EPSRgui v1.0 manual

July 2016

Sam Callear

Contents

- Installing EPSR
- Installing EPSRgui
- Example workflows

Running EPSRgui opens a main GUI window. To see the outputs from short EPSR processes open the messages window in the settings menu. Additional command prompt windows are opened for longer EPSR processes. Closing these windows before an EPSR process has finished will cause it to stop immediately and is not recommended.

EPSRgui will copy .mol files from any directory into the project directory, but other files such as datafiles need to be in the project folder for EPSRgui to be able to use them. (This will be updated in a later version)

After each step, save the project.

Install EPSR

- Go to the Disord Matt Facebook page for links to download EPSR from dropbox. For both windows and Linux make sure the system_commands.txt in the startup folder is appropriate for your computer and operating system. For windows, make sure the java path is set to the java.exe on your computer. For linux make sure the system_termination symbol is ‘/’, make sure the system_mopac path is appropriate fro your computer and make sure java is installed and executable on your computer.

Workflows

- EPSRgui offers a number of ways to build the components (atoms, molecules and lattices) to go into the simulation box:
  - Create new .mol file – create a molecule or single atom in Jmol (including geometry minimisation) and run mopac if desired (equivalent to runjmol and readjmol in EPSRshell)
  - Load existing .mol file – put a .mol file in the project directory and then open it.
  - Create single atom – complete the fields in the dialog box and a single atom .mol file is created (equivalent to makeato in EPSRshell).
  - Create atomic lattice – open a .unit file and/or fill out the fields in the dialog box to generate an atomic lattice. The lattice can be used as the simulation box or as a component.
  - Make .mol in preferred visualiser – if a preferred visualiser is specified in Settings, this can be used to generate any component. Remember to save the .mol and the .ato for the component as both of these are used in EPSRgui.

Workflows

- Once the components have been specified there are currently 2 ways the components can be placed in the simulation box:
  - Mixato – This puts the specified number of each component at the centre of a box that is of a size determined from the atomic number density. Note that all the molecules are positioned on top of each other and have their starting conformation until Randomise is clicked and Fmole is run.
  - Addato – This uses the first component in the list as the container, and adds all the subsequent components to this box. The ‘number in box’ for the container can only be 1. The atomic number density is calculated after the box has been built.
  - Loadato has not been fully implemented yet.

Example workflows

- Simple liquid
  - Create/load .mol files for each component
  - Mixato
- Amorphous atomic glass
  - Create/load atom .mol for each element
  - Mixato
- Amorphous atomic glass from lattice
  - Makelattice – tick ‘use as simulation box’
  - Untick tether in component tab, additional details
- Amorphous molecular glass from lattice
  - Create molecule mol and ato and lattice ato in external software
  - Use as box
  - Untick tether in component tab, additional details

Example workflows

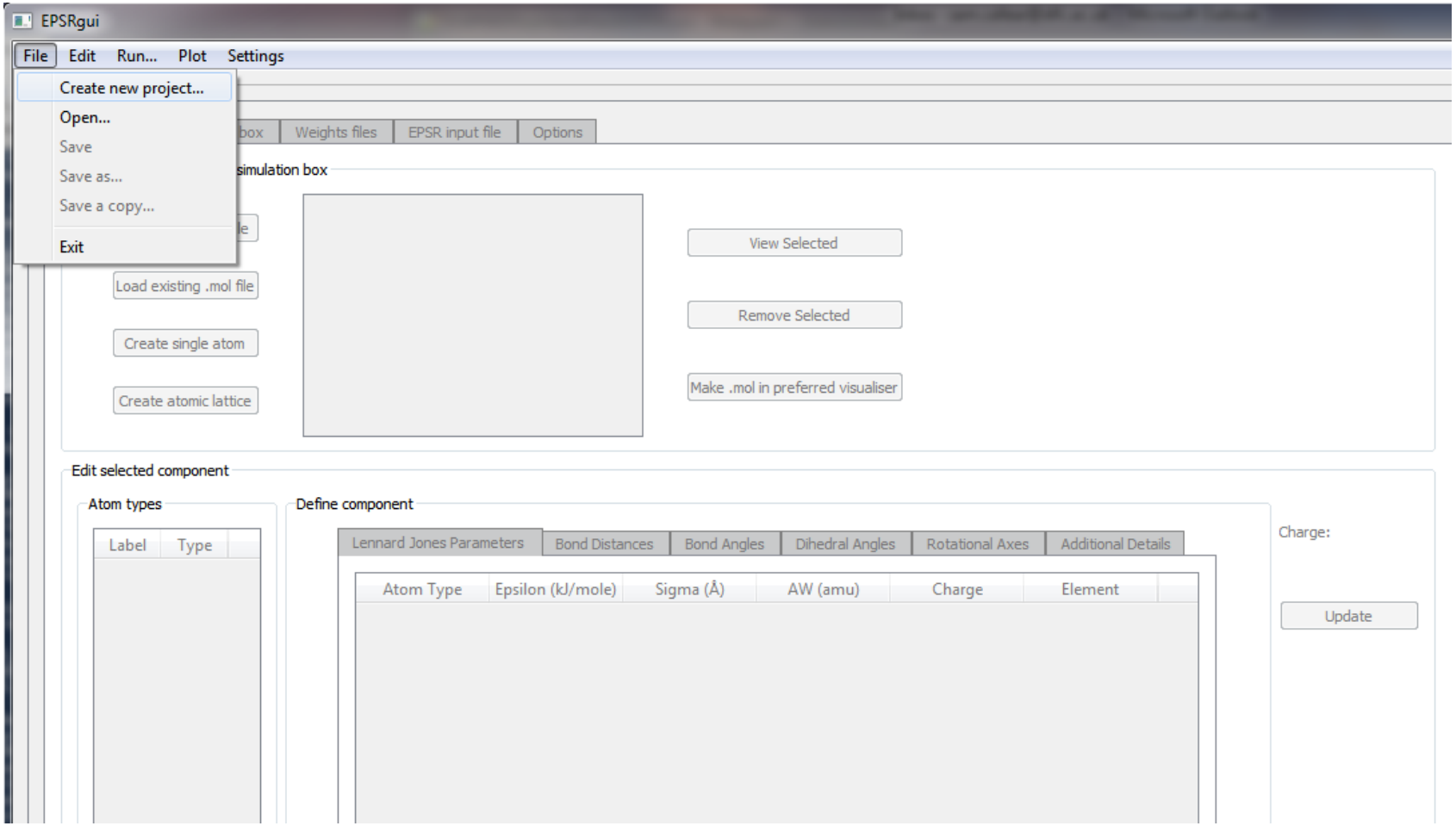
- Crystalline porous material
  - Create lattice mol and ato in external software
  - Load box
  - Changeato on box.ato to tether lattice.
- Loaded crystalline porous material
  - Create lattice mol and ato in external software
  - Create/load .mol file for added molecule
  - Addato
- Amorphous porous material
  - Make lattice of Q points
  - Create/load components for amorphous material
  - Addato
- Loaded amorphous porous material
  - Follow above method and refine to data to make the amorphous porous material
  - Create/load components for loaded molecules
  - Addato (using box as container)
- Liquid with nanoparticles present
  - Create lattice mol and ato in external software, increase the box size to produce the correct density of the final system. Make sure this is the first component in the list.
  - Create/load .mol files for liquid component
  - Addato

