EPSRgui v1.0 manual

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Installing EPSR

- Go to the Disord Matt Facebook page for links to download EPSR from dropbox and install it.
- For both Windows and Linux make sure the system_commands.txt or system_commands_Linux.txt (respectively) in the startup folder are appropriate for your computer and operating system. EPSRgui will copy the file appropriate to your operating system from the startup folder on creating a new project and will rename it to system_commands.txt if using Linux.
- For windows, make sure the java path is set to the java.exe on your computer.
- For linux make sure the system_mopac path is appropriate for your computer and that java is installed and executable on your computer.

Installing EPSRgui

- Windows: Download the EPSRgui folder and copy it to your hard drive. To run ESPRgui, double click the exectuable
- Linux: Ensure the Qt libraries are installed on your system. Download the source code from https://github.com/samcallear/EPSRgui, make a make file using *qmake* and then compile using *make.*

Setting up EPSRgui

- EPSRgui acts as a ‘front-end’ for the EPSR routines, thus reducing the need for cmd/terminal commands. Not all EPSR routines have been fully implemented yet – some still require setting up via the command line. If a routine is missing please let me know (sam.callear@stfc.ac.uk).
- EPSRgui behaves very similarly to EPSR. Simulations are set up as project folders in the EPSR/run directory. For simplicity, the simulation box is automatically named <project folder name>box.ato.
- Component .mol files and data files do not need to be present in the project folder – on clicking load .mol or browse for data file they will be automatically copied to the project folder and any missing .ato files will be created. This is also the case for the box.ato file on clicking load box.
- The path to the EPSR folder containing the run etc folders can be saved as the default directory by clicking Settings->Save default settings. The path to an executable for a preferred visualiser can also be set here. It is not necessary to do this, but it speeds up folder navigation.
- EPSRgui runs many EPSR routines ‘behind the scenes’. If the simulation box is large or the component molecule is complex, this means that some of the processes might take a little longer than usual and the gui will ‘hang’ while it waits for the process to finish. Please be patient while this is happening - messages are given at the bottom of the gui screen and also in Settings->show messages once the process has finished. For longer EPSR processes (fmole and running EPSR) command prompt /terminal windows are opened so the gui can still be used while they are running. Closing these windows before an EPSR process has finished will cause the process to stop immediately and is not recommended.
- The gui will not automatically save the project on exiting. Any files created/edited will still be as such, but the project needs to be saved in order for the gui to remember that they are associated with the project.

Creating molecules

- 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.

Creating the simulation box

- Once the components have been specified there are currently 3 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.
  - Load box – Load a simulation box .ato file made elsewhere. First add the .mol files of the component into the component tab. Make sure the names of the mol files are at the bottom of the box .ato file (in place of moltypeXX) so that changes made to the .mol files are implemented to the box on running fmole. Put the box.ato file in the project folder and rename it <projectname>box.ato Click load box and select the .ato file.

Example workflows

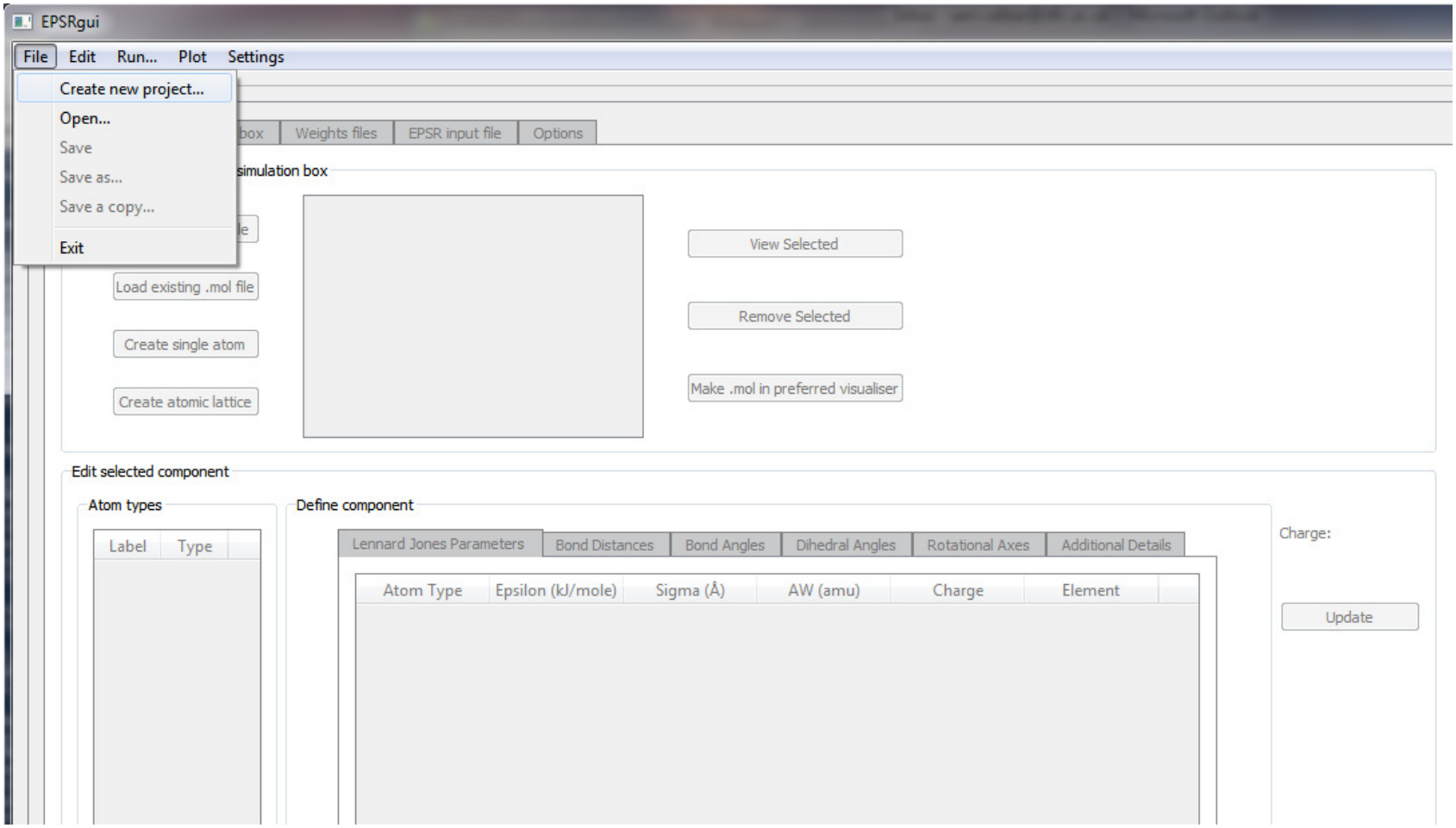
- Simple liquid
  - Create/load .mol files for each component
  - Mixato
- Amorphous atomic glass
  - Create/load atom .mol for each element
  - Mixato
- Amorphous atomic glass from lattice
  - Makelattice – tick ‘use as simulation box’
  - Untick tether in component tab, additional details
- Amorphous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

