



Scientific Computing & Modelling

ADFGUI Reference Manual

ADF Program System

Release 2004.01

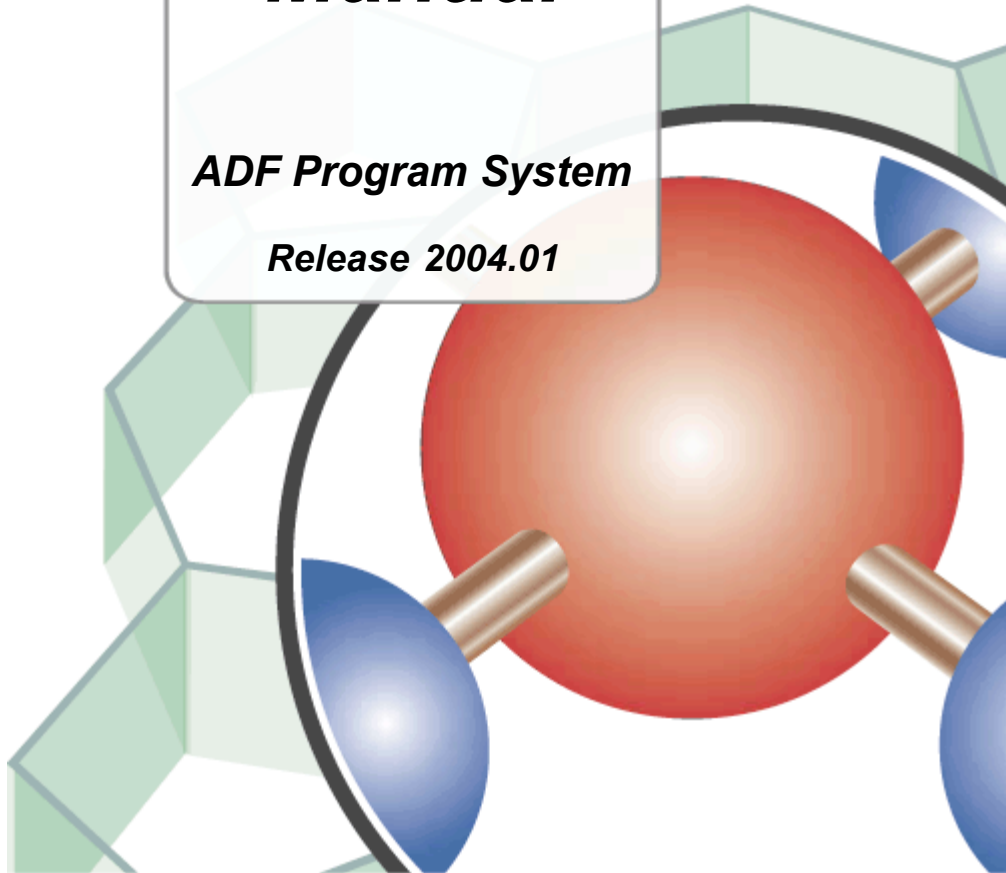


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Introduction

This document will provide a basic reference manual of the ADF GUI. ADF GUI is the Graphical User Interface for the ADF package.

If you are new to the ADF GUI we advise you to study the ADF GUI tutorial.

All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using the SCM menu commands you can easily switch between the different modules of the ADF GUI.

The ADF GUI consists of several modules:

ADFinput

A utility program (`$ADFBIN/adfinput`), which enables ADF users to easily create ADF jobs. You can use ADFinput to define your molecule (geometry), pre-optimize it, and to set details of your ADF job using an easy-to-use graphical user interface. ADFinput will generate the complete job script for you. This script takes care of running ADF and property programs as required. You can also use ADFinput to run these script files on your localhost in the background.

Can be selected with the 'Input' command from the SCM menu.

ADFview

A simple program (`$ADFBIN/adfview`) that displays 3-D (volume) data, such as electron densities, orbitals, electrostatic potentials.

Can be selected with the 'View' command from the SCM menu.

ADFmovie

This program (`$ADFBIN/adfmovie`) follows geometry steps as performed by ADF during geometry optimizations, IRC calculations, etc. Actually, it will display just any series of changing geometries, and is also used to display normal modes calculated with a frequency calculation.

Can be selected with the 'Movie' command from the SCM menu.

