EPSRgui v1.0 manual

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Installing EPSR

- Go to the Disord Matt Facebook page for links to download the latest distribution of 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 where the java.exe is on your computer.
- For linux make sure the system_mopac path is appropriate for your computer (and with correct permissions) and that java is installed and executable on your computer.

Installing EPSRgui

- Windows: Download the EPSRgui folder from ftp://ftp.nd.rl.ac.uk/scratch/EPSRgui and copy the whole folder to your hard drive (username:anonymous password*:your email address*; open with Windows Explorer and click View, Open ftp site in File Explorer to copy the entire folder). To run ESPRgui, double click the executable.
- Linux: Ensure the Qt5 libraries *qt5-default* and *qt5-qmake* are installed on your system (Qt4 is not compatible). 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.
- EPSRgui automatically saves any files added to or removed from the project so that the project can be opened again later and all associated files will be remembered.

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 one of the components in the list as the container, and adds all the remaining components to this box. The 'number in box' column for the container actually means the number of containers and therefore is 1, rather than the number of molecules in that container. The atomic number density is calculated after the box has been built. Note that there can only be 1 component per ato file in the ato files to be added to the container.
  - 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.
- Remember to make the box size big enough so as half the length of the box is larger than the largest g(r) to be studied.

Example workflows

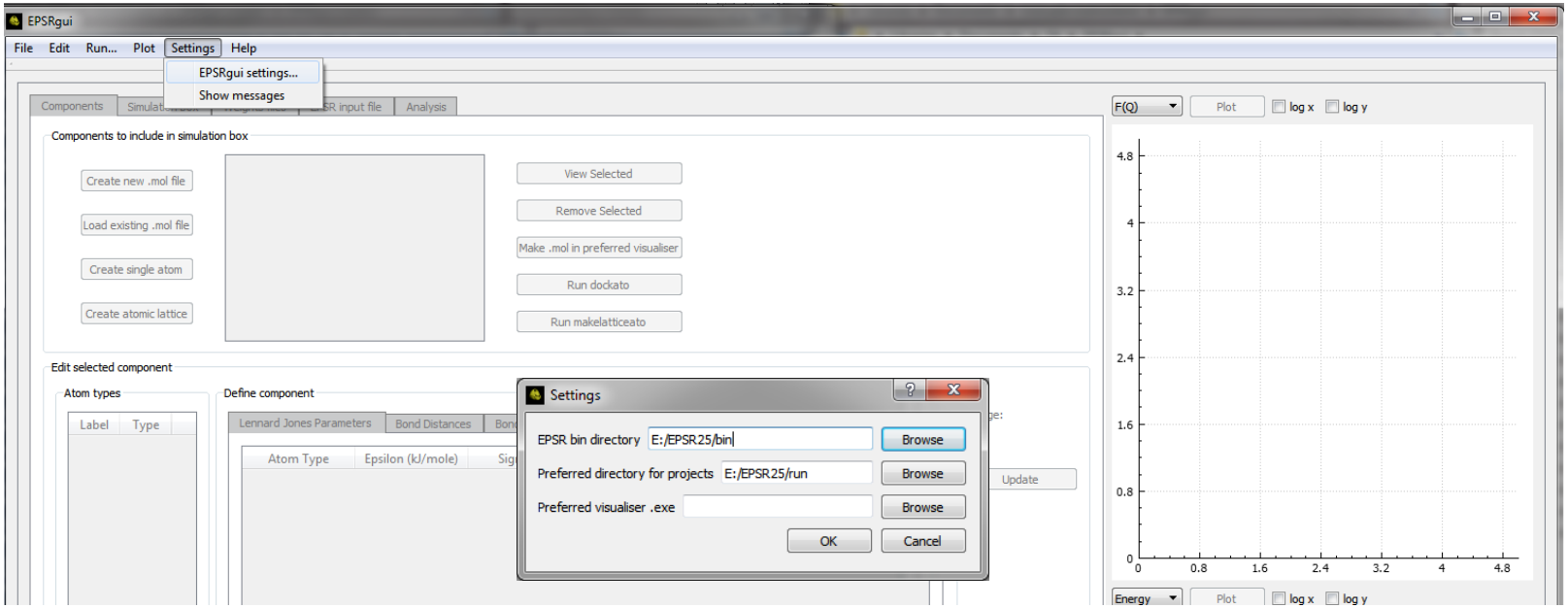
- Simple liquid
  - Create/load .mol files for each component
  - Mixato
- Amorphous atomic glass
  - Create/load atom .mol for each element
  - Mixato
- Amorphous atomic glass from lattice
  - Makelattice – tick ‘use as simulation box’
  - Change ‘Tethered?’ to ‘f’ in tethered components table, simulation box 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

