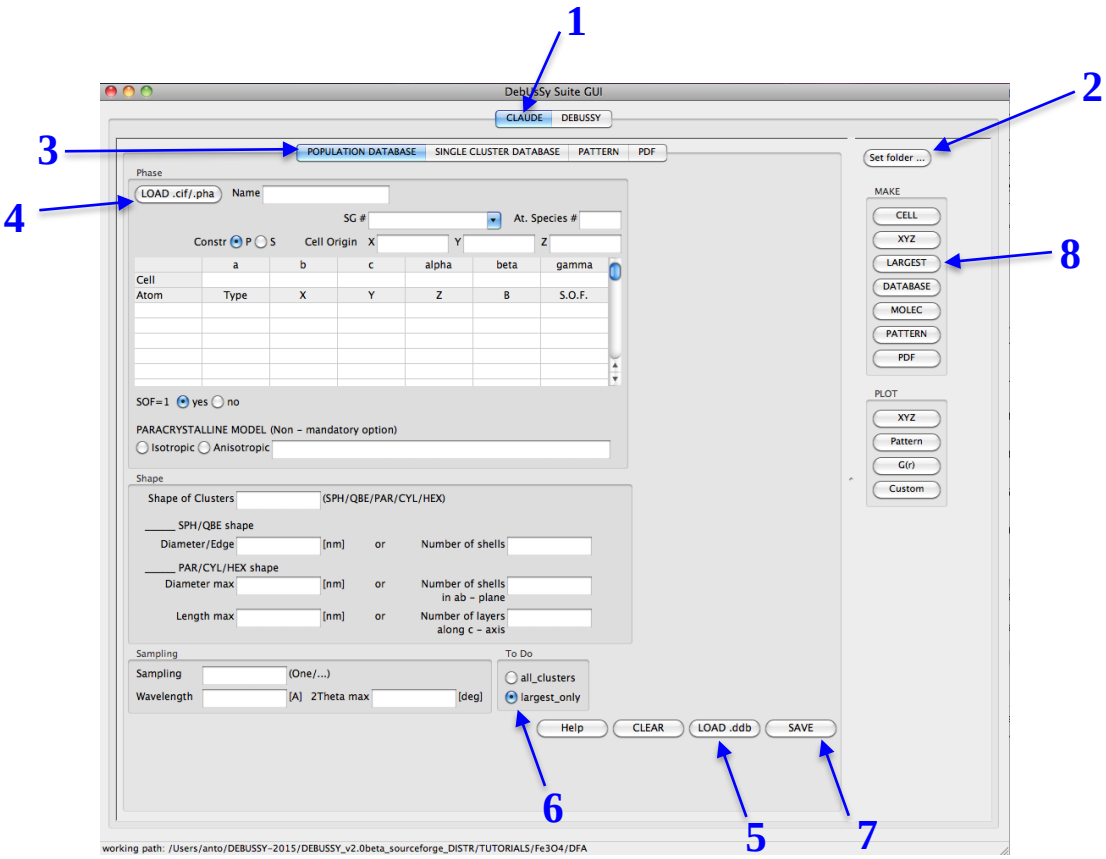
7) Click on **CELL** button of the **MAKE** vertical menu (the unit cell is built starting from the asymmetric unit and from the space group information reported in the *.pha* file).

8) Click on **DATABASE** button of the **MAKE** vertical menu. The DISTANCES/SAMPTO* folder is created in the working folder, including the *.smp* and *.smp_INFO* files of each cluster.

9) Optionally, click on the **XYZ** button of the **MAKE** vertical menu to generate the *.xyz* files containing the atomic Cartesian coordinates of the NCs. It is strongly recommended to limit the maximum number of the NCs for this operation, by editing the *.ddb* file.

10) If step 9 has been performed, click on the **XYZ** button of the **PLOT** vertical menu in order to visualize and manage the atomistic models of the NCs (*Jmol* application will be launched).

