



Scientific Computing & Modelling

GUI Installation Manual

**ADF Program System
Release 2010**

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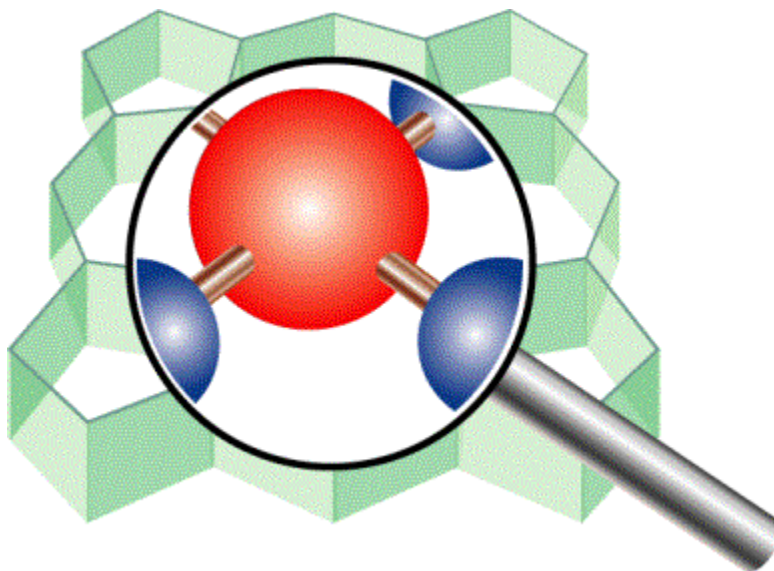


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Introduction

The ADF-GUI and the BAND-GUI are installed as part of the whole ADF package.

ADFinput provides an GUI for Mopac. It can do full Mopac calculations, or use it as a pre-optimizer. Mopac is not included with the ADF distribution, so if you wish to use Mopac you will need to install Mopac yourself.

Mopac can also be used by the ADF package in combination with Quild. It will allow you to perform a multi-level calculation, using Mopac for a big system and ADF for a smaller sub-system.

One of the features of ADFjobs is that queues can be predefined for remote machines. These are called Dynamic Queues.

As a convenience for users, these Dynamic Queues can be pre-configured by the system administrator(s) of the remote machines. To do, you will need to understand the concept of a Queue in ADFjobs, and how ADFjobs detects Dynamic Queues.

Dynamic Queues are also convenient to change the submit commands that users use when using the batch system. Just a change in one place, instead of informing all users and hoping that they change their configuration.

Another detail that might require some configuration by users is proper configuration of ssh for running on remote machines.

Mopac

To use Mopac you will (obviously) need to have Mopac installed. If you do not yet have it, you can get it from OpenMOPAC. Please contact OpenMOPAC for license information. At this moment academic licenses for OpenMOPAC are free.

ADFinput starts MOPAC using the \$ADFBIN/mopac.scm script. It should work if you install MOPAC in the default location, otherwise you will need to adjust it. Alternatively, you can set the SCM_MOPAC environment variable to some command to be executed. You can also use this to run MOPAC on some other machine (mopac.machine.com in this example, and assuming that ADF is installed on that machine as well to get the mopac.scm script):

```
export SCM_MOPAC="ssh mopac.machine.com adfhome/bin/mopac.scm"
```

When using MOPAC as a pre-optimizer ADFinput will import the MOPAC charges and bond orders at the end of an optimization. The bond orders are automatically used to set the bond details (bonds are created and adjusted based on the mopac bond orders). The MOPAC charges can be visualized as other scalar atomic properties.

The current ADFinput version has been tested with MOPAC2009 (from OpenMOPAC) and with MOPAC2006 (from Fujitsu). Not all features are supported together with MOPAC2006. Please make sure you are using a recent Mopac version.

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.

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

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

ADFjobs Queues

When the user runs a job using ADFjobs, he will use a Queue that determines how he will run his job: interactively on the local machine, using a batch system, or on a remote system (either interactively or using a batch system). The queue defines what commands are used to start the job and to monitor the progress.

The queues can be defined by the user using the Queue menu in ADFjobs.

When you use the "Queue:Edit:Interactive" command in ADFjobs, a dialog will popup showing the details of the Interactive queue. In this dialog you will see the essential data that ADFjobs needs to know: on what machine should the job run, what user name, in what directory to store the results, what command should be used to start or queue the job, how to check the progress, and so on.

If you use the command "Queue:New:PBS" the same dialog will popup to show the values that we use on a machine using the PBS queueing system. As batch systems differ a lot, you should check especially the Run command to make sure that it matches the command that a normal user should use to submit a job. Note that \$options will be replaced by a value specified by the user. The default value is specified with the Default Options field. Typically you can use it for a time lime, or number of cpus, or something like that.

When installing the GUI you should start ADFjobs yourself, and set up the queues as the user should do. When you create a queue, the details are saved in a simple text file in the \$HOME/.scm_gui directory. The names of these files are the queue name with a .tid extension.

Dynamic Queues

In the `$HOME/.scm_gui` directory you will find a couple of files, one for each queue that you have defined. The file names should NOT start with Template, and will have a `.tid` extension.

In order to make these available as dynamic queues for a group of users you need to copy these files to a directory on the remote machine that is readable by all users.

Next set the `SCM_QUEUES` environment variable for all users: it should contain the full path of the directory in which you put the queue files. Now ADFjobs will be able to load the dynamic queues automatically

If you do not set the `SCM_QUEUES` environment variable, ADFjobs will search the `$HOME/.scm_gui` directory on the remote platform. This way users can set up their own dynamic queues.

User configuration needed for Dynamic Queues

The user must configure their local copy of ADFjobs to find the Dynamic Queues. To do this:

Start ADFjobs

Select the Preferences command from the SCM menu

Select the ADFjobs page (using the pull-down menu across the top of the window)

Click on the + in front of Dynamic Queues

Enter the host name of the host on which to look for dynamic queues

Optionally: enter a user name to be used on the remote machine.

ADFjobs will use ssh to contact the remote machine and get the dynamic queue information. If no username is specified no username is passed to ssh, and thus ssh will determine what username to use.

Next, when ADFjobs is started again, the remote queues will be visible in the Queues menu with a small arrow in front of them to indicate that they are remote queues.

Example queue configuration file for SGE

```
# hostname: machine.domain
# username:
# jobscript:
# prolog: source $HOME/setup/adf2010
# epilog:
# jobdir: $HOME/jobs
# runcmd: qsub -pe s3_mpich $options -q short3.q "$job"
# batch: no
# options: 2-2
# killcmd: qdel $jid
# jobstatuscmd: qstat | grep " $jid "
# sysstatuscmd: qstat
# label: My SGE queue
# logfile: logfile
```

Example queue configuration file for PBS

```
# hostname: machine.domain
# username:
# jobscript:
# prolog: source $HOME/setup/adf2010
# 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
```