



## **Gaussian 09 for Mac OS X Installation Instructions**

In order to run *Gaussian 09*, several UNIX environment variables must be set in each user's account. If you are comfortable using UNIX, *G09* can be set up using the instructions in the **ReadMe** document on the distribution CD. The following alternate instructions attempt to make minimal use of UNIX commands. These instructions are appropriate for both the full *G09* program and for the *G09* Utilities.

### **Instructions for users who will also install *GaussView***

*Install the program:* Insert the *G09* CD. Open the **tar** folder, and double-click the **Mxx-10yz.tgz** file (**xx** = is the platform version which indicates whether it is for PowerPC Macs, 32-bit Intel Macs, or 64-bit Intel Macs; **y** is a version number; and **z = N, X or U** for the *G09* binaries plus TCP Linda, the *G09* binaries, or the *G09* Utilities respectively). On most systems, *Archive Utility* will be started and the ".tgz" file will be expanded to a folder named **g09** on either your **Desktop** or your **Downloads** folder (if the latter exists). After *Archive Utility* has finished expanding the ".tgz" file, drag the resulting **g09** folder to the desired location for the *G09* binaries (or the *G09* Utilities). Do not rename the **g09** folder. There is no need to modify any files inside the **g09** folder in order to install the *G09* binaries or the utilities. The directory path to the **g09** folder cannot contain spaces.

*Set the UNIX environment variables:* Each user who will run *Gaussian* must perform this step. Mac OS X prevents the user from viewing or editing certain UNIX files from the Finder, but one can run a few simple UNIX commands to get around this limitation for specific files. Open a *Terminal* window (the *Terminal* application is found in the **Applications/Utilities** folder). Type the following commands (without typing the \$ prompt which is included for illustrative purposes):

```
$ cd
$ touch .login
$ ln -s .login my_login
```

Exit the *Terminal* program and open the file **my\_login** with a text editor such as *TextEdit*. Assuming that the **g09** folder was placed in the **Applications** folder, add the following two lines to the file (the file may be empty at this point; if not, add these lines to the end of the file):

```
setenv g09root /Applications
source $g09root/g09/bsd/g09.login
```

You may also want to add a third line to define a destination directory for *G09* temporary files. For example:

```
setenv GAUSS_SCRDIR /Users/name/Scratch
```

You will need to create the specified folder if it does not already exist.

Note that if you already have lines in the **.login** file which refer to *g03*, you should replace these lines with the above lines. Save the file as plain text (not RTF) and exit. It is recommended that you log out of your user account and relogin in order for the changes in the **.login** file to take effect. You are now ready to install *GaussView*, following the steps on its instruction sheet.

### **Instructions for users who need to submit *G09* jobs from a *Terminal* window**

If you are using an application that can create *Gaussian* input files but cannot submit the job, you will need to submit the job using a *Terminal* window. Mac OS X users have one of two default UNIX shells. The setup instructions are different for these two shells.

Determine your default UNIX shell: Accounts originally created using Mac OS X 10.0.x, 10.1.x, or 10.2.x default to using **tcsh**. Accounts created using Mac OS X 10.3.x or later default to **bash**. To determine which shell your account uses, open a *Terminal* window and type the following:

```
$ echo $SHELL
```

- If **“/bin/tcsh”** is returned, follow the “Instructions for users who will also install *GaussView*” above to modify your **.login** file, which will allow you to run G09 from either *GaussView* or a *Terminal* window (you do not need to repeat that process if you have already done it). Then follow the instructions in “Additional Setup Step when Multiple Users will run G09”, if necessary.
- If **“/bin/bash”** is returned, proceed as indicated below (the remainder of this section) in order to be able to run G09 from a *Terminal* window. Remember that in order to run G09 from *GaussView*, you need to perform the steps in “Instructions for users who will also install *GaussView*” even if your default shell is **“/bin/bash”**.

Modify your *.profile* file: Mac OS X prevents the user from viewing or editing certain UNIX files from the Finder, but one can run a few simple UNIX commands to get around this limitation for specific files. Open a *Terminal* window (the *Terminal* application is found in the **Applications/Utilities** folder). Type the following commands (without typing the \$ prompt which is included for illustrative purposes):

```
$ cd
$ touch .profile
$ ln -s .profile my_profile
```

Exit the *Terminal* program and open the file **my\_profile** with a text editor such as TextEdit. Assuming that the **g09** folder was placed in the **Applications** folder, add the following two lines to the file (the file may be empty at this point; if not, add these lines to the end of the file):

```
g09root=/Applications
export g09root
. $g09root/g09/bsd/g09.profile
```

Note that the last line above starts with a period (.), then space and finally (**\$g09root/g09/bsd/g09.profile**). You may also want to add two more lines to define a destination directory for G09 temporary files. For example:

```
GAUSS_SCRDIR=/Users/name/Scratch
export GAUSS_SCRDIR
```

You will need to create the specified folder if it does not already exist.

Note that if you already have lines in the **.profile** file which refer to *g03*, you should replace these lines with the above lines. Save the file as plain text (not RTF) and exit. It is recommended that you log out of your user account and relogin in order for the changes in the **.profile** file to take effect. You are now ready to run *Gaussian* from a *Terminal* window.

### Additional Setup Step when Multiple Users will run G09

If multiple users will log into the Macintosh computer and run G09, then they must all be placed into the same group, and that group must be the owner of the G09 software files. The latter can be accomplished with the **chgrp -R** command.

For example, the following command will set the group ownership of the G09 files to group *chem* (assuming the same installation location as above):

```
$ sudo chgrp -R chem /Applications/g09
```

These steps are especially important for Panther and later systems, where users are placed into separate groups by default. You may need to ask your system administrator to help you set up things properly.