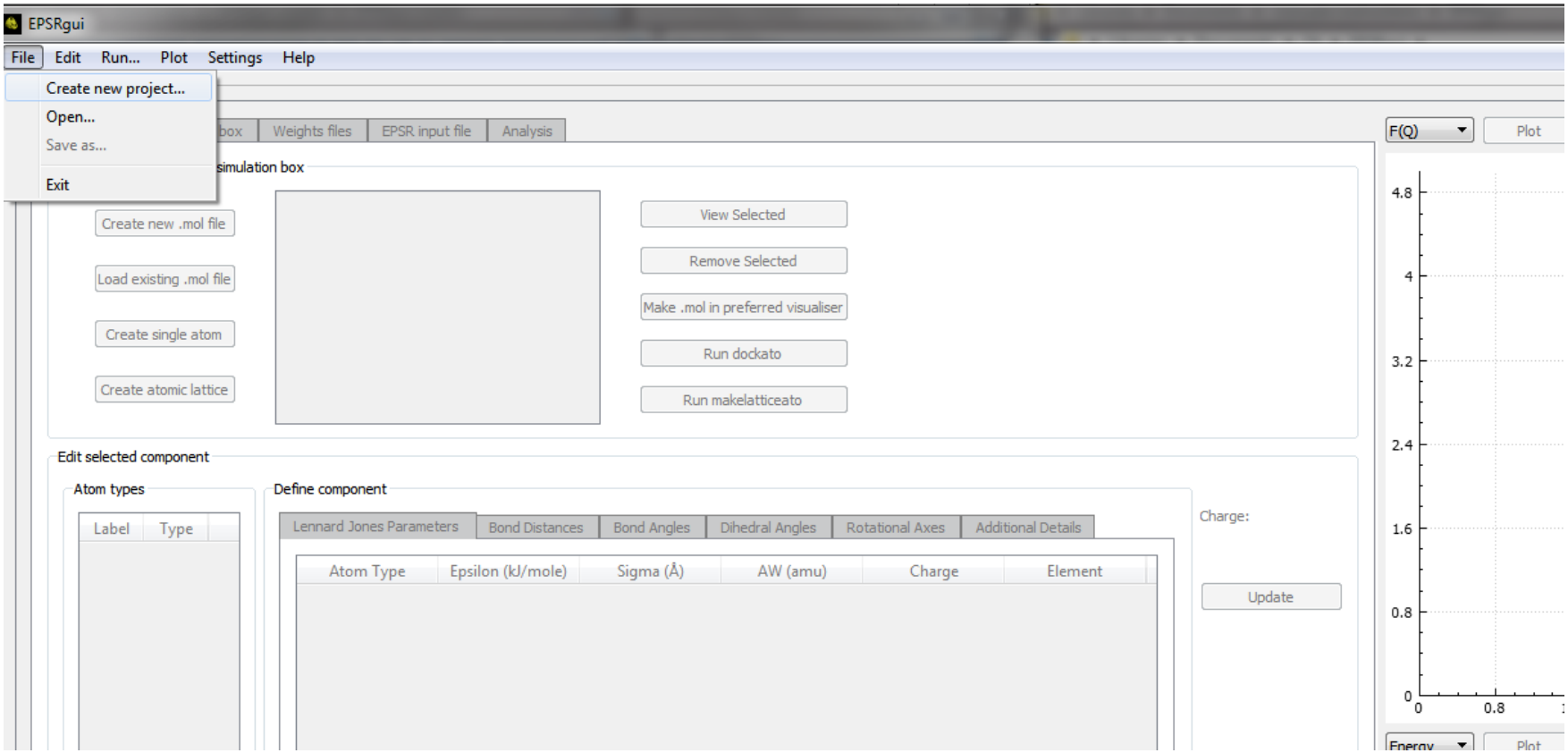
Setting up EPSRgui

In the tope menu bar click Settings->EPSRgui settings…
In the Settings dialog window that opens, click Browse to navigate the to EPSR bin directory. The MUST be defined before EPSRgui can be used.
If you would like to set a default directory where all your projects are kept, navigate to this folder in the preferred directory for projects.
A preferred visualiser executable can also be set.



