



Scientific Computing & Modelling

Installation manual for Windows

**ADF Program System
Release 2008.01**

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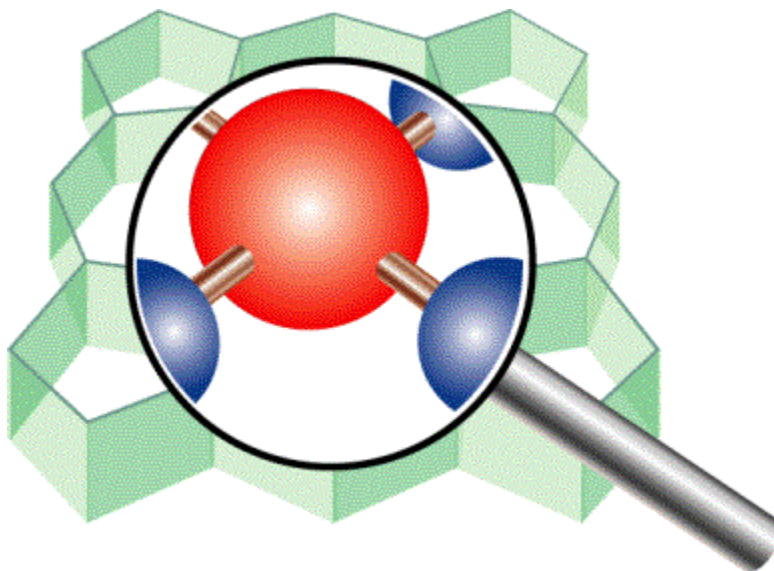


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Quick Start

Requirements

For more details on requirements see the general Installation Manual.

Hardware requirements.

- Intel Pentium 4 or AMD Athlon processor or better
- Minimum 512MB of RAM but 1GB/core is recommended
- Ethernet network card
- 1GB of free disk space for installation, more at run-time (see the general installation manual for details)

Software requirements:

- One of: Windows 2000, 32-bit XP, 32- or 64-bit Vista
- For HP-MPI version: a TCP/IP connection which must be active while an MPI program is running

Installation

VERY IMPORTANT: You must have **ADMINISTRATOR** privileges to install ADF on Windows 2000/XP/Vista!

To install ADF on your Windows computer just execute the setup file and the installation wizard will guide you through the installation process.

License file

You must obtain a license file before you can use ADF programs. If you are a trial user you should have already obtained one together with the download information. Otherwise you need to contact license@scm.com. After you have obtained a license file, save it as `%ADFHOME%\license.txt`. Everywhere in this document `%ADFHOME%` stands for the path where you installed ADF, which is by default `C:\ADF2008.01`. Except for the trial users, the license file is usually host-locked. The information necessary to create a host-locked license file is normally generated automatically by the installer and is saved in the `%ADFHOME%\licinfo.txt` file. It is also displayed using your default text editor so you can easily copy the information and paste it in an e-mail message.

Whenever you get license errors, you should execute the `%ADFHOME%\makelicinfo.bat` file and follow the instructions on the screen.

On a computer running Windows Vista, you may get an error message "VTK has stopped working". This message may also be caused by an invalid license. Therefore, you should execute the `makelicinfo.bat` file if you get this error.

Configuring Putty for Use with ADFjobs

This section explains how to enable ADFjobs to manage ADF jobs on remote computers; you can skip it if you are going to run ADF on the local Windows computer only.

ADF installation script installs the Putty software on your computer in `%ADFHOME%\bin\Putty`, where `%ADFHOME%` should be understood as the ADF installation directory, `C:\ADF2008.01` by default. Putty, or rather its command-line version Plink, serves as an ssh client for communicating with remote Unix- and Linux-based computers. It is very important to configure Putty in such a way that the communication takes place without any interactive prompting. The Pageant utility is used for this purpose. This is how you configure the ssh client for use with ADFjobs to manage remote jobs:

- Pageant must be already running when you start ADFjobs. The easiest way to make sure Pageant is always up is to add a shortcut to `%ADFBIN%\bin\Putty\pageant.exe` to the StartUp folder. In case you already had Putty installed on your computer make sure that both Plink and Pageant are of the same version because otherwise Plink may fail to use Pageant's keys.
- A private+public key pair must be added to Pageant. If you don't already have a key pair, you can create one using the `%ADFBIN%\bin\Putty\puttygen.exe` utility. You can also use this utility to import an OpenSSH private key and save it as a Putty key file. After you have created such a file (it usually has a .ppk extension) you can add it to the list of Pageant keys by right-clicking on the Pageant icon in the Taskbar notification area and selecting "Add key". Select a .ppk file and press "Open".
Type in the passphrase if you have chosen one to protect your key (which is always a good idea) and press Enter.
- A public key from the key pair above must be added to the `~/.ssh/authorized_keys` file on the remote computer. Note that often the `~/.ssh` directory as well as the `authorized_keys` file must have proper permissions (usually 0700 and 0600, respectively) for public key authentication to work.
- Connect to the remote computer at least once with a "`C:\ADF2008.01\bin\Putty\plink {user}@{host}`" command so that plink stores the myhost's host key locally. Of course, you need to substitute correct username and hostname for `{user}` and `{host}`.
- Now make sure you can connect to the remote computer without a password and without host key warnings.
To test the connection, open a Command Prompt window and type (substituting appropriate values for `{user}` and `{host}`):
`C:\ADF2008.01\bin\Putty\plink -batch -agent -l {user} {host} uptime`
When everything is configured correctly you should see output of the uptime command from the remote host.
- After this you can start using the remote computer with your local ADFjobs.

Getting Support

When something goes wrong and you would like to get help, please do the following:

If ADFjobs is working then start it and select "Generate Test Job" in the Job menu. A job named "Test-Job" will be created in the directory. Select it and press Ctrl-R. Press "Yes" button if asked. An ADFtail window will pop up showing the job progress. Send an e-mail to support@scm.com describing the problem in detail and attach the Test-Job.logfile file after the test job has been finished.

In case ADFjobs does not work, please collect the information below manually and send it to support@scm.com.

- Description of the problem and the sequence of actions to reproduce it.
- The file `%ADFHOME\bin\version` containing all information about ADF version.
- Information about environment variables. To obtain it, you can do the following (on Windows 2000/XP, on other systems it should be similar):
 - Click "Start" menu and select "Run".
 - Type `msinfo32` and press Enter.
 - System Information utility will start. Unfold the "Software Environment" item in the left window.
 - Right-click on the "Environment Variables" and select "Save as Text File". Enter a file name. Click Save.
 - Attach the file to the support request.
- Content of the file specified in the SCMLICENSE environment variable.

Background Information

Please see the general Installation Manual for more background information on ADF.

MPI

Starting from ADF2007.01, the Windows version of ADF comes bundled with the HP-MPI runtime environment. This means that you can run parallel ADF jobs on your brand new multi-core Windows machine. By default, if the NSCM environment variable is not defined, ADF will use all logical processors present in the system. Should you decide to use ADF on fewer processors, then you will need to set the NSCM environment variable to 1. You can do this in ADFjobs permanently by adding NSCM with the value 1 to the list of environment variables or on the per-queue basis. Just type "export NSCM=1" (without quotes) in the prolog field of the corresponding queue in ADFjobs. Moreover, you can define two local queues in ADFjobs: one for serial and one for parallel jobs. The queues may be called, for example, serial and parallel. You would then need to change the prolog value for the serial queue only.

Environment Variables

As of ADF2008, the installation procedure does not set system wide environment variables ADFHOME, ADFBIN, ADFRESOURCES and it does not alter the PATH variable. Instead, GUI modules will always set ADFBIN to their own directory and set ADFHOME and ADFRESOURCES accordingly if they are not set. This will ensure that each GUI module uses only programs from the package version with which it was installed but, at the same time, basis sets and other resources from a different installation may be used. **NOTE:** Since ADFHOME and ADFRESOURCES are not changed if present it is important to properly uninstall ADF2007 before installing ADF2008 because the previous version sets the environment variables above globally and, thus, some undesirable effect are possible.

The main benefit of this approach is that one can install different ADF versions (although they must all be 2008 or newer) and use them without the risk of intermixing. There is also a downside to this: it is possible to run jobs under the ADFjobs GUI module only, i.e. associating the .job file extension with sh.exe is not sufficient. However, starting from ADF2008.01d, there has been added a possibility to run ADF jobs on Windows from a command line, see the next section.

Currently, the following environment variables are set by each GUI module on startup:

- ADFBIN is set to the path of the directory from which the GUI module was started.
- ADFHOME and ADFRESOURCES, if absent, are set to appropriate folders based on the value of the ADFBIN variable.
- It is important to ensure that ADF programs find proper files during execution. To this end, the PATH environment variable is updated by adding the following folders:
 - ADF program folder, i.e. the folder in which the GUI module's executable is located (%ADFBIN%).
 - Tcl shell and Tcl/Tk dynamic libraries (DLL's) folder (%ADFBIN%\TclTk\bin).
 - Msys, MinGW mini-system, binary files folder (%ADFHOM%\msys\bin).
 - Putty folder (%ADFBIN%\Putty).
 - For HP-MPI version only: HP-MPI's bin folder (%ADFBIN%\hpmpl\bin).