Example workflows

- Crystalline porous material
  - Create lattice mol and ato in external software
  - Load box
  - tether lattice in box .ato details
- 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.
  - Create/load .mol files for liquid component
  - Addato

Starting a new project

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

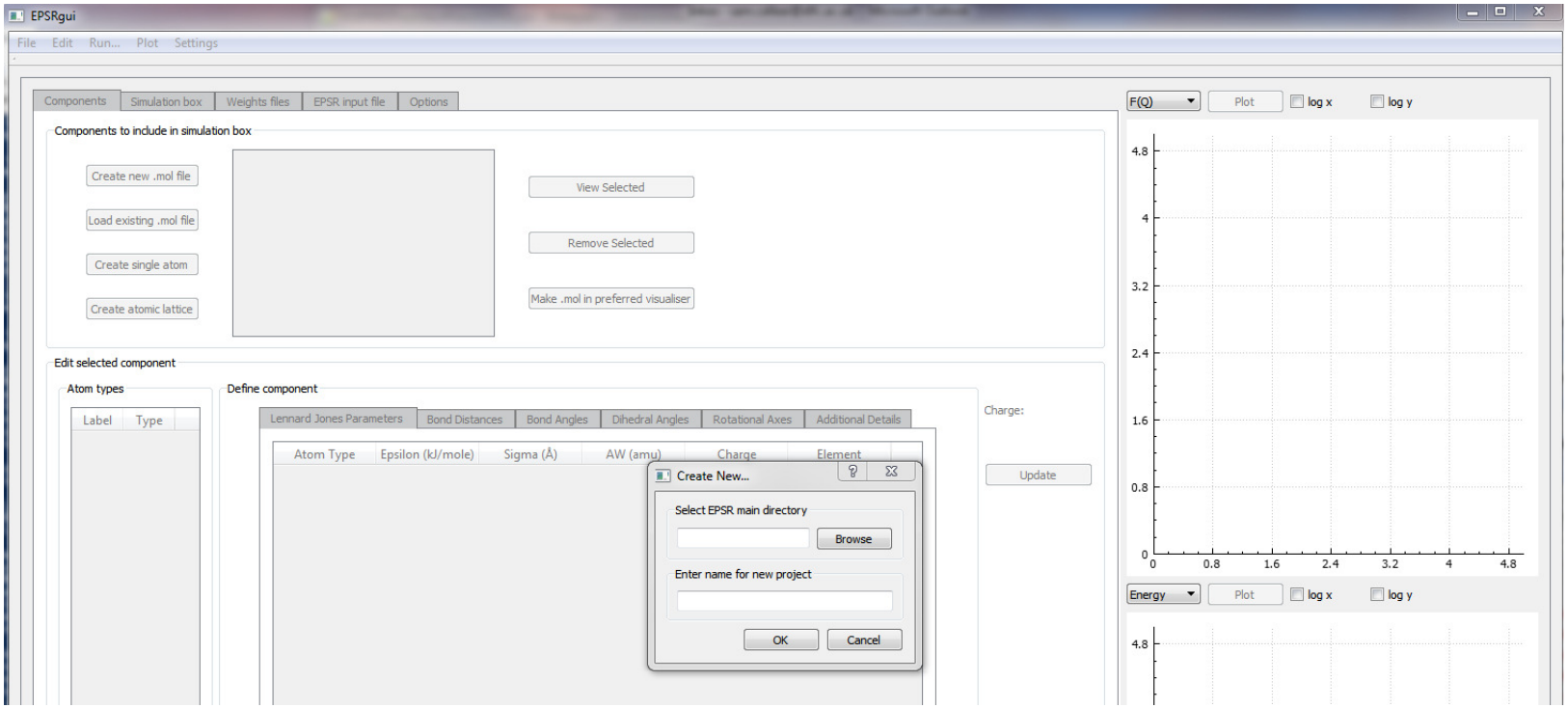


Starting a new project

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

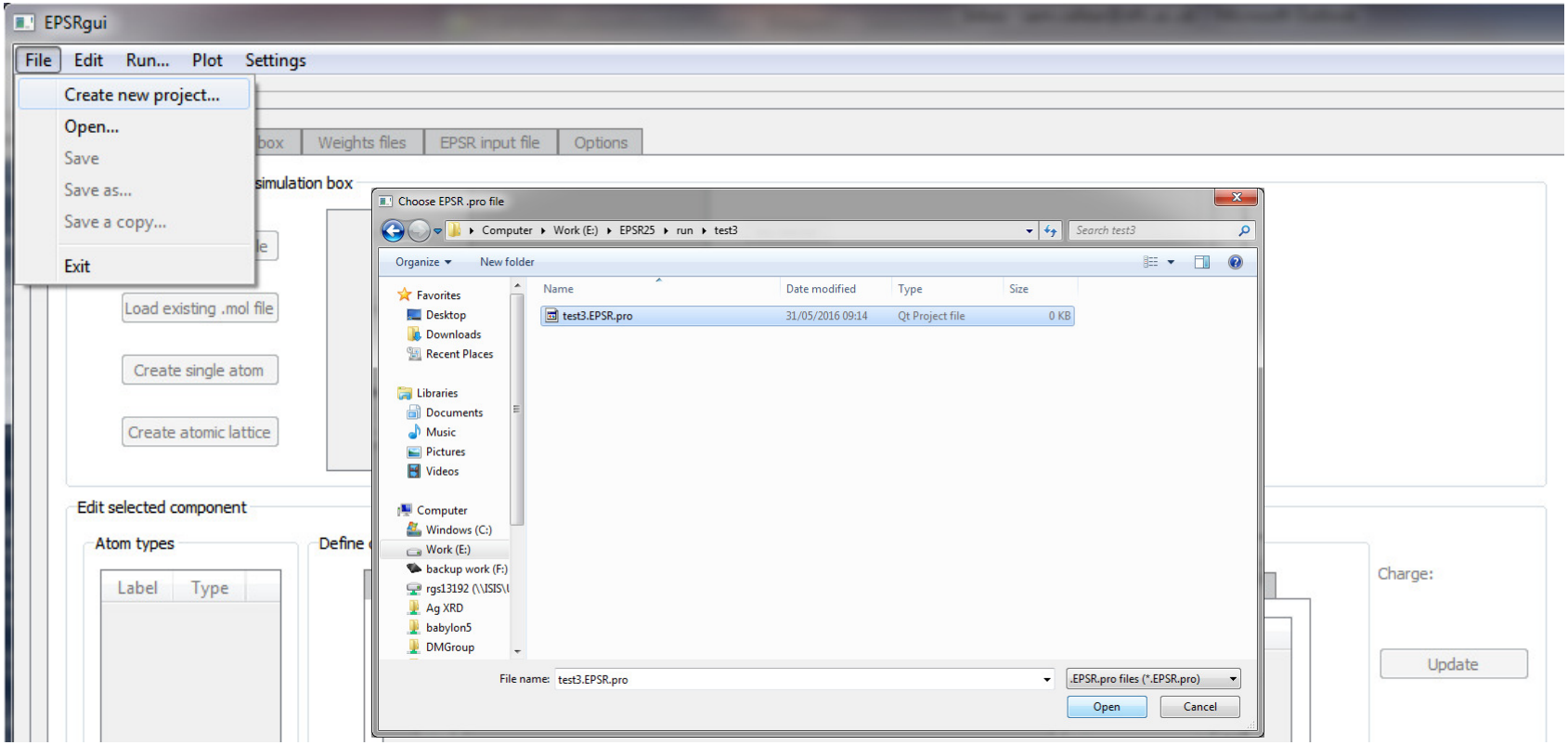
Then type a name for the project (no spaces or special characters) and press enter

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.

