



# **GUI Manual**

***Amsterdam Modeling Suite 2019***

**[www.scm.com](http://www.scm.com)**

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**GENERAL**

## 1.1 Introduction

This document will provide background information for the Graphical User Interface (GUI, ADF-GUI, BAND-GUI and so on), part of the ADF package.

The purpose of this document is to give more detailed background information on how the GUI operates. It will not explain how to use it in detail. For that reason, we strongly suggest that before reading this document, you first check the GUI tutorials.

The current version of the GUI was developed by O. Visser, and L. Groot. Other authors include M. Luppi (artwork), L. Hong (NMR spin-spin coupling in ADFspectra), M. Koenis (VCD tools in ADFspectra), K. Salimans (GUI support for QE CPMD) and the SCM developer team. Thanks to M. Mouthaan for testing and documentation.

## 1.2 Release 2019

In comparison to ADF-GUI 2018, the ADF-GUI 2019 release offers the following new functionality:

- General GUI features:
  - AMS IRC support
- ADFinput:
  - Polymer builder
  - GFN1-xTB support
  - GCMC support for all AMS engines
  - CVHD support for all AMS engines
  - Molecule Gun support for all AMS engines
  - Molecule Sink support for all AMS engines
  - Warn if changes by the user are not in the run script because controls are disabled (for example, changing a geometry optimization detail when performing a single point run). In the GUI Preferences this warning may be turned off
  - Centroids (special dummies, connected to and moving with some atoms, use to control rings etc)
- ADFmovie:
  - Handle AMS MD results
  - Handle AMS Molecule analysis (after MD)

- For remote AMS jobs, update the local copy automatically (frequency in ADFjobs prefs)
- ADFview:
  - Irrep densities
- ADFtrain:
  - New GUI module ADFtrain (to set up training set and force field with ReaxFF)



## 2.1 Mouse

A three-button mouse is also very convenient for using the ADF-GUI, and on a Mac you can use a Magic mouse for this purpose. To get three buttons (instead of the standard one or two), download and install one of the free utilities BetterTouchTool or MagicPrefs, and configure it to add a middle click.

## 2.2 Running Remotely

To use ADFjobs with remote machines, you need to set up ssh first. You should take care to configure things such that you do not need to type a password when you access your remote machine. To do this you need to:

- create **keys**,
- run an **ssh agent**,
- add your public key to the **authorized\_keys** file on the remote machine.
- set up a ssh config file, if needed. This allows you to automatically set options, like the user name to use on the remote machine.

Thus, users (and ADFjobs) should be able to use ssh to log in to the remote machine without ever needing to enter a password.

If you are using OpenSSH (typically on Linux machine or MacOSX) you can make the communication with the remote machine much more efficient by setting the `SCM_SSH_MULTIPLEXING` environment variable to yes (in the GUI Preferences module).

ADFjobs does not store passwords, it always uses the ssh command to communicate with remote systems.

For more information, consult your ssh documentation or one of the many guides on the internet.

## 2.3 OpenGL3.2+, fallback mode

The GUI needs OpenGL 3.2 or later. Using it results in a much better performance, especially for bigger systems. Also some new graphical features depend on it. That OpenGL version may not be available when you are running on old hardware or OS, or when you are running remotely via X11 with GLX or some remote desktop solutions.

When the GUI detects a problem with the OpenGL version it will automatically activate a fallback option. That will normally just run, but it will be significantly slower, and of course the features depending on OpenGL 3.2 will be missing. We advise that you try to update your system to solve this issue. For remote use of a linux machine a solution could be the use of VirtualGL.

For more details please see the Installation manual.

## 2.4 Font issues

The GUI used unicode characters in many places. For example, the proper characters for Angstrom, degrees Celcius, and many more. You can see examples by starting ADFinput, selecting a Geometry Optimization, and then going to the details page (by clicking the ... button). There you should see a couple of Angstrom symbols if everything is working as intended.

On most machines this will just work out of the box. If not, the issue might be that the default font on the machine does not support such characters. Try installing a font line DejaVU Sans and Monospace DejaVu. On Centos you can do this (as root) with the command::

```
yum install dejavu-sans-fonts dejavu-sans-mono-fonts dejavu-serif-fonts
```

## 2.5 ADFjobs Queues

Defining proper queues in ADFjobs will making the GUI much easier. For example, you can run as easily on a remote compute cluster that you have access to as on your local desktop. ADFjobs will handle all the details like transferring input and output files, and you can even monitor the progress of running jobs as if they were running on your local machine.

So you should take some time to set up the queues correctly. It is possible that there are predefined queues on your remote machine. Then you can configure ADFjobs to automatically use those queues. You can find a description of the ADFjobs queues and how to set them up later in *this manual* (page 39).

## 2.6 Quantum ESPRESSO

Quantum ESPRESSO is an open source package that can perform plane wave SCF calculations, among other things. See [www.quantum-espresso.org](http://www.quantum-espresso.org) (<http://www.quantum-espresso.org>) for details.

Quantum ESPRESSO is *not* included in the ADF distribution. The GUI works with the standard Quantum ESPRESSO distribution (version 6.2), no changes have been made.

The easiest way to install it is just to open ADFinput and go to the Quantum ESPRESSO section. Then it will be installed in \$ADFBIN and \$ADFHOMe/atomicdata for the pseudo potentials, or in "\$HOME/Library/Application Support/SCM" (on a mac). The binaries will be in a folder qe6.0, and the pseudo potentials will be in a folder upf\_files.

To force installation of Quantum ESPRESSO (for example to re-install it to make sure you have a clean version), use the **Help** → **(Re)Install Quantum ESPRESSO** command as available in most of the GUI modules. Another way is to run the \$ADFBIN/get\_QuantumEspresso.sh shell script.

Alternatively, the precompiled Quantum ESPRESSO binaries are [available](https://www.scm.com/support/downloads/quantum-espresso-binaries/) (<https://www.scm.com/support/downloads/quantum-espresso-binaries/>) from the SCM web site.

The search path for Quantum ESPRESSO by the GUI and by the run scripts made by the GUI is:

1. \$QE\_BIN (and \$PSEUDO\_DIR for the pseudo potentials)
2. "\$HOME/Library/Application Support/SCM"
3. \$ADFBIN (and \$ADFHOMe/atomicdata for the pseudo potentials)

4. `"/Library/Application Support/SCM"`

On a mac you can make the Quantum ESPRESSO installation available to all users by moving it from the `$HOME/Library/Application Support/SCM` folder to the global `/Library/Application Support/SCM` folder. Obviously all users need proper permissions to access these files.



## SCM MENU

All GUI modules have an SCM menu. The SCM menu is the leftmost menu in all modules, and is represented by either the SCM-logo or the text SCM.

In general, when you select a command from the SCM menu you will switch to the selected module, showing the same job as you have open in the current module. If such a module is already running with that particular job open, it will be brought to the front. If you use the SCM menu to open the same module as is currently active, it will start another blank copy of this module. Thus the SCM menu is very convenient to quickly switch between the already open windows belonging to the same job.

As a shortcut you can also right-click on a job name in ADFjobs, and the SCM menu will appear with the job you clicked on selected.

In ADFjobs the currently selected job will be used with the SCM menu. Thus, if you have one job selected, using the **SCM** → **View** command will start or switch to ADFview, showing the results of the selected job. If you have no job selected, or more than one, the selected module will start blank.

One important exception within ADFjobs: the Input module will always start a new blank version. If you wish to show the input GUI for the selected job you need to click in the icon in front of it (reading 'ADF', 'BAND', or some other job type).

The SCM menu also allows you access to preferences for that are used by all GUI modules: **SCM** → **Preferences**

In some cases a GUI module is able to open several file types. For example, ADFmovie can open the logfile or the .t21 file of a calculation. By selecting a file in ADFjobs (after opening the job by clicking on the triangle) you can force ADFmovie to open the .t21 or the .logfile. In a similar way, you can force ADFview to open a .t21 or a .t41 file.

The **SCM** → **Quit** and **SCM** → **Quit All** menu commands will close windows: the Quit command will close all windows belonging to the current job, the Quit All command will close all open GUI windows, as well as any invisible background processes belonging to the GUI (scmd and scmjobd).



## BACKGROUND PROCESSES WITH NO INTERFACE

### 4.1 scmd: communication between GUI modules

The scmd process should always be running when any of the GUI modules is active. You should have one scmd process (per user, if you are working with multiple users). The scmd process has no window, it should normally be invisible to the user.

The purpose of the scmd process is to handle all communication between GUI modules. For example, if you use the SCM menu to start a GUI module, that command is actually handled by the scmd process. It will figure out if a new module needs to be started, or if an already open module with that particular job should be activated.

Starting jobs, and handling the local Sequential queue is also done by scmd.

Communication between the GUI modules and scmd is done using TCP/IP within the local machine. If such communications are blocked, for example by a firewall, this will make the GUI non-functional! So in case of trouble, make sure you are not blocking TCP/IP traffic within the local machine. The GUI will never accept any TCP/IP connection from outside, only from within the local machine.

### 4.2 scmjobd: monitor running jobs

The scmjobd processes are also faceless background processes that belong to the GUI. They are started and terminated as needed, normally one per queued or running job. Their task is to monitor the progress of jobs, updating the status if it changes, getting logfile results for remote jobs, and killing jobs (if you use the Kill command in ADFjobs). Even if all windows of the GUI are closed they may still continue to be present if you have queued or running jobs.

The scmjobd processes communicate with the other GUI components using TCP/IP, via the scmd process. To monitor remote jobs they will use ssh to connect to the remote machines.





## VIEWING YOUR MOLECULE

### 5.1 Molecule style: Balls and Sticks, Sticks, or Wireframe

The molecule style can be selected via the View menu (**View** → **Molecule** → ...). You can select Balls and Sticks, Sticks, Wireframe or Hidden. This choice will affect the whole molecule. Note that if you use anything else then Balls and Sticks it will become much more difficult to select an atom (as there is no ball representing it).

You can also use different styles at the same time, for different regions. To do that, go to the Regions panel, make regions as you like, and set the molecule style from the pop-up menu per region in the Regions panel (the downward pointing triangle at the end of each region line).

### 5.2 Camera position: view direction

You can use the mouse to view your molecule from a different position.

In some situations you may want to view your molecule from some very specific angle. There are a couple of ways to do this:

- **View** → **View Directions** → **Along X-axes**
- **View** → **View Directions** → **Along Y-axes**
- **View** → **View Directions** → **Along Z-axes**

These commands need no further explanation.

- **View** → **Align Screen**

Using this command, you can align the screen parallel to some plane in your molecule. You need to select three atoms first which will define the plane to align to.

- **View** → **Camera** → **Save... / Load...**

First view your molecule from your favorite position (or use one of the just mentioned commands). Next, you can store the camera position by selecting one of the Save 1-5 commands. That will store the current view in the selected slot. To switch to one of the stored views, use one of the Load 1-5 commands.

The camera positions are saved for all GUI modules to use. Thus, if you start ADFinput (or any other GUI module with a View menu) the stored camera positions are available everywhere. This makes it possible to force the use of the same camera position in different GUI modules.

The Camera menu can be torn off, which is very convenient if you have several views that you wish to switch between frequently. To tear off the menu, select the dashed line in the Camerae menu.

## 5.3 3D

The GUI modules do have support for real 3D viewing. Use the **View** → **3D** menu to select what kind of stereoscopic display you have. The simplest version is having none, but using colored glasses (like the Red-Cyan). The other options are for special hardware. Just try out what works for you. This is a rather new and not completely stable feature, so it may not work for you.

One known but at the moment this is written unsolved problem is that the 3D view does not work on Mac OS X using Lion (it does work with Snow Leopard).

## 5.4 Fly to selection

When you have a big system, it often make sense to zoom in to some particular region. To do this, use the **View** → **Fly To Selection** menu command.

Not only will this zoom in to the selected atoms, but the center of the selected atoms will also become the new center of rotation when you use the mouse to get a different view.

## 5.5 Reset View

You can reset the view using the **View** → **Reset View** menu command. This is especially useful after flying to the selection. Or when the view gets distorted for some reason.

## MOUSE INTERACTION

### 6.1 Rotate, Translate and Zoom

In the modules that provide a 3D view of your molecule (like ADFinput, ADFview and ADFmovie) you can rotate, translate and zoom using the mouse.

Drag with the mouse: press a mouse button, and move it while holding it down. A one-button mouse button is the same as a Left mouse button. Which mouse button, and which modifier key you press at the same time, determines what will happen:

Rotate	Left mouse button
Rotate in-plane	Ctrl with Left mouse button
Translate	Right mouse button
Zoom	Use the scroll wheel on your mouse, or Middle mouse button, or (not on windows) Alt with Left mouse button

The rotate, translate and zoom operations change how you look at the molecule. They do not change the coordinates.

In ADFinput operating with the mouse on the selection will move the selection only. In that case the geometry of your molecule (and thus the coordinates) will change. Zooming the selection will move it perpendicular to the screen, unless you are using the mouse-wheel. You operate on the selection by starting the drag operation with the mouse above a selected object.

In the View menu you can select either 'Mouse as trackball' or 'Mouse as joystick'. If 'Mouse as trackball' is selected, you need to drag with the mouse (move the mouse with a button pressed down). If 'Mouse as joystick' is selected you just need to press and keep the button pressed down. The direction of movement etc will depend on the position of the mouse with respect to the center of the 3D view area.

The mouse handling has changed in the 2013 release: the middle and right buttons have been switched. The right mouse button was used for zooming, now by default it is for translating (and zooming is much more convenient using the scroll wheel). Via the **SCM** → **Preferences** you can switch the mouse handling back to the previous style (use the "Right mouse button" option).

### 6.2 Selecting

In the modules that provide a 3D view of your molecule (like ADFinput, ADFview and ADFmovie) you can make selections using the mouse.

Click on an **object**: make a new selection **with** it

Click **in** space: clear selection

Shift-Click on **object**: add **or** remove it **from the** selection

Shift-Drag **in** space: add **all** objects within the rectangle to the selection

In some modules there are additional ways to select objects using menu commands. Furthermore, in ADFinput one can select atoms from the list in the coordinates window.

## KEYBOARD SHORTCUTS

Many tools and menu commands have keyboard shortcuts associated. For menu command shortcuts, the shortcut is listed in the menu.

In many modules the shortcut to open or add a result file can be combined with the shift key. That allows selection of any file (otherwise a filter will be applied).

On most UNIX systems (including Linux) and Windows you need to use the control key together with some letter. On a Macintosh (running locally) you need to use the `key` (command key) together with a letter.

If you are using a Mac, the GUI uses the X11 program to run. The X11 program itself may intercept the menu-shortcuts like `-C`, `-H`, and so on. You can change this using the Preferences command from the X11 menu (Enable key equivalents under X11 should NOT be checked).

The following table lists all keyboard shortcuts, per module. If no `or ctrl` is specified Just press the indicated key without any modifier keys. On a mac, `should be used` as shown, on other systems use the control key (`ctrl`).

