Modeller

Program for Comparative Protein
Structure Modelling by Satisfaction
of Spatial Restraints

Modeller 9.21 Release Notes

What's new in version 9.21?

9.21 is primarily a bugfix release relative to the last public release (9.20). Major user-visible changes include:

- Add Python 3.7 support.
- Bugfix: first derivatives of SOAP potentials should now be handled correctly (previously those of non-differentiable terms were undefined rather than zero, and those of soap_pp.PairScorer() were applied to the wrong atoms).
- Bugfix: fix double-counting of soap_pp.PairScorer() energy.
- Bugfix: selection.rotate_dihedrals() and sequence_db.search() now respect the random seed set when the environ() object was created (previously they would use a fixed random seed).
- Bugfix: CONECT records in output PDB files should now contain

the correct atom serial numbers in all cases (previously they may have been incorrect for multichain models, or model subsets written out with selection.write()).

See the Modeller manual for a full change log.

Installation

Modeller is free for academic use. To obtain an academic license key, which you will need during the installation, complete the license agreement. The license key will be sent to you in an email from our license server. For commercial or governmental use, licensing is handled by BIOVIA.

Modeller is available for Windows, Mac OS X, Linux, and some Unix variants (see the full list of platforms). Please refer to the relevant section below for installation instructions:

For Anaconda Python ('conda')

Modeller is packaged to use with the Anaconda scientific Python distribution for Windows, Linux and Mac.

To install Modeller using the 'conda' package manager, simply run from a command line

```
conda config --add channels salilab
conda install modeller
```

You will be prompted after installation to edit a file to add your Modeller license key. Alternatively, set the `KEY_MODELLER` environment variable to your license key before you run 'conda install'.

For Windows

1. Log on as a Computer Administrator user (usually the first user you create is an administrator).

2. Download the Windows installer and save it to your Desktop. The 32-bit version should work on any Windows machine; the 64-bit version will only work on 64-bit versions of Windows.

3. Double-click on the `modeller9.21-32bit` or `modeller9.21-64bit` file to start the installer. (Windows Vista or 7 will pop up a User Account Control window at this point warning about an unidentified program - click 'Allow'.)

4. Tell the installer where to install Modeller, and enter your Modeller license key when prompted. This must be typed exactly as given in the email you received from our license server.

5. Once the install is complete, you can run Modeller scripts from a regular Python command line or IDLE GUI, if you install any version of Python between 2.3 and 3.7 from the Python website. (To run a Modeller script in IDLE, right-click on it, select "edit in IDLE", then hit F5 to run it; if you install the 32-bit version of Modeller, this will only work with the 32-bit version of Python, and likewise for the 64-bit version.) Alternatively, you can use the Modeller link from the Start Menu to start a Command Prompt from where you can run Modeller scripts. It is usually **not** a good idea to simply double-click on a Modeller script to run it, as the output will disappear as soon as the script finishes.

6. Examples can be found in the '`examples`' folder. You can type 'run_tests' in this folder to run them all (an 'import site' warning is normal, as is a failure to load the 'socket' module for some examples). Note, however, that if you use NT/2000/XP, and are NOT an Administrator user, or you are using Windows Vista or later with UAC turned on (the default) you will first need to make a copy of this directory elsewhere, as Windows will not allow Modeller to write output files into this directory.

7. To uninstall Modeller, use the 'Uninstall' link on your Start Menu (again, you will need to be logged on as a Computer Administrator).

If you have not used Modeller before, proceed to the Getting started section.

Note: the Windows installer also supports silent (unattended) installation. To install silently, run the installer with the /D flag to specify install location and /KEY to specify the Modeller license key, e.g. `modeller9.21-32bit.exe /S /KEY=xxx /D=C:\Program Files\modeller`. Note that the /D option must come at the end of the command line and the path must not be quoted.

For Mac OS X

If you are using the Homebrew package manager, you can install Modeller by simply running

```
brew tap salilab/salilab
brew install modeller
```

Alternatively, we provide a Modeller installer, which should work on both 32-bit and 64-bit Intel Macs (it does not work on older PowerPC-based Macs):

1. Download the Mac installer to your Desktop.

2. Double-click on the `modeller-9.21.dmg` file to open the disk image.

3. Double-click on the `Modeller 9.21.pkg` file within this image (if your Mac complains that the package is by an unidentified developer, right-click or control-click on it instead and select Open from the dropdown menu, then Open again in the confirmation dialog). Enter your license key when prompted by the installer.

   Note: you can also use Apple's command line `installer` utility to install the package, but this will not fill in the license key; you would need to then manually edit the file `/Library/modeller-9.21/modlib/modeller/config.py` to fill in the `license` variable.