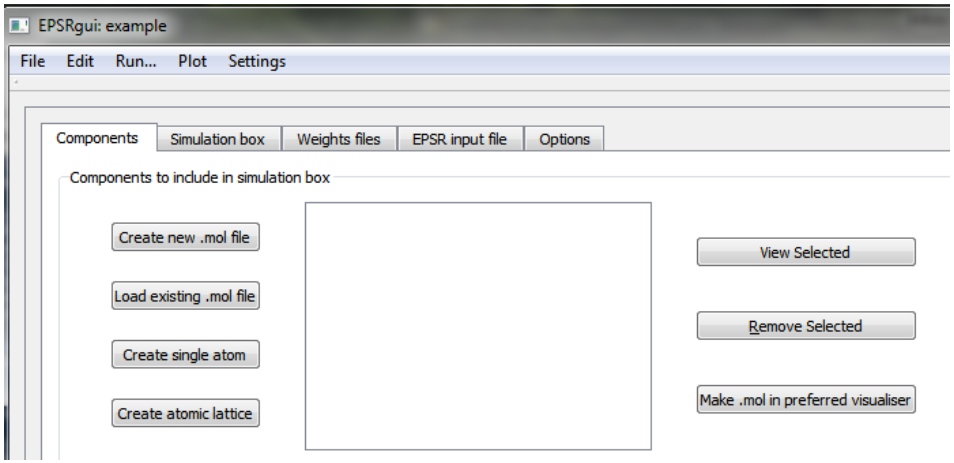


Opening an existing project

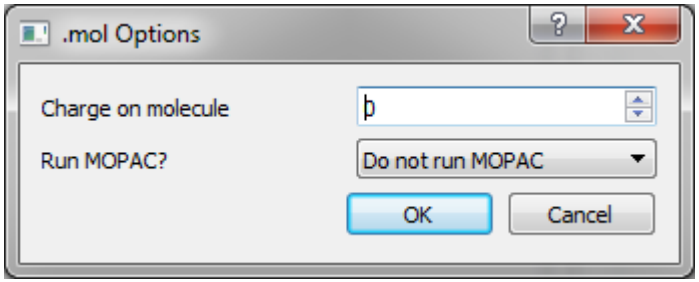
To open an existing project, click File, Open…
In the pop up window navigate to the project folder and select the XXX.EPSR.pro file and click Open



Creating a molecule in Jmol



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.

Creating a molecule in Jmol

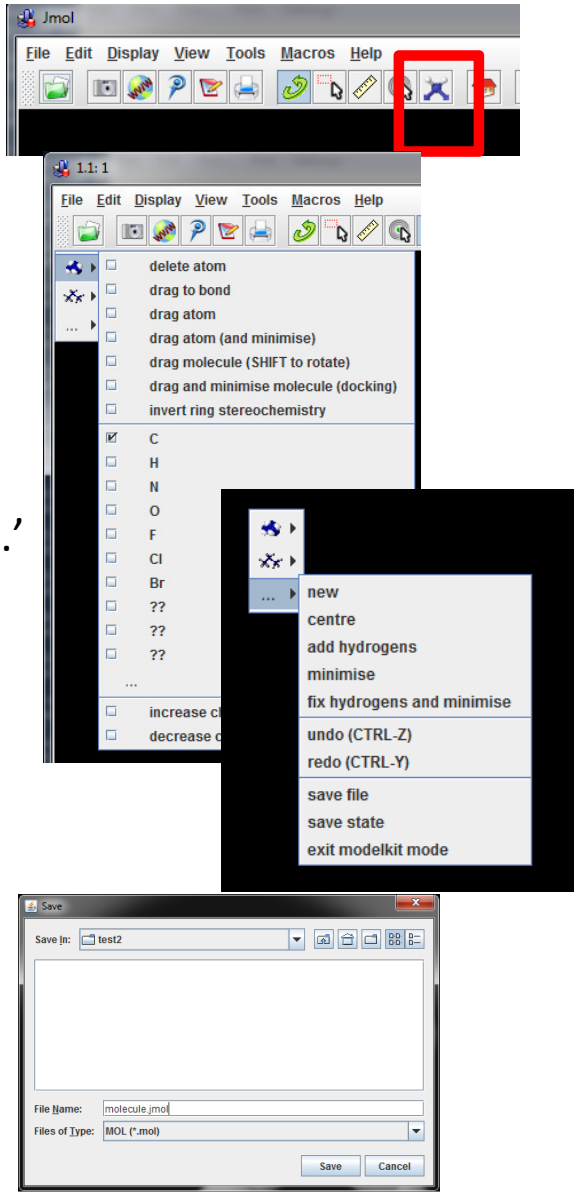
In the Jmol window that has just opened, click the build icon

A toolbar will appear on the left hand side with all the options required for building the molecule.

Draw the molecule with the correct bonding (and preferred conformation if necessary or use the ‘minimise’ option in the ‘…’ menu in the toolbar)

When finished, right click on the background and click on the ‘…’ icon, and then click save file. Save the file as a **.jmol** This is important because jmol and EPSR use different types of .mol files - the .mol file for EPSR will be created from the .jmol file automatically within EPSRProject.