Building the sampled interatomic distances for a single cluster



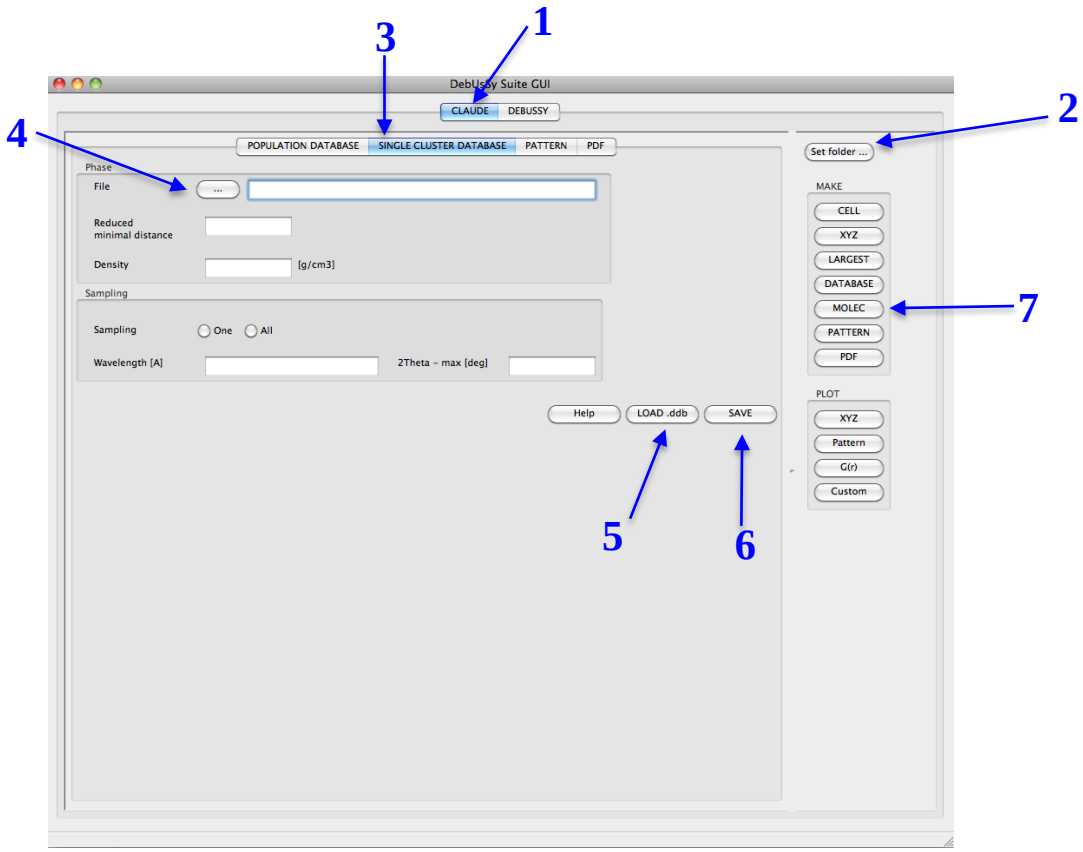
Follow the list of operations from 1 to 5 reported for building the population of NCs.

6) Select the **largest_only** option in the **POPULATION DATABASE** tab.

7) **SAVE** the *.ddb* file.

