Visualizing Results when *GaussView* and *Gaussian* are Installed on Different Machines

Joseph W. Ochterski, Ph.D.
help@gaussian.com

June 21, 2000

Abstract

The purpose of this paper is to describe how to use *GaussView* (or *GaussViewW*) to create jobs and visualize results calculated by *Gaussian*, when *Gaussian* is installed on a different computer (running Unix).

Contents

1 Introduction

There are a variety of reasons you may want to run *GaussView* and *Gaussian* on different computers. The typical reason is that the computer with *Gaussian* has more resources – memory, disks or processors. Throughout the rest of this document, I'll refer to the machine running *GaussView* (if it's a Unix computer) or *GaussViewW* (if it's running Windows) as the *local* machine, and the Unix machine on which *Gaussian* will run as the *remote* machine. Also, I'll use *GaussView* as short had to mean "*GaussView* on a Unix machine, or *GaussViewW* on a Windows machine".

2 The shortcut

For those who don't want to read the entire document, I'll give a sneak peek at the essential point here; the rest of the document will be a description of how to create formatted checkpoint files and how to use them. *GaussView* gets results from *Gaussian* via formatted checkpoint files and log files (i.e. *Gaussian* output files). If you already know how to generate formatted checkpoint files and move them around, then you needn't read further. If you didn't understand all that, don't worry, I'll explain it below.

3 Overview

The whole process of creating jobs, running them, and visualizing the results can be broken down into five essential steps:

1. Create the input file.
2. Transfer the input file to the remote computer.
3. Run the calculation and prepare the output file.
4. Transfer the output file(s) back to the local computer.
5. View the results.

The next few sections describe these steps in detail. First, though, I'll give a brief list of some assumptions I've made about how things (computers and software) are set up.

I'll assume the local machine has the following:

- *GaussView* is installed if it is a Unix machine; *GaussViewW* is installed if it is running Windows.
- Either *Gaussian* or the *Gaussian* utilities are installed. Technically, it is possible to generate cube files on the remote machine and view them on the local machine, but I will not discuss that process in detail.
- The machine should be hooked up to a network, and should be able to run network software such as `ftp` and `telnet`.

The assumptions for the remote machine are similar:

- It should be a Unix-type system, so users can log in.
- Gaussian should be installed, and be accessible for users. This includes setting up the initialization files, as described in the *Gaussian User's Reference*.
- You have an account and password on the Unix system.
- It has a network connection. As for the local system, `ftp` should be available to users.

3.1 Step 1: Create an input file

This can be as simple as firing up *GaussView*, building your molecule, and saving it as an input file (`.com` or `.gjf`). However, if you are interested in visualizing surfaces (electrostatic potential, orbitals, density, etc.), then there will be an additional step you need to take before you save the input file; namely, indicating in the input file that you wish to save a formatted checkpoint file. By formatted, I mean human readable, rather than binary.

GaussView needs to read in formatted checkpoint files, which generally have the extensions `.fch` or `.fchk`, in order to have enough information to be able to calculate surfaces. *Gaussian* does not generate these files by default, but will generate them if the input file indicates that it should.

Modifying an input file is a straight forward procedure, and can be done within *GaussView*, from the **Gaussian Calculation Setup** window. To see that window, from the *GaussView* main menu, choose `Calculate->Gaussian...`, and the **Gaussian Calculation Setup** window will pop up. Exactly what to do in that window is described below. When you've made your modifications, you can save them in a file by clicking on the **Retain** button in the **Gaussian Calculation Setup** window, then choosing `File->Save...` from the *GaussView* main menu. Save it with file type "Gaussian", with either a `.com` or `.gjf` extension. *Gaussian* accepts both `.gjf` and `.com` files equivalently as input. Remember the name of the file and the directory you saved it in, you'll need to know these later.

The easiest way to tell *Gaussian* to generate a formatted checkpoint file is to add the keyword `FORMCHECK` to the "Additional Keywords" box in the **Gaussian Calculation Setup** window. This tells *Gaussian* to create a formatted checkpoint file named `Test.FChk` when the job completes successfully. If the job fails, `Test.FChk` will not be created. The name of the file will *always* be `Test.FChk`. If you need the additional flexibility of a checkpoint file with a different name, then you can simply rename it after the calculation finishes.

There is another way, which is somewhat more flexible, to generate a formatted checkpoint file. If you modify your input file so that it has a `%chk` card (which is described in Chapter 2 of the *Gaussian User's Reference*), then *Gaussian* will not delete the unformatted checkpoint file after the calculation has completed. You can format this checkpoint file using *Gaussian*'s `formchk` utility. Instructions for doing this are included in section 3.3, "Step 3. Run the calculation". You do not need to use the `FORMCHECK` keyword. If you do, then both the unformatted checkpoint file and `Test.FChk` will be available at the end of the calculation.