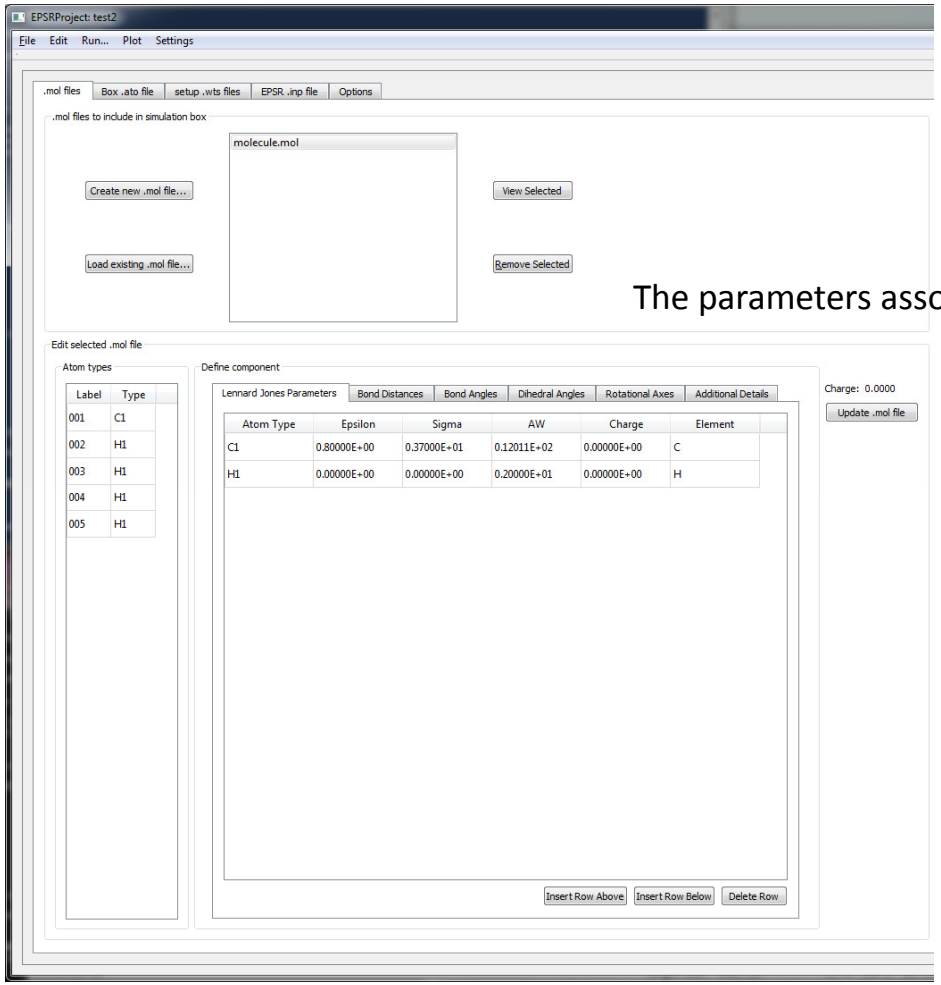
Close the jmol window



Editing the .mol files

On closing the jmol window, or after loading an existing .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 tethering and 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.

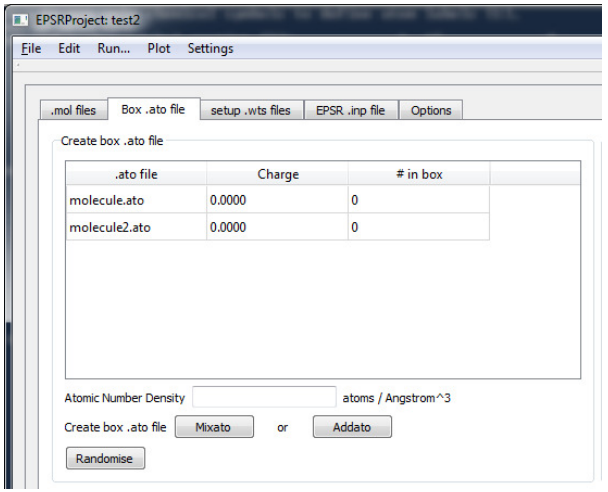
Editing the .mol files

Add as many .mol files as required by creating new, or loading existing.
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 changed 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



To mix the components randomly in the box:

- Edit the number of each component in the box, appropriately for your system and the size of the box you want to create.
- Input an atomic number density.
- Click Mixato to make the simulation box
- Click Randomise to distribute the components throughout the box.
- Check the box details are appropriate for your simulation.
- Run fmole 10000 times

