Restarting an externally terminated Gaussian calculation

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It is possible to restart Gaussian calculations that were terminated externally to the program, i.e. the job was ended not by Gaussian, e.g. when there is a power outage in the building housing the Tiger cluster, or the node running the calculation crashed, etc. This is especially helpful for calculations that take a long time, like freq jobs. Note that when a Gaussian job crashes internally, i.e. the calculation is terminated by Gaussian itself, the restart should be done another way.

Here are the steps to take:

(1) Determine the Tiger node on which the calculation was running. For this, find the **calc.job.o#** file corresponding to the job. Here, "calc" is the name you gave the job, and # is the job-ID, which may be several digits. The node name will be printed on the first line of this file, and will have the format **compute-m-n.local**.

(2) Find the **.rwf** file for the job. This is a Gaussian data file, and it will (hopefully) be found on the node from step 1. Login to the node by opening a command-line terminal and typing **ssh tiger**, and then **ssh compute-m-n** (but use the actual numbers for the node). Then type **cd /scr/username/job-ID**, where username is your MGCF user name, and job-ID is the number in the file suffix from step 1. Then type **ls** to display the files in this subdirectory. If it didn't somehow already get deleted, there should be a file named **Gau-#.rwf**, where # is a number that can have several digits. We will reference this file in the restart calculation. An optional, but probably generally good, step to take is to make a copy of this rwf, because Gaussian will modify the rwf file in the restart calculation, and you may have to backtrack in case your restart calculation doesn't work for some reason. If you do make a copy, do so within this /scr/username/job-ID directory (choose your own file prefix, but end the filename in .rwf), because rwf files can be extremely large.

(3) Make a new .com file for the restart calculation. For this, go into the directory containing the original calculation. Create a new text file called, for example, restart.com (you can choose your own file prefix), and put the following in it:

```
%nproc=16
%mem=120GB
%rwf=/scr/username/job-ID/Gau-100_copy.rwf
%chk=calc_copy.chk
#p restart
```

Ensure that the file ends with a blank line. The actual numerical values used for nproc and mem should match those used in your original calc.com. For %rwf, specify the actual path to your original rwf (or the copy of it, if that's what you chose to do). For %chk, you can either specify the original copy.chk, or you can also make a copy of that file (in the same directory as the original calculation) and use that here. Making a copy of this file is probably advisable for the same reasons mentioned in step 2, and if you do this, after the restart calculation successfully finishes, you'll be able to delete the original chk file to save disk space.

(4) Make a new .job file for submitting the restart. For this, go into the directory containing the original calculation. Then copy calc.job (again, substitute your actual named prefix) to something like restart.job (you can choose your own file prefix, but make it the same as what you're using for the .com file in step 3). Then you'll need to make a few edits to the file:
   (a) Near the top of the file, there will lines starting with **#$ -o** and **#$ -N**. Within these lines, your original "calc" prefix will show up. Change these to be the same as the prefix used for the new .job and .com files.
   (b) At the end of the block of lines beginning with **#$**, add a new line with **#$ -l h=compute-m-n** (again, use the actual numbers instead of m,n).
   (c) Near the end of the file, there should be a line like **/usr/software/gaussian16/g16.revA03_sse4_2/g16/g16 < calc.com > calc.out** Change both instances of "calc" to match the prefix you choose for the new "restart.com".

(5) Submit the restart calculation by typing **qsub restart.job**.

You should check that the restart calculation is proceeding as expected. Here's an example to help with this. I did a freq calculation that was externally terminated at the following stage in the output file:

```
    30 vectors produced by pass  0 Test12= 3.63D-14 3.33D-09 XBig12= 1.47D+02 8.15D+00.
 AX will form    30 AO Fock derivatives at one time.
    30 vectors produced by pass  1 Test12= 3.63D-14 3.33D-09 XBig12= 2.50D+01 9.95D-01.
    30 vectors produced by pass  2 Test12= 3.63D-14 3.33D-09 XBig12= 1.60D+00 3.41D-01.
    30 vectors produced by pass  3 Test12= 3.63D-14 3.33D-09 XBig12= 3.02D-02 2.67D-02.
```

I followed the above steps to restart the calculation, and the "restart.out" file shows:

```
 Resume CPHF with iteration    4.
 AX will form    30 AO Fock derivatives at one time.
    30 vectors produced by pass  4 Test12= 3.63D-14 3.33D-09 XBig12= 3.61D-04 2.95D-03.
    30 vectors produced by pass  5 Test12= 3.63D-14 3.33D-09 XBig12= 3.28D-06 2.10D-04.
    30 vectors produced by pass  6 Test12= 3.63D-14 3.33D-09 XBig12= 2.09D-08 1.87D-05.
    17 vectors produced by pass  7 Test12= 3.63D-14 3.33D-09 XBig12= 1.22D-10 1.49D-06.
     4 vectors produced by pass  8 Test12= 3.63D-14 3.33D-09 XBig12= 8.04D-13 1.17D-07.
     2 vectors produced by pass  9 Test12= 3.63D-14 3.33D-09 XBig12= 5.18D-15 1.10D-08.
```

So the output file is indicating that it's restarting at the 4th CPHF iteration (CPHF is one of the

main parts of a freq calculation), and note the “pass 3” at the end of the original output file. I also did the full freq calculation without a termination/restart, and it prints:

```
    30 vectors produced by pass  0 Test12= 3.63D-14 3.33D-09 XBig12= 1.47D+02 8.15D+00.
 AX will form    30 AO Fock derivatives at one time.
    30 vectors produced by pass  1 Test12= 3.63D-14 3.33D-09 XBig12= 2.50D+01 9.95D-01.
    30 vectors produced by pass  2 Test12= 3.63D-14 3.33D-09 XBig12= 1.60D+00 3.41D-01.
    30 vectors produced by pass  3 Test12= 3.63D-14 3.33D-09 XBig12= 3.02D-02 2.67D-02.
    30 vectors produced by pass  4 Test12= 3.63D-14 3.33D-09 XBig12= 3.61D-04 2.95D-03.
    30 vectors produced by pass  5 Test12= 3.63D-14 3.33D-09 XBig12= 3.28D-06 2.10D-04.
    30 vectors produced by pass  6 Test12= 3.63D-14 3.33D-09 XBig12= 2.09D-08 1.87D-05.
    17 vectors produced by pass  7 Test12= 3.63D-14 3.33D-09 XBig12= 1.22D-10 1.49D-06.
     4 vectors produced by pass  8 Test12= 3.63D-14 3.33D-09 XBig12= 8.04D-13 1.17D-07.
     2 vectors produced by pass  9 Test12= 3.63D-14 3.33D-09 XBig12= 5.18D-15 1.10D-08.
```

From this, you can verify that the restart calculation indeed started where the first calculation left off, and proceeded to use the exact same number of iterations that were expected to be remaining, i.e. nothing was repeated.

After a successful restart, you can login to the node and delete the rwf files.