



Gaussian 09 Source Code Installation Instructions

If you will be using Linda, build the regular *Gaussian 09* program first, and then build the Linda version using the instructions on page 3.

1. Check that you have the correct versions of the OS, compiler, and libraries for your machine, as listed in the platform list file **platform_rev.pdf** on the CD (*rev* represents the revision of the program; replace with the revision you actually use). The latest version of this file is always available on our website at www.gaussian.com/g09_plat.htm.
2. Select a group which will own the *Gaussian* files. Users who will run *Gaussian* should either already be in this group, or should have this added to their list of groups. Consult your system administrator if you need help with this process.
3. Mount the CD. Information about how to do this for various types of computers is given on page 2.
4. Change to the C shell, and set the **g09root** and **mntpnt** environment variables:

```
$ /bin/csh
% setenv mntpnt "/mnt/cdrom"      # Set to wherever CD is mounted.
% setenv g09root "dir"          # dir=install location for G09.
% cd $g09root
```

5. Read the CD, set group ownership, and run the build script:

```
% gunzip -c $mntpnt/tar/*.tgz | tar xvf -
% chgrp -R grp g09              # grp=group from step 1.
% cd g09
% bsd/install
```

6. Compile the program:

```
% source $g09root/g09/bsd/g09.login
% bsd/bldg09 >&make.log          # Will take between .5 and 6 hours.
```

Notes:

- i) A case-sensitive file system is required for building from source on Mac OS X (Intel) systems. Also, for this case, the default is to build for the current (Intel EM64T) processors. In order to build the IA32 version, you must specify:

```
% bsd/bldg09 all mac32 >&make.log
```

- ii) When building from source on IBM Power systems, the default is to build for the current (Power7) processors. In order to build the versions for Power5 or Power6 machines, you must specify:

```
% bsd/bldg09 all ibmp5 >&make.log
```

7. Check the end of **make.log** for successful completion. Confirm that the executables have been built:

```
% ls $g09root/g09/*.exe
```

There should be 79 files.

8. You are now ready to run. Users will want to add the following to their **.login** or **.profile** file:

```
# .login commands                                # .profile commands
setenv g09root "dir"                              g09root="dir"
setenv GAUSS_SCRDIR "sdir"                        GAUSS_SCRDIR="sdir"
source $g09root/g09/bsd/g09.login                 export g09root GAUSS_SCRDIR
                                                    . $g09root/g09/bsd/g09.profile
```

The *dir* in the first command is the location of the **g09** directory. For example, if the path to this directory is **/usr/local/g09**, then set **g09root** to **/usr/local**. The *sdir* in the second command is a directory to be used by default for *Gaussian 09* scratch files. There should be plenty of disk space available at this location.

Building G09 with Linda

Note: Building Gaussian 09 with Linda requires Linda version 8.2; the executables will not build with previous version of Linda.

1. First install G09 from source
2. Mount the Linda CD using the same location as above. Now install Linda:

```
% cd $g09root/g09
% gunzip -c $mntpnt/tar/*.tgz | tar xvf -
% bsd/install                                # repeat command for Linda
% source $g09root/g09/bsd/g09.login          # repeat command for Linda
% mg linda
```

3. You are now ready to run. Users will need to set the **%LindaWorkers** Link 0 command in their input files to specify the list of nodes to use for the parallel Gaussian calculation (or use **-W-** in **Default.Route**). Consult the *Gaussian 09 User's Reference* for detailed information about Linda parallel Gaussian jobs.

Mounting CDs

This page reviews the methods for mounting CDs on various UNIX systems.

LINUX:

Most Linux machines allow ordinary users to mount CDs into **/mnt/cdrom**, using a command like this one:

```
$ mount /mnt/cdrom          # Prompt is % if you use tcsh.
```

HP/COMPAQ TRU64:

The **mount** command varies with the hardware configuration but is usually something like:

```
# /sbin/mount -rt cdrfs /dev/disk/cdrom0c /mnt
```

The command must be run by *root*. You can mount the CD from your ordinary user account using the following command:

```
$ su -c /sbin/mount -rt cdrfs /dev/disk/cdrom0c /mnt
```

You can also use the **sudo** command if it is in use at your site. Finally, if you do not have *root* access, ask the system administrator to mount the CD for you.

IBM AIX:

The **mount** command is typically of the form:

```
# /sbin/mount -v cdrfs -o ro /dev/cd0 /mnt
```

The command must be run by *root*. You can mount the CD from your ordinary user account using the following command:

```
$ su -c /sbin/mount -v cdrfs -o ro /dev/cd0 /mnt
```

You can also use the **sudo** command if it is in use at your site. If you do not have *root* access, ask the system administrator to mount the CD for you.