Starting Jobs from Checkpoint Files

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It is often desirable to restart a failed calculation or start a new calculation using the structure, wavefunction, and/or the force constant matrix from a previous calculation. For example, if SCF convergence was a problem, you might run a single point calculation using keywords helping SCF convergence, that would hurt efficiency in a geometry optimization. You would then start a geometry optimization specifying that the previously-determined wavefunction should be read from the checkpoint file as an initial guess.

Note: if you change the geometry of the structure or add/delete any atoms, you cannot use previously-calculated wavefunctions or force constant matrices from a checkpoint file! However, you *can* add/subtract electrons, just remember to correspondingly change the multiplicity.

In Gaussian 16, use the **oldchk** keyword to specify the previously computed checkpoint file that is used to restart the calculation. In GaussView, go to the **Calculation Setup** and then go to the **Link 0** tab. Go to **OldChk File:** and change **No** to **Specify…** [tips_oldchk.png] Be careful not to select the box for **Chkpoint File:** here. If you already had the previous calculation file open in GaussView, the corresponding checkpoint filename will automatically appear. Otherwise, you can type in the name of the previous .chk file (this was “previous.chk” in the above example image file). If only the .chk filename is put here (and not the full path to the file), Gaussian will assume this file is in the same directory as the new calculation. If you want to restart from a .chk file that is in a different directory, use the … button to the left of where it says “Full Path”, and browse for the desired .chk file. [tips_oldchk_fullpath.png] GaussView will then insert the full path to the desired .chk file.

Some options for each keyword that specify reading from the checkpoint file are: **Opt=ReadFC** [tips_readfc.png] (reads force constant matrix if it existed in the checkpoint file, also works with Freq, see below); **Guess=Read** [tips_guess_eq_read.png] (reads the wavefunction from the checkpoint file, uses it as an initial guess for SCF); **Geom=Checkpoint** [tips_geom_eq_check.png] (reads the structure from the checkpoint file, you still need to specify charge and multiplicity); **Geom=AllCheck** [tips_geom_eq_allcheck.png] (reads the structure, charge and multiplicity from the checkpoint file); **Geom(Step=*N*)** [tips_geom_eq_step.png] (reads the N^{th} structure from a previous geometry optimization checkpoint file); **chkbasis** [tips_chkbasis.png] (reads the basis-set specification from the previous .chk file, which is especially useful for user-defined basis-set specifications). The last 4 arguments are useful if you are constructing the new input file in a text editor, as it eliminates the need to copy/paste atomic coordinates and complicated basis-set specifications.

Gaussian 09 note:

The oldchk keyword only works for Gaussian 16. For G09, start by making a copy of the checkpoint file (**cp original.chk restart.chk**) of the failed/failing/previous calculation. The copied checkpoint filename should reflect the name of the new calculation you are about to start from the failed/failing/previous calculation state. This prevents overwriting the old checkpoint file (which you may need later on) while allowing the restart to get needed information from the previous calculation. Read the copied checkpoint file into Gaussview and start where you left off by saving a new input file (**restart.com**) matching the new checkpoint file name.