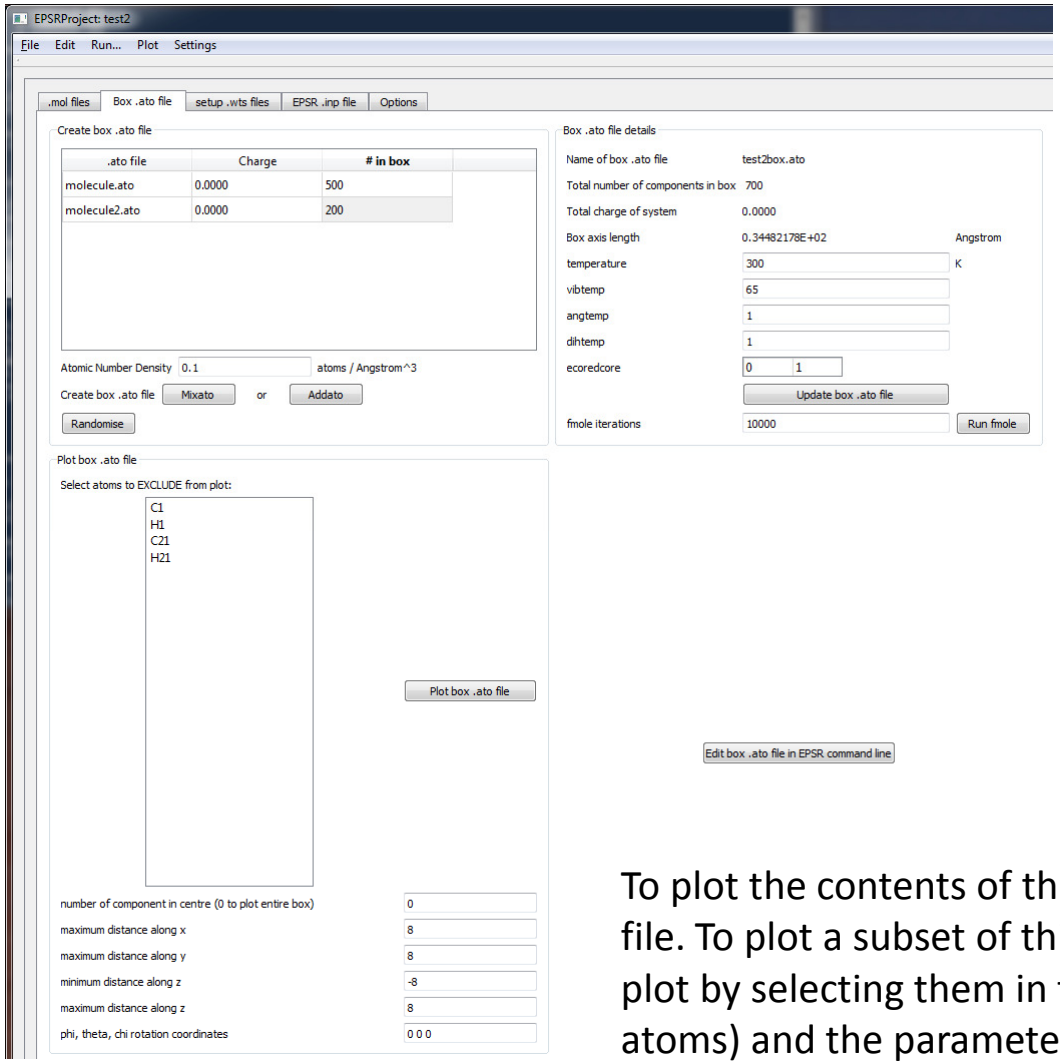
To add 1 or more components into a 'container' component:

- 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).
- Click Addato and choose the container and how many of the component molecules you want to add to the container (ensure the container is the correct size for the number of molecules you want to add as the atomic number density is not used during addato).
- Check in the Settings->Show messages window that all of the components were added to the box.
- The atomic number density will show the resulting density of the simulation box after addato.
- Check the box details are appropriate for your simulation (particularly any tethering).
- Run fmole 10000 times.

To load an existing box .ato file (e.g. generated from an external program):

- Load the .mol files appropriate to the box and ensure they are listed at the bottom of the box .ato file (in place of moltypeXX) so as any changes made to the .mol files are implemented in the box.
- The atomic number density will show the density of the simulation box after it is loaded.
- NB the '#in box' column will not be correct for boxes with more than one type of component present. (this does not affect the simulation)
- Check the box details are appropriate for your simulation (particularly any tethering).
- Run fmole 10000 times