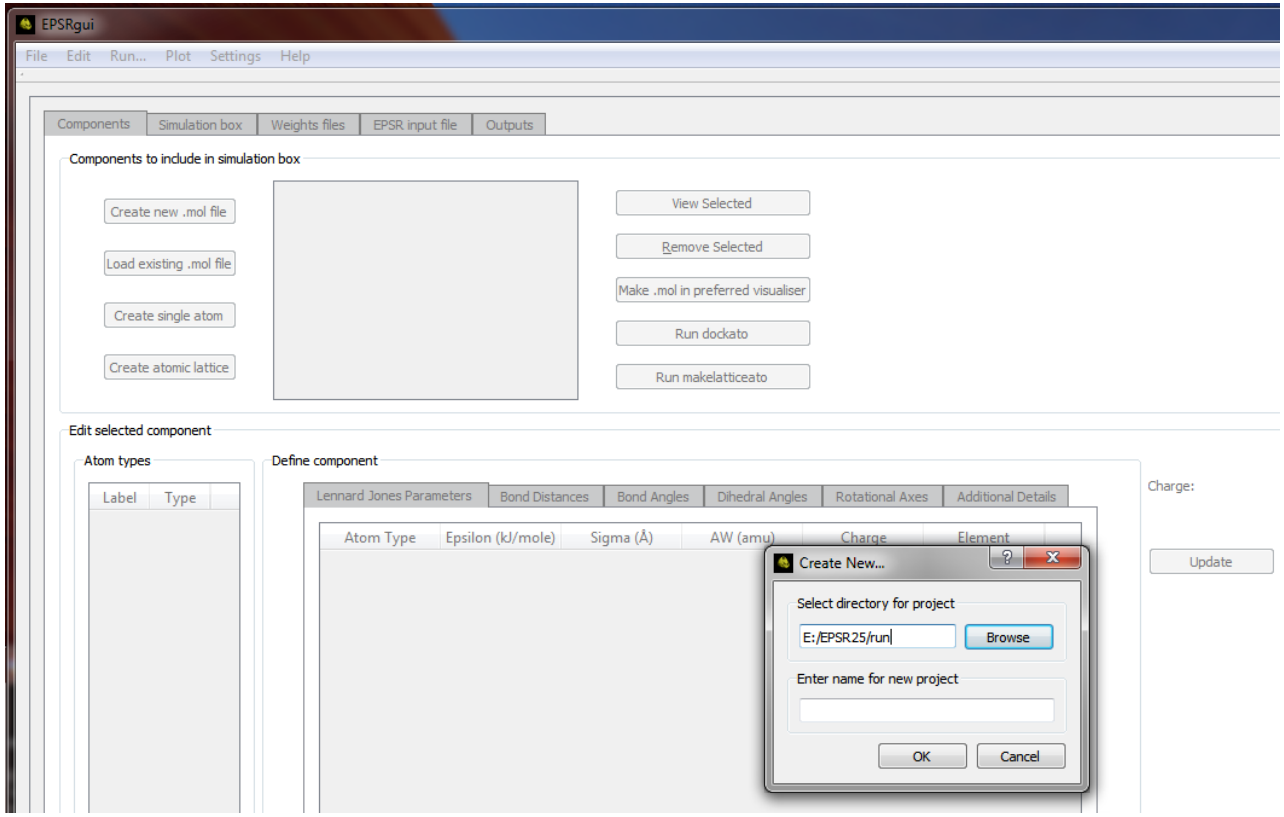
Starting a new project

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



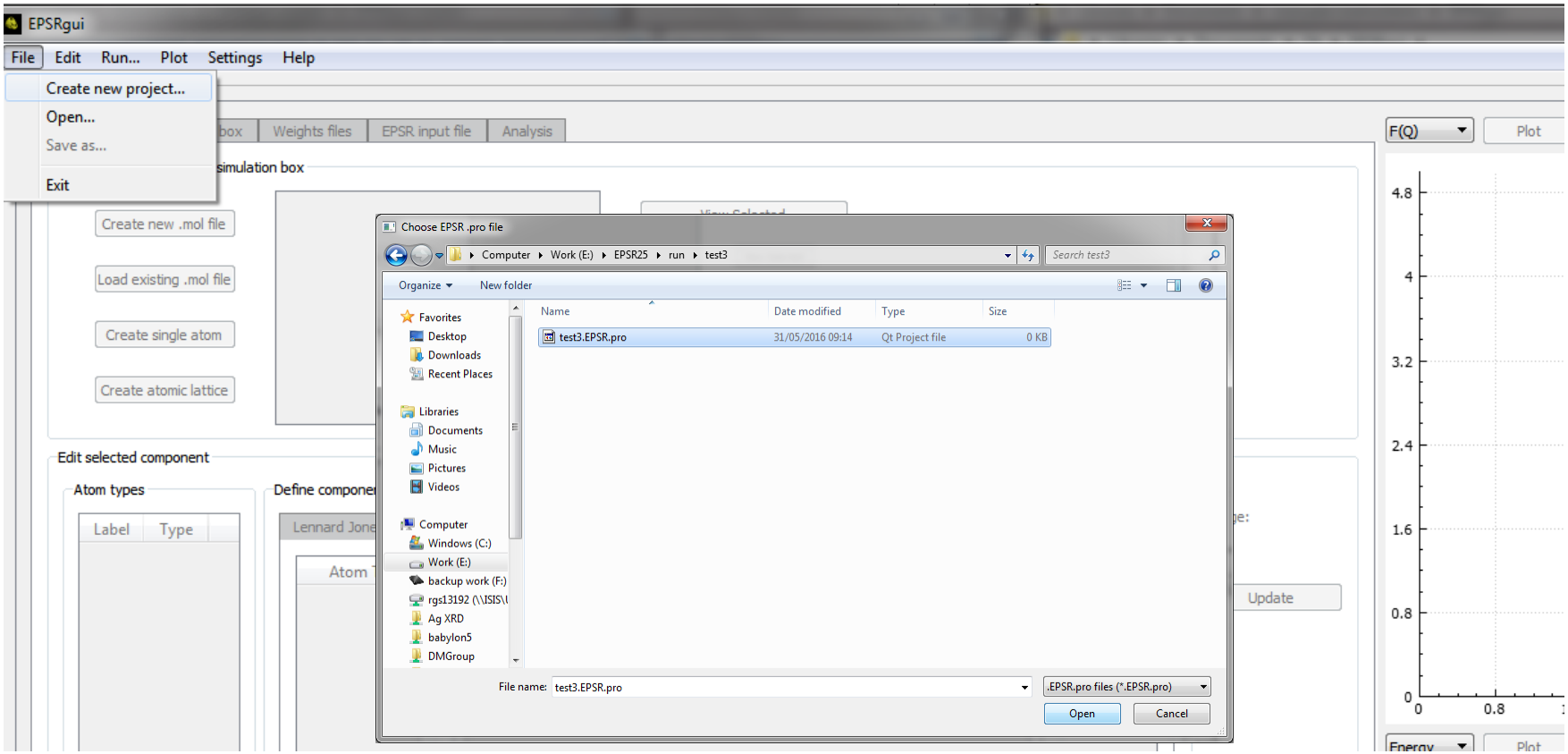
Starting a new project

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.

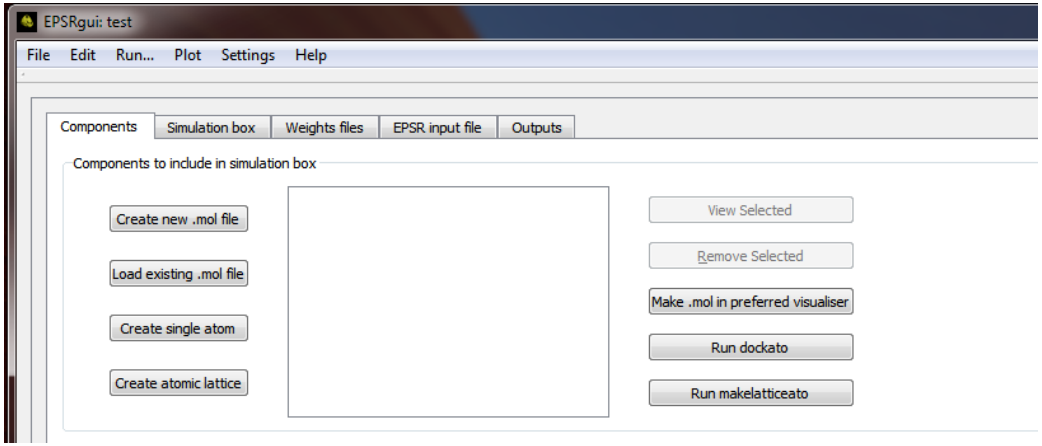


Opening an existing project

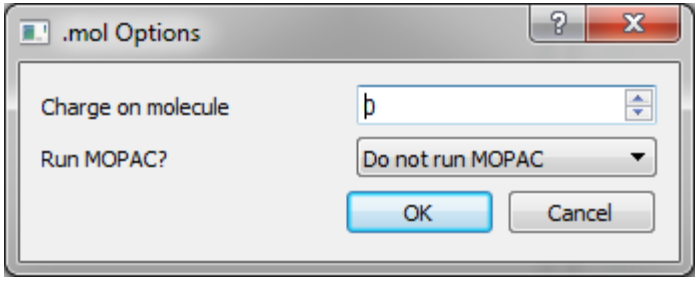
To open an existing project, click File, Open…
In the pop up window navigate to the project folder and select the XXX.EPSR.pro file and click Open



Creating a molecule in Jmol



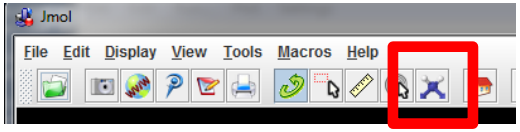
To create a new .mol file using Jmol click Create new .mol file.
In the pop up window input the charge on the molecule and whether you want to run MOPAC on the molecule, and if so which option to use (provided it exists) then click OK

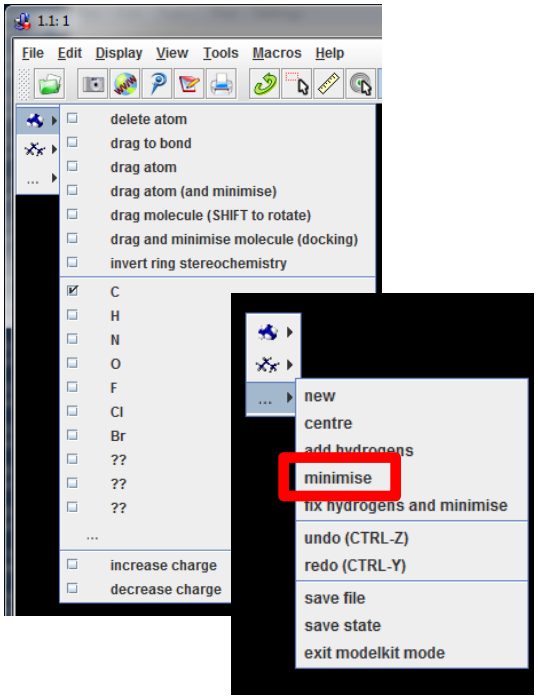


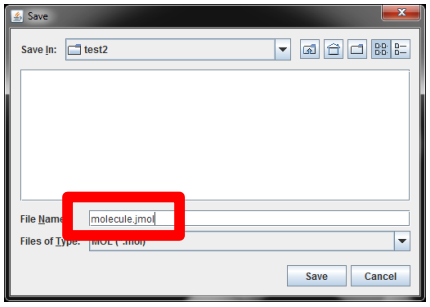
To load an existing .mol file, first put the .mol file and .ato file for the molecule in the project folder and then click load existing .mol file and select the .mol file.