### 7.1 ADFinput

Key	Function
arrow-up/down in search results	highlight the previous or next search result
backspace	Delete selection
delete	Delete selection
Return in search results	open the currently highlighted search result
Esc	Select-tool (end other tool), clear search, active Main page
1	Single bond
2	Double bond
3	Triple bond
4	Aromatic bond
-1	View Direction → Along X-axis
-2	View Direction → Along Y-axis
-3	View Direction → Along Z-axis
-a	Select → Select All
-b	Edit → Builder...
-c	Edit → Copy
-d	Select → Select Connected
-e	Atoms → Add Hydrogens
-f	Search
-g	Atoms → New Region From Selected Atoms
-i	View → Properties (Estimated)
Continued on next page	

Table 7.1 – continued from previous page

-j	Transparency Periodic Cells → Increase Transparency Periodic Cells
-k	Transparency Periodic Cells → Decrease Transparency Periodic Cells
-l	Bonds → Add Bond
-m	Select → Select Molecule
-n	File → New
-o	File → Open...
-q	Quit
-r	File → Run
-s	File → Save
-v	Edit → Paste
-w	File → Close
-x	Edit → Cut
-z	Edit → Undo
--B	Generate Super Cell...
--e	Atoms → Remove Hydrogens
--g	Atoms → Remove Selected Atoms From Regions
--r	Show RunScript panel
--z	Edit → Redo
Space	Structure Tool
c	Carbon
f	Fluorine
h	Hydrogen
n	Nitrogen
o	Oxygen
p	Phosphorus
s	Sulfur
x	Element (type to select element and then return)
-	Molecule Smaller
=	Molecule Bigger

## 7.2 ADFview

-1	View Direction → Along X-axis
-2	View Direction → Along Y-axis
-3	View Direction → Along Z-axis
-a	Select → Select All
-d	Add → Isosurface: Double (+/-)
-d	Select → Select Connected
-f	Fields → Calculated
-i	Add → Isosurface: Colored
-j	Transparency Periodic Cells → Increase Transparency Periodic Cells
-k	Transparency Periodic Cells → Decrease Transparency Periodic Cells
-l	Add → Add Bond
-m	Select → Select Molecule
-n	File → New
-o	File → Open...
-p	Add → Cut Plane: Colored
-q	Quit
-s	File → Save Picture...
-w	File → Close
--o	File → Open... (no filter)
-	Molecule Smaller
=	Molecule Bigger

## 7.3 ADFmovie

-1	View Direction → Along X-axis
-2	View Direction → Along Y-axis
-3	View Direction → Along Z-axis
-a	Select → Select All
-j	Transparency Periodic Cells → Increase Transparency Periodic Cells
-n	Transparency Periodic Cells → Decrease Transparency Periodic Cells
-k	Scale Displacements → Smaller
-l	Scale Displacements → Bigger
-o	File → Open...
-q	Quit
-s	File → Save Geometry...
-t	File → Update Geometry In Input
-w	File → Close
--o	File → Open Any... (no filter)
-	Molecule Smaller
=	Molecule Bigger

## 7.4 ADFlevels

-	Interactions → Decrease # Significant
=	Interactions → Increase # Significant
-a	View → Hide/Show All Fragments
-i	File → Add...
-o	File → Open...
-p	File → Save Postscript...
-q	Quit
-w	File → Close
--i	File → Add Any... (no filter)
--o	File → Open Any... (no filter)

## 7.5 ADFtail (Logfile)

-c	Edit → Copy
-o	File → Open...
-q	Quit
-w	File → Close

## 7.6 ADFoutput

-c	Edit → Copy
-o	File → Open...
-p	File → Print...
-q	Quit
-w	File → Close

## 7.7 ADFspectra

-i	File → Add...
-o	File → Open...
-p	File → Save Postscript...
-q	Quit
-w	File → Close
--i	File → Add Any... (no filter)
--o	File → Open Any... (no filter)



## 7.8 BANDstructure

-1	View Direction → Along X-axis
-2	View Direction → Along Y-axis
-3	View Direction → Along Z-axis
-j	Transparency Periodic Cells → Increase Transparency Periodic Cells
-k	Transparency Periodic Cells → Decrease Transparency Periodic Cells
-o	File → Open...
-p	File → Save Postscript...
-q	Quit
-w	File → Close
--o	File → Open Any... (no filter)
-	Molecule Smaller
=	Molecule Bigger

## 7.9 ADFdos

-1	View Direction → Along X-axis
-2	View Direction → Along Y-axis
-3	View Direction → Along Z-axis
-a	Edit → Select All
-d	Edit → Select Connected
-j	Transparency Periodic Cells → Increase Transparency Periodic Cells
-k	Transparency Periodic Cells → Decrease Transparency Periodic Cells
-m	Edit → Select Molecule
-o	File → Open...
-q	Quit
-w	File → Close
--o	File → Open... (no filter)
-	Molecule Smaller
=	Molecule Bigger

## 7.10 ADFjobs

-a	Tools → Add To SDF...
-b	Edit → Clear
-c	Edit → Copy
-n	SCM → New Input
-q	Quit
-r	Job → Run
-s	Queue → Status
-v	Edit → Paste
-w	File → Close
-x	Edit → Cut



## INPUT

This version of the GUI has unified the input modules for ADF, BAND, ReaxFF and other packages. The new input module, typically called ADFinput, can now prepare the input for all of the old methods, as well as for new methods like DFTB, Mopac, UFF and so on.

After starting ADFinput, you will notice a bright colored menu ‘ADF’ on the left of the panel bar. Depending on your license, it might read ADF, or BAND, or one of the other methods. If you click there, you will get a pull-down menu that allows you to switch the method. Thus effectively you can turn ADFinput into BANDinput, or ReaxFFinput, and so on.

In the SCM menu you will find a New Input command. This command will start ADFinput. Next you can switch to BAND mode, etc, as just described.

In this release the list of available packages includes both ReaxAms and ReaxFF. ReaxFF is the original ReaxFF as in the previous release, with some new features. It will run the standalone reaxff executable. ReaxAms is the same ReaxFF code, but executed (and linked) via AMS. Thus you can use the AMS features (the AMS geometry optimization, MD, nD-PES scan etc) with the ReaxFF force field. Once the conversion of ReaxFF to AMS is complete this situation will change, only the AMS version of ReaxFF will remain.

The unified interface makes it possible to do things like reading a crystal structure file (which will cause ADFinput to switch one of the methods supporting periodicity automatically). Next you can build super cells, cut out clusters, and switch back to ADF without periodicity. No need for extra licenses, and no need to copy/paste between GUI modules.

The Main panel for some methods (like DFTB and UFF) contain a ‘Run’ button. If you press that, the current method will be started interactively, with the geometry of your system updating on the fly. The main use for this is as a pre-optimizer, no files will be saved and only the geometry will be updated.

## 8.1 Input: options

### 8.1.1 Normal Options

On the right side of the ADFinput window you have the panels with input options.

Most of the options presented in the different panels are generated automatically from configuration files that define the input for ADF, BAND etc. This ensures that all options are up-to-date, and that the descriptions in the help balloons (when your mouse pointer is over an option) are also up-to-date (and identical to the information in the user manuals).

The options are logically grouped together, the most important are on the Main panel.

Options regarding the physical Model are in the Model section, options that determine how and what properties are calculated are in the Properties section, and many other options that are details relating to the calculation are in the Details section.

If you cannot locate the option you are looking for, use the search field at the top right of the ADFinput window.

## 8.1.2 Expert Options

Some options are either hardly ever used and have not been put explicitly on some panel. And similar it might happen that the compute codes have some new options that have not yet been explicitly added to ADFinput. All such options are added to the Expert Options panel in the Details section (again automatically generated).

Most users will not need to use these, but all options are available in this way.

The Expert Options panel is available for all SCM software, except for ADF (this will be fixed in a future release).

Again, if you cannot locate the option you are looking for, use the search field at the top right of the ADFinput window.

## 8.1.3 Units

Often options have some unit associated with them. The units are clearly presented in the panels.

A hidden feature is that in most cases in ADFinput you can change the units. Just click on the unit with your mouse, and a menu will pop up that you can use to select the units that you like.

The units that are selected without moving the mouse are the default units.

When you make a change, that change is saved when you quit ADFinput (in the \$HOME/.scm\_guirc file). The next time you start ADFinput, that particular field will use the units you selected. To revert everything to the default units, use the Preferences module, and select the 'Reset ADFinput units' command from the File menu.

## 8.2 Input: buttons

### 8.2.1 Searching

At the top right in the panel bar you will find a Search tool. You can activate it by clicking on it, or by using the ctrl/cmd-F shortcut.

After activating it, a small field will pop-up that allows you to enter your search text.

When you enter some text in the search field, the search will start immediately and the results will be presented below the search text. The results are divided in several sections:

**Panels:** a list of all panels that match the search text. All texts on a panel will be searched: titles, menus, help text and associated keys. When you click on one of the panel search results that panel will be activated, and the items matching your search query will be marked. This is a very convenient way to find a particular input option. The search is restricted to panels belonging to the currently active method (thus, while in ADF input mode you will not find BAND input panels).

**Documentation:** a list of matching documentation pages. If you click on it, that page will be shown in your browser. Note that this uses the local documentation, it does not contact the SCM web site. Again, the search is restricted to documentation that belongs to the currently active method.

**Molecules:** a list of matching molecules. The match may for example be in the name or in the molecule formula. If you click on a match, that molecule will be imported. The list of molecules is a mix of some ADF optimized molecules, and of results taken from the NCI-Open database (see <http://cactus.nci.nih.gov>). Again, all information is contained in the ADF distribution, the search will not contact external sources. In total about 35000 molecules are included.

**Crystals:** a list of matching crystals. The match may be in the name or formula. Most of the crystals are simple common crystals are found in many textbooks. On the MOPAC web site there is a list of crystals that have been optimized using MOPAC. Those are also included. Finally, the zeolite frameworks from the *IZA-SC database* (<http://www.iza-structure.org/databases/>) are available.

When starting, at most five matches will be shown in each section. At the right side of the section headers (Panels, Documentation, Molecules) you will spot a triangle pointing to the right. If you click on it, you will open that particular section and many more results will be shown, if available.

Pressing the “i” (to the right of the search text field) will bring up a detailed description of the search facility. It will explain how to do more complex searches.

If you move your mouse above one of the search results, without clicking on it, a balloon will pop up showing more details about that particular match. For the documentation matches it will tell you from what manual the result is, and from which chapter. For molecules it will give some more information about that molecule, like names, sometimes a CAS number, and what the source of the data is (for example, optimized using ADF, or from the NCI-Open database).

After typing a search text, you can also use the up and down arrow keys to select a particular search result, and then press the Return key to open that result. When starting with ctrl/cmd-F this means you can perform the search and accept result without using the mouse.

### 8.2.2 The “...” details buttons

In many panels in ADFinput you will find white oval buttons with three dots in them. These buttons will activate a panel showing more details for some particular feature.

For example, the “...” button to the right of the Task option in ADFinput will activate a panel that allows you to set details for the current task. Thus details for a geometry optimization, or details for a transition state search.

It depends on the context and sometimes on the active options to which panel the buttons link. In all situations it should be intuitive, just try it out.

### 8.2.3 Using the “i” info buttons

Some panels in ADFinput have an “i” button (just as the search pop-up). When you press the “i” button, a new page will open with much more background information on some feature.

For example, the “i” button in the search pop-up will show a description of the search syntax. And the “i” button next to the basis set (in the Basis detail panel) will show more information about the basis sets.

## 8.3 Searching

In ADFinput there is a search icon in the top-right corner. Click on it to bring up a search box. Searching will be performed automatically when you enter text in the search box.

You will search multiple things at the same time:

- matching panels with input options in ADFinput (from the panel bar)
- documentation
- molecules

The search will be restricted to panels and documentation that belong to the currently selected program (ADF, BAND, DFTB, ...). In these panels, it will find any panel that contains your search string, including the matching program key.

Prefix: key

If you start your search with “key ” (without quotes), you will restrict your search to fields related to matching input keys only. This will allow you to locate an input option very quickly.

Prefix: all

If you start your search with “all ” (without quotes), the search will be global for both the panel search and documentation search. Thus it will not be restricted to the currently selected program.

The molecule search will search a (local) database with some common molecular structures. Currently it consists of a roughly 1800 molecules optimized with ADF for use with COSMO-RS, and of the molecules found in the NCI database (NCI-Open\_09\_03.sdf, see <http://cactus.nci.nih.gov>). The molecules in the NCI database have been filtered to include only molecules with names and xyz coordinates, and most CAS numbers have been removed for legal reasons. Also periodic structures are available: zeolites (from the [Database of Zeolite Structures](http://www.iza-structure.org/Databases) (<http://www.iza-structure.org/Databases>)), many simple crystal structures, and a set of complex crystals included with the MOPAC distribution.

As the structures come from an external source we can not guarantee that the found structures will be correct. So please check them!

In total roughly 35000 molecules are available.

To clear the search results at any time, also when the search box is no longer visible, use the Escape key.

Only the locally included documentation and molecule structures will be searched. No internet search will be performed.

### 8.3.1 Panel search details

All text belonging to the panels will be searched: panel titles, labels for input options, headers, text in pull-down menus, and text in help balloons.

You can use the \* and ? wildcards: the \* matches anything, the ? matches any single character. The search string will be broken into words, and only results containing all words will be found. Use double quotes (") around text to search for exactly that phrase. The words to search for are implicitly surrounded by \* wildcards, so text matching will happen even in the middle of a word.

The names of the found panels will be listed. When you click on one of them, it will be activated. Options not matching the search string will be dimmed. If an option is not dimmed, it matches either directly, by its help text, or by the page title.

Use the arrows next to the search loupe to quickly loop through the found panels.

### 8.3.2 Key search details

To search for input fields that have to do with a particular input key, you can use the key search. To do this, start your search string with “key ” (without the quotes). This will restrict the panel search to find only items that set or change the matching key.

You can use the \* and ? wildcards: the \* matches anything, the ? matches any single character. The search string will be broken into words, and only results containing all words will be found. Use double quotes (") around text to search for exactly that phrase. The words to search for are implicitly surrounded by \* wildcards, so matching will happen even in the middle of a word.

For example, searching for

key integration

will show you what input options in the GUI will set the INTEGRATION key.

The names of the found panels will be listed. When you click on one of them, it will be activated. Options not matching the search string will be dimmed. If an option is not dimmed, it matches either directly, by its help text, or by the page title.

Use the arrows next to the search loupe to quickly loop through the found panels.

### 8.3.3 Documentation search details

The included documentation (in html format) will be searched using the Swish-e search engine. You will be searching for words. If you specify more you will get matches that contain both words, in any order.

The (shortened) titles of the found documentation pages will be listed. If you point at an item with your mouse, it will show the full title. Click on it to open that item with your default browser. Note that you will be viewing local documentation, not the SCM web site.

When staring, only the first 5 documentation matches will be shown. To view all results, click on the arrow on the right side of the 'Documentation' header in the search results. Click on the same arrow again to show only the first 5 results again.

You can use the \* wildcard to match anything, but only at the end of an word. You can use the ? wildcard to match a single character, but NOT at the beginning of an word. You can also perform complex searches using logical operators (and, or, not) and parenthesis. If no operator is specified between words, the and operator is used (both words need to be found) Finally, you can search for an exact phrase using quotes.

**For example: integration and not accuracy** integration or accuracy integration key "integration key"

The search will be restricted to the parts of the documentation relevant to the module you are using. Thus, when searching from ADFinput with ADF active, the BAND documentation will not be searched.

If you prefix your search with "all" (without the quotes), all documentation will be searched.

For more information on Swish-e: <http://swish-e.org/>

### 8.3.4 Molecule search details

The included database of molecules will be searched. You can search for the IUPAC name, the molecule formula, the CAS number, and sometimes alternative names. Note that the CAS number search will often fail as only a few CAS numbers are included.

You can use the \* and ? wildcards: the \* matches anything, the ? matches any single character. The search string will be broken into words, and only results containing all words will be found. Use double quotes (") around text to search for exactly that phrase. The words to search for are implicitly surrounded by \* wildcards, so text matching will happen even in the middle of a word.

When you start your search string with "=" (an equal sign, no quotes), no wild cards will be added automatically.

When you move the mouse over one of the found molecules, you will get full details including the origin of the entry (optimized by ADF, or from the NCI database).

When you click on the desired search result, that particular molecule will be imported.

## 8.4 Crystals and Slabs

### 8.4.1 Periodicity

Many GUI modules support periodicity. Some menu commands (like the **Edit** → **Crystal** command in ADFinput) will only be available when you have a periodic system.

To set up periodicity you first need to switch to a method that supports periodicity. For example BAND, DFTB, Mopac, or UFF. Some of these, like UFF, are currently available without extra license.

On the Main panel of a method that supports periodicity, you will find a 'Periodicity' pull-down menu. Use it to use periodicity in 1 (Chain), 2 (Slab) or 3 (Bulk) dimensions. Once periodicity is enabled, menus like the Crystal menu will also be enabled.

The tool bar below the molecule editor also changes when you have a periodic system. The structures tool gets replaced by the crystal tool (represented by a snowflake), followed by the Slice tool. At the right side of the tool bar you find buttons to orient the camera, toggle perspective and toggle the display of periodic images.

To set up the lattice vectors, press the "...' details button next to periodicity, or go to the Lattice panel (in the Model section).

When editing the lattice vectors: changing the 1,1 element also adjusts the 2,2 and 3,3 element. Changing the 2,2 element also adjusts the 3,3 element (but leaves the 1,1 as it is).

### 8.4.2 Building crystals

After setting the periodicity and lattice vectors, you can build your own crystal by adding atoms at the proper position. For many crystals this is a lot of work.

You can also build crystals using the **Edit → Crystal** command. The first list of options (Cubic, Hexagonal and so on) have sub-menus for some common crystals. If your crystal is not in there, you can use the "From Space Group..." command in the same menu. This brings up a dialog that will help you build any crystal.

The crystal tools are not only available from the Edit menu, you can also press the 'Snowflake' button in the molecule editor tool bar (next to the element button, if periodicity is enabled). It has the same options as the **Edit → Crystal** menu.

### 8.4.3 Build slabs

Building a slab is done most conveniently using the Slice tool: first build a crystal, next use the "Generate Slab..." command from the Crystal menu to make a slab. Next you will need to enter the Miller indices of the plane that will define your slab.

The Slice tool is available from the **Edit → Crystal** menu, or in the periodic toolbar (next to the snowflake).