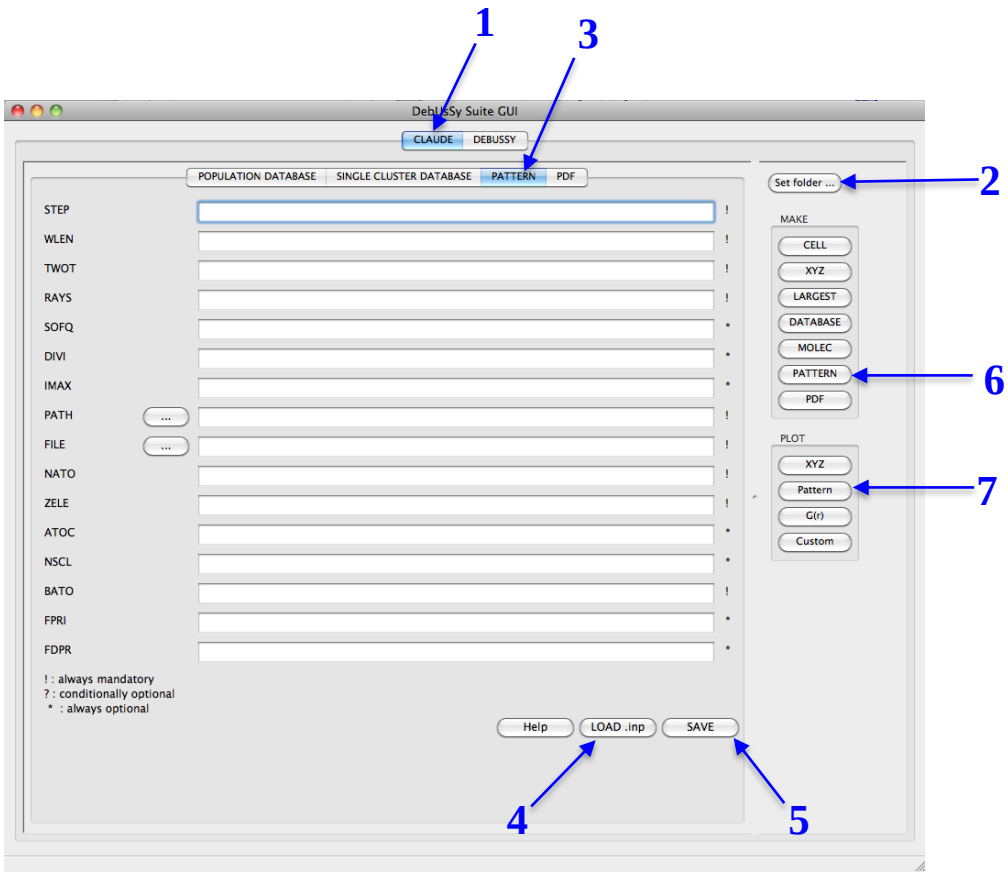
8) Click on **LARGEST** in the **MAKE** vertical menu to generate a single cluster database (single *.smp/smp_INFO* in the case of a monovariate population, single base size combined with all the possible lengths along *c* for bivariate populations of NCs), having the largest size specified in the *.ddb* file.