Creating a molecule in Jmol

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







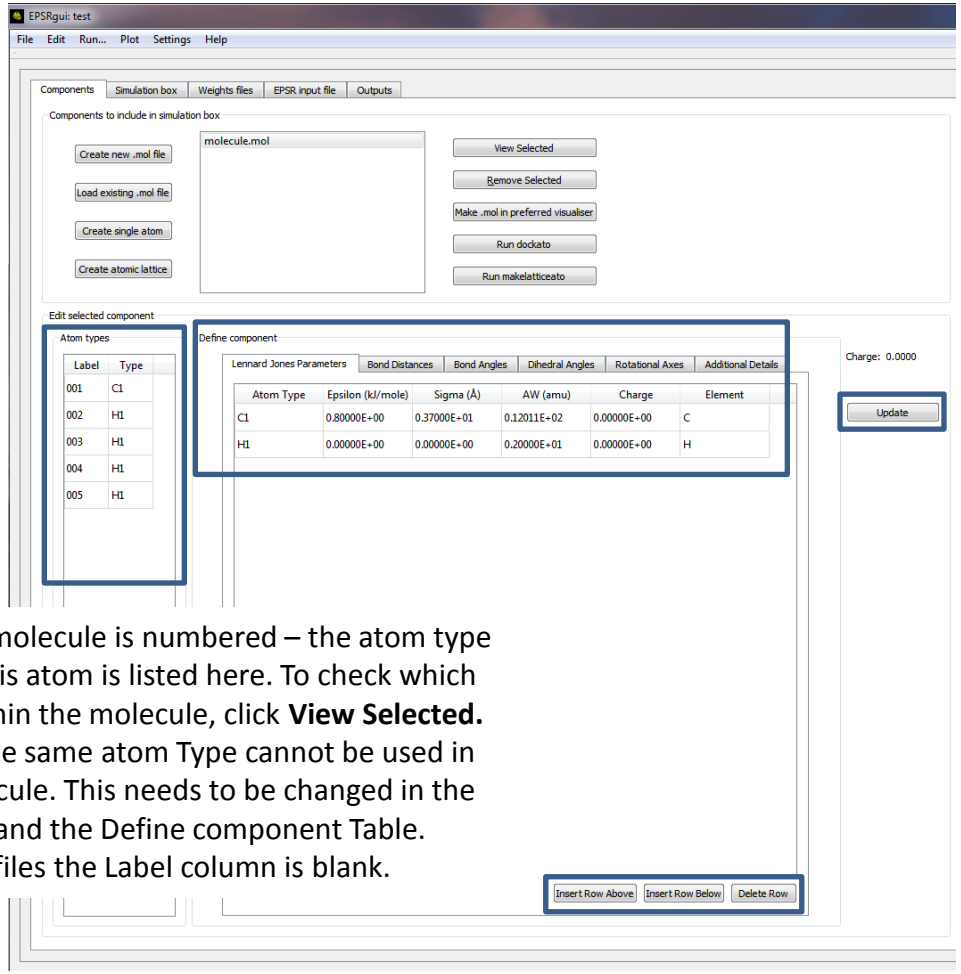
A toolbar will appear on the left hand side with all the options required for building the molecule. It auto-hides so click on the pink line or right click on the background to see the toolbar again.

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 EPSRgui.

Editing the .mol files

On saving the .jmol file, or after loading an existing .mol file, the .mol file is read into EPSRgui and if an equivalent .ato file doesn't exist, it is created. The details are shown in the tabs below:



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.** Remember that the same atom Type cannot be used in more than 1 molecule. This needs to be changed in the Atom types Table and the Define component Table.
For old style .mol files the Label column is blank.

Fill out the LJ parameters and charges appropriately, remember an atomic weight of 2 is generally used for H and D. Click update to implement the changes and recalculate the charge on the molecule (shown above the Update button).

Edit/insert/remove bond distances, angles and dihedrals to define the molecule as appropriate. Rotational axes, .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

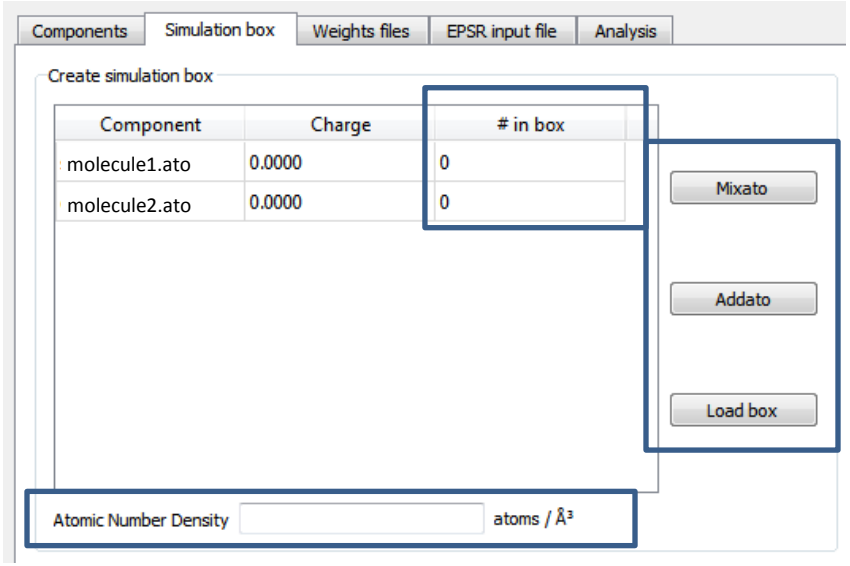
Add as many .mol files as required by clicking **Create new .mol file** or **Loading existing .mol file**.

To remove a .mol file, click **Remove selected**.