### 8.4.4 Crystal menu

#### Generate Super Cell...

In the dialog that appears when using this command you determine how the super cell should be created.

When editing the setup: changing the 1,1 element also adjusts the 2,2 and 3,3 element. Changing the 2,2 element also adjusts the 3,3 element (but leaves the 1,1 as it is).

#### Map Atoms To (-0.5..0.5)

##### **Edit → Crystal → Map Atoms To (-0.5..0.5)**

Using the translational symmetry, the atoms are mapped to the cell centered around the origin. Thus with fractional coordinates between -0.5 and 0.5 for each lattice direction.

#### Map Atoms To (0..1)

##### **Edit → Crystal → Map Atoms To (0..1)**

Using the translational symmetry, the atoms are mapped to the cell in the positive quadrant. Thus with fractional coordinates between 0 and 1 for each lattice direction.



### Set (0.5, 0.5, 0.5)

#### Edit → Crystal → Set (0.5, 0.5, 0.5)

The selected atoms define some point. This point will be translated to the point with fractional coordinates 0.5, 0.5, 0.5. All atoms will be adjusted according to this translation.

Related, to shift the point defined by the selected atoms to the origin use the Set Origin command.

## 8.5 Builder (packmol)

To build systems consisting of many different molecules, randomly put together, the GUI includes the Builder. This is a graphical interface to the packmol program, using only a few possibilities of it. The most common use will be to set up a big system for Molecular Dynamics with ReaxFF or DFTB.

If you find using the Builder (and thus packmol) useful, please give proper credit via the following reference

L.Martínez, R. Andrade, E. G. Birgin, J. M. Martínez. Packmol: A package for building initial configurations for molecular dynamics simulations. *Journal of Computational Chemistry*, 30(13):2157-2164, 2009.

The Builder allows you to compose your system of many replicas of some predefined molecules. These molecules are replicated as often as you want, giving a simulation box full with these molecules. Thus it is very easy to generate a liquid or a gas.

To activate the Builder, use the **Edit** → **Builder** menu command.

First you need to define the box into which the molecules will be generated. In the Builder panel you define the lattice vectors that define the unit cell.

Next you define what molecules to add to your system. Press the + button to add more molecules, or press the - button in front of a line to remove that particular molecule.

The 'Current' option will include whatever you have manually created on the left side. For example, some molecules to be solvated. Or some slab imported from BANDinput.

The 'Fill box with' option allows you to select what molecule to use for filling. The geometry of the molecule must be available in a file with .xyz extension, and it should contain the coordinates and atom types of your molecule in XYZ format. Many typical molecules are included with ReaxFFinput. When you press the folder button at the right side you will be able to select your molecule via a file-select browser. Or you can start typing a text in the field, and below it matching molecules will be shown (similar to the molecule search).

As you may have more than one kind of molecule, you can also make mixtures of different molecules.

Once you press the 'Generate Molecules' button, the actual packing of the molecules is done using [Packmol](http://www.ime.unicamp.br/~martinez/packmol/) (<http://www.ime.unicamp.br/~martinez/packmol/>).

## 8.6 Building molecules

Building molecules with ADFinput is very simple, just draw them with the appropriate tools. Please check the tutorials for extensive description of this.

Here we will just note some details that may not be obvious.

### 8.6.1 Bonding mode

After creating an atom, it will be selected (the 'bond atom'). When you still have an atom tool and one atom is selected, you are in bonding mode. This is indicated by a line from the bond atom to the mouse cursor. If you next click to create a new atom, it will automatically be bonded to the bond atom.

To stop bonding mode, click once on the bond atom. This will switch to the select tool, and as a result you are no longer in bonding mode.

### 8.6.2 Atom Details: Connectors (valency) and Lone Pairs, Atom mass

Each atom you make has the possibility to connect to other atoms. The number of connections depends on the atom type. Some of the 'connectors' may be used by lone pairs and not be available for bonding to other atoms.

For example, carbon has 4 connectors and no lone pairs, oxygen has 4 connectors and 2 lone pairs.

When you use the Add Hydrogen menu command, all unsaturated connectors will be saturated with hydrogen atoms. The number of connectors will determine the geometry (2 linear, 3 flat, 4 tetrahedral). So if you plan to use this command it is essential that the number of connectors and the number of lone pairs is correct.

You can view and change these via the **Atoms** → **Details (Color, Radius, Mass...)** menu command. It will activate the Atom Details panel, in which you can change the number of connectors and lone pairs for each atom. Note that only selected atoms will be visible in the Atom Details panel.

You can also see and change other atom properties like the type, screen radius, nuclear charge, mass, color, Amber and Tripos atom types and more.

Right click on one of the fields to propagate that value to all selected atoms (for example to change the color of all selected atoms).

### 8.6.3 Pre-optimization

After drawing a molecule you will typically run a pre-optimization.

On the right end of the molecule editor tools you will see a cog wheel. If you click it your system will be optimized using the UFF method.

If you right-click the cog wheel you will get a pop-up menu that allows you to specify which method to use as a pre-optimizer: UFF, Mopac, DFTB or SimpleMM. UFF, Mopac and DFTB are identical to these methods within ADFinput, SimpleMM is a very primitive force field like method that used to be the only available pre-optimizer. It is mainly included for compatibility.

Alternatively you can just switch ADFinput into UFF, Mopac or DFTB mode (by using the orange method menu in the panel bar). For each of these you will find a 'Run' button on the Main panel. If you press it, it will run the current set up interactively, updating the coordinates and possibly the bonds on screen automatically. This is very similar to clicking the cog wheel, but it allows you to set details of the calculation. For example, for DFTB you can select what parameter set to use.

### 8.6.4 Geometry adjustments

#### Sliders

Select two, three, four or five atoms.

Below the molecule, a horizontal slider will appear, just above the toolbar.

You can drag the thumb inside the slider to change the distance, angle, dihedral, or plane angles.

The order in which you select the atoms determines what atoms will move. The selection order is shown in the molecule editing window. The last atoms selected will move (together with things connected to those atoms). However, if you press the control key and then move the slider, the smallest group will move. You can force this behavior (so you do not need to press the control key) by setting the `SCM_GEOMODSBYSIZE` environment variable (via the Preferences or via the command line). Note in the 2017 version the default was the reverse (smallest group moving, by order with control key).

You can use regions to group atoms. Atom in a region will move together when using a slider to change distance or angle.

### Edit box

Select two, three, four or five atoms.

Above the slider on the right side you will get an text entry box next to the atom labels. For example, after selecting two atoms it might look like H(8)-C91) (pm): 149. The 149 in this example is editable. Instead of using the slider, you can type some specific number in this box instead.

### Centroids

A centroid in ADFinput is defined as a dummy which is (and will stay) in the geometrical center of the atoms to which it is bonded. They are useful to control the geometry for molecules like ferrocene, as you can easily set the distance between the central atom and the center of a ring.

To make a centroid, select the atoms that should define the center, and use the **Edit** → **Add Centroid** menu command.

As an example, to change the distance between a ring and the Fe atom in Ferrocene:

1. Use the structure tool to load Ferrocene.
2. Select the carbons in one ring.
3. Add a centroid.
4. Delete the bonds between Fe and the carbons belonging to the centroid (otherwise you will not be able to change the distance)
5. Select the centroid and the Fe
6. Use the slider to set whatever distance you want (or set it in the input field).

Thus the centroid functions as a fixed manipulation point.

Another example, to change the angle ring - Fe - ring in Ferrocene, adjusting the planes of the rings as well:

7. Make a similar centroid in the second ring (also with Fe - C bonds removed).
8. select centroid - Fe - centroid.
9. Change the angle using the slider.

### Move an atom (possibly perpendicular to the screen)

First select the atom that you want to move.

Next, translate (middle mouse button, or alt left mouse button), but start with the mouse on the atom that you want to move.

If you wish to move the atom perpendicular to the screen: use the right mouse button (or command left mouse button) and move the mouse up or down). This is equivalent to zooming.

## Rotate or translate the selection

First make your selection.

Next rotate, translate or zoom as usual, but start with the mouse in the selection. So if you click and drag the selection, **ONLY** the selection will be rotated or translated. If you click and drag anywhere else the whole molecule will be rotated or translated (actually, only your viewpoint).

If you 'zoom' the selection you are really moving the selected objects perpendicular to the screen (in or out the screen).

## Coordinates

In some situations you want to set the coordinates of the atoms exactly to some value. You can do this via the Coordinates panel (in the Model part of the panel bar).

If you first select the atoms of interest, they will be highlighted in the Coordinates panel. The coordinates in that panel can be edited, and the molecule on the left side will immediately reflect the changes.

## Z-Matrix

In some situations you want to set the coordinates of the atoms via a Z-Matrix. You can do this via the Z-matrix panel (in the Details part of the panel bar).

If you first select the atoms of interest, they will be highlighted in the Z-Matrix panel. The values for the distances and angles in that panel can be edited, and the molecule on the left side will immediately reflect the changes.

The connectivity can not be edited, but you can effectively do this by reordering the atoms. That way you normally can create the Z-Matrix coordinate that you are after.

## Set Center Of Mass

The **Edit** → **Set Center Of Mass** command translates all atoms so that the mass-weighted center of the selection will be the new origin. If nothing is selected, the center of mass of the whole molecule will be the new origin.

The atoms are really translated, thus the coordinates are changed. It is not a change of the camera.

When symmetry is used, the origin will also be the origin of symmetry.

## Set Origin

The **Edit** → **Set Origin** command translates all atoms so that the center of the selection will be the new origin. If nothing is selected, the center of all atoms will be the new origin.

The atoms are really translated, thus the coordinates are changed. It is not a change of the camera.

When symmetry is used, the origin will also be the origin of symmetry.

## Symmetry

To symmetrize your molecule, click on the **star tool** in the tool bar below the molecule editor. This is equivalent of the **Edit** → **Symmetry** → **Symmetrize Using Symmol** menu command. In most cases this just works, and is the preferred method of symmetrizing your molecule.

The **Edit** → **Symmetry** menu gives access to a less automatic but more power-full symmetry code. Using it is somewhat complicated, and sometimes it does not work as expected.

To use it, follow this procedure:

- Select the symmetry group
- Set the (symmetry) origin of your molecule via the SetOrigin menu command
- Define one or two operators for the selected group. In the symmetry menu you can see what operators you need to define.
- Use one of the symmetry commands:

## Rotate 90

The **Edit** → **Rotate 90** commands (select an axes via the submenu) will rotate your system around some axes.

Not only the coordinates of the atoms, but also the lattice vectors (if any) will be rotated.

Thus, for example, if you get some .cif file with a nanotube structure and want to treat it with BAND as a one-dimensional periodic structure (a chain), you must ensure it is oriented along the x axes. If the structure in the .cif file is oriented along another main axes, these commands make it very easy to fix that.

## Align

The **Edit** → **Align** command contains commands to align your molecule to the indicated axes or plane.

If you are aligning to an axes, you need to select which atoms to align. If you select one atom, the molecule is rotated around the origin such that the selected atom is on the specified axes. If you select two atoms, first the molecule is translated such that one of the selected atoms is on the origin. Next, the molecule will be rotated such that the other selected atom is on the specified axes.

If you are aligning to a plane, you need to select a plane to align. If you select two atoms, these will define the normal of the plane to be aligned. If you select three atoms, these define the plane to be aligned.

This Align command does change the coordinates of your atoms, unlike the Align Screen command in the View menu.

Not only the coordinates of the atoms, but also the lattice vectors (if any) will be rotated.

Typically the Align command will change your origin. You can always set the origin as you like after-wards.

## Mirror

The **Edit** → **Mirror** command contains commands to mirror the selected atoms (or all atoms if no atoms selected) in a plane parallel to the indicated plane, through the center of the selected atom(s), or through the center of the molecule if no atoms selected.

The Mirror command does change the coordinates of your atoms. Also the lattice vectors (if any) will be mirrored.

## Update coordinates via ADFmovie

If you have performed a calculation that saves multiple geometries, for example a geometry optimization or a linear transit run, you can use ADFmovie to see how the geometry changes. You can go to a particular geometry, and then use the **File** → **Update Geometry in Input** menu command in the Movie window to adjust the geometry in the matching ADFinput window.

## 8.6.5 Bonds

Bonds are normally made while drawing the molecule. There are several other options to handle bonds:

- Make a bond via an atom tool: Take one of the atom tools. Next click once on the first atom you want to connect. You will enter the bonding mode (the line to the mouse position from the atom you just clicked on will be your visual cue for the bonding mode). Next click on the atom you want to make the bond to. The bond will be created, and you will revert to the normal select mode.
- Make a bond using the Add Bond command: Select the two atoms that you wish to be bonded together, and then use the **Bonds** → **Add Bond** command.
- Via Guess Bonds Use the **Bonds** → **Guess Bonds** menu command. This command uses an algorithm that looks at bond distances to guess the bonds and bond orders. The bond orders are adjusted based on the known number of connectors and lone pairs.

## 8.7 Importing and exporting your molecule

### 8.7.1 Importing your molecule

**Importing from file: .adf, .t21, .xyz, .mol, .mol2, .pdb, .runkf, .band, .cif, .dmol, .rkf, .rxi, .rxkf ...**

You can also import your molecule from a file using the **File** → **Import Coordinates...** command.

Many formats are handled explicitly. They are typically recognized by the file extension:

- .adf, .band, .rxi** These files have been saved by ADFinput, BANDinput or ReaxFFinput. Every detail belonging to atoms or bonds will be imported: not only the coordinates and bonds, but also things like atom properties (for example the color, the force field atom type, number of connectors, bond orders, and so on).
- .t21, .runkf, .rxkf, .rkf** These are all results files produced by the ADF package. The coordinates and bond information will be read, if present. The files are binary, and will be recognized even if having a different extension.
- .pdb, .mol2** Importing from a .pdb or .mol2 file will get the coordinates and the protein information (residues, PDB atom names and so on). For PDB files, only the ATOM information is read, thus no bond information. For MOL2 files, also the bond information is read.
- .mol** Importing from a .mol file will get the coordinates and bond information.
- .cif** Importing from a .cif file (Crystallographic Information File) will import the proper crystal structure. No bonds will be read.
- .dmol** Files from the DMol program can also be read, and atom positions and periodic information is properly handled. No bond information will be read.
- .xyz, any file type not recognized** Importing from an unknown text file, or a file with .xyz extension is rather flexible: ADFinput needs three real numbers next to each other. These will be interpreted as x, y and z coordinate. One additional integer or the abbreviation of an element is also needed to identify the kind of atom.  
To be recognized as real, the real number must contain a '.' (dot), and at least one digit before or after the dot. Real numbers with exponents (E or D) are **not** recognized.  
If an integer is used to specify the element (the nuclear charge), it may **not** contain a '.' (dot).  
No bond information is read.

If no bond information has been read, ADFinput tries to guess the bonds between the imported atoms. Guessed bonds might be completely wrong, or have the wrong bond order.

Z-matrix import (internal coordinates) is not available.

After using the 'Import Coordinates...' command the newly imported atoms are selected. This makes it easy to reposition them with respect to other atoms that may already be present, remove the automatically guessed bonds, or use other operations on the newly imported atoms and bonds.

If you are importing many atoms, the molecule visualization will switch to wire-frame for the newly imported atoms. By default this happens when importing 50 atoms or more. You can change this limit via the **SCM** → **Preferences**.

## 8.7.2 Copy/Paste between GUI modules, XYZ coordinates, SMILES or InChI strings

When Copying or Pasting with ADFinput, you need to make sure that the molecule editor has focus. Otherwise you will be copying or pasting one of the text input fields. To be sure, just click once in the drawing area before pasting.

You can copy an XYZ-formatted geometry (for example from an ADF output file), and use the **Edit** → **Paste** command to import coordinates. Pasted text will be handled as when it had been import as .xyz or .cif file via the Import Coordinates command.

Copy/Paste also works between the GUI modules, for example if you have several ADFinput windows. This will copy all information about your molecule: xyz, bonds, but also things like color of atoms or number of connectors. Only selected atoms will be copied.

If you have the SMILES or InChI string of your molecule on your clipboard (for example, from wikipedia) you can just paste it in ADFinput. It will automatically be converted to a 3D structure (via OpenBabel). It works often, not always, so be sure to check your structure.

## 8.7.3 Exporting your molecule

### Exporting to file: .xyz, .mol, .cif or .bgf

Use the **File** → **Export Coordinates...** to export your current system.

In the file select box you will have the option to select the format. Currently supported are .xyz (default), .mol, .bgf and .cif (for periodic systems).

You can also Copy your system via the Copy menu. The contents of the clipboard will be identical to the .xyz file that would have been exported. For periodic systems, the lattice vectors are included as special atoms VEC1, VEC2 and VEC3.