Settings

- EPSRgui settings can be stored for ease of use and also to enable additional methods to create components. Run EPSRgui and click Settings and navigate to the preferred EPSR directory and visualiser executable.

Starting a new project

To start a new project, click File, Create New Project.

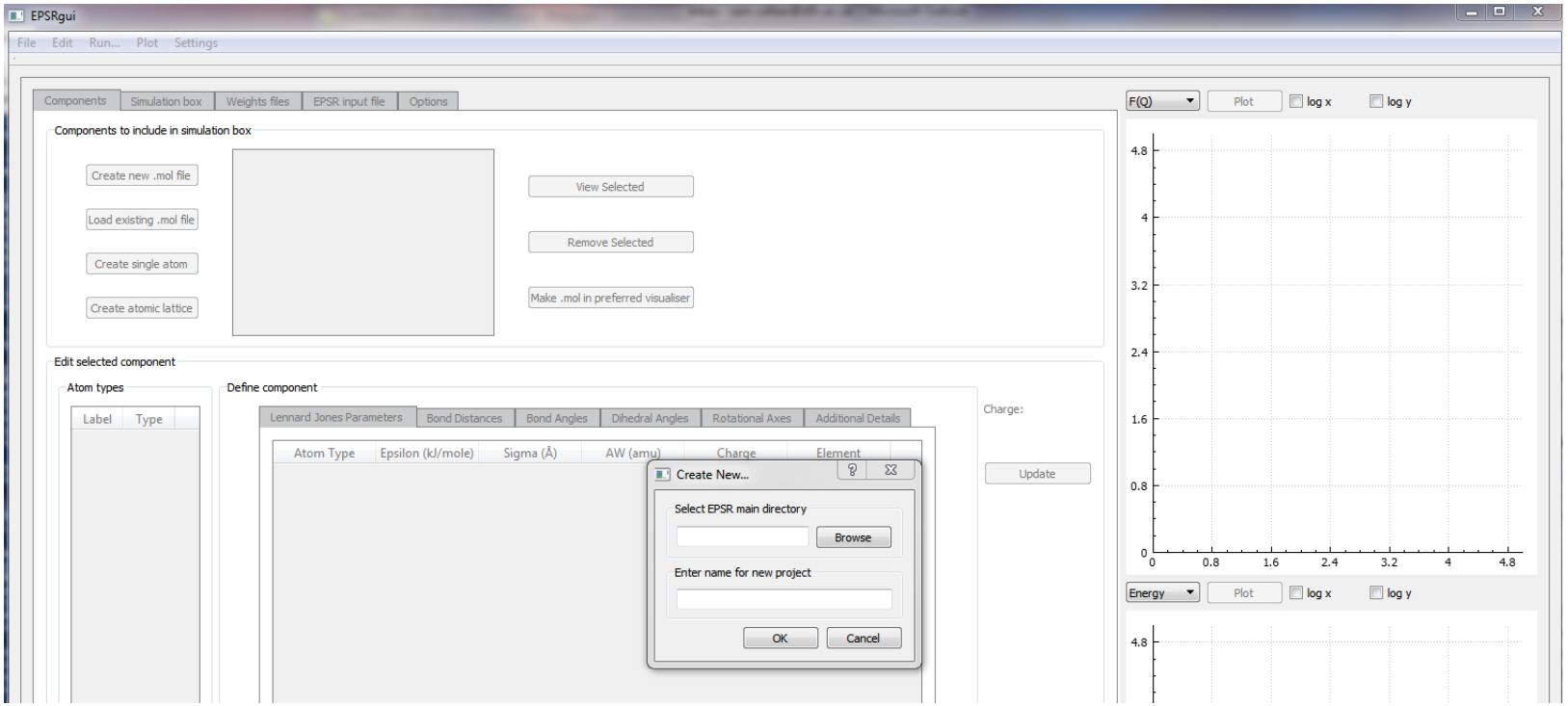


Starting a new project

In the pop up window, click Browse and navigate to the EPSR root directory e.g. C:\EPSR25