If opening an existing old style .mol file where all the atoms are positioned on 0,0,0 (check this by clicking **View selected** - if you see only 1 atom when you should see more then do the following) you will need to run fmole on the .mol file before making a box with it. To do this, click on the *Additional Details* tab and click **Run fmole on molecule**. This implements all the bond and angle etc restraints that are in the .mol file. You can then check the molecule looks as it should be clicking **View Selected** again.

For components that will be the container when using Addato, the size of the container can be seen in the *Additional Details* tab – to change the size of this box, click **Run changeato for selected file**. If the component needs to be tethered, tick the **Tethered?** check box and input the number for the tethering atom (use 0 for the centre of mass of the component), the tethering tolerance (a small number is more tightly tethered) and the tethering origin coordinates (use 0.0 0.0 0.0 for the centre of the box). Then click **Update** to implement the changes.

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.

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

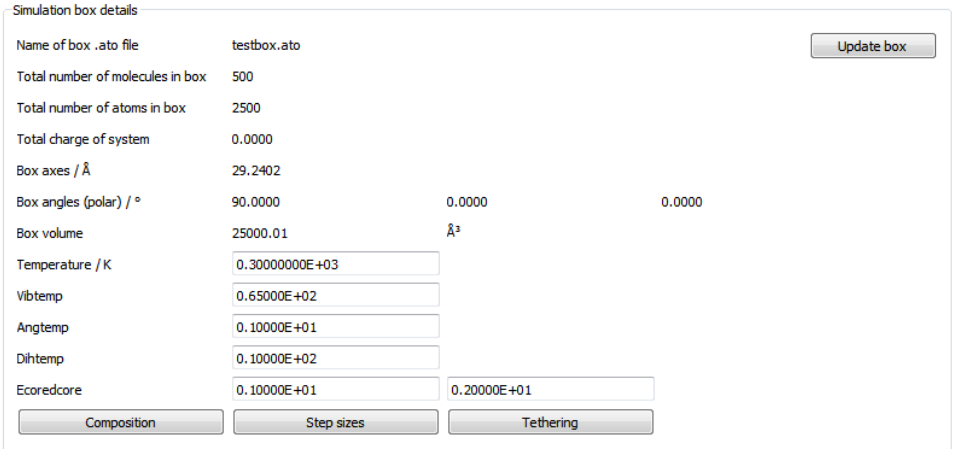
- Click **Addato** and choose the container and how many of the component molecules you want to add to the container (ensure the container is the correct size for the number of molecules you want to add as the atomic number density is not used during Addato).
- Check in the messages window (*Settings*->Show messages) that all of the components were successfully added to the box.
- The atomic number density will show the resulting density of the simulation box after Addato.

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

- In the *Components* tab, load the .mol files applicable 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.
- Click **Load Box** and choose the box .ato file.
- 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)

Simulation box details

Once the simulation box has been created, the details of the box are listed at the bottom of the Simulation box tab:



To make changes to the simulation settings such as the level of bond and angle restraints and ecoredcore, change the values here and then click **Update box**.

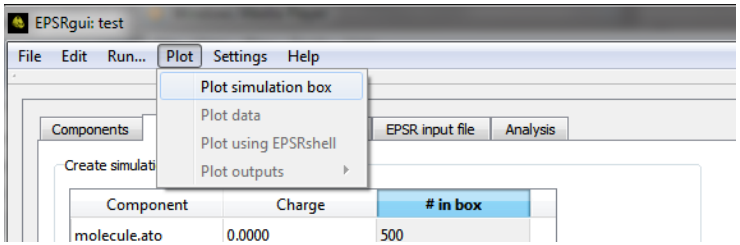
For additional settings such as step size, click the step sizes button.

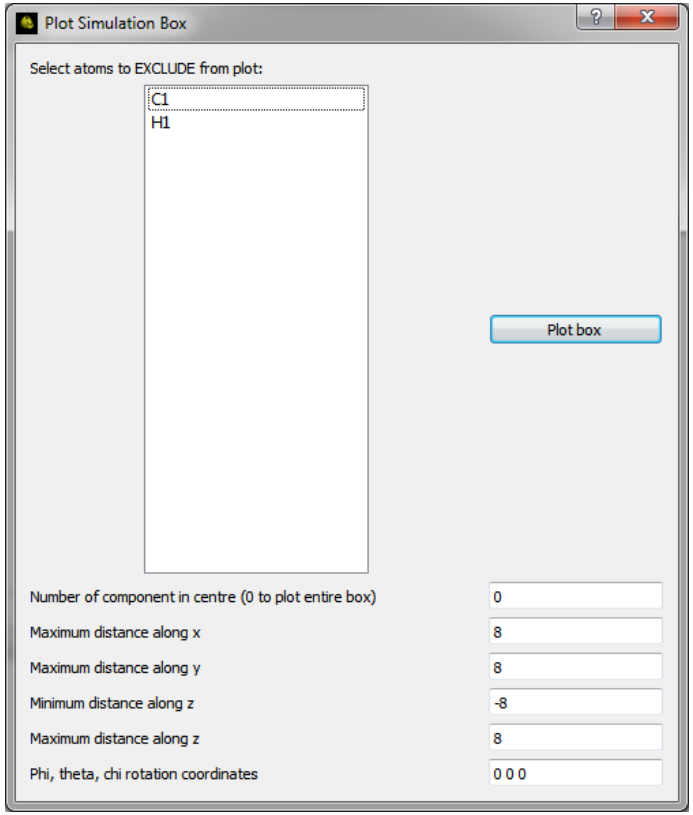
If a component in the box is tethered this will be shown on clicking the Tethering button which shows/hides the tethered components. To un-tether a component, type F in the Tethered? column and delete the Tether atom. To tether a component, type T in the Tethered? Column and type 0 to use the centre of mass of the component, or the numerical atom label to specify an atom as the point to tether. Then type a small number for the tethering tolerance.

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.

For any additional changes not listed here, click **Run changeato for box -** note that this will run changeato in a command prompt/terminal window.

Plotting the simulation box





In the top menu bar, click Plot->Plot simulation box. The dialog window that opens gives options as to which atoms and how much of the box to plot.