## 8.8 Regions

A Region in ADFinput is defined as a collection of atoms. Atoms may be present in one or more region.

Within the GUI they are used for many purposes. For example to change the visualization style for part of the molecule, to set up fragment calculations, or to set up other multilevel calculations like QUILD, QMMM or FDE.

When using the slider to change distances or angles you can use regions to group atoms (so they move as one).

When you select the Regions panel (in the panel bar Model section) you will find that one region has already been defined: All. This region consists of all atoms of your molecule, and is always present.

To add a new region, click the + button. If any atoms are selected when you press this button, they will automatically be added to this new region. With this new region you can do a couple of things:

- Click the - button: delete the region. Note that only the region is deleted, not the atoms in it.
- The check box: this selects all atoms currently in the region. In your molecule display you can easily see what atoms are in it, and it will also tell you how many atoms are contained in this region.

- Click in the region name to change the name
- Click the check box (the V-like shape) to show the region graphically
- The + button (on the right hand side): add the currently selected atoms to this region
- The - button (on the right hand side): remove the currently selected atoms from this region
- Click the triangle to get access to a pop-up menu with a number of commands that apply to that region.

The pop-up menu per region has the following options:

- **Split By Molecule:** split the region in many regions, based on the connectivity. Thus parts that are not bonded together will all be put in a separate region. The typical use is for solvents: first add a solvent with explicit molecules. The solvent molecules will automatically be put in their own region. Next, use the Split By Molecule command to split this into many small regions. If all your solvent molecules are identical, this leads to a very big time saving with fragment or FDE calculations. As the typical use is for replicated fragments, the naming of the newly generated regions will use the /n name, with n a number. Currently ADFinput does not check if the fragments are really identical!
- **Invert Selection Within Region:** perform an invert selection command, but just within the atoms part of this region.
- **Region Color:** set the color used to visualize the region
- **Balls And Sticks:** show the atoms and bonds in this region using Balls and Sticks
- **Sticks:** show the atoms and bonds in this region using Sticks only (that is, atoms not visible)
- **Wireframe:** show the atoms and bonds in this region using a wire frame only (again, no atoms visible)
- **Hidden:** do not show the atoms and bonds in this region

Regions can also be used in the Numerical Quality and Basis panel: you can change the basis per atom type per region. For example, give all carbon atoms in an outer region a smaller basis. Or you can set the Quality per region (the Becke / Zlm fit options and/or Basis and Core).

A quick and easy way to make a new region containing the current selection is to use the **Atoms → New Region From Selected Atoms** menu command (cmd/ctrl-G).

## 8.9 Proteins (from PDB or mol2 files)

ADFinput can read a protein from a PDB file or from a mol2 file.

The atom information is read (element type, coordinates, PDB name, residue to which the atom belongs, and chain information).

The PDB atom names are also essential to properly add hydrogens, in case your PDB or mol2 file does not have any hydrogens.

In the **Regions panel** for each chain detected in the PDB file, there will be a new line. This gives you a couple of visualization options (Ribbon, or all C, CA, N or O atoms connected). If you click on the triangle to the right you get a pop-up menu with some additional commands:

- **New Region From Chain:** make a new region, and put all atoms belonging to this chain into the new region
- **Select Residue:** select all atoms in a given residue (which you select from the menu)
- **Residue Protonation:** change the protonation state of some residues
- **Add Hydrogen:** add hydrogen atoms to this chain
- **Add Selection To Chain:** the selected atoms are marked as belonging to this chain



- **Add Selection To Residue:** the selected atoms are added to the specified residue

Many of these features depend on the proper PDB names and residue information for the atoms. If they are not correct, or non-standard, ADFinput may for example add hydrogens to the wrong positions, or visualize things incorrectly.

For the protonation state of some residues it is essential that their proper names are used: **LYN/LYS, ASP/ASH, GLU/GLH, HID/HIE/HIP**.

You can use the **Atoms** → **Details (Color, Radius, Mass, ...)** command to check and change the PDB names of the atoms.

Having the proper PDB atom names and residue types (including the proper protonation state) is essential. The atom types generated for MM (Amber95) depend on them, as well as the algorithm that adds hydrogens (if needed).

The hydrogens that are added by ADFinput do not use a very advanced algorithm. For the protein itself it should be correct in most cases, assuming you have made sure that you have the proper protonation state of the residues. However, if you have solvent molecules in your PDB file the hydrogens will be added properly but the solvent molecules will be oriented randomly. So no hydrogen bond structure in water for example.

To avoid problems with the primitive algorithm ADFinput uses to add hydrogens you can obviously use some other tool to first make a proper PDB or mol2 file for your protein including hydrogens.

Once read in, you can use in principle all tools within the GUI as you like. For example, perform MM, QMMM or QUILD calculations for the protein structure.

## 8.10 Presets and Defaults

All input options have default values. ADFinput presets are simply a collection of input values to be used.

A preset may set all or just a few input options. After you have selected a preset, fields that are set by the selected preset will be show with a green color.

If you next use another preset, only the input options included in the preset will be changed. Other input options will remain as they are. Thus the order in which you apply presets is important.

### 8.10.1 Using a preset

ADFinput always first uses the Defaults preset as included by SCM. Next the Defaults preset defined by the user (if any). Finally, a preset matching the current task will be loaded (either from SCM or defined by the user).

When you switch the Task, ADFinput will try to load a matching preset.

If you have saved matching presets yourself these will be used instead of the standard presets, thus allowing you to set your own defaults as you like them. A matching preset is a preset that has the same name as the Task selected, user-defined presets are searched first. If no matching preset is found, ADFinput will load a preset matching the Single Point task (which is always available). For presets to match, spaces and minus signs are ignored.

You can also load any preset you like using the Preset command from the File menu. This preset will be applied just as the other presets, so it does make a difference when you load the preset.

### 8.10.2 Color Code

The input fields use a color coding to warn you they have been modified:

- No special color: the field has its original default value.
- Yellow: the field has been changed by the user (only).

- Green: the field has been changed by the preset (only).
- Red: the field has been changed by the preset, and next by the user.

The pull-down menus in the panel bar use a similar color-coding to point you to fields that have been changed:

- No special color: all fields in the panel have their original default value.
- Yellow: some fields have been changed by the user.
- Green: some fields has been changed by the preset.
- Red: some fields has been changed by the preset, and some (possibly also) by the user.

### 8.10.3 Make your own presets

It is very easy to make your own presets, collecting all or a few default values for the typical jobs you like to perform.

By default presets are saved in the `$HOME/.scmgui/Tpl` directory. This can be changed by setting the `SCM_TPLDIR` environment variable.

To make your own preset, follow these steps (in ADFinput):

- edit all the fields as you would like them to be stored in a preset.
- select ‘Save as preset...’ from the Preset menu, or ‘Save as full preset...’
- specify a name
- click on Save

If you now check your Preset menu you will find a new entry.

The name of the preset is the file name you have chosen, but without the `.tpl` extension.

The difference between a Full Preset and a ‘normal’ Preset is that a Full Preset will save all input options, and a ‘normal’ preset will save only the yellow, green or red fields (options that have been changed by the user or by the active template).

If you wish to store only fields that you have changed yourself in the preset, make sure you start with the None preset.

If you save a preset with the same name as one of the default presets, it will effectively replace that preset. One exception: the SCM supplied Defaults are always read first, and thus cannot be replaced.

Some presets are only available for specific methods. For example, the Fragment Analysis preset is only available for ADF. You can get this behavior for your own presets by pre-pending the name of your preset by the name of the method for which it should be available. For example “`ADF_My_Defaults`”, or “`BAND_My_band_Defaults`”.

To delete your own preset(s), use the ‘Delete Preset’ command from the Preset menu.

### 8.10.4 Multiple presets are used

The default values that are used when you start ADFinput are generated as follows:

- Use the Defaults preset supplied by SCM
- Use the Defaults preset that the user has defined, if any
- Use the ‘Single Point’ preset, either supplied by SCM or one that is defined by the user (if any)
- Any user selected preset, directly or implicitly (by changing the Task).

## 8.10.5 Input options remarks

### Empty fields

Some input fields do not have a value from the default Preset. In those cases ADFinput does not specify the value, but leaves the value to be determined by the ADF program.

You can use the 'Explicit Defaults' preset to see the typical values. However, depending on details of your calculation the actual default used by ADF may be different.

### Spin and Occupation

The spin and occupation panel allows you to specify the occupations of the orbitals per symmetry. In case of an unrestricted calculation you can also specify the occupations per spin type.

To show the available symmetries, ADFinput needs the result of an ADF calculation. If a previous calculation is available (without specifying the occupations), it will use the information from that calculation to generate the proper options in this panel. If such results are not available, ADFinput will suggest to run a short guess calculation: a preliminary run with an inaccurate grid, only a few SCF cycles and stopping immediately after the SCF. Hopefully this guess calculation will allow you to generate sensible occupation.

The energy levels of the guess calculation (or previous calculation if available) will be shown using ADFlevels. Be aware that it is the result of the guess calculation, and not your proper results!

### User Input

You can use the User Input field to specify any kind of text. The text will be put without any change at the beginning of the ADF input. This way, you may access some keys that are not (yet) available in ADFinput.

Alternatively, and more flexible, you can obviously edit the .run file after saving it with ADFinput.



**ADFJOBS**

## 9.1 Jobs

### 9.1.1 Job list: per folder or global

When ADFjobs starts, it will generate a list of jobs for you by scanning the local directory. All files that have the same file name, with only a different extension, will be considered to be one job. A job may also contain a directory, it should have the .results as extension.

ADFjobs can also show a global list of jobs. All recent jobs that it knows about (by previously scanning a directory, or by running them) are shown. This typically can be a huge list, and it is limited (currently) to 500 most recent jobs. The big advantage is that you do not need to remember where you saved a job, it will automatically show in the global list. To switch between the two modes (showing only jobs in the current directory, or showing all known jobs) use the toggle switch at the right bottom corner.

If you are viewing the global list of jobs, you can use the **View** → **Job Location** menu command to show where on your disk the jobs are located. For each job one extra line will be displayed with this information.

The job list refreshes automatically when needed. You can force a refresh via the **Job** → **Refresh List** menu command, or by pressing F5. For each job you will see:

The Filter command determines what kind of jobs will be shown. For example, you can choose not to show directories, or only ADF jobs.

At the bottom right you will find a toggle button. This button will toggle between the two modes of ADFjobs: show all jobs, or show the jobs per folder.

### 9.1.2 Job status (including WARNING and ERROR info)

The status icon is the icon on the right side of the job. It tells you if the job is a new, queued, running, terminated, ready, ready with a warning, or ready with an error condition.

The warning and error condition is determined from the logfile of the job. If it contains a WARNING, the icon will display a warning triangle. If the logfile contains ERROR, the status icon will change into a red stop sign. If the standard error output of a job contains unexpected information this will also be reported as an ERROR.

The details of the error or warning will be shown in a color just below the job. Obviously, when a job has ended with an error you will normally not have useful results. If a warning has been printed, you should make sure you understand the warning, and that the ADF did perform the calculation that you intended.

### 9.1.3 Selecting Jobs

You can select one or more jobs with:

- left click - select that job
- shift left click - select a range of jobs
- right click (or control left click) - toggle that job to be selected or not selected
- click on the search icon - clear the selection

To clear the selection, press the ESC key, use the **Job** → **Clear Selection** menu command, or click somewhere in white space on the bottom or in the selected job (thus not on the name, queue, or one of the icons).

### 9.1.4 Running a job: `.run` and `.job`

When saving your job, ADFinput saves a `.adf` file and a `.run` file. The `.adf` file contains all information for ADFinput, and if you wish to make changes to your job use ADFinput to make them. ADFinput will read the `.adf` file.

The `.run` file contains the basic commands and input to run your calculation. It is intentionally kept as simple as possible.

However, typically some more administrative things need to be done: make empty working directories, make some links to follow a running calculation, etc. This used to be done by the run script, but not any more. If you wish to use the run script yourself you are responsible of taking care of such details.

To run your calculation, use the Run command from the File menu. This will tell ADFjobs to run your job. Alternatively, you can switch to ADFjobs, select your job (that you should have saved from ADFinput), and select Run from ADFjobs Job menu.

ADFjobs will create the real job script (with `.job` extension). This is a the `.run` script as saved by ADFinput, with the administrative things included at the front and at the end.

**As the `.run` script is simply included, you may edit it if you wish, and ADFjobs will automatically include your changed `.run` script.**

If the environment variable `SCM_RESULTDIR` has been set, the job script will change into that directory. Next it will run from there, and all result files will be stored in that directory.

If the environment variable `SCM_RESULTDIR` has not been set, the job script will execute in the directory where it is located, and the result files will also be located in that place.

The exact command given to run the job depends on the queue configuration.

### 9.1.5 Job files

#### Local files

The local files section lists all files that ADFjobs found. They all have the same name (the name of the job), and different extensions. Here you can see what files belong to a job, including modification date and time, and the size of the files.

Double clicking on some of the extensions will open that file. For example, double clicking a `.adf` file will open it in ADFinput. Double clicking a KF results file will open it in the KFBrowser.

One useful application is double click on the `.run` file. This will open the `.run` file in a text editor, depending on your operating system. In this editor you can actually make changes to the `.run` file. When you save it this modified run file will be used when you run the job. The `.job` file will be overwritten, thus you need to change the `.run` file if you wish to make manual changes.

You can also first select a local file. Next select one of the GUI modules from the SCM menu, and the selected file will be opened by that GUI module, if possible.

Within the local files you may also find a directory called 'results'. This will be created when result files are present other than the standard result files. For local jobs they will always be present, for remote jobs it will be created when using the Transfer from Remote command or when you click on one of the remote files in the remote .results folder, as displayed in ADFjobs.

You can select multiple files using click followed by shift-click (for a range), or using control-click to add the clicked file to the selection. Once multiple files are selected, you can open all of them at the same time via the SCM menu (either from the menu or via a right-click in the selection). Alternatively, you can use the Backspace or Job->Delete menu command to delete the selected files.

## Remote files

This is a similar list of files as the local files list, but these files reside on a the remote machine as specified in the job details. If you are preparing a new calculation it will be empty. When a calculation is complete, it will show all the result files on the remote machine.

At the top of the list the name of the directory in which the files live on the remote machine is shown.

You can select a remote file by clicking on it. This will cause the file to be transferred to the local machine, replacing any local file with the same name. If you click on any of the remote files in the .results directory all remote files belonging to the job will be transferred (overwriting local files with the same names).

After selecting the remote file it will be used by GUI modules started from the SCM menu.

### 9.1.6 Clean Up

After a calculation many files may be saved. Some of them might not be of interest for you, or only temporarily. You can use the **Job** → **Clean Up** command to remove files no longer needed. It will present a dialog where you can select exactly what files to remove. The most important result files will by default be saved.

Note that you can also just select the files you want to delete and press backspace.

### 9.1.7 Archive jobs

You can use the **Job** → **Archive** command to collect most files belonging to a job and put them in a gzipped tar archive. This will significantly reduce the amount of space used by the job. The command will operate on all selected jobs.

If you use an archived job in ADFjobs (or any GUI module) will recognize it as archived, and automatically unarchive it before using. So in practice you can just archive many (or all) of your jobs and forget about it. This will save a lot of disk space.

### 9.1.8 Import / Export jobs

If you want to share jobs with other users (or SCM support) there is an easy way to do this. Just select your job in ADFjobs, and use the **Job** → **Export...** command. A dialog will appear that allows you to specify where to save the packaged job. The packaged job is in principle just a gzipped tar file containing all job files, with some extra data so that ADFjobs recognizes it as a packaged job.

Use the **Job** → **Import...** command to open such a packaged job and add it to your ADFjobs listing.

### 9.1.9 Find job files

After some time you may have a lot of result files collected in the same folder. The **Job** → **Show Files** command will show the files belonging to the selected job on your computer. How it does this exactly depends on your operating system. Typically a window will open showing the files in the directory, with the files of the job selected.

### 9.1.10 Test Job

When you have trouble running jobs, either locally or via some queue you have defined, it is sometimes not easy to figure out what the problem is. To help you (or us, when you ask for support) diagnose the problem ADFjobs can make a test job.

Use the **Job** → **Generate Test Job**, select it in your ADFjobs window, assign the queue you want to use (or skip this step if you want to test the default queue), and use the **Job** → **Run** command.

The logfile of that job will contain a lot of diagnostic information, like the environment, license details, adf version details and more. Some consistency checks are performed. This information might help you to solve the problem. If not, contact us, explain the problem and include the output of the test job.

## 9.2 Queues

A queue tells ADFjobs how to run the selected job: where (possibly on a remote system!), how and by whom.

In the Queue menu you see a list of queues. Select one of them to use that queue when running the selected jobs.