ADFspectra

This program (`$ADFBIN/adfspectra`) the spectra calculated by ADF. Currently it can show IR and excitation spectra, as well as a DOS plot. For some spectra (for example for IR spectra) it can also provide additional information, like a visualization of the normal modes (using ADFmovie). More types of spectra will follow in future versions.

Can be selected with the 'Spectra' command from the SCM menu.

ADFTail

A minor GUI utility (`$ADFBIN/adftail`) that will just show the contents of a text file, updating when the text file grows. It is used to follow the progress of an ADF calculation (similar to the UNIX tail -f command).

Can be selected with the 'Logfile' command from the SCM menu.

BOB

A Basic Output Browser (`$ADFBIN/bob`) for the output generated by ADF.

Can be selected with the 'Output' command from the SCM menu.

Automatic bug-reports

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of the GUI module having some problem, but do not contain personal information.

You can enable this by setting the global environment variable `SCM_ERROR_MAIL`, for example in your login script:

```
SCM_ERROR_MAIL=errors@scm.com
export SCM_ERROR_MAIL
```

This will ensure that the bug report will be sent to the mail address you specify. If you specify your own email address you can see exactly what kind of information is contained in the error report. And of course we would like you to forward that report to errors@scm.com.

Your comments and bug reports are very welcome. Please send them to support@scm.com.

ADFinput

Introduction

ADFinput is a utility program, which enables ADF users to easily create ADF jobs. You can use ADFinput to define your molecule (geometry), pre-optimize it, and to set details of your ADF job using an easy-to-use graphical user interface. ADFinput will generate the complete job script for you. This script takes care of running ADF and property programs as required.

The documentation of ADFinput consists of two main sections.

The first part is a very basic hands-on tutorial section in the ADF GUI tutorial. Its purpose is to make some simple job scripts, and to have a simple and fast tour of the main features of the utility. We estimate that you should be able to finish this section including the hands-on activities within 30 minutes.

The second part explains in detail many of the possible options, buttons and so on. This material is mainly included as a reference. We hope that the utility is easy to use, and that the options, together with the help information popping up, will not require you to use the reference manual.

At this point in time, ADFinput is still under development and is being tested. It is now released as a first version as a service to our customers. Your suggestions and bug reports are valuable to us for making an improved and extended next release available as soon as possible.

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of ADFinput, but do not contain personal information.

You can enable this by setting the global environment variable `SCM_ERROR_MAIL`, for example in your login script:

```
SCM_ERROR_MAIL=errors@scm.com
export SCM_ERROR_MAIL
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Your comments and bug reports are very welcome. Please send them to `support@scm.com`.

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Starting ADFinput

If you have installed the ADF package correctly, the ADFinput is located in \$ADFBIN.




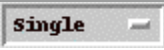



If \$ADFBIN is included in your PATH environment variable, you can start the ADFinput program with the following command:

```
adfinput [filename]
```

The filename is optional. ADFinput can only handles files that were created by ADFinput before, which have a .adf extension.

There is a second possibility to start ADFinput if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu ADFinput can be started by selecting the 'Input' command.

Buttons and Tools

Button	Description
	Select Tool: used to select, and to rotate, translate or zoom (with modifier keys or mouse buttons).
	C-tool, O-tool, N-tool, H-tool, Cl-tool: atom-tools used to <ul style="list-style-type: none"> • create a C, O, N, H or Cl atom, • change an existing atom, • create bonds between existing atoms. <p>The ?-tool is used with the Element menu.</p>
	Display button: toggle the display between a very simple but fast picture, or a photographic quality picture of your molecule
	Bond Type menu: <ul style="list-style-type: none"> • for new bonds • change selected bonds
	Connector menu: number of connectors <ul style="list-style-type: none"> • on new atoms • change selected atoms
	Optimizer buttons: use to <ul style="list-style-type: none"> • start or stop the optimization • replay the optimization • kill a running optimization
	Mouse-mode buttons: <ul style="list-style-type: none"> • S: normal mouse button • R: rotate with left mouse button • T: translate with left mouse button • Z: zoom with left mouse button

Templates and Defaults

All input options have default values. However, the default values depend on the main task you have chosen, and on further properties you may select to calculate. ADFinput uses templates that are simply a collection of input values to be used together as defaults.

ADFinput has a couple of templates for typical calculations (currently Single Point, Geometry Optimization, IRC, Frequencies, and Transition State Search). You may also define your own templates.

Use a template

Select the template you want to use from the Template menu, located in the main input options area.

All input values will change to the values specified in the template you select.

Yellow fields: different from template value

After you have selected a template, you can make changes to any input field you like.

The background color of that field turns yellow. This is just feedback for you so you know what fields you changed with respect to the default value specified in the current template.

Red fields: error in template

If you happen to see an input field with a red background, this means that the default value for that field is NOT specified in the current template. If you are using one of the original templates, please notify us so we can fix that template (email to support@scm.com).

Revert to template values

If you want to undo your changes and get back to the default values as specified in the current template, simply select the template again from the Template menu.

Make your own templates

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

If you set the `SCM_TPLDIR` environment variable, ADFinput will look for additional templates (when starting up) in the directory `$SCM_TPLDIR`.

In a terminal window:

- make a directory where you want to store your templates
- set the environment variable `SCM_TPLDIR` to the complete path to this directory

In ADFinput:

- edit all the fields as you would like them to be stored in a template.

- select 'Save as Template' from the File menu
- select the directory in which you want to store your template
- specify a filename, ending with '.tpl'
- click on Save.

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

The name of the template is the filename you have chosen, but without the .tpl extension.

Molecule Editor Tricks

Selecting

You can select parts of your molecule (atoms and / or bonds) with the mouse, using a combination of the following techniques:

- Click on the item you want to select. If you want to extent the selection with more items, hold the Shift key and click on the item to add.
If you want to remove an item from the selection, hold the Shift key and click on the item to be removed.
- Click with the mouse somewhere in the empty space, and drag a selection rectangle by moving the mouse while holding the mouse button down. Release the mouse button when the items to be selected are included within the rectangle.

When extending or reducing the selection by shift clicking, take care not to move the mouse while clicking. Moving in combination with the shift key will rotate the selection.

When selecting does not react as described, make sure you are using the select tool, and that the mouse mode is the normal 'S' mode:



Delete an atom

Select the atom (click on it), and press the Backspace key.

Delete a bond

Select the bond (click on it), and press the Backspace key.

Delete the selection

Make your selection, and press the Backspace key,.

Make a bond

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 (if possible), and you will revert to the normal select mode.

Change the bond type

Select the bond or bonds to change.

Chose the required bond type from the Bond-type pull down menu.

The bond type will be visible in the picture by the color used.

Rotate or translate the selection

When you try to rotate or translate while you have some items selected, only the selected items will be rotated or translated.

Run Script

Save your input using the Save or Save As ... menu commands.

Your input will be saved in a file with the name you specify, and at the same time a run script will be saved. It has the same name, but with '.run' appended.

To execute your calculation just execute this run script.

In the panel 'Files (Restart)' you can specify what files to save at the end of the run script.

By default, TAPE21 (result data), TAPE41 (grid data for visualization) and TAPE13 (checkpoint information) are saved.

If the environment variable SCM_RESULTDIR has been set, the run 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 run script will execute in the directory where it is started, and the result files will also be located in that place.

Menu Commands

Print...

The Print command will generate a file containing the picture of the molecule (only).

The input options are not printed.

If the simple picture quality is currently in use, a postscript file is generated.

If you have activated the photographic picture mode, a ppm file is generated.

Preferences...

The Preferences... menu command gives access to the 'Preferences' input panel. You may also select this panel from the pull-down menu on top of the input panels.

This panel is used to set a number of preferences for the ADFinput program.

To save the preferences, click on the Save button in the Preferences panel.

Reset View

When you use the 'Reset View' menu command, the translation, zoom and rotation settings will be adjusted such that the entire molecule is visible.

Use it for example when you translate the molecule 'out of view'.

Bond Lengths constrained

When creating new atoms bonded to existing atoms, ADFinput will constrain the bond length to the textbook value.

If you do not wish this to happen, select this menu command to toggle this behaviour.

Add Hydrogen

The 'Add Hydrogen' menu command will add hydrogen atoms to your molecule until every connector is connected. The number of connectors and the number of lone pairs determine the geometry. For example, the Oxygen atom has four connectors and two lone pairs in a tetrahedral arrangement.

Import Molecule...

Use this menu command to import the geometry of your molecule from file.

Currently ADFinput has little knowledge about other formats, it can only read text files, and it assumes to find x, y, z coordinates on a line, and some indication of the atom type (an element name or an atom charge). Most popular formats will work fine, just try with your favorite format.

Bond information is not imported.

Guess Bonds

Roughly guess what atoms are bonded together, depending on the distance between the atoms compared with text book values. The bond type is currently always set to single, so you probably need to make some changes.

Only ADFinput uses the bond information. The ADF program itself does not use any of the bond information.

Input options remarks

Empty fields

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

Coordinates

The coordinates panel shows the coordinates corresponding to the molecule visible in the molecule display. You may edit the coordinate values here as well.

You may select to use Cartesian or Internal coordinates. For internal coordinates you can currently only edit the values for bond lengths and angles, not the connection information.

If you will optimize the geometry (with ADF), the program will perform this optimization in the coordinate type you have selected here. Thus, the Cartesian or Internal pull-down menu is not only for display purposes, but determines the optimization method used.

By checking the check boxes next to the coordinates you will freeze those coordinates during a geometry optimization.

User Input

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

Note that at this point in time you can only add text to the ADF input file, not to the input of any of the property programs.

Environment Variables

Name	Meaning
SCM_ERROR_MAIL	email address for error reports
SCM_GUIRC	location of the preferences file
SCM_TPLDIR	location of the templates directory
SCM_RESULTDIR	location of the results directory
DISPLAY	X-window display to use

ADFview

Introduction

ADFview is a small utility program, which provides some basic volume visualization tools. It will enable ADF users to visualize their results: SCF densities, orbitals, electrostatic potentials, and any other property that is available as a scalar value over a grid.

The documentation of ADFview consists of two documents.

The first document is a very basic hands-on tutorial section in the ADF GUI tutorial. Its purpose is to help you create some pictures, and to have a simple and fast tour of the main features of the utility. We estimate that you should be able to finish this section including the hands-on activities within 30 minutes.

The second document explains in detail all possible options, buttons and so on. This material is mainly intended as a reference. We hope that the utility is easy to use, and that the options, together with the help information popping up, will not require you to use the reference manual.

At this point in time, ADFview is still under development and is being tested. Your suggestions and bug reports are valuable to us for making an improved and extended next release available as soon as possible.

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of ADFview, but do not contain personal information.

You can enable this by setting the global environment variable `SCMERRORMAIL`, for example in your login script:

```
SCM_ERROR_MAIL=cwyourmail@your.institute.com
export SCM_ERROR_MAIL
```

This will ensure that the bug report will be sent back to us, and also to the mail address you specify. Thus you can see exactly what kind of information you are mailing to us. If you do not want to receive a copy yourself, please set `SCMERRORMAIL` to `'errors@scm.com'`, without quotes.

Your comments and bug reports are very welcome. Please send them to support@scm.com.

Reference Manual

Starting ADFview

If you have installed the ADF package correctly, ADFview is located in \$ADFBIN.

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

```
adfview [filename] [-var varname]
```

The filename is optional. ADFview only handles TAPE41 files, such as produced by the densf program. These files should be named properly, with a .t41 extension. The variable name varname is also optional.

There is a second possibility to start ADFview if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu ADFview can be started by selecting the 'View' command.

Data file

The data file is a KF file, which is the ADF binary file format. The Utilities document describes the KF utilities that can be used to manipulate these KF files (e.g. to convert it into an ASCII format and vice versa).

The data file is divided into sections containing the property values on a grid, for all properties you have selected in densf. Currently only scalar fields are supported. The data file also contains a specification of the grid used.

ADFview is not restricted to the properties calculated by densf. You can use the program to visualize any kind of scalar field. Just calculate its values on the grid, and save the result in a KF variable in the format used by densf. To view this data field, specify the name of the KF variable (including the section) on the commandline with the -var flag.

If you have specified a filename at the invocation of ADFview, that file will be used as data file. Alternatively, you may select the "Open..." command from the File menu. A standard file select dialog box will appear, and you will be able to select the data file (with extension .t41) you want to use. The title of the adfview window will change into the name of the file being used.

If you want to use a different file without restarting ADFview, use the File:Open... menu command to select another file.

Main property

The main property is one of the data fields available on the selected data file, and will be used to generate isosurfaces and the MIP and AVE pictures.

You can select any property available on the data file using the pull-down menu. ADFview shows only known data fields in the pull-down menu. If you have another property (field) you want to visualize, you need to let ADFview know this by specifying it using the -var commandline flag.

Secondary property

The secondary property is also one of the data fields available on the file. You can select it with the pull-down menu.

Secondary Options

The pull-down menu to the right of the secondary property pull-down menu determines what the secondary property is used for.

- not used -

The secondary property will not be used at all.

as Color field

The secondary property will be used to paint the main isosurface with colors determined by the secondary property. The range of colors used corresponds with the horizontal color bar, and is mapped to the range of scalar values that occur in the secondary field.

Typical use is to display the values of the electrostatic potential as different colors across an iso-density surface.

as Difference field

The secondary field will be subtracted from the main field.

For example, use this option to see the differences in density between the final SCF density and the sum of fragments density. Another application might be to visualize the difference between alpha and beta spin densities.

A more advanced use would be to view changes that result from using a different basis set or Hamiltonian. To do this you would need to combine the results from two different densf runs. This is easy to do using the KF utilities.

as Sum field

The secondary field will be added to the main field.

For example, use this option to see the total density in a spin unrestricted calculation. On the .t41 file only the total density per spin is available, and you can use the Sum field to calculate the total density.

as Product field

The secondary field will be multiplied into the main field.

For example, use this option to see the spatial shape of orbital products.

as Pos Diff field

This option is similar to 'as Difference field', but this time only the positive part of the difference is retained. The negative part of the difference has been set to zero.

Use this option to clean up a complex situation, or in combination with MIP or AVE. These visualization modes can only handle positive fields.

as Neg Diff field

This option is similar to 'as Difference field', but this time only the negative part of the difference is retained, with inverted sign. The positive part of the difference has been set to zero.

Use this option to clean up a complex situation, or in combination with MIP or AVE. These visualization modes can only handle positive fields.

Visualization modes

Isosurface

Construct an isosurface and show it, using shading and reflections based on the (numerical) gradient. Only one isosurface is visible, no colors.

The isosurface value used is the number in the box to the right of the Isosurface mode box. You may enter any numerical value you like, including negative values.

Isosurface with Color field

When an isosurface is combined with a secondary 'Color field', the same surface is displayed, but painted with colors based on the secondary field. The color range used is determined by the horizontal color bar.

Double Isosurface

Two isosurfaces are constructed: one for the value entered, and one for the opposite value. The extreme colors of the horizontal color bar are used to distinguish the two surfaces. Shading and reflections are done the same as with a single isosurface.

Since color is already being used to distinguish between the two surfaces, there is no possibility to use a color field.

MIP grayscale / color

The Maximum Intensity Projection images are a nice way to have a look at your molecule: you will be able to see many details that would be difficult to view using only an isosurface.

The construction of MIP images is simple but expensive. From your eye, a ray is cast through the data set. The maximum intensity of the data set along this ray determines the intensity or color. For coloring, the horizontal color bar is used again.

Most fields used in combination with ADF have very large differences in numerical values around nuclei and the rest of space. So ADFview always takes a logarithm of the field values before calculating a MIP image.

For that reason, only positive fields can be displayed.

AVE grayscale / color

The AVErage intensity projection images are similar to MIP images.

The construction is as for a MIP image, but now the average value along the ray is used. In this case also the logarithm of the field value is used.

Mouse interaction

Following is a description how to rotate, translate or zoom the picture. We assume the Standard mouse mode is active, as described later. To ensure this, click on the S button just below the picture.

If you have a mouse with only one button, this button is always equivalent to the 'left' button.

Rotate the image

Click in the window, somewhere on the picture shown, and hold down the right mouse button. The picture will change to a simple cube. If you move the mouse around within the window, the picture will rotate. When you release the mouse button, the cube will disappear and ADFview will recalculate the isosurface of the density in the new orientation.

Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you are rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle) the rotation will be around an axis perpendicular to the screen.

Alternatively, you may use the left mouse button together with the shift key.

Zoom the image

Click in the picture using the right mouse button while holding the control key, and move the mouse to the right: you will zoom in. Moving the mouse to the left (with the right mouse button and control key pressed down) will zoom out.

Alternatively, you may use the left mouse button together with the control and shift keys.

Translate the image

Click in the picture using the middle mouse button and drag the mouse in some direction. The image will be translated following the mouse.

Alternatively, you may use the left mouse button together with the control key.

The SRTZ mouse mode buttons

You may change the reaction to mouse clicks completely by changing the mouse mode using the S, R, T, or Z buttons.

The S button is the Standard mouse mode. Mouse interaction is exactly as described before. If you want to return from any of the other modes, just press the S button again.

If you click the R button, the Rotate mode is active. Dragging with the left mouse button will rotate the image.

If you click the T button, the Translate mode is active. Dragging with the left mouse button will translate the image.

If you click the Z button, the Zoom mode is active. Dragging with the left mouse button will zoom the image.

The mouse mode will change only by clicking in one of the S, R, T, or Z buttons.

Resize window

You can resize the window as usual, by grabbing the lower right corner of the window with your mouse, and dragging it. You may have to use a different technique, depending on the window manager you are using.

The picture area will enlarge as much as possible, and the picture will be rescaled.

A bigger picture will take more time to calculate and to draw, since more pixels need to be handled.

If you need a high-resolution picture you can use this technique: make the window big, save the picture in a file, import that file into your graphics program, and finally rescale the image to get an image with a resolution better than the screen resolution.

Color range

Using the horizontal color bar, you can change the color range used for different images. Change the number on the left or right by selecting and typing the new number, and pressing return. Alternatively, you can change the numbers by clicking on the arrows next to the numbers.

The color range is used to visualize the value of a color field on a single isosurface, or to display the value of the field in a MIP or AVE picture.

The extreme colors (left and right side) are used to distinguish the two isosurfaces in case the double isosurface option is active.

Menu commands

File:Open...: open a new data file (in TAPE41 format). A file select box will appear which allows you to select the data file. At first only files with .t41 extension will be shown. You can also open other files using the pulldown menu. However, even in that case the file should be a TAPE41 file as produced by densf.

File:Save As PPM...: save the current picture in ppm format. This format is a color bitmap format and can be handled by many image manipulation programs to convert it into your preferred graphic format. Since the bitmap contains all pixels in the picture, the resulting quality is better when you increase the size of your window.

Save As PS...: save the current picture in postscript format. Again, you can get a better quality by increasing the size of your window.

File:Quit: quits ADFview.

Efficiency and Quality

The pull-down menu just below the picture determines how the picture quality is improved. It has effect only on the calculation of the displayed picture. Another important factor is of course the density of the grid used as input for ADFview.

Simple Cube

The most basic picture is a picture of a cube only. This is very fast, and contains only information about the orientation and scaling of the data set.

Coarse

This will produce the real picture but in a very coarse resolution: the image is calculated in block of 16 x 16 pixels at a time.

Medium

This will produce an acceptable but still low-quality image. The image is calculated in blocks of 4 x 4 pixels at a time.

Fine

This will produce a picture at the best possible quality given the current data set and grid quality. The color of each pixel in the image is calculated individually. This gives the best quality, but may require some patience.

Auto refine

Starts the display with a coarse picture, and updates the quality if you are not doing anything. The updating will continue until the picture has been recalculated at the best possible quality ('Fine').

Quick Rotate

This check box determines what to do when rotating, zooming or translating: temporarily replace the picture with the picture of a cube, or continue with the current picture.

Displaying the cube while rotating and so on of course greatly improves the interactive response.

Isosurface properties

The line with 'DSPQG' in front of it determines some properties of the isosurfaces generated. The first number corresponds to the D, the next one to the S, and so on.

D: amount of directed light.

100 means only directed light, 0 means only diffuse light.

S: amount of specular reflections

These are the 'highlights' reflecting from the surface.

100 means specular reflections only, 0 means no reflections.

P: power of the specular reflections.

This determines the 'size' of the bright reflecting spots.

Q: quality setting.

To speed up things, ADFview uses an algorithm where the isosurface is calculated first in a coarse resolution. When all four corners of a square in this resolution have the surface at the same distance, ADFview uses that value for the entire square. A great speed up is achieved for surfaces parallel to the screen, and for empty space.

The quality setting is the numerical threshold on these distances to determine if they are equal.

Increasing the value from the default 1.0 speeds up the algorithm at the expense of artifacts, especially with surfaces with small details or disconnected surfaces.

Reducing the value slows things down but removes any artifacts introduced. Setting the value to a negative number ensures that no approximations in this respect are used.

G: gamma value.

This determines the overall 'contrast' of the picture. Adjust to your taste.

Status field

In the lower right corner you will see a status field. This informs the user what ADFview is currently doing.

The percentage number is the percentage of the image currently being calculated which has been completed. Thus, 100% shows you that the calculation is complete.

The number within parentheses shows the current resolution. If the number is n , the picture has been calculated with blocks of $n \times n$ pixels. Thus, (1) indicates that the picture being calculated is a picture at the highest possible resolution (corresponding to the 'Fine' option in the pull-down menu).

ADFSpectra

Introduction

ADFSpectra shows the spectra calculated by ADF. Currently it can show IR and excitation spectra, as well as a DOS plot. For some spectra (for example for IR spectra) it can also provide additional information, like a visualization of the normal modes (using ADFmovie). More types of spectra will follow in future versions.

No export options are available, and also no possibilities to change peak shape or width. Such features will probably follow in a later release.

Reference Manual

Starting ADFSpectra

If you have installed the ADF package correctly, the ADFSpectra is located in \$ADFBIN.

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