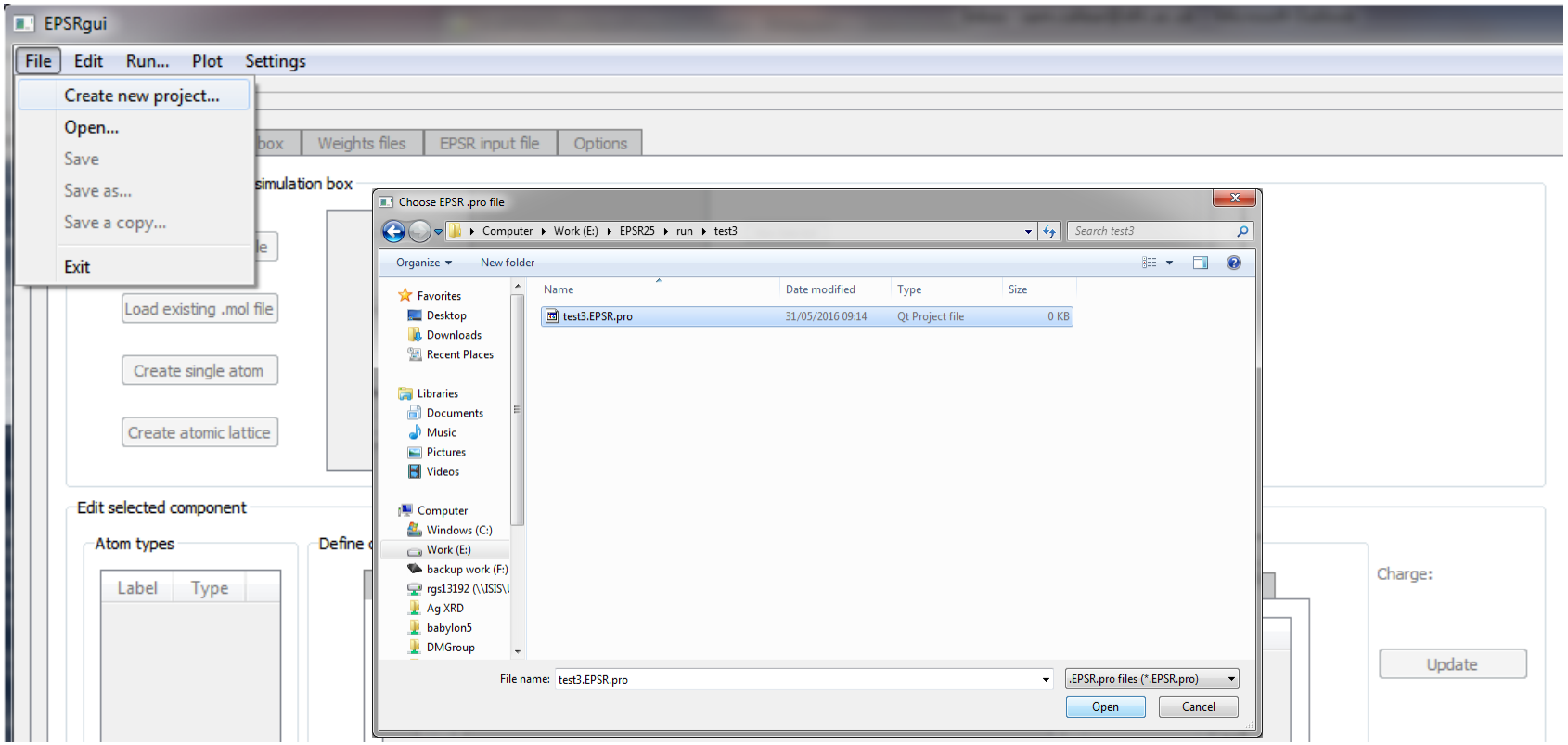
Then type a name for the project (no spaces or special characters) and press enter

The new project will then be saved as a new folder in the EPSR\run directory and the project details are saved into the XXX.EPSR.pro file.