Building the sampled interatomic distances starting from an .xyz file



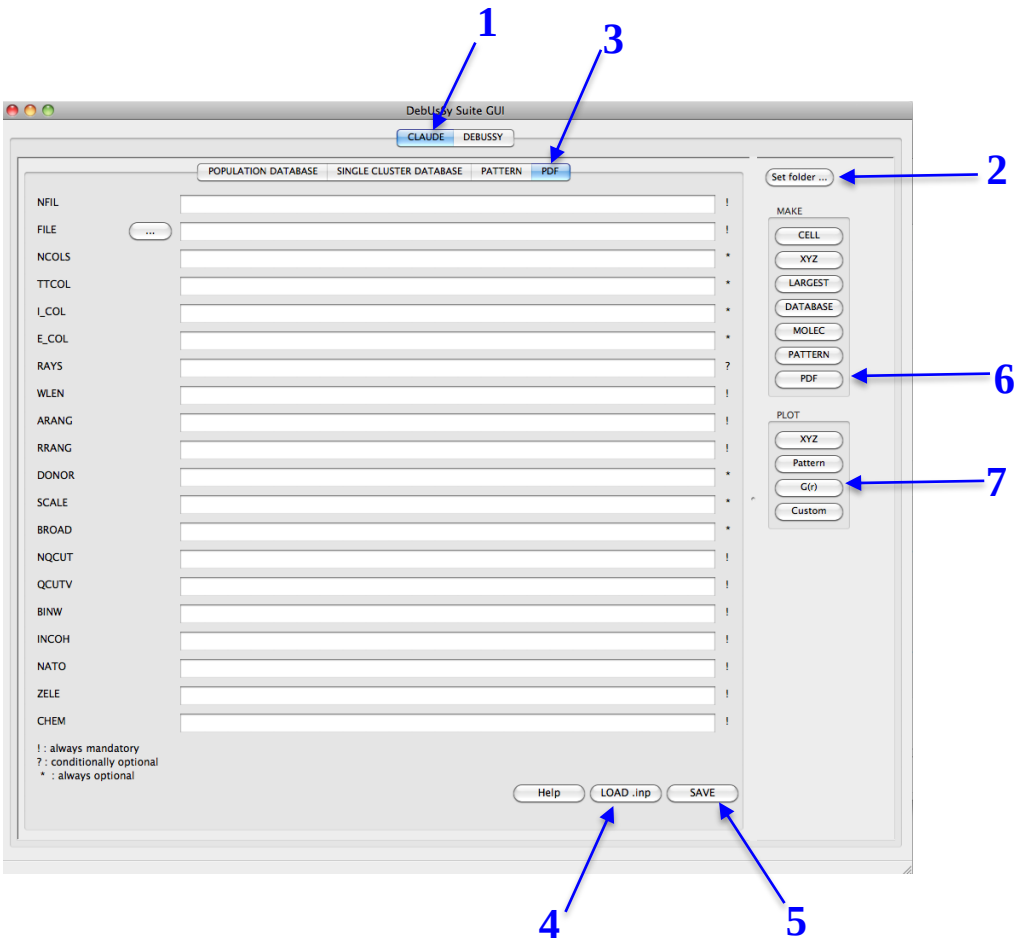
2) Select your working folder by clicking on Set Folder button.
3) Select the **SINGLE CLUSTER DATABASE** tab:
4) Upload the *.xyz* file of the cluster by clicking on the **…** button.
5) Fill the **SINGLE CLUSTER DATABASE** tab with the information about the phase and the sampling (see the *Claude User's Manual* for details) or load an existing *.ddb* file by clicking on **LOAD .ddb.**
6) **SAVE** the *.ddb* file.
7) Click on the **MOLEC** button of the **MAKE** vertical menu. The DISTANCES/SAMPTO* folder is created in the working folder, including a *.smp* and a *.smp_INFO* files.

Computing a powder pattern from a single cluster (.smp file)



2) Select your working folder by clicking on **Set Folder** button.
3) Select the **PATTERN** tab.
4) Fill the **PATTERN** tab or load an existing *diffractor.inp* file by clicking on **LOAD .inp** button and edit it, if necessary.
5) **SAVE** the *diffractor.inp* file.
6) Click on the **PATTERN** button of the **MAKE** vertical menu, in order to compute the pattern from the *.smp* indicated in the *diffractor.inp* file.
7) The output file with the *.tqi* extension is created and can be visualized automatically using the **PATTERN** button of the **PLOT** vertical menu.