Simulation box details



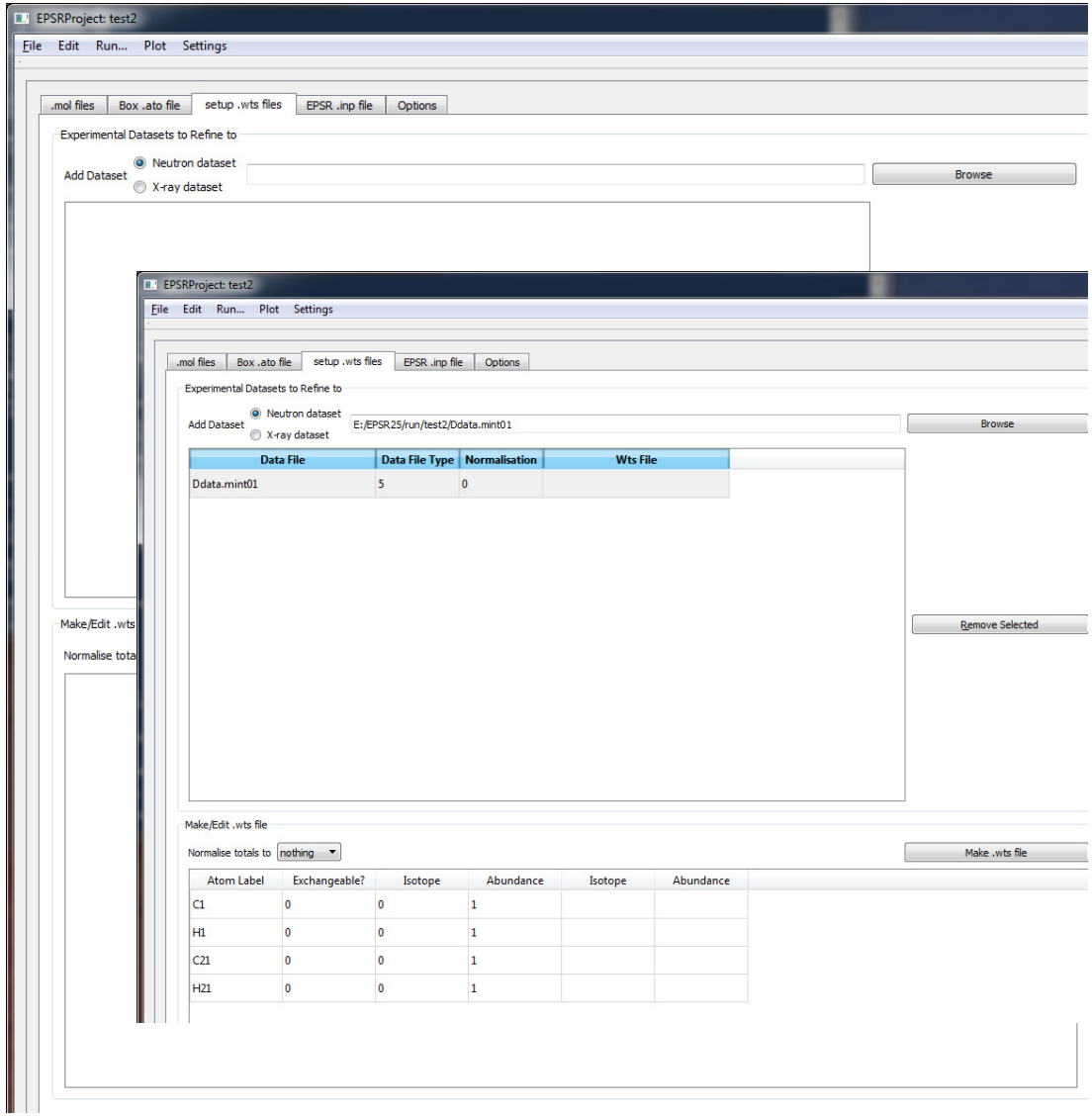
Once the simulation box has been created, the details of the box are listed here.

To make changes to the box parameters, 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.

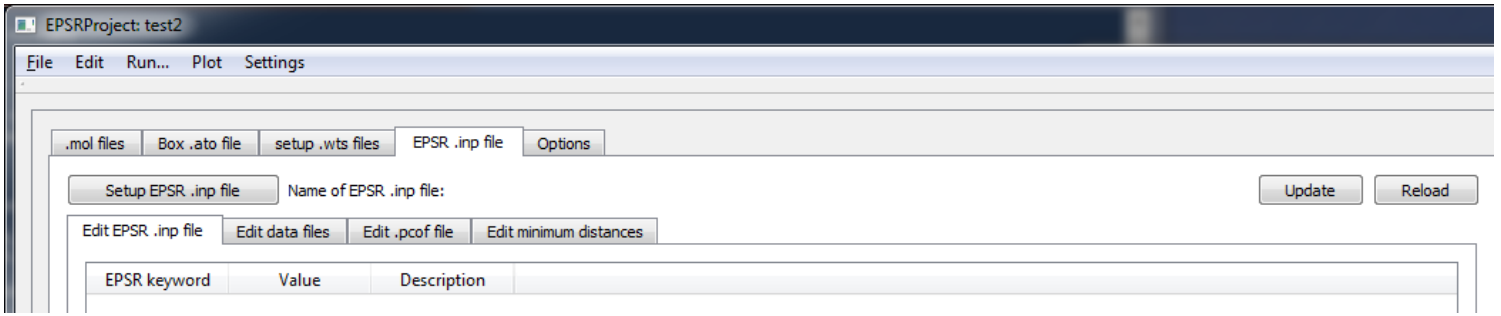
Select how the data are normalised from the drop down menu. Edit the exchangeable hydrogens (use 1 for exchanges, 0 for non-exchangeable) and the isotope (use 2 for D, 0 for natural H) and the abundance.