3.2 Step 2: Transfer the input file to the remote computer

Now that you've saved the input file, you need to transfer it to the remote computer so Gaussian can use it. One way to do this is to use `ftp`, which is included with Windows, and is available on most Unix machines. Here are the steps to take to transfer the file:

1. *Get a command prompt.*

    - *Windows:* From the Windows task bar (the one on the bottom of the Windows screen), click `Start->Programs->Command Prompt`, and a command prompt window will pop up.

- *Unix:* Hopefully, an xterm, or it's equivalent is already running. If *GaussView* is running in the xterm, you can either exit *GaussView*, or make it a background process by typing `Ctrl-Z`, then `bg` at the prompt.

2. *Change directories on the local machine.* Change directories (using the `cd` command) to the directory on the local machine where you saved your input. Remember that on Windows machines, the slashes point the opposite way from Unix machines (Windows: \; Unix: `/`).

3. *Start* `ftp`. Type `ftp` *machine* where *machine* is the name (or IP address) of the remote machine where you'll run the *Gaussian* calculation. When `ftp` asks for them, enter your username and password.

4. *Change directories on the remote machine.* With `ftp`, use the `cd` command to the directory where you want the input file to go on the remote machine (remembering the different Unix/Windows slash conventions:(Windows: \; Unix: `/`).

5. *Copy the input file to the remote machine.* Once you are in `ftp`, connected to the remote machine, and in the proper directory there, you can copy the input file to that machine using `ftp`'s `put` command, like this: `put` *`name`*`.gjf`. The file will then be copied to the remote machine.

6. *Quit from* `ftp`. That's it – now you can leave `ftp` using the `quit` command.

3.3 Step 3. Run the calculation

For this step, you need to be connected to a command prompt on the remote machine. Typically the `telnet` program is used to do this.

1. *Log into the remote machine.* Again, you'll need your username and password. Type `telnet` *machine*, where *machine* is the same computer you `ftp`'d the file to, and enter your username and password when prompted.

2. *Change directories.* Use the `cd` command to change directories to the directory you put the file in on the remote machine.

3. *Run the job.* How you actually do this depends a bit on how *Gaussian* was set up on the remote computer. Generally, you can run *Gaussian* as described in the *Gaussian User's Reference*; however, on computers which use batch queues, you'll have to contact your administrator to find out how to run *Gaussian* if you don't already know. If your remote machine does use queues, you may have to modify the script you submit to the queue to make it copy the *Gaussian* log file and the `Test.FChk` file to a safe place until you copy them to the local machine.

   Once the job has successfully finished, you can rename the `Test.FChk` file, if you wish to, using the Unix `mv` command. Generally, formatted checkpoint files have the extension `.fchk` (`.fch` on Windows). Using this extension will make it somewhat more convenient to load the file into *GaussView*. *Warning:* if you choose not to rename it,

remember that you may accidently overwrite an older `Test.FChk` file when you run another job using the `FORMCHECK` keyword.

If you did not use the `FORMCHECK` keyword, but chose to use a `%chk` card, then you need to take the extra step of formatting the checkpoint file now, so that *GaussView* can read it. The `formchk` utility, which is part of *Gaussian*, is the correct tool for doing this. Just type: `formchk` ***name***`.chk`, and `formchk` will create ***name***`.fchk`. This is just one way to use `formchk`; other ways are described in the Gaussian User's Reference.

4. Exit from `telnet`. If your job is a long running one, you may which to exit from `telnet`, and come back from time to time to check on it. If it's a short one, you can check to make sure it has completed successfully, and then exit. You may leave `telnet` with the `exit` command.

3.4 Step 4. Copy the output files back to the local machine.

This is essentially the same process as moving the input file to the remote machine.

1. *Get a command prompt.*

2. *Change directories on the local machine.* Change directories to the directory on the local machine where you want the output to end up.

3. *Start* `ftp`.

4. *Change directories on the remote machine.* Again, use the `cd` command to the directory where the output files are.

5. *Copy the output file(s) from the remote machine.* You can copy the output file(s) from the remote machine using `ftp`'s `get` command, like this: `get input.log` or `get input.fchk`. The files will then be copied from the remote machine.

   The formatted checkpoint file and the log (`.log`) file hold slightly different (but overlapping) information. Here's a brief summary of what is in each (as of *Gaussian* 98 Revision A.9), assuming the appropriate calculation was run for that type of information.

Information	Formatted Checkpoint	*Gaussian* log file
Atomic coordinates	X	X
Normal mode vibrations	X	X
Atomic charges		X
MO coefficients	X	
Summary	X	X

6. *Quit from* `ftp`.

3.5 Step 5. View the results.

If it's not already running, start up *GaussView* again. Then select `File->Open...` and after selection the corresponding file type, enter either the log file or formatted checkpoint file name in the **Open File** window. You may need to change directories in **Open File** window to find your output files. Once you click **Open**, the molecule you ran the calculation on will appear in the main *GaussView* window.