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 **plat_list_a01.htm** on the CD. 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/*.taz | 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.
    ```

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

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

    There should be 78 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.

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 cdfs /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 cdfs /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.

Building G09 with 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/*.taz | tar xvf -
    % bsd/install                       # repeat command for Linda
    % source $g09root/g09/bsd/g09.login   # repeat command for Linda
    % mg linda
    ```

3. If your default shell is **csh** or **tcsh.cshrc** file on**,** your each node used as a Linda worker should contain:

    ```
    if (! ($?LD_LIBRARY_PATH) ) then
            setenv LD_LIBRARY_PATH  full_path_to_g09
    endif
    ```

    g09root is not set at this point, so the complete path (e.g. **/home/software/g09**) should be used.

4. You are now ready to run. You will need to set the **%LindaWorkers** Link 0 command to the list of nodes that you want 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.