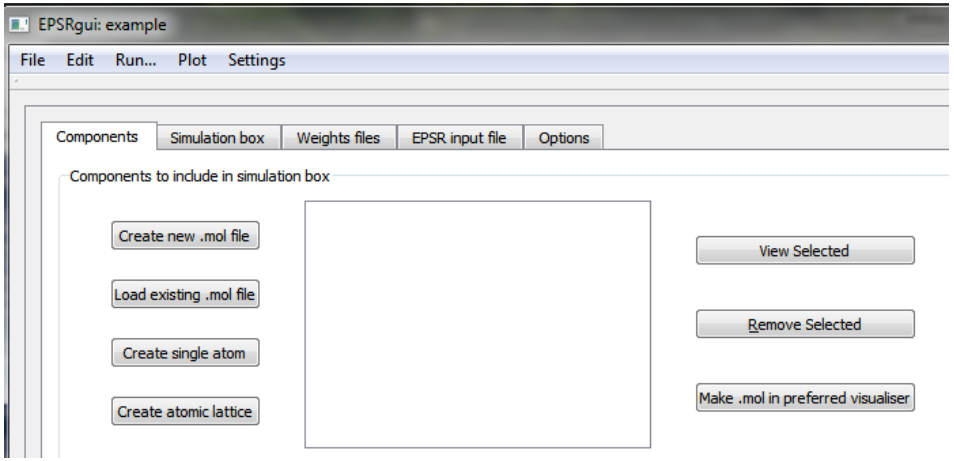


Opening an existing project

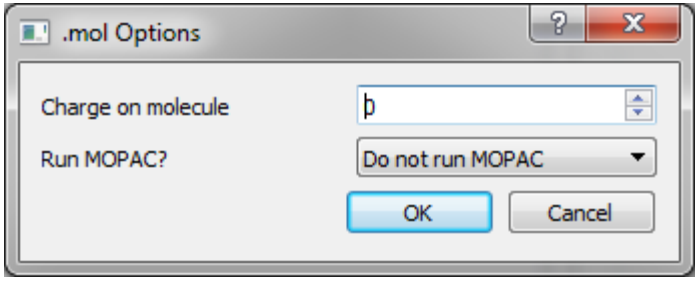
To open an existing project, click File, Open…
In the pop up window navigate to the project folder and select the XXX.EPSR.pro file and click Open



Creating a molecule



To create a new .mol file using Jmol click Create new .mol file.
In the pop up window input the charge on the molecule and whether you want to run MOPAC on the molecule, and if so which option to use (provided it exists) then click OK



To load an existing .mol file, first put the .mol file and .ato file for the molecule in the project folder and then click load existing .mol file and select the .mol file.

Jmol

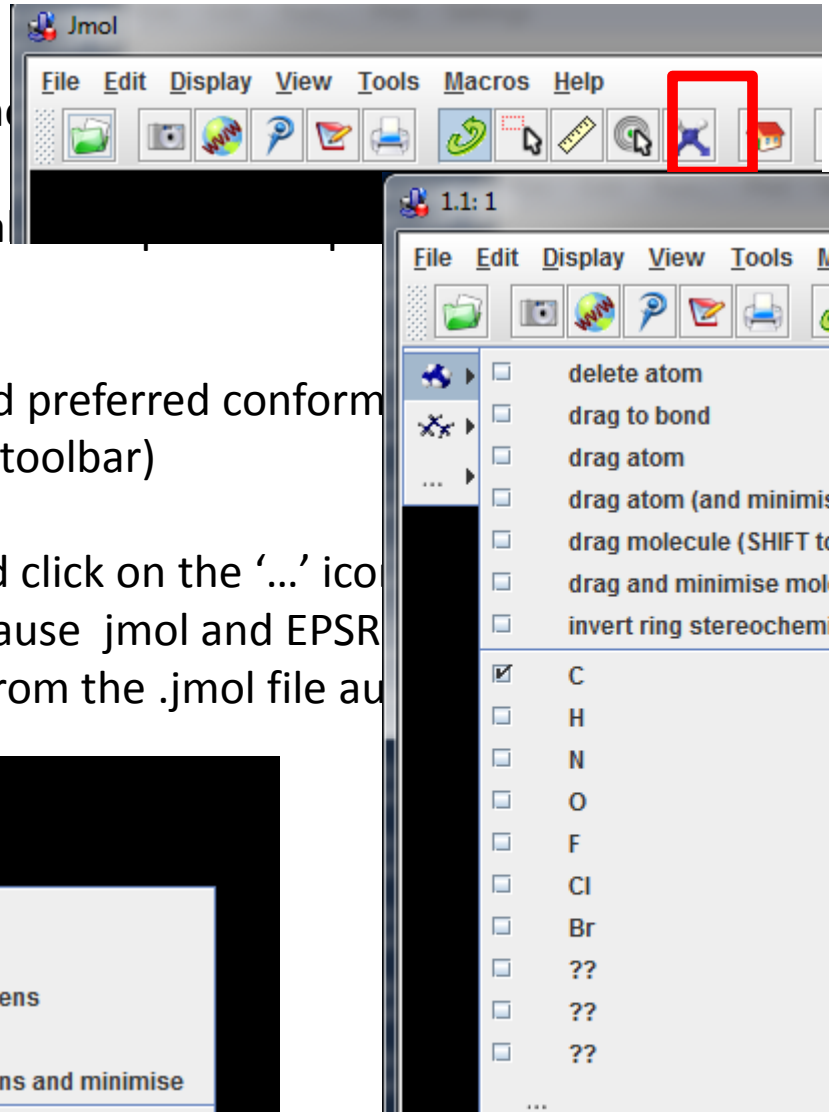
In the Jmol window that has just opened, click th

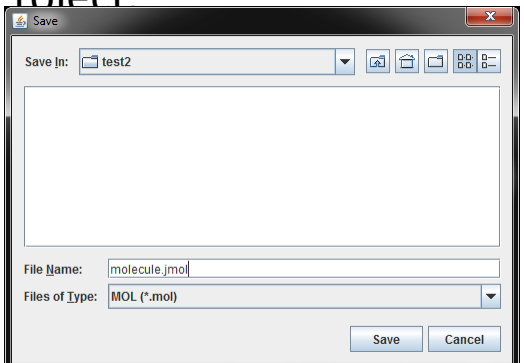
A toolbar will appear on the left hand side with a
molecule.