```
adfspectra [filename]
```

The filename is optional. ADFSpectra handles the ADF binary TAPE21 files (.t21).

There is a second possibility to start ADFSpectra if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu ADFSpectra can be started by selecting the 'Spectra' command.

DOS (density of states)

Select the 'DOS' command from the 'Spectra' menu. Part of the results of the calculation is typically a large number of orbital energies. These may be graphically represented as a DOS (density of states).

After the DOS is shown the little red arrow along the horizontal energy axis corresponds to the Fermi level (the highest occupied orbital). The height of the peaks depend on the number of peaks close together (real or accidental degeneracies). The orbital energies, with their symmetry and occupation numbers, are also available from the menu.

By dragging a rectangle on a certain region in the spectrum you can zoom in.

Vibration (IR spectrum)

Select the 'Vibration' command from the 'Spectra' menu. This is only possible if ADF has calculated the IR frequencies.

After the IR spectrum is shown the red arrows on the baseline indicate the peak positions as calculated by ADF. The peak positions, with their symmetry and intensity information, is also available from the menu.

By dragging a rectangle on a certain region in the spectrum you can zoom in.

To scale the frequencies one may enter a number other than 1.0 in the scale box.

View normal modes

Click on a peak to get more detailed information. Below the spectrum some information will be printed, and ADFmovie will start showing the corresponding normal modes.

If one clicks on a different peak, the ADFmovie windows showing the current normal modes will be closed, and new windows corresponding to the new peak will appear. By control-clicking on a peak the new windows will appear, but the old windows will not be closed.

Excitation

Select the 'Excitation' command from the 'Spectra' menu. This is only possible if ADF has calculated the excitation energies.

After the excitation spectrum is shown the excitation energies are listed in the menus, together with details like intensity. Select a peak using the menu or click on it to get more detailed information, including the composition of the corresponding transition. This will be printed in the lower part of the window.

By dragging a rectangle on a certain region in the spectrum you can zoom in.

ADFmovie

Introduction

ADFmovie is a small utility program, which follows geometry steps as performed by ADF during geometry optimizations, IRC calculations, etc. Actually, it will display just any series of changing geometries, and is also used to display normal modes calculated with a frequency calculation.

Reference Manual

Starting ADFmovie

If you have installed the ADF package correctly, the ADFmovie is located in \$ADFBIN.

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