4. Once the install is complete, you can run Modeller scripts like any other Python script: for example, you could run the Modeller script `foo.py` by typing "`python foo.py`" from a Terminal window. Alternatively, you can type "mod9.21" to run Modeller. (See below for example scripts.) (Modeller itself can be found in the `/Library/modeller-9.21/` directory.) Note that Modeller is set up to work with the standard Apple-provided Python, i.e. `/usr/bin/python`; to make it work with other versions of Python installed on your system, you may need to modify PYTHONPATH.
5. To uninstall Modeller, run the following from a Terminal window (all on one line): '`sudo rm -rf /Library/modeller-9.21/ /usr/local/bin/mod9.21 /Library/Python/2.?/site-packages/modeller.pth /var/db/receipts/org.salilab.modeller.*`'.

If you have not used Modeller before, proceed to the Getting started section.

For Linux (RPM)

The Linux RPM installer should install on any modern RPM-based Linux system, such as RedHat Enterprise, Fedora, or SuSE. It can also be installed on non-RPM systems such as Gentoo. (For .deb-based systems such as Debian or Ubuntu, we recommend the Debian/Ubuntu package instead.)

If you do not have root access to your Linux system, or wish to install in a non-standard location, you can use the generic Unix installer instead.

Prerequisites: **glibc >= 2.3** (although it may work with glibc 2.2; see below); and **glib >= 2.2** (installed on most Linux systems by default; can be obtained from the GTK+ website if your distribution doesn't have a 'glib' or 'glib2' package.) For old operating systems such as RedHat 8.0, see this page in the Modeller wiki.

1. Download the correct RPM file for your architecture. (If in doubt, run '`uname -m`' from a terminal on your Linux box. "i386" (or

i586/i686) is for 32-bit machines such as the Pentium. x86_64 is for most 64-machines such as the Opteron or Intel Xeon64.) For the security conscious, all of these files are GPG signed.

2. Install the RPM file by running the following command (either logging in as the `root` user, or by prepending the command with '`sudo`'), replacing `XXXX` with the Modeller license key (and i386 with x86_64 if necessary).

   ```
   env KEY_MODELLER=XXXX rpm -Uvh modeller-9.21-1.i386.rpm
   ```

   On a built-from-source system such as Gentoo, the original 'rpm' command should work, although you will probably need to build the rpm package itself first, and append the `--nodeps` option to the command.

3. If you have any version of Python between 2.3 and 3.7 installed on your system, you should be able to use Modeller from a regular "python" interpreter. For example, you could run the Modeller script `foo.py` by typing "`python foo.py`" from a command line (e.g. a GNOME terminal window, KDE Konsole window, etc.). Alternatively, you can run Modeller by typing "mod9.21" from a command line. (See below for example scripts.)

4. Documentation and examples can be found in the `/usr/lib/modeller9.21/` directory. Note that you will need to make a copy of the `examples` directory in order to use it, e.g. "`cp -a /usr/lib/modeller9.21/examples ~`".

5. To uninstall Modeller, run the following command: '`rpm -e modeller`'.

If you have not used Modeller before, proceed to the Getting started section.

For Linux (Debian/Ubuntu)

The Debian/Ubuntu package should install on any modern .deb-based system. (It was, however, built and tested on an Ubuntu 14.04 (Trusty Tahr) machine, so may not work on older systems.) If you do not have root access to your Linux system, or wish to install in a non-standard location, you can use the generic Unix installer instead.

1. Download the correct Debian/Ubuntu package for your architecture.

2. Install the package by running the following command, replacing `XXXX` with the Modeller license key (and i386 with x86_64 if you are using the 64-bit installer).

```
sudo env KEY_MODELLER=XXXX dpkg -i modeller_9.21-1_i386.deb
```

3. If you have any version of Python between 2.3 and 3.7 installed on your system, you should be able to use Modeller from a regular "python" interpreter. For example, you could run the Modeller script `foo.py` by typing "`python foo.py`" from a command line (e.g. a GNOME terminal window, KDE Konsole window, etc.). Alternatively, you can run Modeller by typing "mod9.21" from a command line. (See below for example scripts.)

4. Documentation and examples can be found in the `/usr/lib/modeller9.21/` directory. Note that you will need to make a copy of the `examples` directory in order to use it, e.g. "`cp -a /usr/lib/modeller9.21/examples ~`".

5. To uninstall Modeller, run the following command: '`sudo apt-get remove modeller`'.

For generic Unix

This installer contains binaries for Linux and AIX. If installing for Linux, the prerequisites are the same as for installing the RPM.

1. Download the generic tarball (.tar.gz) file into a temporary directory on your computer.

2. Open a console or terminal (e.g. xterm, Konsole, GNOME terminal) and change to the directory where you downloaded the `.tar.gz` file. Unpack the file with the following commands:

   ```
   gunzip modeller-9.21.tar.gz
   tar -xvf modeller-9.21.tar
   ```

3. Go to the `./modeller-9.21` directory and run the installation script:

   ```
   cd modeller-9.21
   ./Install
   ```

   Answer several questions as prompted. If you make a mistake, you can re-run the script.