Draw the molecule with the correct bonding (and preferred conform
use the 'minimise' option in the '…' menu in the toolbar)

When finished, right click on the background and click on the '…' ico
file. Save the file as a **.jmol** This is important because jmol and EPSR
.mol file - the .mol file for EPSR will be created from the .jmol file au
EPSRProject

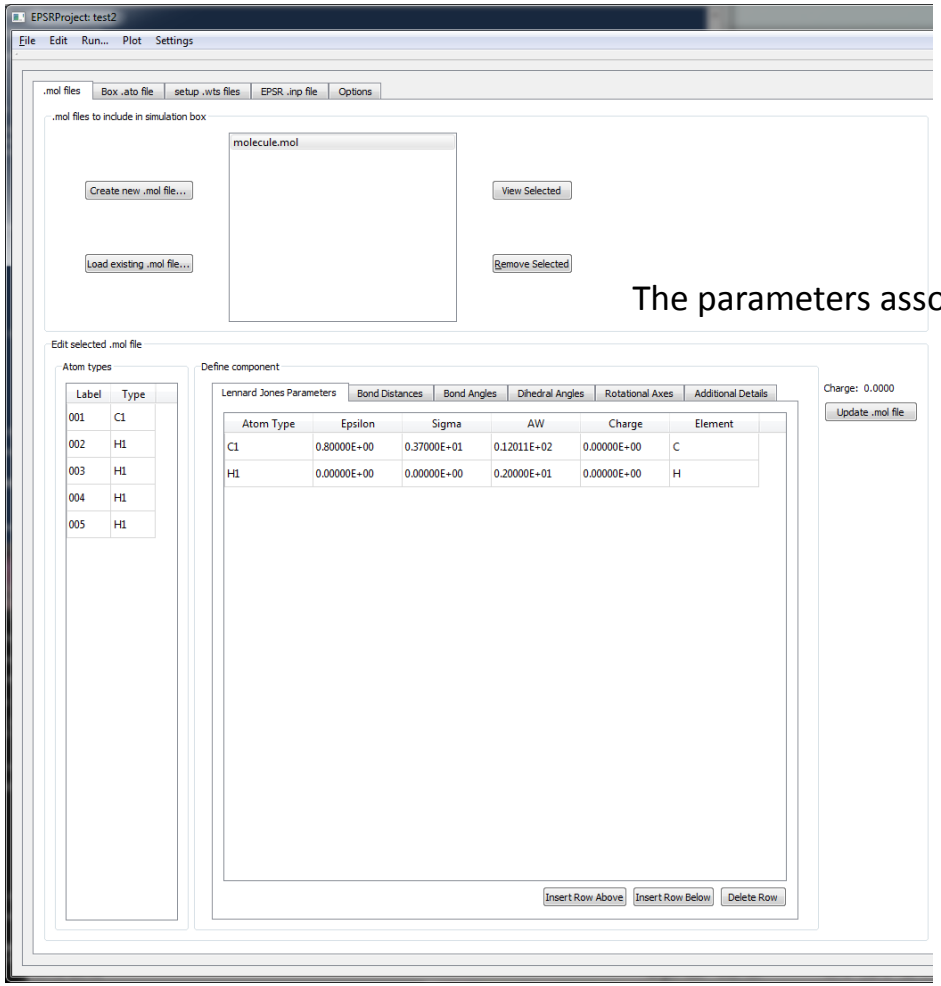
Close





.mol file

On closing the jmol window, or after loading an exisiting .mol file, the .mol file is read into EPSRProject.



Each atom in the molecule is numbered – the atom type associated with this atom is listed here. To check which atom is which within the molecule, click view selected

The parameters associated with each molecule are listed here.

Fill out the LJ parameters appropriately, remember an atomic weight of 2 is generally used for H and D.
The charge on the molecule is shown here. If the charges are edited, click update .mol file to recalculate the charge on the molecule. Edit/insert/remove bond distances, angles and dihedrals to define the molecule as appropriate. Rotational axes and .mol file ecordcore values can also be inputted.

Click update .mol file to save the changes to the .mol file. Don't click on another .mol file before doing this otherwise the changes will be lost.

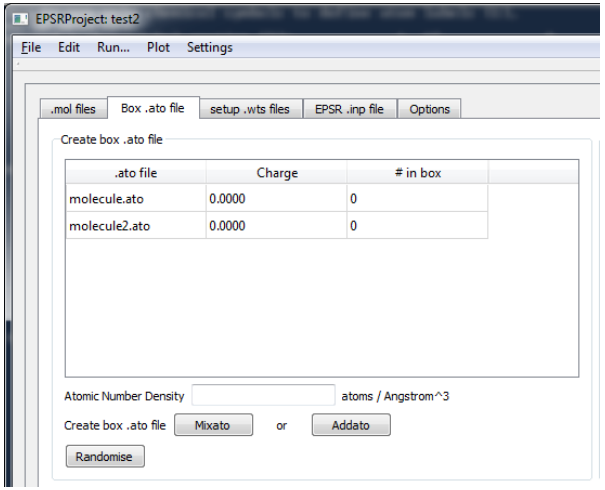
.mol files

Add as many .mol files as required by creating new, or loading exisiting.
Remember that no 2 atoms (including 2 atoms on separate molecules) can have the same atom type so the atom type in the LJ parameter tab needs to change d according to the type in the atom types table.