If you have configured queues for remote machines, you will be able to use those remote machines just as easily as your local machine. ADFjobs will take care of copying files to and from the remote machine. It will also start or submit your job, and inform you of the progress of your job.

If you have defined your own queue, for example to run on some remote cluster, you can make that the default queue (instead of the Sequential queue) by using the **Queue** → **Set Default** menu command.

For each job, you can specify some extra text in the options field next to the name of the queue (with the gray rectangle around it). How this text is used depends on how your queues are set up. For example, the Interactive queue uses it to specify the number of tasks to use in your job. For batch systems, it might be the number of nodes to use, or some time limit or batch queue name.

When starting ADFjobs the first time, you will see the Interactive and the Sequential queue. Both will run jobs on your local machine, using as many tasks as possible. You can enter a number in the options field of the job (with the gray rectangle) to set the number of tasks use explicitly.

Via the GUI Preferences, you can also configure ADFjobs to automatically pick up queues stored in a central location. They need to be defined once, and any ADFjobs user can import them. Such queues are called 'Dynamic queues'.

**Warning:** The `Job status` command in default queues have been updated, to avoid excess load on the batch system.

For PBS the `qstat` command has been changed into `qstat $jid`. And a similar change for the other batch systems, the syntax depends on your batch system.

You may want to change your own queue in the same way.



### 9.2.1 Interactive Queue

When you run ADFjobs for the first time, it will make sure that an Interactive queue exists. If not, it will automatically create such a queue for you.

When you use the interactive queue to run a job, your job will run immediately on the local machine. Thus you can run many jobs at the same time.

To specify how many tasks to use, enter a number in the options field. If you leave it empty all cores will be used.

As you could be overloading your machine it may not be what you want, but it is great if you have some job running and want another small one to run at the same time. Another use would be to run several single-core jobs on a multi-core desktop machine at the same time.

### 9.2.2 Sequential Queue

When you run ADFjobs for the first time, it will also make sure that a Sequential queue exists. If not, it will automatically create such a queue for you.

When you use the Sequential queue to run a job, your job will run interactively on the local machine as soon as no other job is running. Thus you can give the run command in ADFjobs for many jobs at the same time, but they will actually run one after the other.

To specify how many tasks to use, enter a number in the options field. If you leave it empty all cores will be used.

Normally, this is the most convenient and efficient way to run jobs on your local machine. For that reason it is the default queue (unless you change that).

### 9.2.3 Setting up your own Queues

You can define a queue in several ways:

- **Queue** → **New...** based on one of the included example queues,
- **Queue** → **Edit...** change details of a queue (or make a new one if you change the queue name as well),
- **SCM** → **Preferences** → **ADFjobs** → **Dynamic Queues** import queues stored on some central system

When using the **Queue** → **New...** command, you can select what configuration to start with:

- **Interactive**: make a new Interactive queue. For example, to make a special version that will force your job to use only 1 task.
- **LSF, PBS, SGE**: make a new queue that will submit your job to the selected batch system. The configuration of these batch systems can be quite different. The included examples should server as an example only, you will need to fix the details. In the included examples the options field is used to specify the number of nodes to be used.

When using the **Queue** → **Edit...** command, you select what queue configuration to edit.

Using either of these commands, a dialog will appear requesting you to set the details of the queue you are creating (or modifying).

Often it requires some experimentation to set up all the details correctly. You can use the **Help** → **Trace Commands To Remote** menu command in ADFjobs to trace the commands given to communicate with the remote host (typically the ssh or putty command with arguments), and to see the responses to these commands received from the remote host. This trace will be shown in via ADFtail.

The following details may be set when configuring a queue:

**Remote host** Name of the machine on which you wish to issue the command to run (or submit) your job. You should be able to connect to that machine using ssh, and the host name as specified here. If you wish to run on your local machine, leave this field empty or specify localhost.

**Remote user** The username that you need to specify in the ssh command, if any. Typically, this is your username on the remote machine. If you have configured ssh to log in on your remote machine without specifying a user name, you can just leave this field empty. That is also the most convenient way to set up a queue that is to be used by other people as well (with their own accounts on the remote machine).

**Remote job directory** On the remote machine, ADFjobs needs to set up your input files and run script, and needs to collect the results. For that purpose ADFjobs will make its own directories within the directory you specify. A typical value would be something like \$HOME/jobs.

**Run command** The command **on the remote host** to be executed. ADFjobs will always first ssh into the Remote machine, and then issue the Run command. The run command should start the job interactively, or submit the job using some batch system. If the remote host field is empty or localhost, the run command will be executed on the local machine.

\$job will be replaced by the full path to your job script on the remote machine.

\$jobname will be replaced by a jobname based on the value of \$job, but truncated and with spaces removed.

\$options will be replaced by the contents of the Options field. The Options typically will be used to specify the number of tasks, a time limit, or a batch queue name.

If you use the run command to submit a job to some batch system, it should return a number. This number will be assigned to \$jid, and may be used by the kill and job status commands.

To run interactively, just enter “sh \$job”. To submit your job to a queue, specify the submit command (for example, qsub, or some other special submit tool). For example, check the pre-configured queues for Interactive and batch systems (via the **Queue** → **New...** menu command).

The job script that is automatically generated accepts an optional parameter. This parameter is ‘eval-ed’ at the start of the script. Thus, you can use it to set environment variables (like NSCM) or other things.

When the run command is issued, the working directory will be \$SCM\_RESULTDIR or the location of the .job script if no SCM\_RESULTDIR has been defined. The results (output file and so on) will also be saved in that location. Note that the computational engines (ADF, BAND, ...) will automatically change their working directory when started to \$SCM\_TMPDIR. You should make sure that SCM\_TMPDIR points to the proper location as you want to make sure you are writing to a fast local disk, and not to the (typically shared) disk where the results are stored.

**Use Local Batch** If yes, jobs will be queued on the local machine. Only one job will be running at a time. This is set for the Sequential queue (which is default). Currently this value is ignored when the job will be queued or run on a remote system.

**Kill command** The command to use to kill a queued or running job. In this command \$jid will be replaced by the job id (from the output of the run command), or by the process id. For interactive jobs, killall \$pid should work fine. This killall is actually replaced by a special script that takes care to kill adf and all child processes.

**Job status command** This command will be used to determine if a job is still queued or running. If a job is no longer queued or running, it should return an empty string. Anything else will server as indication that the job is alive.

For interactive jobs ps -p \$pid | grep \$pid works fine.

For batch jobs the command typically is qstat \$jid | grep -w \$pid (note: the \$jid after the qstat was added recently, and the exact syntax depends on your batch system).

The job status command is issued every 5 minutes by default, per job, while the job is running or queued. You can change that by setting the SCM\_STATUSINTERVAL environment variable on the remote machine (where the batch commands are executed).

**System status command** The command to use to determine the system status. This might be uptime, or some qstat command for batch systems.

**Prolog command** The command to execute by the job script, just before the included .run script. This will be used to set up the environment properly. For example, you would source a script file to set all environment variables for ADF like ADFHOME, ADFBIN etc. This is especially important if you are working with different versions of ADF at the same time. Note that the job script is started using /bin/sh, so you should use sh-like syntax (an not csh-like). If your environment is already set up correctly for running ADF on the remote host, without issuing any commands, you can leave this field empty.

In your prolog command you can use environment variables that are defined by the job script. Most importantly, the environment variable SCM\_OUT points to the output file of the job, SCM\_LOG points to the logfile, and SCM\_ERR points to the error output. This makes it easy to print some additional information to those files.

You can put multiple commands here separated by ";". However, in most cases it is easier to source a file with commands. By sourcing it you make sure that changes in the environment defined in the sourced file will also be available by the job script.

**Epilog command** This is the command to run by the job script, just after the included .run script. You can use it to copy save result files, or to perform some cleanup action. Again, use sh-style syntax, and the same environment variables are still defined..

**Synchronize jobs** If this field is set to 'yes', jobs on the corresponding remote host will be used for job synchronization (via the ADFjobs Synchronize Jobs command).

## 9.2.4 Dynamic queues

Dynamic queues are updated automatically when ADFjobs starts.

ADFjobs will check with the hosts that you have specified in the Preferences:

```
Open GUI preferences: SCM → Preferences
Panel bar Module → ADFjobs
Click the + button in front of Dynamic Queues
Enter the host name of the host on which to look for dynamic queues
Optionally: enter the username of the remote machine on which to look for dynamic_
→ queues
Click the 'Save' button at the bottom of the panel, and restart ADFjobs
```

If the username is left empty (or to the value (username)), no username will be used when connecting to the remote machine. Then your ssh configuration determines what username to use.

On the remote hosts listed, ADFjobs first checks the \$SCM\_QUEUES environment variable. If it is set, it will import the queues defined in the \$SCM\_QUEUES directory. If it is not defined it will try to import queues from \$HOME/.scm\_gui. This is the location where ADFjobs stores the queue information.

To define the dynamic queues, first figure out what queue settings you (and/or others) want to use. You can do this by configuring a normal queue with ADFjobs as described. As dynamic queues typically will be used by many users, you should not specify a username (unless you want all users to use the same account on some system). Make sure it works properly.

Next make a directory on the remote system where you want to store the dynamic queue definitions.

Set the SCM\_QUEUES environment variable system wide on remote system for all users. If SCM\_QUEUES is not defined, ADFjobs will search the \$HOME/.scmgui directory on the remote platform. This way users can set up their own dynamic queues.

Locate the files that define your queue: you can find these files in the \$HOME/.scm\_gui directory. They have the name of the queue, with a .tid extension, and are plain text files. Next, copy these files into the \$SCM\_QUEUES directory

on the remote system. Make sure all users have permissions to read the \$SCM\_QUEUES directory and the files in it.

Note: the server that stores the dynamic queues need not be the same machine on which the jobs will run.

Note: the ADFjobs user needs to have access to the server via ssh

## 9.2.5 Example Queue configurations for SGE and PBS

Here you will find example .tid files for SGE and PBS. They will not work without change, you need to set at least the proper hostname and runcmd, and most likely the prolog needs to be changed (or just made empty).

The contents of the .tid file for a SGE queue might look something like this:

```
# hostname: machine.domain
# username:
# jobscript:
# prolog: source $HOME/setup/adf2017
# epilog:
# jobdir: $HOME/jobs
# runcmd: qsub -pe s3_mpic h $options -q short3.q "$job"
# batch: no
# options: 2-2
# killcmd: qdel $jid
# jobstatuscmd: qstat | grep " $jid "
# sysstatuscmd: qstat
# label: My SGE queue
# logfile: logfile
```

Similar, for a PBS queue it might look something like this:

```
# hostname: machine.domain
# username:
# jobscript:
# prolog: source $HOME/setup/adf2017
# epilog:
# jobdir: $HOME/jobs
# runcmd: qsub -lnodes=2:ppn=2:infiniband -lwalltime=$options "$job"
# batch: no
# options: 0:15:00
# killcmd: qdel $jid
# jobstatuscmd: qstat | grep $jid
# sysstatuscmd: qstat -q
# label: My PBS queue
# logfile: logfile
```

## 9.3 Tools: set up many jobs and collect data from many jobs

You can use the Prepare tool to set up batches of jobs. For example, first set up an ADF calculation with your preferred basis set, XC potential and so on using ADFinput. Next, use the Prepare tool to generate a batch of similar jobs, but for different molecules (taken from .xyz files for example). Or you could set up a calculation for your molecule, and generate a set of jobs with different XC potentials and / or integration accuracies.

The Reporting tool is to generate a report of one or more calculations. This report will contain the information that you select when you define a 'report template'. Most of the properties that have been saved to .t21 will be available. And you can generate images as well (like HOMO or SCF density). These results will typically be collected in an HTML table: one row for each molecule, and one column for each property.

A report template defines what information to put into the report.

### 9.3.1 Prepare: set up many jobs at once

You activate the Prepare tool via the **Tools** → **Prepare...** menu command.

A window will appear that you can use to specify how to generate a set of jobs.

Three main list fields are presented: the Run field, the coordinates field, and the input options field. In each of these lists you can specify multiple options. When pressing 'OK' ADFjobs will generate the jobs by combining the options in all possible ways.

**Run list** Select one or more .adf files to run. A .adf file is just a calculation that has been set up using ADFinput before. Alternatively, one may use one of the predefined .adf files as present in the pull-down menu when you press the '+' button. To add a .adf file, use the pull-down menu, or specify a file name in the text field and press return. You may use wild card in the text field, so the default value (\*.adf) will expand to all .adf files in the current directory. To remove something from the list, select it and press the '-' button.

**Coordinates list** When this list is empty, the molecule as found in the .adf files will be used. When one or more sets of coordinates is present in this list, the molecule in the .adf file(s) will be replaced by the molecules as defined in the coordinate files. You may use .adf files, .xyz files, .t21 results files, .mol files, .pdb files or whatever other format ADFinput can use with the 'Import Coordinates' function. By listing multiple files here your .adf files (that you listed in the Run: list box) will all be executed with each of the molecules in turn. Thus, if you specified two run files (for example a Single Point calculation, and a Geometry Optimization), and three molecules, you will end up with 6 jobs.

**Input options list** In this list you may define alternative input options. The corresponding input options in the .adf file will be replaced by the values that you specify here. So if you specify two different basis sets, each job will be replaced by two new jobs, one with each basis set that you specify. You may also specify other things, like integration accuracy and so on. If you specify only one value, that value will be used in all jobs. If you specify multiple values (by repeatedly adding the option) you will generate multiple jobs.

The text field may be used to add additional keywords, or replace existing ones, with the value specified. These options will be added to the list of options by pressing return in the text field. The values will be used as the '-k' argument to the adfprep command. For detailed information about this please check the adfprep documentation.

**Produce jobs options** The final fields will tell the prepare tool where to generate the jobs (the directory is relative to the current directory, and will be created if it does not yet exist). Also one big job will be created that is just a concatenation of all the individual jobs. When running interactively it might be more convenient to run this job instead of all the individual jobs. The results should be identical, the big job will produce files that look as if they have been produced by the individual jobs.

### 9.3.2 Report: collect data from many jobs

To make a report of calculation results, you first have to set up a 'Report Template' that defines what information should be collected for the report. You manage these report templates via the New, Edit and Delete Report Template menu commands in the Tools menu.

When editing a report template, a dialog box will appear with many options. Just check the options for the information that you wish to collect in your report. Note that you can also include images (of orbitals, and so on) in the report.

If you wish to include something that is not present in the dialog, you can use the last field: Extra ADFreport command line options. Whatever you specify here will be passed to ADFreport to generate the report. This allows you to get any information that is available on a .t21 result file into your report. Check the ADFreport documentation for syntax details.

Once you have your Report template set up, you can use the Build command to actually generate a report. The data for the report will be taken from the currently selected jobs. You can update the report with new data from other jobs

by using the Update Last Report command, with one or more different jobs selected. These jobs may even be located in a different directory. This allows you to collect information from jobs a few at a time.

## 9.4 Series of jobs depending on each other

In ADFinput you can specify (in the Coordinates panel) that it should use the molecule from some other file or job. Then a job is created that depends on another job or on some other file (for example a .sdf file).

ADFjobs shows such dependencies when you select a job.

To run such a series of jobs that depend upon each other, you can just run the last job in the series. ADFjobs will determine what other jobs need to be run as well, and automatically start them (using the same Queue as the job you started yourself).

In the Tutorials you will find several examples of such jobs.

## ADFVIEW

The ADFview module of the GUI is used mainly to visualize field data like orbitals, densities and potentials. Additionally, it can also visualize some scalar atomic data, tensor data, and Bader (AIM) results.

### 10.1 Visualization methods

Via the Add menu you can select a visualization tool. This tool (an isosurface, or a cut plane for example) can be used with any kind of field. After selecting the command to add the visualization tool you will get a new extra control bar at the bottom of the window.

The following visualization tools are available:

- Isosurface: a simple isosurface through a scalar field
- Colored Isosurface: an isosurface through a scalar field colored by a second field
- Isosurface with Phase: an isosurfaces through a scalar field, colored by the complex phase (or sign for a real field). Typically used for orbitals.
- Multi Isosurface: multiple isosurfaces colored by isovalue
- Colored cut plane: a plane through some field, colored by the values of the field
- Contours cut plane: a plane through some field, with contour lines on the plane to show the values of the field
- Contours(+/-) cut plane: a plane through some field, with contour lines on the plane to show the values of the field, with negative contours using dashed lines
- Vector Field: many vectors on a grid, pointing as directed by some vector field. You can get a vector field by calculating the gradient of some other field for example. You can do this via the Calculated Fields menu command.
- StreamLines: an alternative to visualize a vector field.

In the control bar you select what field to visualize. The fields will be calculated on the fly. The leftmost field of the control bar (containing the name of the visualization method) also is a pull-down menu that you can use to access details, or to delete that particular visualization tool.

