



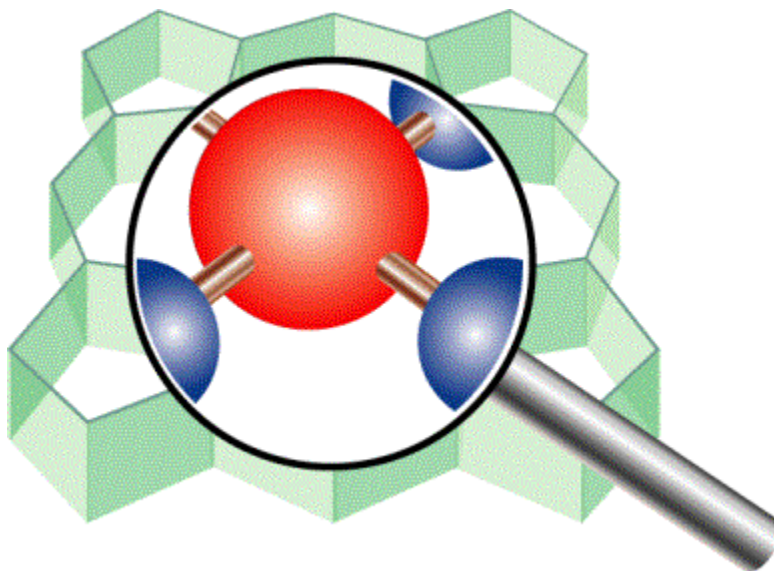
Scientific Computing & Modelling

# Installation manual for Windows

**ADF Program System  
Release 2009.01**

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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:

- Supported operating systems: Windows 2000, 32-bit XP, 32- or 64-bit Vista;
- For the HP-MPI version: a TCP/IP connection which must be active while a parallel calculation 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

Before you can use ADF programs, you must obtain a license file and save it as %ADFHOME%\license.txt. Everywhere in this document %ADFHOME% stands for ADF installation directory, which is by default C:\ADF2009.01.

**Trial users:** If you are a trial user you should have already obtained license.txt together with the download information. Your license file will allow you to use ADF on any computer.

**Other users:** Your license file is usually host-locked. In order to generate the information necessary to create a license file, execute the %ADFHOME%\makelicinfo.bat file. This information is saved in the %ADFHOME%\licinfo.txt file and is displayed using your default text editor so you can easily copy the information and paste it in an e-mail message to [license@scm.com](mailto:license@scm.com).

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.

The ADF installation script installs the Putty software on your computer in %ADFHOME%\bin\Putty. 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. Follow the steps below to configure plink for use with ADFjobs:

- 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 %ADFHOME%\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 %ADFHOME%\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 the ~/.ssh directory as well as the authorized\_keys file must have proper permissions (usually 0700 and 0600, respectively) for the public key authentication to work.
- Connect to the remote computer at least once with a "plink user@host" command so that plink stores the host's 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):  
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 ADF on the remote computer with your local ADFjobs.

## Getting Support

When something goes wrong and you need help, please remember that in addition to a (comprehensive) description of the problem we often need additional information. This information should be obtained as follows:

If ADFjobs is working then start it and select "Generate Test Job" in the Job menu. A job named "Test-Job" will be created. Select it and press Ctrl-R. Press "Yes" button if asked. An ADFtail window will pop up showing progress of the job. Send an e-mail to support@scm.com describing the problem 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 a sequence of actions to reproduce it.
- The file %ADFHOME%\bin\version containing all information about version of the ADF installation.
- Content of the file specified in the SCMLICENSE environment variable.
- 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.

# Additional Information

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

## Environment Variables

As of ADF2008, the installation procedure does not set system wide environment variables ADFHOME, ADFBIN, ADFRESOURCES and 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 uninstall ADF2007 or any earlier release before installing ADF2009 because the previous version sets the environment variables mentioned 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. There is, however, 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%\hpmpi\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.

- SCMLICENSE is set to the full path of the license.txt file in the ADF installation directory, by default C:\ADF2009.01\license.txt. Thus, you need to save the license.txt file in the root of the installation directory for it to be found by the programs of the ADF package.

## Running jobs from the command line

In order to run ADF without ADF-GUI, 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, `cd` 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 dummy network "card" called Microsoft Loopback Adapter. Doing so will add an extra network interface to the system and assign a private IP address to it, thus enabling MPI jobs regardless of whether the computer is connected to other networks or not. Please note, however, that a running MPI job may still stop when the computer gets disconnected from a real network if the job was started when the computer was still connected to this network. This happens because the IP address that MPI used for communication has suddenly become invalid. This situation is common when using a laptop so laptop users should be aware of this issue.

## Killing jobs does not work under Windows 2000

ADFjobs uses the Windows' 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 (normally 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".