To remove a .mol file, click remove selected.

If an old .mol file is used which doesn't include a changelabel section in the .mol file, the atom types box will be blank. This is not a problem – the .mol file will still work with EPSR but no changes can be made to the atom label.

Creating a simulation box



The .ato files for each of the .mol files loaded are listed in this table.

Edit the number in box column appropriately for your system and the size of the box you want to create.

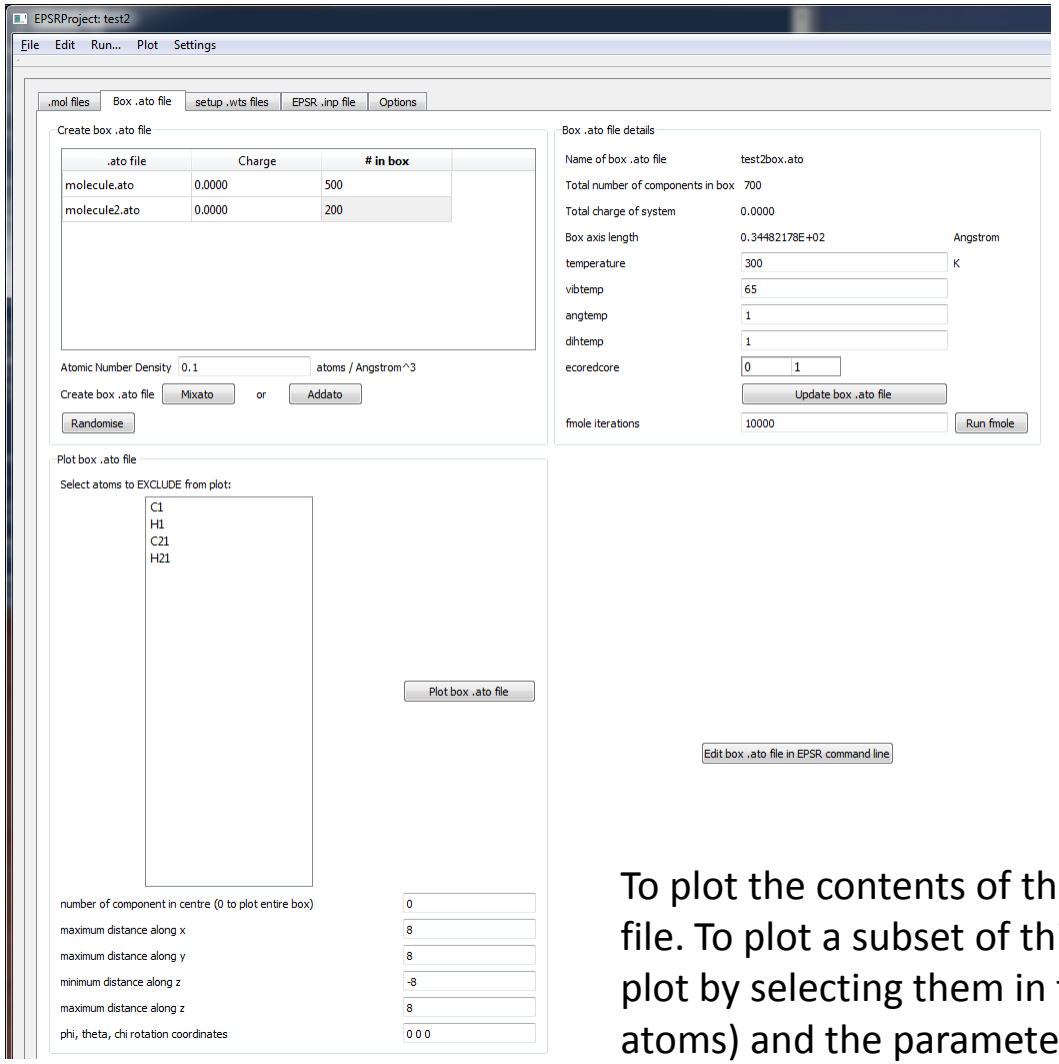
If either of the .ato files contains a molecule that needs to be fixed in specific position in the simulation box, put a t (for tethered) in the tethered? column, otherwise use f (for free).

Input the atomic number density in atoms/Angstrom^3

Click mixato to create the box. Then click Randomise to distribute the molecules randomly throughout the box.

If a more complicated system is being created, use addato to add the 2nd and all subsequent .ato files to the first .ato file in the table (the order here is important!) Remember if you are using addato to have already made the box the correct size for the number of molecules you want to add and the atomic number density is not used during addato.