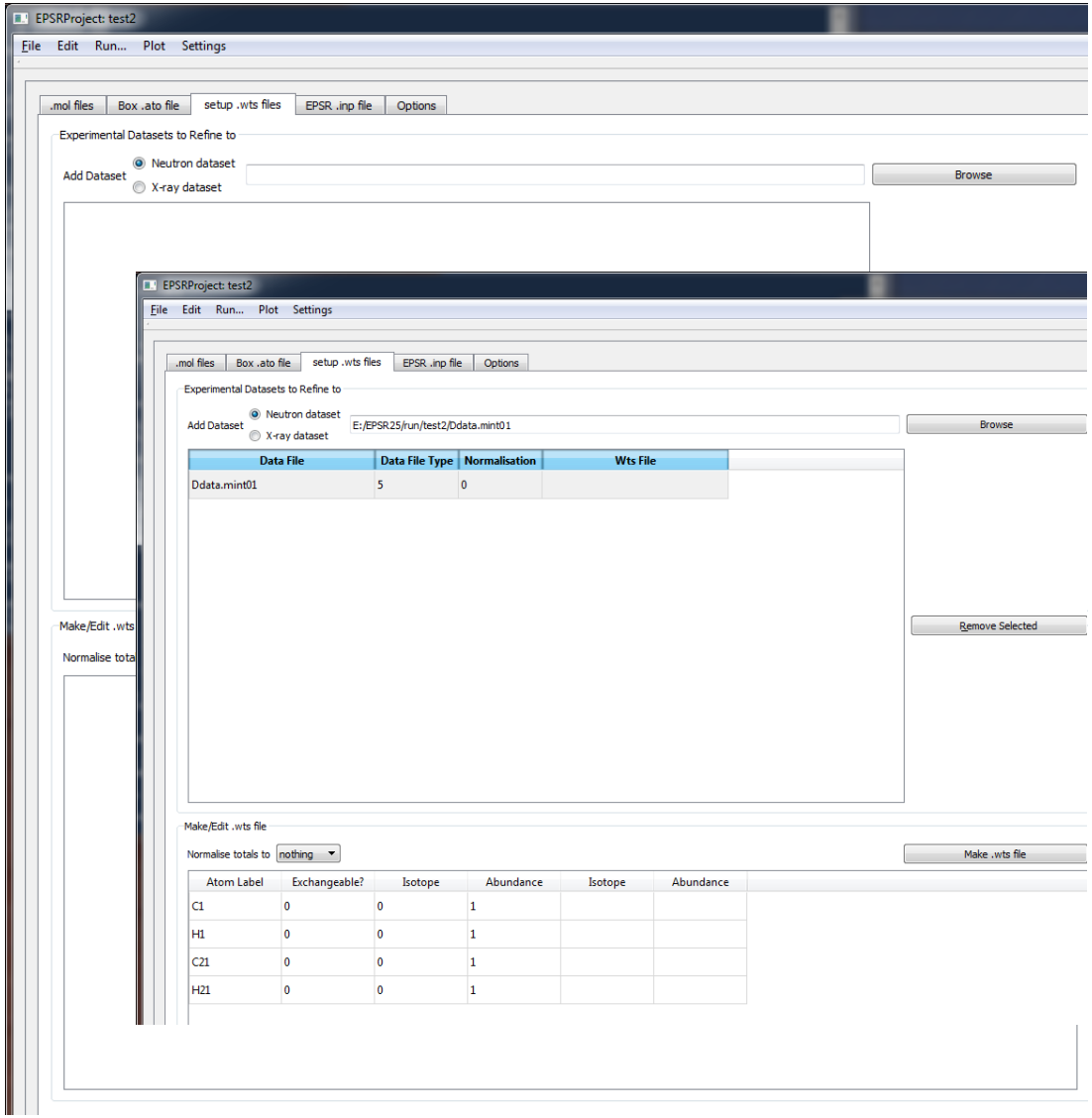
To plot the whole box click **Plot box.**

To plot a subset of the box, click on the atoms to be excluded from the plot (use Ctrl to select multiple atoms) and click **Plot box**.

To plot only a part of the box, input the numerical atom label for the atom that you want in the middle of the box and then edit the distances along x, y and z to specify how much of the box is to be plotted. To rotate the box, edit the phi, theta, chi coordinates. Then click **Plot box**.

This shows a snapshot of the current simulation and does not update as the simulation is running.

Weights files



To prepare the weights files for the system, select whether the data are neutron data or X-ray data, then click **Browse** and select the data file (if it is not in the project directory it will automatically be copied to the project directory)

Select how the data are normalised from the drop down menu. Edit the exchangeable hydrogens (use 1 if the atom exchanges and 0 for non-exchangeable) and the Isotope (use 2 for D and 0 for natural H) and the Abundance of each isotope (as a fraction of 1).

Then click **Make .wts file**.

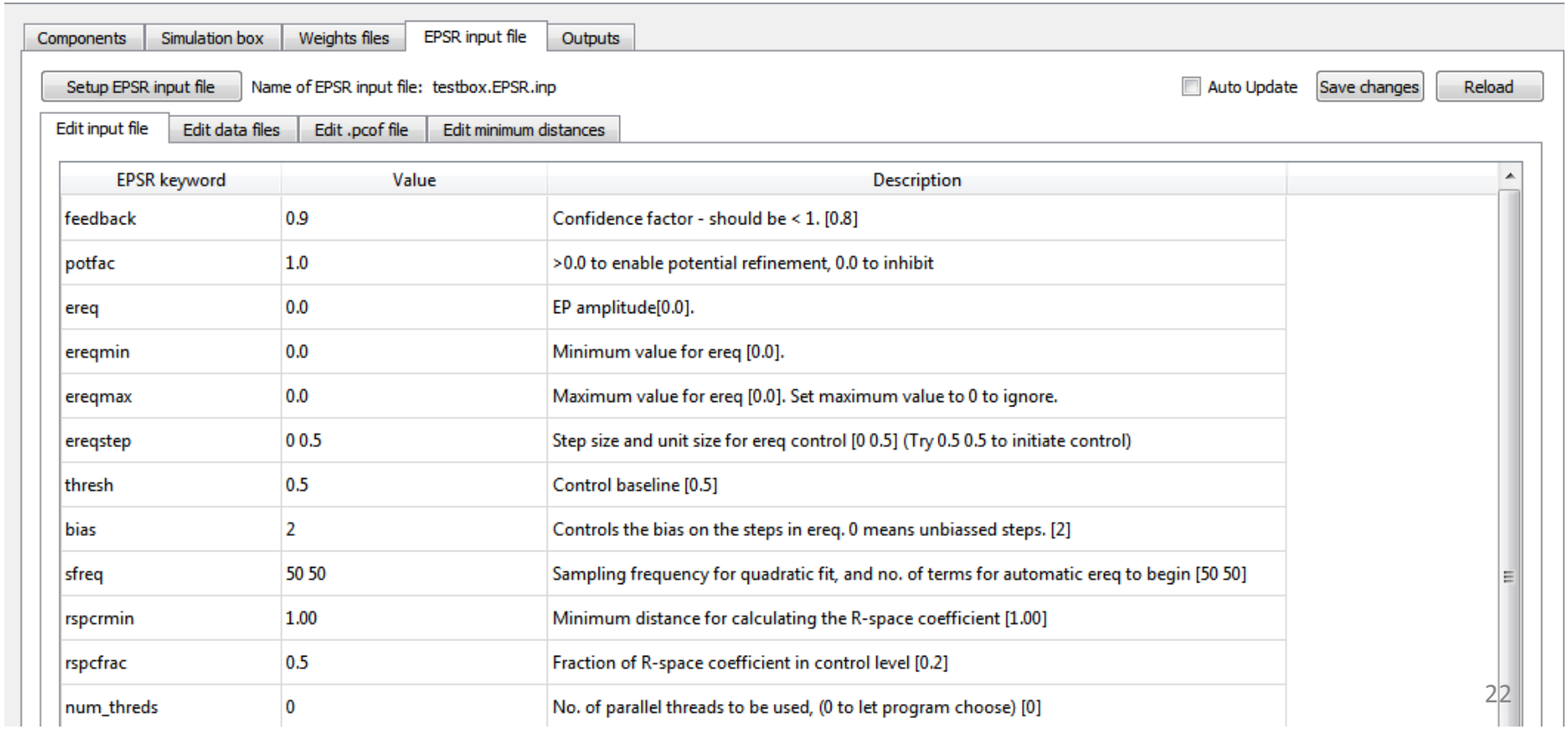
Repeat for all data files. If a mistake is made, click on the data file you want to change and edit the scattering weights table as necessary and then click **Make .wts file** again.