#### 10.1.1 Spinor: spin magnetization density

Spinors are a result of spin-orbit coupled calculations. Visualization of spinors is more difficult than visualization of orbitals. A spinor  $\Psi$  is a two-component complex wave function, which can be described with four real functions  $\phi$ :

real part  $\alpha \phi_\alpha^R$ , imaginary part  $\alpha \phi_\alpha^I$ , real part  $\beta \phi_\beta^R$ , imaginary part  $\beta \phi_\beta^I$ :

$$\Psi = \begin{pmatrix} \phi_\alpha^R + i\phi_\alpha^I \\ \phi_\beta^R + i\phi_\beta^I \end{pmatrix}$$

The density  $\rho$  is:

$$\rho = \Psi^\dagger \Psi$$

The spin magnetization density  $m$  is:

$$m = \Psi^\dagger \sigma \Psi$$

where  $\sigma$  is the vector of the Pauli spin matrices  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$ . A spinor is fully determined by the spin magnetization density and a phase factor  $e^{i\theta}$ , which both are functions of spatial coordinates.

The (square root of the) density and spin magnetization density are visualized as a double isosurface and a vector field respectively. The phase factor  $e^{i\theta}$ , reduced to a plus or minus sign, is visualized with the double isosurface and with the color of the vector field.

The main control bar is identical to the control bar of a normal isosurface. If you show the details, you will find that in addition to the controls available for a normal isosurface, you can also specify coloring information. In this case, the two numbers for the HSV colors define the colors of the minus and plus sign.

## 10.2 Fields

Fields can be things like orbitals or densities. You select them from the field pull-down menu in the control bars. In the Fields menu the Grid option determines on what kind of grid the field will be calculated.

As a convenient short-cut, you can switch fields using the up/down arrow keys

For many fields, like orbitals, transition densities etc selecting the option from the field pull-down menu brings up a window where you can select the field of interest. As an example, selecting 'Occupied Orbitals' will bring up a window that lists all occupied orbitals.

In these field select windows you can sort the fields by clicking on a column header. Clicking again on the same column header will reverse the sort order. When you use another command from the field pull-down menu the select window will close, unless you check the 'Keep Open' check box. That allows you, for example, to show all orbitals (both occupied and virtual) at the same time.

You can also create new fields out of these basic fields by combining them (calculated fields, for example the difference between two fields), or by interpolating them to get a finer or less dense field.

### 10.2.1 Steric Interaction

The Steric Interaction field is generated using Van der Waals radii to visualize steric bulk. The field is the minimum distance to the Van der Waals surface of the selected atoms. The radii are taken from the MM3 method by Allinger (N.L. Allinger, X. Zhou, J. Bergsma, *Molecular mechanics parameters*, *Journal of Molecular Structure: THEOCHEM* 312, 69 (1994) ([https://doi.org/10.1016/S0166-1280\(09\)80008-0](https://doi.org/10.1016/S0166-1280(09)80008-0))). An isovalue of 0 corresponds to the Van der Waals surface.



## 10.3 Properties

In the Properties menu you find commands to visualize scalar atomic info. Either by displaying the numbers, scaling the atom radii by these numbers, or by using the scalar values to color the atoms.

You also find some short-cuts to generate orbital plots: HOMO-1, HOMO, LUMO, LUMO+1, Density and Spin=Density. These commands will generate a double isosurface, and select the appropriate field for it.

Next are commands to visualize some tensor data, depending on what tensor data is available. The tensor is visualized as a sphere scaled in the directions of the eigen-vectors of the tensors by the eigenvalues of the tensors. For each visualized tensor type you will get a control bar that allows you to tune the visualization.

Finally, the properties menu allows you to visualize some Bader results. The Bader sampling shows you the integration grid, but with all the grid points colored that are together in the same Bader basins. The AIM (Bader) command visualized the critical points and critical paths.

## 10.4 Comparing data from several molecules

ADFview can handle more than one molecule at the same time. You can show fields for different molecules in the same window, you can create calculated fields to see differences, and so on.

The different molecules may come from different files, or from one result file containing multiple geometries. An example of the first situation would be two different calculations, with different XC potential, resulting in two different .t21 files. An example of the second would be the .t21 file from a NEB calculation. That file contains the information for all images, so you can see how (for example) the HOMO changes from image to image.

To add a new molecule from a different file, just open an additional file using the Open menu command from the File menu.

ADFview has a 'current' geometry. The molecule shown will be the one for the current geometry only.

To change the 'current' geometry, use the horizontal slider below the molecule window.

The visualization items (surfaces) might be filtered in such a way that only items related to the current geometry are shown. This is the default when visualizing NEB results: you want to see how the density or an orbital changes going from one image to the next (using the slider). If you open different files the default is to show visualization items for all geometries at once. Thus you might compare orbitals from one fragment with those from another. You can switch this behavior using the 'Show All Geometries' menu command from the View menu.

You can easily compare calculations on the same molecule that differ in something else than geometry. Just open both result files (.t21). Next, you can calculate differences between similar things. If you add a calculated field, you will find that the first command in the field select menu is used to select the geometry from which to take the data. Thus, you can select the same property from different files and compute the difference.

**Warning:** The current implementation has no possibility to adjust the orientation or the grid. In practice this means that you need to take care that the fields that you compare actually make sense to compare. This is only the case if the geometry of the molecules is identical and thus the grid is identical. Though this is very restrictive, you can make interesting comparisons for a given molecule: change due to different XC, basis sets or integration accuracy for example.

## 10.5 Temporary Files

ADFview normally will run DENSF or BAND in the background. This means that it needs scratch space to store inputs and result files to be visualized. After normal termination of ADFview (using Quit) all scratch files will be removed.

The scratch files will be created in the following location:

- If \$SCM\_TMPDIR is defined : use the \$SCM\_TMPDIR directory
- else, if \$HOME is defined: use the \$HOME directory
- else, if \$TMPDIR is defined: use the \$TMPDIR directory
- else try to use the current working directory.

## 10.6 Calculating Fields

ADFview will show you a progress dialog with some options when calculating fields.

In front of the progress bar you will notice a right-pointing arrow. If you click on it the progress dialog window will enlarge, and you can follow the progress of the field calculation (by DENSF) in detail. If you scroll back in that window you can also examine the input given to DENSF. Obviously this output is also very useful when there is some problem calculating the field. Click the Close button at the right of the progress bar to close the progress dialog.

You will also see a Run button, and before it a pull-down menu that you can use to select a queue. When the calculation of a field is slow (for a fine grid or big molecule) you can press Run, and the calculation will be saved as a job in ADFjobs, and will then automatically be started to run in the specified queue. After the calculation has started you may quit ADFview if you wish, the results should automatically be picked up when you start ADFview again (and when the fields are available). As you can select the queue to use, you can also calculate the fields on some remote machine if you wish. See the ADFjobs documentation about the use of queues.

While a field is being calculated via ADFjobs, it will be visible in ADFjobs as a new job. The results will be stored with that job. When you start ADFview for your original molecule it will detect the newly available fields automatically. It will move the newly calculated fields to it self, and delete the job that was used to calculate the fields.

When you close ADFview after calculating some fields, ADFview may ask you to save the field. If you save the field it will automatically be available the next time you start ADFview (for this job). Be warned that saving many fields may take a lot of disk space. You can use the Clean Up command in ADFjobs to delete them.

## ADFMOVIE

The ADFmovie module of the GUI is used mainly to visualize molecular geometries, and graphs related to it. For example, follow the progress of a geometry optimization, the trajectory of an MD run, or visualize the Potential Energy Surface.

Additionally scalar atomic data (like names, charges, atomic temperature, etc) and vector atomic data (forces, gradients, velocities) may be visualized when available.

### 11.1 Geometries

When opening a results file, ADFmovie will show the current geometry of the system. If multiple geometries are available, there will be a slider and buttons that allow you to play a movie, and to move to a specific frame.

If the calculation is a PES (Linear Transit) calculation, there may be many unconverged geometries as well as converged geometries. In the View menu you can toggle if you want to see all geometries, or just the converged geometries.

### 11.2 Scalar Atomic Properties

If atomic properties are available for a geometry, you can show them using the View menu:

- Atom Info: show the selected property as a text label
- Color Atoms By: use the selected property to color the atoms
- Atom Radius From: use the selected property to scale the atoms

Properties may be things like Name, AtomType, Charge (actually many different kinds of charges), ...

### 11.3 Atomic Vectors

If atomic vectors are available for a geometry, you can show them using the View menu: use the Vectors command in the View menu to select which vectors to show.

Examples of atomic vectors: gradient, force, velocity

When doing a geometry optimization via AMS, or an MD calculation via AMS or ReaxFF these may be present.

With the Scale Vectors menu command in the View menu you can make the vectors bigger or smaller (often needed to see very small vectors at all).

## 11.4 Graphs

ADFmovie can also make graphs of many properties (like energy, temperature, selected distances, angles etc) that change with the geometry. Check the tutorials for many examples.

Note that you can have multiple curves in one graph, and you can have multiple graphs.

You can save the graph in many different formats, and you can export the graph data.

## 11.5 Trajectory Analysis

ADFmovie also provides an interface to some tools to analyze MD trajectories, apart from the graphs.

- Histograms
- Radial Distribution Function
- Molecule Fractions: make graphs of specific molecules detected
- ChemTraYzer: use the Reaction Event Detection command in the Properties menu to analyze reactions happening

## KFBROWSER

With the Kfbrowser you can inspect all KF files produced by the ADF package. It has two modes: the default non-expert mode, and the expert mode.

### 12.1 Non-expert mode

You will see a sub-set of the data contained on the KF file. It may be empty, depending on the KF file. For KF files that the Kfbrowser knows about (t21, runkf, rkf and rxkf) it will show the results that may be of use for users.

If you select values you can use double click on the selection or use the **Selection As Graph** menu command to see the values in a graph.

You can use Copy/Paste to copy the selected data and paste it in a different program, for example Excel. The data will be copied as tab-separated so it will be pasted nicely formatted in your editor or spreadsheet.

### 12.2 Expert mode

In expert mode you will see all data on the KF file. This is mainly intended for developers. You should not assume any meaning to anything shown here unless you are familiar with the code that produced the KF file.



## CONFORMERS

The GUI has an option to handle multiple conformers of molecules.

Conformers may be created using RDKit (see [www.rdkit.org](http://www.rdkit.org) (<http://www.rdkit.org>)) via ADFinput. There is now a Conformers job method (just like ADF, BAND, DFTB etc) that will show a panel with options to generate the conformers. The algorithm used by RDKit for conformer generation will only work properly for single molecules, and the proper connectivity needs to be present.

After setting the proper options, just run the job like any other job. So it may also be running in the background.

The conformer geometries are stored in an .sdf file. This is in principle a series of xyz structures, with bond information and some other data. The energy is stored in the comment line, and in the extra fields there is also information like what program calculated the energy, and sometimes a pointer to the matching input file (.adf file) and results file (.t21 file).

You can use ADFmovie to open the .sdf file and see the molecules in there. Open the Energy Graph in ADFmovie to get a graph of the corresponding energies.

With ADFinput you can set up your calculation as usual (single point, geometry optimization, or anything else). In the Coordinates panel (in the Model section) you can specify that you want to use the molecules from the .sdf file (Use Selected File, and specify the .sdf file generated by the Conformers job). You can select what entries to use from the .sdf file using the SDF Filter panel (click on the ... button after Use Selected File, or go to the SDF Filters panel in the Details section directly). You can filter based on count or energy. In this panel you can also select what post-processing options will be applied to new sdf files generated by a calculation.

When you save your setup in ADFinput, a run script is created that will execute your job for all the conformers. Results of the individual calculations will be saved in the .results directory, and the original .sdf file will also be put there (with a time stamp). After running a new .sdf file will be created that has the results of the calculations, with pointers to the result files. Technically this is done using adfprep and adfreport in the run script.

Based on this new sdf file you can now do other things, if you want. Thus you can chain a series of calculations, for example first optimizing with DFTB or MOPAC, next optimizing with ADF, and finally calculating some property with ADF.

If you have calculated some spectrum (IR, NMR, UV/Vis) for all conformers in this way, you can visualize the averaged spectrum via ADFspectra. If it finds an .sdf file with the job, it will use it and the pointers in it to calculate averaged spectra. In ADFspectra there will be extra controls on how this averaging is done, most importantly the Temperature. In the View menu in ADFspectra you can also show all individual spectra, put together in one plot.

As the individual result files are present in the results directory, you can also visualize results from any specific conformer by selecting that t21 result file in ADFjobs, and then using the tools in the SCM menu as usual.





## FUKUI FUNCTION

The Fukui function describes the electron density after adding or removing some amount of electrons. It can predict where the most electrophilic and nucleophilic sites on a molecule are.

Fukui functions can be easily calculated using the GUI, as shown in the Fukui tutorial.

The Fukui function is implemented as a finite charge change. By default a whole electron is added or removed, however the calculation is not restricted to this amount. Fractional amounts of electrons are allowed.

The Fukui equation for the electrophilic attack,  $f^-$ , is given for when 1 electron is removed.

$$f^- = \rho(N) - \rho(N - 1)$$

Equally, the Fukui function for the nucleophilic attack,  $f^+$ , is given for when 1 electron is added.

$$f^+ = \rho(N + 1) - \rho(N)$$

Do note that in all cases the geometry of the neutral state is used to get the electron density.

The Dual Descriptor is a way to combine the two Fukui functions. It has a positive value where it is electrophilic and negative where it is nucleophilic. It is implemented as the difference between the Fukui plus and Fukui minus functions.

$$f(r) = f^+ - f^-$$

The Fukui function can be used to describe local chemical reactivity. This can even be done per atom by using the condensed Fukui function.

$$f_k^- = q_k(N) - q_k(N - 1)$$

$$f_k^+ = q_k(N + 1) - q_k(N)$$

Atomic charges are used to get the condensed Fukui function. There are several ways to partition the atomic charges. The Fukui calculation prints the condensed Fukui functions for Hirshfeld, Mulliken, Voronoi, and if calculated, Bader charges.

The condensed Fukui function is normalized, so that atomic Fukui values sum to one.

$$\sum_{k=1}^{N_{atoms}} f_k(\mathbf{r}) = 1$$

The local softness can be calculated as the product of the condensed Fukui function and the global softness. An approximation for the global softness is given as the inverse of the HOMO-LUMO gap.

$$S = \frac{1}{E_{LUMO} - E_{HOMO}}$$

The local softness is then simply

$$s_k^-(\mathbf{r}) = Sf_k^-(\mathbf{r})$$

$$s_k^+(\mathbf{r}) = Sf_k^+(\mathbf{r})$$

## MINIMUM ENERGY CROSSING POINT

The Minimum Energy Crossing Point (MECP) is the lowest point where two potential energy surfaces cross. These two potential energy surfaces can be any two orthogonal states. The situation for different spin states is implemented in the GUI, which takes the current state and the next spin state, e.g. singlet and triplet. This can be used to find the most likely location for a spin forbidden chemical reaction.

The model menu in ADFinput has the option to calculate the MECP. The same convergence criteria as for ADF is used for the MECP optimization.



## QUANTUM ESPRESSO

The GUI also supports setting up, running and visualizing results from Quantum ESPRESSO. For installation of Quantum ESPRESSO see the *Set up* (page 3) section in this manual.

The Quantum ESPRESSO code has not been developed by SCM. We cannot give support for Quantum ESPRESSO issues other than use via our GUI.

### 16.1 Input

ADFinput can make run scripts for Quantum ESPRESSO. To do that just go to the Quantum ESPRESSO section in ADFinput, it should be self-explaining how to run jobs.

On the Main panel you can set the task type (with Geometry Optimization doing the same as the relax and vc\_relax options in Quantum ESPRESSO).

The XC, Type and Relativity options are used to select pseudo potentials. They work by filtering all pseudo potentials available to match the selected options, for your current system. Thus it depends on your system what options are available in the XC and Type menus. Click on the ... next to Type, or go to the Pseudopotentials details page to have ultimate control: select any file as a pseudo potential file.

When you save your setup, ADFinput will generate a run script. You can preview this script in the Run Script panel (in Details). You can even edit it, and then your edited run script will be used (note that this will block other changes you may make in ADFinput until you turn Auto update back on).

### 16.2 Running

You should run the job preferably via ADFjobs, in the usual way.

That way you can also run on remote machines, and ADFjobs takes care to copy the files needed to the remote machine. The selected pseudo potential files will also be copied to the remote machine, unless they live in upf\_files (then it is assumed they are already on the remote machine). Obviously you should install Quantum ESPRESSO on the remote machine as well if you want to run jobs there.