Simulation box details



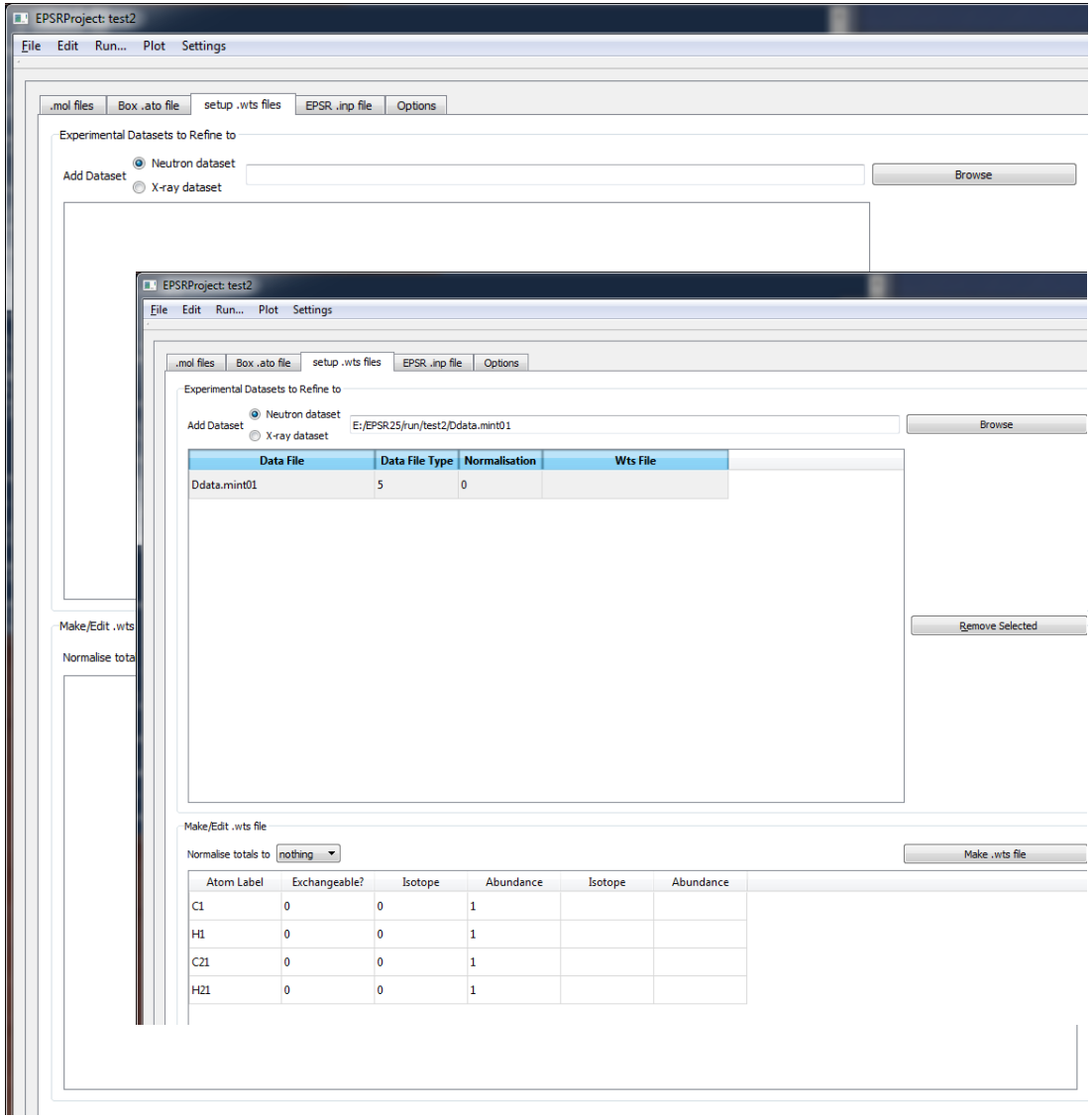
Once the simulation box has been created, the details of the box are listed here.

To make changes to the box paramters, change the values here and then click update box.ato file.

For a system where mixato has been used, fmole needs to be run ~10000 times in order to introduce some disorder to the molecular structure. This will not always be appropriate, depending on your system. Fmole runs in a separate window so the simulation can be prepared further while it is running.

To plot the contents of the simulation box click plot box .ato file. To plot a subset of this, atoms can be excluded from the plot by selecting them in the list (use Ctrl to select multiple atoms) and the parameters at the bottom of the plot window can be used to only plot part of the box.

Wts files



First copy all the datafiles appropriate to the simulation into the project folder.

To prepare the wts files for the system, select whether the data is neutron data or xray data, then click browse and select the data file.

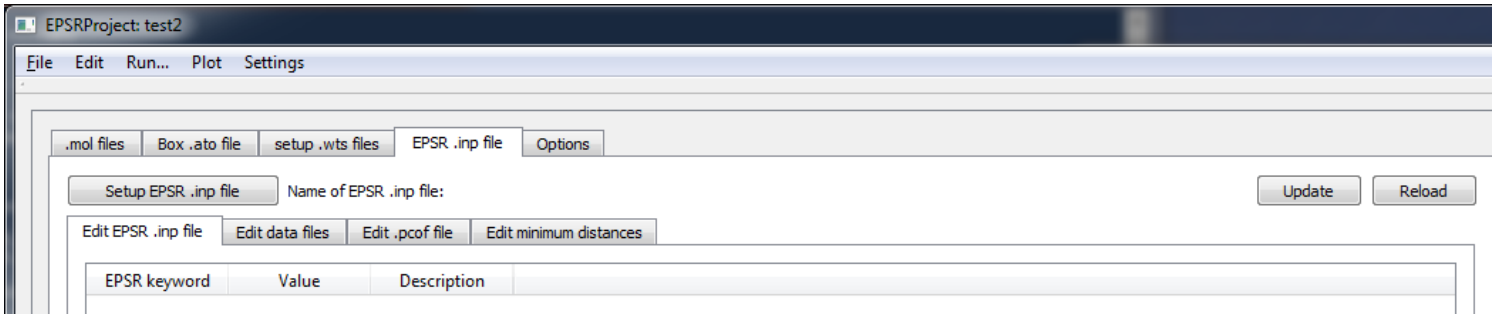
Select how the data are normalised from the drop down menu. Edit the exchangeable hydrogens (use 1 for exchanges, 0 for non-exchangeable) and the isotope (use 2 for D, 0 for natural H) and the abundance.