Computing the Pair Distribution Function from a powder diffraction pattern



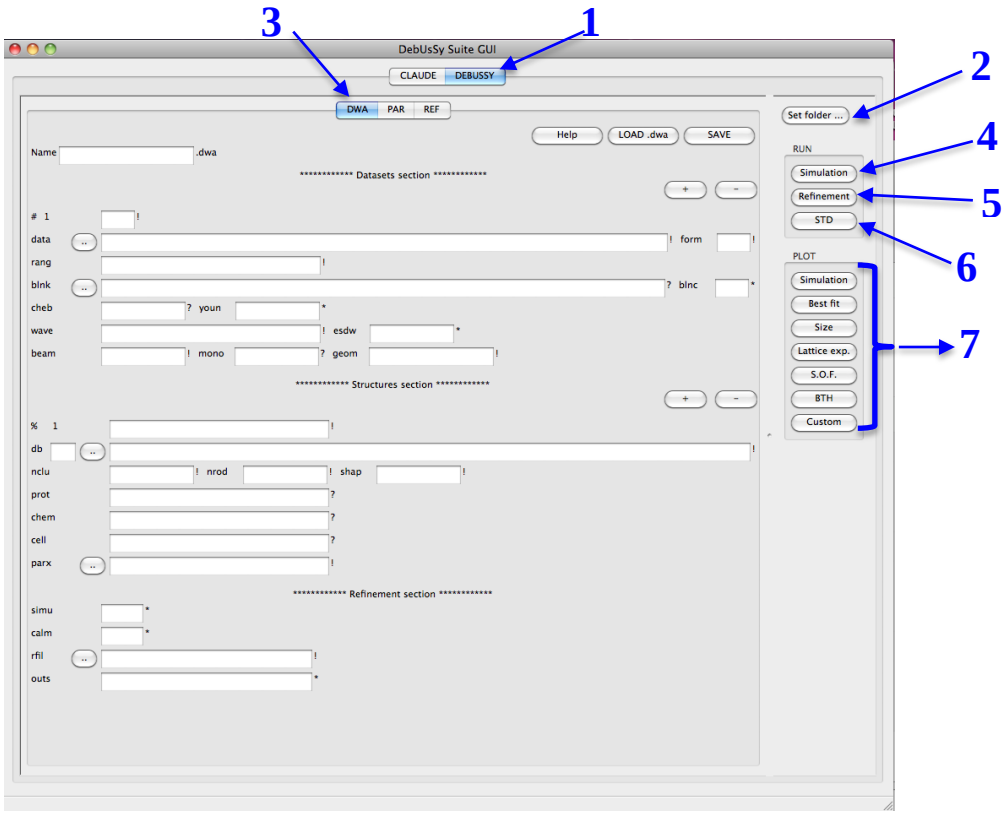
2) Select your working folder by clicking on **Set Folder** button.
3) Select the **PDF** tab.
4) Fill the **PDF** tab or load an existing *dopdf.inp* file by clicking on **LOAD .inp** button and edit it, if necessary.
5) **SAVE** the *dopdf.inp* file.
6) Click on the **PDF** button of the **MAKE** vertical menu. Several files can be created, according to the options selected in the input file (see the *Claude User's Manual* for details)
7) In order to automatically visualize the reduced G(r) computed, the **G(r)** button in the **PLOT** vertical menu can be used.

Quick guide for the *DEBUSSY_GUI*

The Debussy program can be used for the following tasks:

- simulating a powder diffraction pattern by the DSE in the absence or in the presence of an experimental pattern;
- refining a model powder pattern against the experimental data;
- calculating the e.s.d. of the refined parameters.

A database of sampled interatomic distances is necessary for any of the previous listed tasks (see the *CLAUDE_GUI* section).



1) Select the *DEBUSSY* tab of the D*ebUsSy Suite* GUI.

2) Select your working folder by clicking on **Set Folder** button.

3) Fill the required input files (*.dwa*, *.par*, *.ref*) using the related tabs or load the existing ones using the **LOAD .dwa/.par/.ref** buttons.

4) Click on the **Simulation** button of the **RUN** vertical menu in order to compute the model pattern described by the set of parameters written in the *.par* file(s). This action does not perform any refinement of parameters and can be used to preliminary testing the starting model.

5) Click on the **Refinement** button of the **RUN** vertical menu in order to perform the refinement of the model parameters.

6) Click on the **STD** button of the **RUN** vertical menu, compute the e.s.d. of the refined parameters, once the minimum of the χ^2 function is reached.

7) Use the **PLOT** buttons in the vertical menu to visualize all the graphical outputs generated during and at the end of the refinement or the simulation:

Simulation to plot the pattern calculated by the **Simulation** run.
Best fit to plot the pattern calculated by the **Refinement** run
Size to plot the mono- or bivariate size distributions.
Lattice exp. to plot the lattice parameter(s) as a function of the NCs size.
S.O.F. to plot the atomic site occupancy factors as a function of the NCs size.
BTH to plot the atomic Debye Waller factors as a function of the NCs size.