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

EPSR.inp file

Once the box and weights files are setup the simulation parameters can be setup. Click **Setup EPSR input file**. All of the parameters in the previous tabs are carried forwards into the EPSR.inp file.

To make changes edit the Value column as appropriate - changes can also be made to the .pcof file, the minimum distances list between atom pairs (intermolecular) and the data file details. To save the changes without running EPSR, click **Save changes**. Otherwise, the changes will be saved on running EPSR.



EPSR keyword	Value	Description
feedback	0.9	Confidence factor - should be < 1. [0.8]
potfac	1.0	>0.0 to enable potential refinement, 0.0 to inhibit
ereq	0.0	EP amplitude[0.0].
ereqmin	0.0	Minimum value for ereq [0.0].
ereqmax	0.0	Maximum value for ereq [0.0]. Set maximum value to 0 to ignore.
ereqstep	0 0.5	Step size and unit size for ereq control [0 0.5] (Try 0.5 0.5 to initiate control)
thresh	0.5	Control baseline [0.5]
bias	2	Controls the bias on the steps in ereq. 0 means unbiassed steps. [2]
sfreq	50 50	Sampling frequency for quadratic fit, and no. of terms for automatic ereq to begin [50 50]
rspcrmin	1.00	Minimum distance for calculating the R-space coefficient [1.00]
rspcfrac	0.5	Fraction of R-space coefficient in control level [0.2]
num_threds	0	No. of parallel threads to be used, (0 to let program choose) [0]

Running the simulation

To run the simulation, click *Run…->Run* EPSR. This first saves the values in the tables to the EPSR .inp and .pcof files before running EPSR:

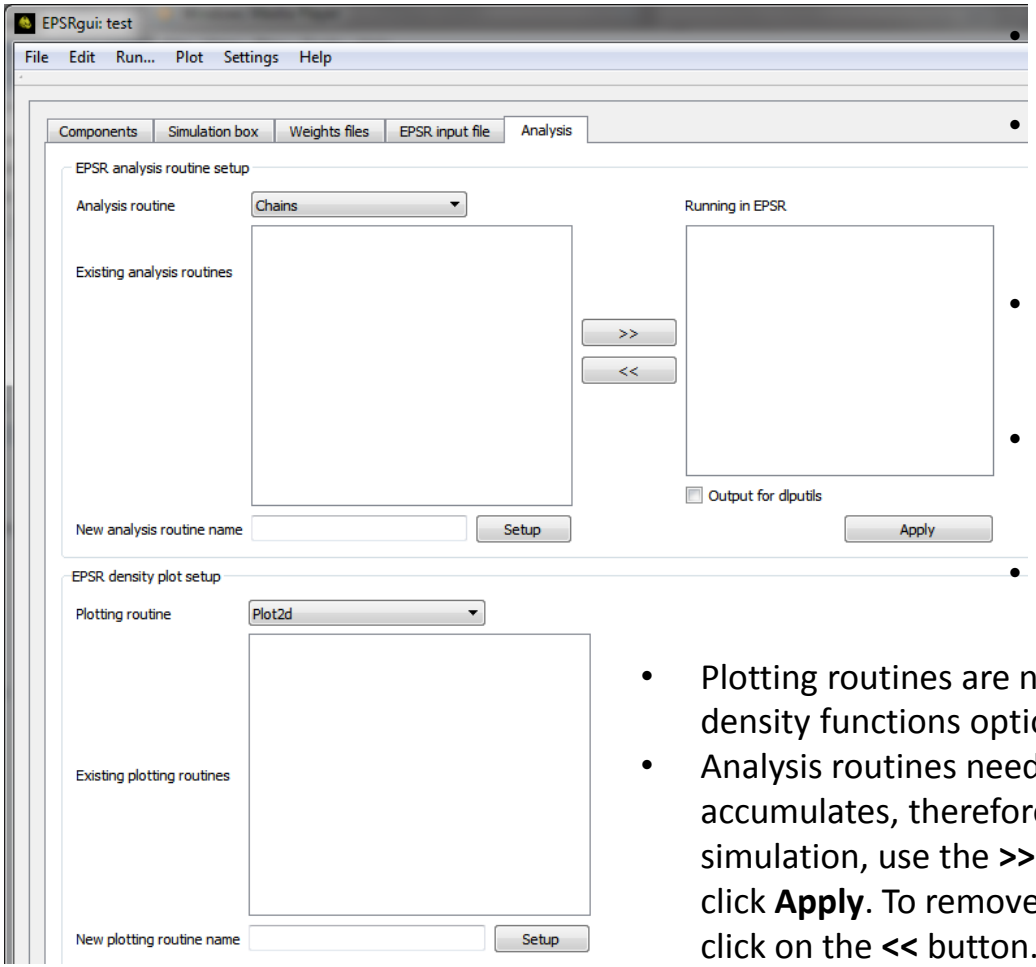
- To run the simulation once as a check, click *Run…->Run epsr check*.
- To run EPSR iteratively, click *Run…->Run EPSR*.
- To stop EPSR running iteratively, click *Run…-> Stop EPSR*.

EPSR will then 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. Note that most things are not editable while EPSR is running.