Note that while the job is running you can monitor its progress in ADFjobs, or via the logfile (which in this case is identical to the output file).

### 16.3 Visualization of results

After the calculation the Quantum ESPRESSO results are parsed to generate an RKF file. Preferably data from the data-file.xml is used, but many pieces of information are taken from the standard output file as they are not available

on the xml file. For that reason there is a chance that things will fail to use if you use a different version of Quantum ESPRESSO.

The RKF result file can be used by all the SCM GUI modules to visualize results. Thus you can use the SCM menu to:

- **View:** visualize the system and fields (density, potential, deformation potential, spin density, ...). ADFview uses the post processing tools from Quantum ESPRESSO to generate the fields. For that the Quantum ESPRESSO results need to be available (in the .results folder), not just the RKF file. When your calculation is a remote calculation ADFview will automatically generate jobs to calculate fields as needed on the remote machine (thus no need to transfer the ofther big .results directory)
- **Movie:** the geometry changes during your calculation (for geometry optimizations with or without lattice optimization). As usual you can plot the energy as function of the geometry step, or any geometric data (distances, angles, cell axes, etc).
- **Logfile:** the standard text output.
- **Output:** the standard text output.
- **Band Structure:** visualize the band structure and (partial) DOS, if calculated
- **DOS:** visualize the (partial) DOS
- **KF Browser:** many pieces of output results collected, ready to copy to some spreadsheet or make graphs inside KF Browser

## 16.4 Scripting support

Using Quantum ESPRESSO via adfprep and adfreport is fully supported.

Use `$ADFBIN/adfprep -h` and `$ADFBIN/adreport -h` for details. For more information on what QE results are available via adfreport, specify the result file name (the .rkf file) as well.

For example: `$ADFBIN/adfreport -h qejob.rkf`

## ADFTRAIN

### 17.1 General

#### 17.1.1 Overview

ADFtrain is a graphical user interface (GUI) to handle Training sets and ReaxFF force field files.

When optimizing a force field, one has to define a training set and initial force field file, and decide on what parameters to optimize (and in what range).

ADFtrain shows you the training set and force field, and allows you to make adjustments:

- adjust the training set (new systems, remove systems, define what to include in the objective function, weights, etc.)
- adjust the force field (add or remove terms, initial values for parameters, optimization details)

After saving, you will have a trainset.in and geo file. These define the training set. You will also have a ffield and params file. These define the force field and how to optimize it.

The next step would be to actually optimize the ffield, using all these files as input. That is currently not handled by ADFtrain.

Finally, the results of the training (new ffield and fort.99) can be shown with ADFtrain. The fort.99 contains the contributions to the objective function, and they will be shown together with the training set.

Based on the results, one can adjust the optimization: improve the training set, or focus on other parameters of the ffield to optimize.

#### 17.1.2 File handling

##### Open

Use the Open command in the File menu to open a specific file. Alternatively, one can start ADFtrain via the command line and specify the file to open as argument.

The current setup will be cleared (that is, the New command is automatically used).

ADFtrain will try to determine what kind of file you have selected to open. Possible options are a trainset.in file (must be named trainset.in), a geo file (either named geo or with the .bgf extension), a force field file (named ffield or with the .ff extension), or a params file (must be named params).

The names of the other files to open are the default names (trainset.in, geo, ffield, params and fort.99) in the same directory as the file you selected to open.

### Add

When using the Add command in the File menu, the selected file will be added to the current ADFtrain window. Only the selected file will be imported, and you can add only trainset.in, geo or ffield files.

### Save

First it will be suggested to save with the same names as has been used while opening.

If you do not like that (probably you want to save your original files), click 'No'. You will be asked to select a directory in which to save the files. All files will have their default names.

## 17.1.3 Tables

Both the training set and force field are shown as a table.

### Header menus: sort and filter

On top of the tables is an header. All the items in the header are pull-down menus, you can use them to sort the table (by the values in the corresponding column).

The left-most item in the headers are 'Type' menus. They offer the same sorting options, but you can also filter by specific types. You can select which types of data to show, one or more types, or all.

### Search

Both tables have a Search field on the bottom. Use cmd/ctrl-F to go there, or click in the field. While you type, the data shown in the corresponding table will automatically be filtered by whatever you type. The spaces in your search string will automatically be replaced by wild-cards.

### Selection

To make selections in the tables use your mouse.

In the training set table you may click anywhere, in the force field table click somewhere in the left two columns to make a selection.

Left click: set the selection to the clicked line,

Shift-left click: extent the selection up to and including the clicked line,

Control-left or right click: toggle the clicked line in/out the selection.

The backspace key: delete the selected lines.

The Escape key: clear the selection.

All lines in the training set correspond to one or more systems (molecules). If only one system is selected (or multiple lines with the same system) it is displayed on the left. When a single line with an Energy term is selected, all systems in that energy expression are shown on the left. Use your arrow keys (left and right) to go through the different systems in the energy expression.

You can move the selected line in the tables using up and down arrow keys.



## 17.2 Training set

### 17.2.1 Systems

A training set needs one or more systems. A system is a molecule or a crystal, together with details on how to run a calculation with it. So it might be a single point calculation, a geometry optimization, with extra details (like constraints, maximum number of geometry iterations, ...).

If you select a System line, and if it is the only selected system, the molecule will be shown on the left.

You can use the commands in the View menu to change details of what is shown on the left, just as in other ADF-GUI modules. Of course you can use the mouse to rotate, zoom, and select atoms.

Systems cannot be created inside ADFtrain, they are imported from various sources:

- ADFtrain: select a file to import, all formats that the ADF-GUI can read are supported (for example .adf, .xyz, .bgf, .sdf, .pdb, but also result files like .t21, .rkf etc)
- ADFinput: use the 'Add Coordinates To ADFtrain' menu command (in the File menu)
- ADFmovie: use the 'Add Coordinates To ADFtrain' menu command (in the File menu) to add the current frame to ADFtrain. Note you can do this repeatedly, for any frame you like to use as a test system
- ADFjobs: select one or more jobs, and use the 'Add To ADFtrain' menu command (in the File menu). In this case the selected job(s) is (are) added, not just the coordinates. ADFtrain will try to handle the job as best as it can. For example:
  - when adding a Linear Transit or PES Scan job ADFtrain will convert it into a series of geometry optimizations with constraints, and will also add Energy entries to match the corresponding LT/PES.,
  - jobs using SDF files will be added using all entries of the SDF file as a separate system.

Shortcut: cmd/ctrl-T (in ADFtrain, ADFinput, ADFmovie and ADFjobs).

In a system line in the training set table you can see the details of the system:

- SystemID,
- Runtype (with possible extra details),
- File from which the current system is used.

More information can be seen by moving your mouse over the line, and keep it there without moving. A balloon will popup with details.

When saving your setup, the systems are saved in BGF format, in a file called geo or in a .bgf file selected by you (via the Open command).

Currently ReaxFF has a restriction that SystemIDs may have at most 20 characters. To make renaming your SystemIDs easier, there is a menu command 'Change SystemIDs' in the 'Training Set' menu. Use this command to replace some text in all of your selected Systems (or all systems if none are selected) at once with some other text. You will be asked for a string to search for, and for a string to replace it with.

The 'Smart System Status' will adjust the status of all systems: if a system is used, the status will be active, if a system is not used the status is disabled.

### 17.2.2 Training set

A training set also defines the objective function that will be minimized with the parameter optimization. The objective function consists of many terms, each line in the table is one term (with the exception of comment lines and system lines).

To add terms to your training set, use the Add menu. Typically the selected systems and the selected atoms are used when adding terms.

As an example, to add a distance terms to your training set:

1. select the system for which you want to add a distance term,
2. select two atoms in the system,
3. use the Bonds command from the Add menu.

One distance term will be created in your training set. Obviously, when you are going to use a distance term your system will need to be a geometry optimization. If it would be a single point calculation, the distances will always remain the same so this term would just be a constant (probably zero).

The atom selection determines what distance terms are added:

- If no atoms are selected (thus step 2 is skipped), all bonds found in the system will be added.
- If two atoms are selected (as in the example): the distance between those atoms will be added (even if they are not bonded directly).
- If more than two atoms are selected: all selected bonds in the system will be added (thus existing bonds between selected atoms).

If more than one system is selected, the above is repeated for all selected systems. The atom selection criterion will still be used, note that this makes no sense if the systems do not have the same atoms in the same order. This way of handling the atom selection is used for all geometric tests.

In the distance term line you can see:

- the Type ('Geometry: distance'),
- the systemID (some name, identical to the name of the selected system),
- the Accuracy (inverse of weight factor, to set the relative contribution of this term to the objective function),
- the Details (the atom numbers and atom types involved in this particular distance),
- the Value (the reference value, calculated using the current system),
- the Error (when opening a training set after optimizing, the actual contribution to the objective function of this term).

The Error column will be filled with results from the training (read from a fort.99 file). It shows the contribution to the objective function for each term in the training set. It is especially convenient if you sort by this column.

Term types that can be added are evident from the Add menu:

- distances (Bonds)
- angles
- dihedrals (Torsions)
- several types of charges
- energy expression
- energy curve
- force
- heat of formation
- cell parameters

An energy curve is special: select two or more systems, and use the Energy Curve command. This will add a set of energy records, one for each system, that test the energy differences between the selected systems. All differences will be with respect to the system with the lowest energy.

You can also add Comments, which are added just before the selected line. They are attached to that selected line, which is important when you are sorting the training set table.

When saving your setup, the systems are saved in a file called 'trainset.in'.

### 17.2.3 Mouse interaction

In addition to the general mouse interactions for selection (already mentioned):

- Double click item to edit
- Right click on system
- Mouse over to see details, error info etc (you will get a popup if you do not move the mouse).

### 17.2.4 Editing

To edit something, double click on it (or single click on a selected item). Next you can edit it in place, or in a window that appears.

Depending on what you are editing, the changes you make will be applied to the full selection! So when selecting multiple terms and editing the Accuracy, that field will be set for all your selected items. Similar, when changing runtime options, like runtime or maximum number of iterations, it applies to all selected systems. Constraints are not propagated as they depend on a particular system.

When editing SystemIDs, you can use the tab key to cycle through all SystemIDs matching what you have been typing. Add a space to use the current suggestion, or type more letters to narrow the search down. This works when changing SystemIDs as well as when editing energy expressions.

When you edit the runtime (double click on the Details field of a system), a window will appear that enables you to select the runtime and a couple of options. You can also add or remove constraints in this window. If you have made changes that are not visible in the Details field (like constraints), this will be graphically indicated.

### 17.2.5 Show

In the Show menu you can choose if you want to show comments, active or disabled items. With the Activate and Disable commands in the Training Set menu you can make an item active or disabled.

A disabled item will still be saved to the trainset.in file, but it will be commented out (with a special comment to distinguish it from a comment line).

In the table the lines can have different colors:

- Yellow background: selected
- Light red background: warning or error
- Red background: warning or error AND selected
- Gray foreground and background: disabled
- Gray foreground, light yellow background: disabled AND selected

This should be intuitive, if you remember yellow for selected, and red for warnings/errors.

## 17.2.6 Warnings and errors

If you hover with your mouse over a red line you will get extra information on why it is red, what kind of error.

For example, checking a distance for a system which is not optimized is useless, or having systems that are not used in any term. For energy expressions there is a check that the stoichiometry is correct (thus the net amount of all atom types should be zero).

Disabling an item makes it unavailable, thus for error testing this is the same as the item not being present at all.

You can also detect duplicate lines using the Duplicates command in the Show menu. They will also be marked as warning/error. This option is not on by default as it may be slow for big training sets.

You can use the ‘Select All Not In Force Field’ command in the Training Set menu to select all items in the training set that have specific atoms mentioned (geometry tests, charges, etc), and where the corresponding explicit term is not present in the Force Field. So when you select a C-H distance in the training set, and the Force Field does not have any C-H bond records, that line will be marked in the training set. It is up to you to consider if extra entries in the Force field are required.

In the Force Field menu there is a similar command to select force field entries that are not in the training set.

## 17.2.7 Reference data

### Generating reference jobs

Use the ‘Generate Ref Jobs...’ command from the ‘Training Set’ menu to generate reference jobs for your selected systems.

You will first be asked to select an example job. This is an .adf file created with ADFinput, which has the calculation setup you want to use. That may be using ADF, DFTB, etc., with basis, parameters and all other options as you like.

Next you need to select a directory in which the reference jobs are created.

Once they are created they are also added to ADFjobs (visible if you have ADFjobs open).

### Running reference jobs

To run the reference jobs, use ADFjobs (just select the jobs and use the Run menu command). With ADFjobs you can also decide to run these jobs on some other computer system.

### Importing results from reference jobs

Use the ‘Get Data From Ref Jobs’ menu command from the ‘Training Set’ menu to update all selected items in the training set with data from the reference jobs (if they are available). If you have no selection, all items in the training set will be updated.

## 17.3 Force field

### 17.3.1 Type: IgDispersion, ACKS2 or eReaxFF

If your force field uses IgDispersion, ACKS2 or eReaxFF you need to specify this. To do this, use the Type command in the Force Field menu.

You can turn on or off each of these options as you like. When using eReaxFF, ACKS2 will always be turned on automatically.

The type of force field (especially lgDisperion) determines how many parameters are saved to the force field file.

### 17.3.2 Force field parameters

For a description of the records in the force field file, please check the ReaxFF documentation. They should be self-explaining as presented in ADFtrain.

Note that when you hover with your mouse over a parameter value, a balloon will appear with the long name of that parameter, and with statistical information collected from all force fields in the force field directory.

#### Adding records

In the Force Field menu you will find many commands like

- Add xxx (Training Set)

These will add an xxx record (Atom, Bond, Angle etc) for each matching item in the Training Set. Thus, if the Training set has a 'Geo: distance' term for atoms C-H, a Bond C-H record will be added to the force field. Records already in the force field will not be added again.

Only the selected lines in the training set will be considered, if no selection the full training set will be considered.

- Add xxx (All)

These commands will add all possible Atoms, Bonds etc that can be made by combining the atoms types found in the training set. The selection in the training set is ignored. Records already in the force field will not be added again.

- Add Any...

This command will show a window where you can select what to add. You need to specify a type, and an atom string (something like H-C-H). You have the option to explicitly allow duplicate records (sometimes needed for angles or torsions).

The atom string may use some special characters:

- a '\*' to match anything (will also be a wildcard in the force field file)
- a '#' to loop over atom types in the force field file
- a '@' to loop over atom types in the training set

So:

1. Add Any Torsion H-C-O-N
2. Add Any Bond #-#
3. Add Any Angle #-#-#
4. Add Any Torsion #-#-#-#

will result in a force field file with many records, all combinations of H, C, O and N. This will be too much for a good force field, and also the Off-diagonal an Hydrogen bond records need to be considered.

The Force Field menu also has a command 'Select All Not In Training Set'. For each line in the force field file, the corresponding geometric tests are searched for in the training set. Thus is you have a Bond C-H line in the force field, this command will check if some Distance C-H occurs in the training set. If not, the line in the force field is selected. This is just a convenience feature, it is possible that lines are used for example in energy expressions and not

in geometric tests. It is up to you to consider to add extra terms to the training set, or to remove lines from the force field, or leave things as they are.

### Editing parameters and optimization details

When adding record to the force field file, values need to be specified for all parameters. The values used by ADFtrain are the values reported by rxffutil. These are the average values of a specific parameter in all force fields in the force field directory. For reasonable values you probably need to set up your own force field library (the default is the collection of all ReaxFF force fields distributed with our software).

With the 'RXFFUtil Options...' command in the Force Field menu you can set the options to use with the RXFFUtil program, especially the force field directory. For more info about rxffutil see the ReaxFF documentation.

For the force field optimization not only the parameters need a value, you also need details like the allowed range for a parameter, a delta per parameter, and a flag to indicate if a specific parameter needs to be optimized.

Select one or more parameters using Left Click and Shift Left Click. The first selected parameter will be shown with a black outline, the other selected parameters will be shown with a tiny outline. The Shift Left Click action will extent the set of selected parameters with all parameters inside a rectangle with respect to the first selected parameter (the one with the black outline). Click on a selected parameter to edit these values (thus if no selection double click on a parameter). If you leave a value empty, the value suggested by RXFFutil will be used.

A very common editing operation is to change the optimize flag. A convenient shortcut for this is to Control-left-click or Right-click on the parameter. When using the shortcut, the optimize status will propagate to all selected parameters if it is changed for a selected parameter.

The optimize flag is indicated with a color (orange when optimized, no special color otherwise).

When you make changes to other optimization values for a parameter, this will be indicated graphically.

When saving the force field with parameter values will be saved to the ffield file, and the details regarding optimization will be saved to the params file.