Then click make .wts file

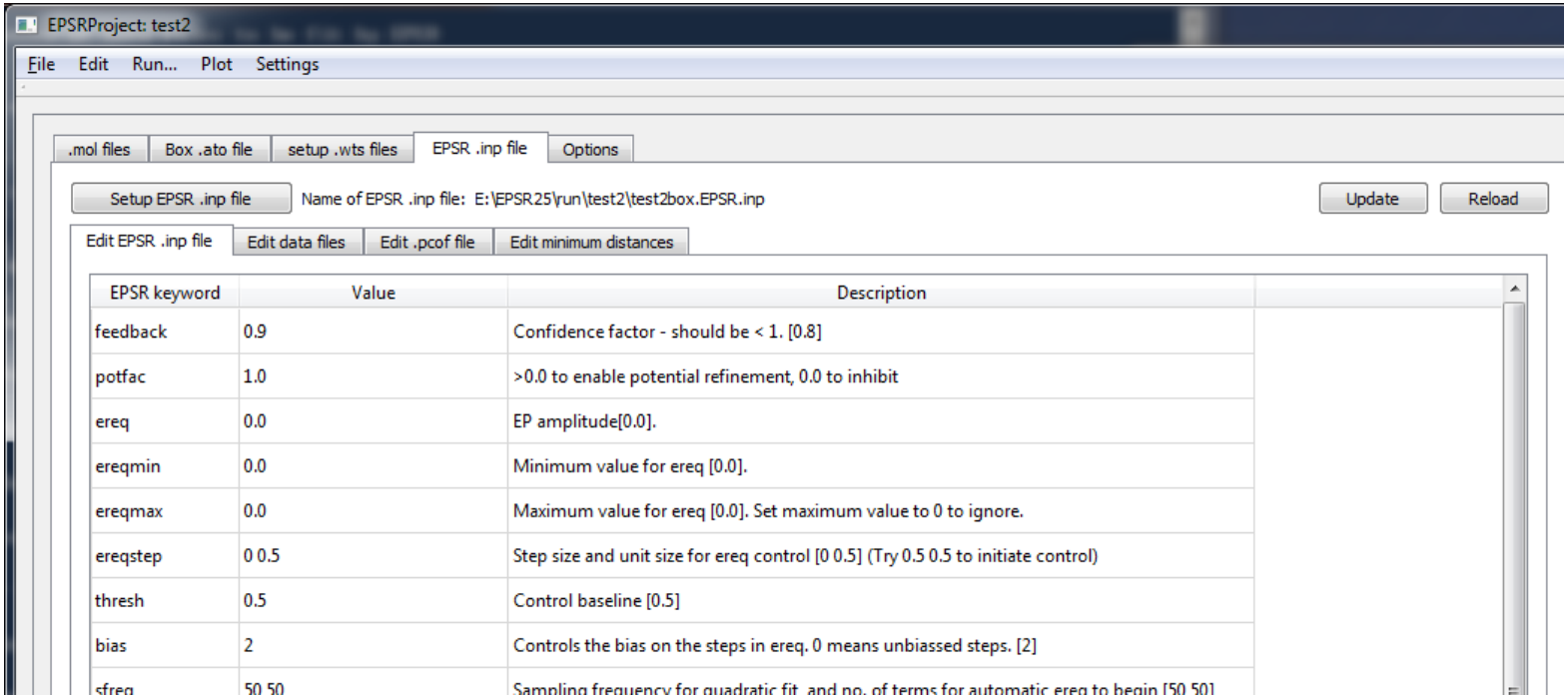
Repeat for all data files. If a mistake is made, just edit the table as necessary and then click make .wts file again.

Click remove selected to remove the data file from the list.

EPSR.inp file



Click Setup EPSR.inp file. All of the parameters in the previous tabs are carried forwards into the EPSR.inp file.



EPSR.inp file

To make changes edit the Value column as appropriate and then click update. Changes can also be made to the .pcof file, the minimum distances list between atom pairs (intermolecular) and the datafile details. To remove or add a datafile, first delete the EPSR.inp file (Edit, delete EPSR .inp file) and then add/remove the dataset and then setup the EPSR.inp file again.

Running the simulation

The epsr inp and pcof files are automatically updated from the GUI on clicking run EPSR.
To check the simulation is setup in a way EPSR understands, run epsr check.
To run EPSR iteratively, click Run, Run EPSR.
To stop EPSR running iteratively, click Run, Stop EPSR.
EPSR will stop at the end of the current iteration.
The ESPR inp and pcof files will be automatically reloaded into the GUI at the end of the last iteration. To reload them while running EPSR click Reload.

Troubleshooting

- Gnuplot not running – check wgnuplot.exe is in the correct place in the system_commands.txt file in both the startup folder and the project directory.
- Check messages window after addato – if there is insufficient space in the container, then not all (or none) of the added .mol files will have been added even though the box will have been made anyway.
- If an inappropriate isotope mass is used, EPSRgui will crash while making the wts files.