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

Setting up EPSR analysis routines

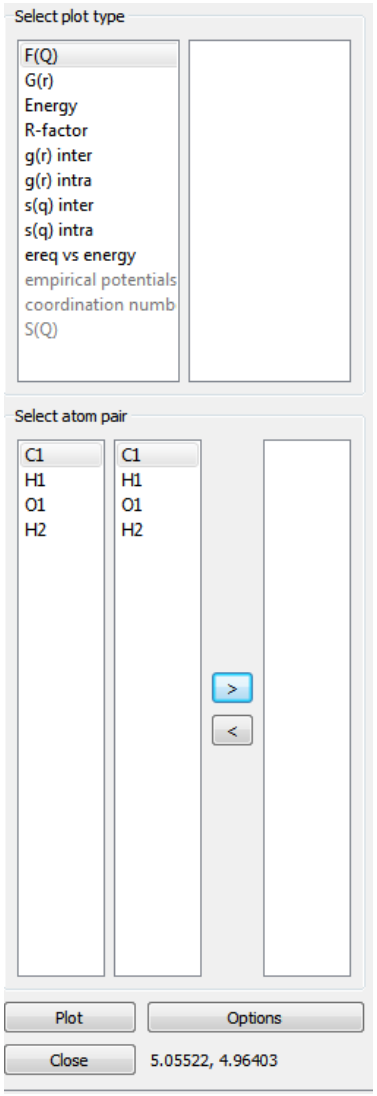


Once the simulation fits the data well, analysis of the simulation box can be started.

To setup EPSR to run with the analysis or plotting routines available within EPSRshell, click on the *Analysis* tab and then select the appropriate routine from the dropdown menu.

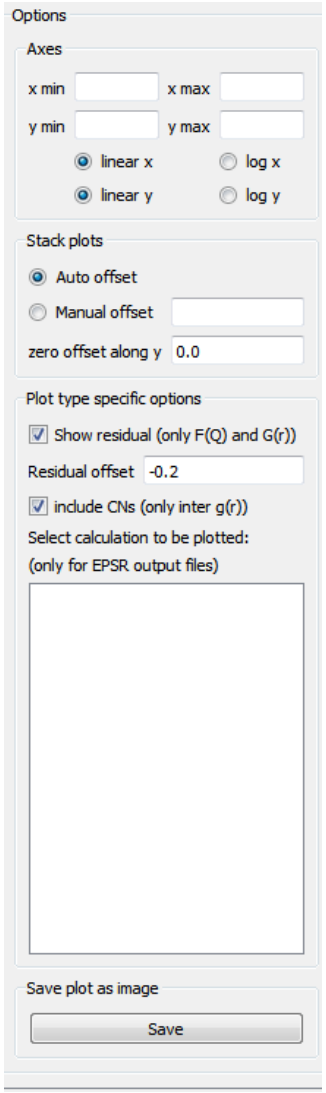
- Either enter a name for a new output routine or select an existing output routine from the list and then click **Setup**.
- In the dialog window that appear, fill in the appropriate settings for the setup file and click **Ok**.
- The new/edited routine name will now be visible in the existing routines column.
- Plotting routines are now setup and can be plotted from the Plot->Plot density functions option in the top menu bar.
- Analysis routines need to be run for multiple iterations while EPSR accumulates, therefore, 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**. To remove a routine from the EPSR script, select it and then click on the **<<** button.
- Now, when EPSR is run as usual, the routine will also run (note this might not be on every iteration, depending on the routine).
- To write an accumulated file of many frames of the simulation for analysis with the dlputils package, tick the Output for dlputils box and click **Apply** to write the xyz file while also incrementing nsumt.

Plotting



- In addition to the two small graphs in the main window, there are additional plotting options:
  - To plot with gnuplot from EPSRshell click *Plot->Plot using EPSRshell*.
  - To plot 3d surfaces (e.g. after running sharm) click *Plot->Plot in Jmol.*
  - To make larger plots and also plot partials etc click *Plot->Plot data.*
- Select the plot you want to plot from either the left hand column which are the standard plots from EPSR, or the right hand column which lists the EPSR output calculations that have been run.
- These plots will never automatically update, so click **Plot** again to update them.
- To plot anything that requires a pair of atoms to be specified, first select the first atom of the pair from the first column of atoms and then select the 2nd atom from the second column. Then click the **>>** button to add the pair to the list of pairs to be plotted. Repeat this until all the pairs you want to plot are listed, then click plot. To remove a pair from the list, click on it and then click **<<**.
- To zoom in and out by equal amounts in the x and y axis, use the roller button on the mouse.
- To move to a different area of the plot, left click on it and drag the plot to see the area you want to view.
- To zoom in or out along the x axis only, hold down shift and use the roller button on the mouse.
- To zoom in or out along the y axis only, hold down control and use the roller button on the mouse.

Plotting



- For additional plotting options, click the **Options** button at the bottom right hand corner of the window. To hide the options menu click the same button again.
- To set the axes limits, enter a number into the appropriate axis box – if the box is blank a default value will be used.
- To change between linear and log axes, click the log or linear buttons.
- For the stack plots in the F(Q) and G(r) plots, the offset between the datasets can be automatically chosen (Auto offset) or chosen manually selecting Manual offset and entering an offset. This offset will be used between each of the datasets.
- To shift all the datasets along the y axis (e.g. for use when plotting on a log scale), change the zero offset along y.
- To show/hide the residual or difference curves for the F(Q) and G(r) plots, tick/untick the Show residual tick box. The offset of the residual with respect to the calculated and experimental datasets can also be changed.
- For the intermolecular partial radial distribution functions (g(r) inter) the coordination number can be displayed on the plot or not by ticking the include CNs tick box.
- When plotting the EPSR output calculations, often there is more than one calculation per file – the first will be plotted by default, so to plot a different calculation select it from the list.
- The plot can be saved as a .jpg/.png/.bmp by clicking Save.

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.
- If a simulation is run in Linux and then run in Windows (or vice versa), note that the system_commands.txt might not be appropriate for the operating system and this will prevent the gui from running the EPSR routines. Either try to avoid doing this, or make sure the system_commands.txt is relevant to the operating system when working on the simulation.
- If using an 'old style' .mol file where all the atom coordinates are 0,0,0, run fmole on the .mol file before using it to make a box. This will quickly move the atoms to the correct positions in the component .ato file. (Running fmole on the box in order to do this will take so many fmole iterations that it is likely the molecule won't be in the correct configuration.)
- To remove or add a datafile after having setup the EPSR input file, 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. To save any settings in the input file, copy the input file and rename it before deleting the original via the gui. The settings can then be copied into the new input file. [This process will be tidied up in a later release.]

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!