Use the following menu commands to reset the changes you made to the values calculated by the rxffutil:

1. Reset Param Values in the Force Field menu: reset the parameter values used in the ffield file (the values that are visible)
2. Reset Param Ranges in the Force Field menu: reset the optimization ranges, as set by double clicking on a parameter

### 17.3.3 Mouse interaction

In addition to the general mouse interactions for selection (already mentioned):

- Mouse over to see distribution of values, defaults etc (info from rxffutil)
- Control-left or right click on a parameter: toggle optimize flag, propagate to all selected parameters
- Click a selected parameter to edit it
- Left click on a parameter: set anchor (shown with an outline)
- Shift left click on a parameter: select a block of parameters (wrt the anchor) (selected parameters are visually marked)
- Left click on a selected parameter (or double click on a non-selected parameter): select and edit it
- Control-left or right click on atoms field: filter the training set with these atoms

## ADFcrs: COSMO-RS

ADFcrs is a utility program (`$ADFBIN/adfcrs`), which enables ADF users to easily create COSMO-RS jobs. You can use ADFcrs to add compounds, choose the desired property, and to set details of your COSMO-RS job using an easy-to-use graphical user interface. ADFcrs will generate the complete job script for you. This script takes care of running COSMO-RS. You can also use ADFcrs to run these script files and visualize the results.

The description of a compound that you want to use should be on a file, and should be a result file of quantum mechanical calculations using COSMO. In ADF such a COSMO result file is called a TAPE21 (.t21) file, or a COSKF (.coskf) file. ADFcrs might also be able to read a result file, for example a .cosmo file, from other programs.

If you have installed the ADF package correctly, the `adfcrs` command is located in `$ADFBIN`.

If `$ADFBIN` is included in your `PATH` environment variable, you can start the ADFcrs program with the following command:

```
adfcrs [filename filename2 ...]
```

The file names are optional. ADFinput handles files that were created by ADFinput before (which have a .crs or .crskf extension), use only one file name in these cases. One can add multiple files, which correspond to different compounds, if these files contain results of quantum mechanical calculations including COSMO on these compounds. these result files should have .t21, .coskf, or .cosmo extension. The file can also be a plain text file with a list of file names (.compoundlist), which contains on each line the filename of a .t21, .coskf, or .cosmo file.

An alternative method to start ADFcrs: select the COSMO-RS command from the SCM menu, or use ADFjobs to start ADFcrs.

Under windows you can start ADFcrs by double-clicking the icon on the desktop.

## 18.1 Menu Commands

### 18.1.1 File menu

**New** Same as quitting ADFcrs and starting again without specifying a file name.

**Open . . .** Open an existing ADFcrs file (with .crs) or an ADFcrs result file (with .crskf).

Same as quitting ADFcrs and starting again with specifying a file name. When you open a .crs file ADFcrs also tries to add all compounds that are specified in this .crs file and tries to open all .crskf files that belong to this .crs file. If you open a .crskf file only this file is read.

**Save** Save the current state of what is present in ADFcrs. If you have not saved before, ADFcrs will ask you to specify a file name.

A run file will not be saved.

**Save As . . .** Save the current state of what is present in ADFcrs in a file with a name of your choice.

A run file will not be saved.

**Save Runfile** Not only the .crs file will be saved, but also a matching .run file which is a run script corresponding to your input (for the selected property).

**Run** Start the COSMO-RS calculation as selected in all the input options.

You will first be asked to save the changes. The run script (with the .run extension) for the selected property is created. Next your job is run. When the run is finished the results will be visualized by ADFcrs and the .run file will be deleted.

**Kill** Kill the COSMO-RS calculation if one is running. The .run file will be deleted.

**Close** Stop ADFcrs, ask you to save changes if you made any.

## 18.1.2 Compounds menu

**List of Added Compounds** Shows a list of all the added compounds, including a possibility to set some input parameters, specific for a certain compound.

On the left side of the window the list of the compounds is given with the full path name to the file from which the quantum mechanical results data are read. Part of this quantum mechanical data is given in the right window for the selected compound. In this right window one can also write some pure compound input data. For ring compounds it is important to write the number of ring atoms. For example, this number should be 6 for benzene.

**Add Compound(s)** Use this menu command to add one or more compounds to the list of compounds. The selected files should be of type:

- .compoundlist: List of compounds
- .coskf: COSMO kf file
- .t21: ADF result file
- .compkf: COMPKF file
- .cosmo: COSMO file

The added file(s) should be either ADF result files (.t21), COSMO kf files (.coskf), COMPKF kf files (.compkf), or ASCII COSMO files (.cosmo). These files should be result files of a quantum mechanical calculation including COSMO, which contains COSMO segment data, or a result of the Fas Sigma prediction (.compkf). In case of ADF the ADF result file (.t21 or .coskf) will contain COSMO data if the ADF calculation was done with COSMO. The added file can also be a plain text file with a list of file names (.compoundlist), which contains on each line the filename of a .t21, .coskf, or .cosmo file.

**Install COSMO-RS database . . .** Download and install the COSMO-RS database ADFCRS-2018.

**Select Compound(s) from COSMO-RS database** If the COSMO-RS database was downloaded, it is easy to select with this menu compounds from this database.

## 18.1.3 Method menu

The methods and its parameters are described in the COSMO-RS manual.

**COSMO-RS** Select this menu command to set the method that will be used in the calculation to COSMO-RS.

**COSMO-SAC** Select this menu command to set the method that will be used in the calculation to COSMO-SAC.

**UNIFAC** Select this menu command to set the method that will be used in the calculation to UNIFAC.



**Parameters** Change the COSMO-RS or COSMO-SAC parameters and technical parameters that are used in the calculation. The COSMO-RS and COSMO-SAC model have general and element specific parameters. Technical parameters are, for example, convergence criteria and thresholds.

### 18.1.4 Properties menu

How the properties are calculated and definitions used can be found in the COSMO-RS manual.

**Vapor Pressure Pure Solvents Vapor Pressure Mixture** In case of a mixture, the mixture can be composed of up to five compounds, and the mole fraction of each compound of the solvent should be given, and it should add up to 1.

It is possible to calculate the vapor pressure for a temperature range, if the first temperature (from:) is different than the last temperature (to:).

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method.

**Boiling Point Pure Solvents Boiling Point Mixture** In case of a mixture, the mixture can be composed of up to five compounds, and the mole fraction of each compound of the solvent should be given, and it should add up to 1.

It is possible to calculate the boiling point for a pressure range, if the first pressure (from:) is different than that the last pressure (to:).

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method.

**Solvent Flash Point** The mixture can be composed of up to five compounds. The mole fraction of each compound of the solvent should be given, and it should add up to 1.

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method. However, for the compounds in the solvent the flash points of the pure compounds should be given as input, since COSMO-RS does not calculate these.

**Activity coefficients** The solvent can be a mixture of up to five compounds. The mole fraction of each compound of the solvent should be given, and it should add up to 1. One can use an input value for the density of the solvent instead of a calculated value, which can influence the calculated Henry constants.

The activity coefficients will be calculated for the selected compounds in the listbox, on the bottom-left side of the window. Compounds not present in the solvent are considered to be infinitely dilute.

**Log partition coefficients** The log of the partition coefficient (logP) of a solute in 2 phases of a solvent. Both phase 1 and phase 2 can be a mixture of up to three compounds. The mole fraction of each compound in phase 1 and phase 2 of the solvent should be given, and for both phases it should add up to 1. For example, if one wants to calculate partition coefficients for Benzene/Water, which are 2 immiscible liquids, phase 1 of the solvent will be purely Benzene, and phase 2 will be purely Water. Another example is the calculation of partition coefficients for 1-Octanol/Water, which are partly miscible liquids, phase 1 of the solvent will be a mixture of 1-Octanol and Water, and phase 2 will be purely Water (the solubility of 1-Octanol in Water is small).

One can use an input value for the quotient of the molar volumes of phase 1 and phase 2 instead of calculated values.

The logP will be calculated for the selected compounds in the listbox, on the bottom-left side of the window. Compounds not present in the solvent are considered to be infinitely dilute.

**Solubility in Pure Solvents Solubility in Mixture** In case of pure solvents one can select any number of different pure solvents, but only 1 solute.

In case of a mixture, the mixture can be composed of up to five compounds, and the mole fraction of each compound of the solvent should be given, and it should add up to 1. In this case can select any number of different solutes, but they should not be present in the solvent. In case of a mixture one can also use an input value for density of the solvent.

It is possible to calculate the vapor pressure for a temperature range, if the first temperature (from:) is different than the last temperature (to:).

For the solubility of a gas in a solvent one has to set the vapor pressure of the gas.

For the solubility of a solid compound it is necessary to include the melting point, the enthalpy of fusion, and optionally, since it is often not so important, the  $\Delta$  heat capacity of fusion of the pure compound (default  $\Delta$  heat capacity of fusion is zero). These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window.

**Binary mixture VLE/LLE** Exactly two compounds should be selected. One can select an isothermal, an isobaric, or a flash point calculation of the binary mixture. The binary mixture will be calculated for a list of molar fractions between zero and one.

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method.

**Ternary mixture VLE/LLE** Exactly three compounds should be selected. One can select an isothermal, an isobaric, or a flash point calculation of the ternary mixture. The ternary mixture will be calculated for a list of compositions.

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method.

**Solvents s1 - s2 Composition Line** Linear interpolation between the compositions of solvent 1 and solvent 2, which both could be mixtures. The solvents s1 and s2 can be a mixture of up to five compounds. The mole fraction of each compound of the solvent s1 and s2 should be given, and it should add up to 1. One can select an isothermal, an isobaric, or a flash point calculation.

One can use input values for the vapor pressure of the pure compounds at a given temperature. These input values can be set by selecting **Compounds** → **List of Added Compounds**, select the desired compound, and set input values for the pure compound in the right window. If these values are not specified (if they are zero) then they will be approximated using the COSMO-RS method.

### 18.1.5 Solvent Optimizations menu

**Optimize Solubility** Optimize the solvent (mixture) in order to maximize or minimize the mole fraction solubility of a solid solute in the liquid mixture.

**Optimize Liquid-Liquid Extraction** Optimize a mixture of immiscible solvents in order to maximize or minimize the distribution ratio (D) of two solutes between the two liquid phases.

### 18.1.6 Analysis menu

**Sigma Profile Pure Solvents Sigma Profile Mixture** The  $\sigma$ -profile is calculated for COSMO charge densities between minus the maximum value for sigma and the maximum value for sigma. In case of pure solvents one can select any number of different pure solvents. In case of a mixture, the mixture can be composed of up to five compounds.

**Sigma Potential Pure Solvents Sigma Potential Mixture** The  $\sigma$ -potential is calculated for COSMO charge densities between minus the maximum value for sigma and the maximum value for sigma. In case of a mixture, the mixture can be composed of up to five compounds.

### 18.1.7 Graph menu

**Graph X Axes** Use one of the submenu commands to change the X axes of your graph.

**Graph Y Axes** Use one of the submenu commands to change the Y axes of your graph.

**Graph Z Colormap** Use one of the sub-menu commands to change the colormap of your graph. Only available for **Properties** → **Ternary Mixture**.

**Save As PostScript** If you have any graphs, you can select one of the graphs. It will be saved in a postscript file.

**Save As XY** If you have any graphs, you can select one of the graphs. It will be saved in a text file as XY pairs. Next you can use most other plotting programs to make the graph just as you want it to be.

### 18.1.8 Help Menu

The help menu provides an easy way to get to information about the ADF-GUI. It will start a browser on your local machine, and opens a local copy of the documentation on the SCM web site.



## GUI ENVIRONMENT VARIABLES

As of the 2016.102 version, if you start the MacOSX ADF-GUI application the environment defined by your shell startup scripts is ignored. Instead the bundled ADF is used, and environment variables may be defined in a file `$HOME/.scmenv` and/or `/Library/Application Support/SCM/scmenv`.

In the following list the environment variables that are specific for the ADF-GUI are listed (the normal environment variables like `ADFHOME`, `ADFBIN` and `SCMLICENSE` are also used by the ADF-GUI):

**DISPLAY:** X-window display to use, when using ssh normally you should NOT set it manually. It is required (for all X11 programs) except on Windows.

**PSEUDO\_DIR:** Path to the folder containing Quantum ESPRESSO pseudo potential files. If not set, a *standard search path* (page 4) is used.

**SCM\_ADFREPORT\_PLAIN:** No labels or units in adfreport output. Not set by default.

**SCM\_BROWSER:** The HTML browser used for both local and remote documents (not for Windows or Mac). Default value: none (the PATH will be searched).

**SCM\_DEBUG:** Turn on many debug items in ADF and avoid clean-up by GUI. Not set by default.

**SCM\_DEBUG\_SSH:** Set to yes to debug communication issues: all non-multiplexed ssh commands will be printed to stderr. Set to all to see all SSH commands, even if multiplexed. Not set by default.

**SCM\_ERROR\_MAIL:** E-mail address for error reports. Default value: `errors@scm.com`.

**SCM\_DOCINDEXDIR:** Location of the directory in which the index for the documentation will be stored. Setting it makes it possible to share this index and save some space. Default value: `$HOME/.scm_gui/doc.index`.

**SCM\_FFMPEG:** The ffmpeg program to use to generate movies. Default value: none (the PATH will be searched).

**SCM\_FFMPEG\_ARGS:** The arguments to pass to ffmpeg. Default value: none. The `-i` and `-t` (for looping movies) will always be added automatically.

**SCM\_GEOMODSBYSIZE:** The geometry slider will always move the smallest group of atoms. Default value: none (the last selected atoms will move).

**SCM\_GUIRC:** Location of the preferences file. Default value: `$HOME/.scm_gui.rc`.

**SCM\_GUIPREFSDIR:** Location of the preferences directory. Default value: `$HOME/.scm_gui`.

**SCM\_SCMJOB\_RESTART:** Force a restart of the scmjobd job monitors every this many milliseconds. Not set by default (600000 which is every 10 minutes).

**SCM\_KFBROWSER\_EXPERT:** Define it to make the expert mode in the Kfbrowser the default. The non-expert mode will be the default mode.

**SCM\_LOG:** Set to the full path of a file to log some stuff the GUI does (mainly invocation of other modules/programs). Not set by default.

**SCM\_LOG\_SCMJOB:** Set to the full path of a file to log some what scmjobd is doing. Not set by default.

**SCM\_NO\_RSYNC:** do not use rsync to transfer files to/from remote machines, but use the previous implementation (with tar/gz). Not set by default.

**SCM\_NO\_LOGIN\_SHELL\_FOR\_MONITOR:** the scripts to monitor a running job normally run in a new login shell. Setting this env var will not force a login shell. Note it must be set on the machine where the monitor script is running, and you need to make sure that the queue commands (as defined in the ADFjobs queues) will work properly.

**SCM\_NO\_SSH\_MULTIPLEXING:** If set SSH multiplexing (bundle multiple ssh connections in one) will be avoided. Not set by default.

**SCM\_OFFSCREEN:** Set it to some value to force the GUI modules to run offscreen. Used for testing.

**SCM\_OLD\_TRANSFERS:** If set files are transferred one by one instead of in a tar archive (turn on when you run into tar compatibility issues). Not set by default.

**SCM\_PACKMOL:** The packmol program to used by the Builder. Default value: none (the PATH will be searched).

**SCM\_RESULTDIR:** Location of the results directory. Default value: none (directory where the .adf files etc live is used).

**SCM\_STRUCTURES:** Location of the structures directory. Default value: none.

**SCM\_TITLEVERSION:** Show SVN revision number in title. Not set by default (show only version number).

**SCM\_TMPDIR:** Temporary files will be made in this directory (should exists if set). Default value, if not set \$TMPDIR \$TMP /tmp \$HOME or the current directory is used (in that order).

**SCM\_TPLDIR:** Location of the presets directory. Default value: none.

**SCM\_STATUSINTERVAL:** The time in seconds between the job status commands used to detect killed jobs (like qstat). Default value: 600.

**SCM\_QUEUES:** Path to the dynamic queues directory. Default value: none (ADFjobs will search the remote \$HOME/.scmgui).

**SCM\_QEDIR:** Path to the folder containing Quantum ESPRESSO installation (binaries and pseudo potentials). Set it to force the installation of QE somewhere outside your \$ADFHOME. If not set, a *standard search path* (page 4) is used.

## REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications.

### 20.1 General References

The current version of the GUI was developed by O. Visser, with many contributions from L. Groot and O. Carstensen. Other (past) authors include M. Luppi (artwork) and the SCM developer team. Thanks to M. Mouthaan for testing and documentation.

**If you used the GUI you may optionally include the reference:** GUI 2019, SCM, Amsterdam, The Netherlands, <http://www.scm.com>

### 20.2 External programs and Libraries

Click [here](#) for the list of programs and/or libraries used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.