The following variables are set by the setup script and are system-wide:

- SCM_STRUCTURES is set by default to C:\ADF_DATA\Structures. You can save your own .adf files in this folder and they will be added to the ADFinput's Structure Tool.

- SCM_TPLDIR is set by default to C:\ADF_DATA\Templates.
You can create your own presets in ADFinput and save them there.
- SCM_TMPDIR is set to the value specified at the installation time and the folder is created if it does not exist. This is where ADF will create temporary files at run time.

Running jobs from the command line

If you have ADF2008.01d or later installed, navigate to the ADF installation directory and double click the `adf_command_file.bat` file. It will start a Windows command interpreter and set up the environment specific for that installation of ADF. Once it has started, go to your jobs directory by entering the following commands at the prompt:

```
C:
```

```
cd \ADF_DATA
```

Then, run your job as follows (assuming the job is called `h2o`):

```
sh h2o.job
```

You can also prepare a job from a `.adf` file and run it using only two commands:

```
sh adfprep -t h2o.adf -j h2o > h2o.job
```

```
sh h2o.job
```

Please note that you do need to use `sh` in the commands above because both `h2o.job` and `adfprep` are shell scripts and, thus, they must be interpreted by a shell.

Known Limitations and Problems.

Below is the list of known limitations and problems.

Parallel calculations are not possible without a valid IP address

The HP-MPI runtime environment has a limitation: it fails to start a parallel job if the computer does not have a valid IP address. For this reason, in order to run a parallel job the computer must be connected to a network (note: it does not have to be connected to Internet, any local network will do). Parallel ADF jobs run on a computer without network will appear to hang after "create" runs are finished before starting a molecular calculation. This issue can be avoided by installing a special network adapter called "Microsoft Loopback Adapter".

You may get license errors after installing the adapter. If this happens, you need to change the order of network adapters and lower the priority of the loopback adapter in the list. To do this, open the "Network Connections" control panel and select menu Advanced|Advanced Settings, select the connection corresponding to the loopback adapter under "Connections:" and move it down the list by clicking on the down-arrow button.

Killing jobs does not work under Windows 2000

ADFjobs uses the system taskkill utility to terminate a running job. This utility does not exist on Windows 2000. For this reason it is not possible to kill a running job on this system. A work-around is to terminate running processes, which are usually called adf.3.exe, band.3.exe, etc., from the Windows Task Manager. To open a Task Manager window, right-click on the taskbar and select "Task Manager" from the pop up menu.

Very large calculations

Due to a hard limit imposed by Windows on the program stack size it is possible that very large calculations crash with Segmentation Fault. This mainly applies to spin-orbit relativistic and TDDFT calculations. If this happens then you should report this case to the SCM support and repeat the calculation under Linux or UNIX.

Spaces in file and directory names

It is recommended to never use any path names that contain spaces with ADF. That is, the ADF installation folder must not contain any spaces. For this reason C:\Program Files\ is not a suitable location to install ADF into. It is also not recommended to run ADF from a folder with spaces in the path name, e.g. "C:\Documents and Settings\Default User\My Documents\", although it might work in some cases and might fail in others. The same applies to names with spaces, for example "Iron Chloride.adf".

ADF 2008.01 and Cygwin

Cygwin is no longer needed for ADF to work; moreover it will cause problems if Cygwin binaries are executed from within ADF and/or MinGW programs. MinGW is a Windows port of Unix utilities and Msys is a subset of it provided with ADF for convenience. It is necessary for ADF to work and it replaces Cygwin needed in the previous versions of ADF (version 2003.01 and earlier). If you have Cygwin installed on your

computer, make sure that its binary files folder is placed **after** Msys folder in the PATH environment variable (normally the ADF Setup program takes care of this).

Do not run ADF from Cygwin programs (Emacs, xterm, etc.). Cygwin adds /cygdrive/ to pathnames in some of the important environment variables, including PATH, which prevents some non-Cygwin programs, including ADF, executed from inside Cygwin from working properly.

If you would like to keep using Cygwin in parallel with ADF you have a choice depending on your personal preferences. If you prefer to work from Unix shell command line, then you can create a shortcut for C:\ADF2008.01\msys\bin\sh.exe and place it on the desktop. You can then use it instead of Cygwin's shell to run ADF programs. However, if you prefer to use Windows native tools, i.e. Windows Explorer and alike, you can, using an editor of your choice, create a shell script that executes ADF; save the script with .run extension and execute it by double-clicking in the Windows Explorer (ADF Installation procedure associates files with .run extension with C:\ADF2008.01\msys\bin\sh.exe).

If you want to know more about MinGW and Msys, visit [their website](#).