4. You can run Modeller by using the `modpy.sh` or `mod9.21` scripts in the `bin` directory under the directory you installed Modeller in. For example, if you installed Modeller in `/opt/mod/`, then if you have any version of Python between 2.3 and 3.7 installed, "`/opt/mod/bin/modpy.sh foo.py`" will run Modeller with a script file called `foo.py`. If you don't have Python installed, "`/opt/mod/bin/mod9.21 foo.py`" will run Modeller on the same script. (See below for example scripts.)

If you have not used Modeller before, proceed to the Getting started section.

Getting started

Once Modeller is successfully installed, please refer to the documentation, in particular the online manual and the Modeller tutorial for information on using the program and example scripts. You will also find several example scripts in the `examples` directory after you install Modeller.

Please also check periodically at the patches page in the Modeller wiki for hotfixes to the current release.

Known issues and questions with 9.21

Please also check the Modeller FAQ and the mailing list archives.

1. **Standard Python libraries like `os` aren't available** or **I get warnings such as '`'import site' failed`' or '`Could not find platform independent libraries <prefix>`'**
   The `mod9.21` script uses a built-in copy of the Python 2.3 interpreter, but not the accompanying modules. To fix this problem, you could install Python 2.3 on your system (however, you only need the Python 2.3 modules if you are trying to import non-Modeller modules; you don't need them to run regular Modeller scripts, so you can ignore these warnings). Alternatively, don't use the `mod9.21` script to run Modeller, but see the instructions above for running Modeller with Python.

2. **Trying to load Biopython (or some other Python modules) in a Modeller script gives errors about `PyUnicodeUCS2`**
   The built-in Python interpreter in the `mod9.21` script is compiled with 4-byte Unicode support ('`UCS4`') on most platforms and is not compatible with any modules compiled with 2-byte Unicode ('`UCS2`'). This is a Python limitation. To avoid this problem, don't use the `mod9.21` script to run Modeller; see the instructions above for running Modeller with Python.

3. **I get an error similar to the following when starting Modeller: '`error while loading shared libraries: libmodeller.so.5: cannot restore segment prot after reloc: Permission denied`'**
   Linux builds of Modeller rely on the Intel Fortran libraries, which are not compatible with strict SELinux policies enforced in the latest versions of Fedora and RedHat Linux. You can make Modeller work by enabling the `allow_execmod` SELinux boolean, disabling SELinux entirely, or labeling the Modeller libraries as containing text relocations using the `semanage` utility. (The last is preferable, and should have been done automatically for you

already if using the RPM installer.) More technical details (see the **execmod** section).

Tested platforms

MODELLER runs on Pentium PC's (Linux and Windows), Apple Macintosh (OS X), Linux x86_64 systems, and workstations from IBM (AIX). The actual platforms which 9.21 has been tested on are shown below:

Platform	Modeller executable type	Tested systems
Linux i686 PC (Intel Pentium, AMD Athlon etc.)	i386-intel8 or i386-absoft	Fedora 29, RH 9[1], RH Enterprise 5 & 6, Ubuntu 14.04, FreeBSD-4.11[2] [3]
Windows i686 PC (Intel Pentium, AMD Athlon etc.)	i386-w32	Windows 7 (32-bit and 64-bit), Vista (32-bit), XP Service Pack 3
Windows x86_64 PC (Intel Xeon 64 etc.)	x86_64-w64	Windows 7 (64-bit)
Apple Mac (Universal)	mac10v4	10.6 (Snow Leopard), 10.11 (El Capitan) and 10.14 (Mojave) on Intel (32-bit and 64-bit)
Opteron/Intel Xeon64 (AMD64/EM64T)	x86_64-intel8	RH Enterprise 5, 6 & 7, Fedora 29, Ubuntu 14.04
AIX	rs6000	AIX V5.1 on a PowerPC p630

[1] A bug in RPM on RedHat 9 causes it to crash with a segmentation fault when trying to install the Modeller RPM (at least on our test system). Upgrade to a more recent Linux distribution, or use the .tar.gz installer instead.

[2] The Linux Modeller binary is linked against glibc-2.3. To make it work on glibc-2.2 systems, you will need to install some glibc-2.3 libraries; see the comments in the `bin/mod9.21` script after installation for one way to do this.

[3] The default Linux binary uses SSE instructions, and thus to run it on a FreeBSD machine you must enable SSE support in your kernel ('`options CPU_ENABLE_SSE`'). If this is not possible, you can use the alternative Linux binary (i386-absoft) which is slower but which does not use SSE.