Then click make .wts file

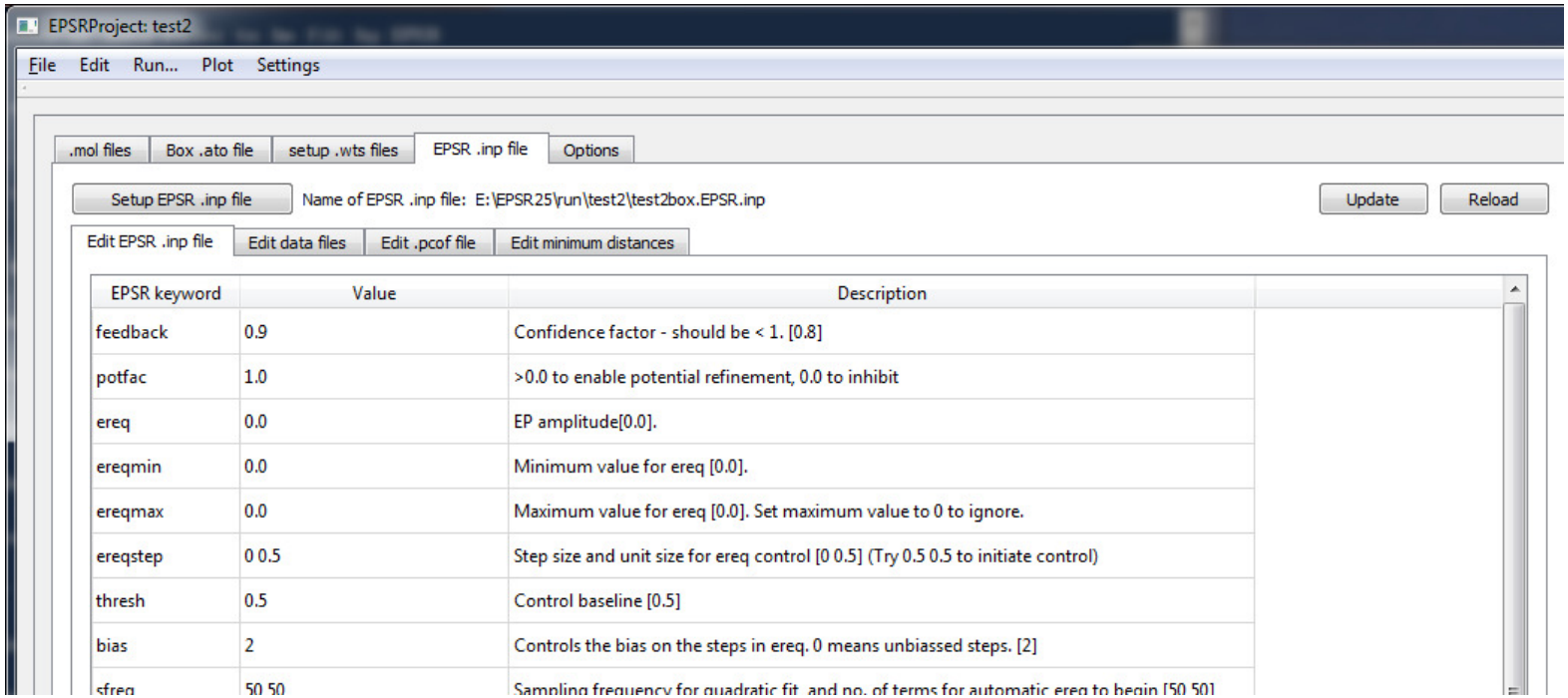
Repeat for all data files. If a mistake is made, just edit the table as necessary and then click make .wts file again.

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 run the simulation once as a check, click Run->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.

Once the simulation has been run once, the plotting windows become enabled.

Setting up EPSR outputs

- To setup EPSR to run with the output routines available within EPSRshell, click on the outputs tab and then select the appropriate routine from the dropdown menu.
- As with EPSRshell, the routine first needs to be setup correctly before it can be run.
- Either enter a name for a new routine or select an existing routine from the list and then click Setup.
- This will open a command line window where the routine can be setup in precisely the same way as it is in EPSRshell. Once the changes have been made exit the setup and save the changes.
- The new/edited routine name will now be in the existing outputs column.
- To get EPSR to run this routine while running the simulation, use the >> button to add it to the running in EPSR list and click Apply.
- Run EPSR as normal and the routine will also run (with the same frequency as in EPSRshell).
- To write an accumulated file of many frames of the simulation for analysis with the dlputils package, tick the output for dlputils box while also incrementing nsumt.

Troubleshooting

- If gnuplot is 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.
- After running addato, check the messages window (Settings->Messages window) – if there is insufficient space in the container, then some (or all) of the added .mol files will **not** 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.
- If an external program is used to make the .mol or .ato file and EPSRgui cannot open the file or errors while running the next routine, check the format of the .mol or .ato file.

Bug reporting

- EPSRgui is still in its infancy – if it crashes/doesn't do what you expect it to, please let me know (email sam.callear@stfc.ac.uk) with a few details about what you were doing before it crashed. Thanks!