```
adfmovie [-loop] [filename]
```

The filename is optional. ADFmovie handles ADF movie files (.amv) and ADF logfiles (.logfile), both types are text files, and the ADF binary TAPE21 files (.t21).

If the -loop commandline option is chosen ADFmovie will display the series of the geometries in the specified file over and over again.

There is a second possibility to start ADFmovie if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu ADFmovie can be started by selecting the 'Movie' command.

Buttons

Button	Description
	Buttons to <ul style="list-style-type: none"> rewind the movie, step one picture backward, play the movie, pause the movie, step one picture forward, skip to the end of the movie.
	Display button: toggle the display between a very simple but fast picture, or a photographic quality picture of your molecule
	Mouse-mode buttons: <ul style="list-style-type: none"> S: normal mouse button R: rotate with left mouse button T: translate with left mouse button Z: zoom with left mouse button

Input Files

TAPE21 and logfile

If a TAPE21 file (ADF binary) or an ADF logfile (text file) is selected ADFmovie displays the series of the changing geometries in the specified file. Typically this will be the change in geometry of a molecule as a result of a geometry optimization, an IRC run, or a frequency run.

If it is generated with ADFinput the ADF logfile file will have a .logfile extension, and the ADF data result file TAPE21 will have the .t21 extension.

ADF movie files

At the moment the ADF movie files (.amv) are generated only by ADFspectra, if the vibrational spectrum is shown and one of the normal modes is selected. If this is the case the -loop option of adfmovie is selected.

It is easy to make an ADF movie file yourself, since it is just a text file with series of coordinates, for several frames of the movie.

Example with rather arbitrary coordinates:

```
water geometry 1
H 0.0 0.0 0.0
H 1.0 0.0 0.0
O 0.0 2.0 0.0
```

```
water geometry 2
H 0.0 0.0 1.0
H 0.0 1.0 0.0
O 3.0 0.0 0.0
```

```
water geometry 3
H 0.0 0.0 0.0
H 0.0 1.0 1.0
O 6.0 0.0 0.0
```

Note: a title (like water geometry 1) should be provided for each new geometry, and an empty line should separate the different geometries.

ADFTail

Introduction

ADFTail is a (very) small utility program, which makes it possible for ADF users to follow the progress of an ADF calculation (similar to the UNIX tail -f command) by showing the end of the ADF logfile.

Reference Manual

Starting ADFTail

If you have installed the ADF package correctly, the ADFTail is located in \$ADFBIN.

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

```
adftail [filename]
```

The filename is optional. ADFTail only handles text files, but is mainly useful for the logfile generated by ADF. If it is generated with ADFinput the ADF logfile file will have a .logfile extension.

There is a second possibility to start ADFTail if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu ADFTail can be started by selecting the 'Logfile' command.

Logfile

The ADF logfile is generated during an ADF calculation and flushed after (almost) each message that is sent to it by the ADF program. Consequently the user can inspect it and see what is going on without being delayed by potentially large I/O buffers. Each message contains date and time of the message plus additional information on how far the calculation has progressed.

In the ADFTail main window the last part of the ADF logfile is shown. Using the scroll bar you can move around in a linear version. At this point using ADFTail is equivalent to using any WYSIWYG(what you see is what you get)-editor. If the logfile file grows during a calculation, ADFTail will update itself and show the text file as it grows (similar to the UNIX tail -f command).

BOB

Introduction

BOB is a small utility program, which makes it easier for ADF users to browse through the output of an ADF calculation.

When loading a file, either at startup or by using the File/Open command, BOB scans the entire file and locates many special points of interest in this file. All these points are linked to menu entries. These menu entries are organized to make it easier to find the entry you are looking for. Furthermore, still during this initialization phase, BOB will try to detect the different parts in an output file. For example, many outputs will consist of the output from one or more ADF Create runs followed by one or more molecular runs. BOB will find these parts and put them in its 'Include' menu.

Reference Manual

Starting BOB

If you have installed the ADF package correctly, the Basis Output Browser BOB is located in \$ADFBIN.

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

```
bob [filename]
```

The filename is optional. BOB only handles text files, but is mainly useful for the output file generated by ADF. If it is generated with ADFinput the ADF output file will have a .out extension.

There is a second possibility to start BOB if one of the GUI modules has already been started. All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using this SCM menu BOB can be started by selecting the 'Output' command.

Main window and Menu commands

Main Window

In the BOB main window the complete output file is shown. Using the scroll bar you can move around in a linear version. At this point using BOB is equivalent to using any WYSIWYG(what you see is what you get)-editor.

Click on Marked Items

The points of interest in the file have also been marked visually. Clicking on one of them will jump to the next point of interest of the same kind. Shift-Clicking will do the same but backwards.

Include Menu

The Include menu is often very informative since it provides at a glance the overall structure of the file you are looking at. If you select any of the parts BOB will jump to that part in the file, *and* it will restrict all operations (except a new Restrict command) to this part. This makes it very easy to study a single part of

the output file without getting lost in another part.

Other Menus

The other menus (Properties, Iterations..., except File and Edit) contain the special markers ('Points of Interest') which have been detected when opening the file. Choosing one of their menu items will jump to that item, or beep if that is not possible (because you included only part of the output to view using the Include menu). The search will wrap around.

Using the BOB menus you can find easily what you are looking for. The property menu gives access to all calculated properties, including excitation energies, polarizabilities, NMR results and bonding energy analysis.