4.24 - Running Dynamics Calculations

Initial test, on the Comet or Bridges XSEDE cluster. The following instructions are related to setting up molecular dynamics trajectory calculations using *Progdyn* (a set of scripts developed by Dan Singleton) on the Comet or Bridges supercomputers. The point of this instruction is to allow the user to perform a preliminary test trajectory calculation using a monoterpene related transition state. Once the test is complete, you will be able to modify the files to fit your system. All the files needed for setting up the test trajectories can be found on strider.ucdavis.edu in the "Dynamics" folder.

After obtaining the necessary supercomputing accounts with Comet/Bridges and the Gaussian permissions, you'll need to place some files in your home directory on Comet/Bridges. Create a "bin" folder in your home directory and place into this folder the files molden and randgen. Next, copy the files progSI, progSIb, progSIc, and progSId into your home directory. These 6 files will be used along with 9 other files to generate your trajectory. To be safe, it's probably best to make each of these files executable using the chmod command. Type "chmod 755 filename" to make a file an executable.

Now that the 6 files are in your home directory, we are able to setup a test trajectory. Create a folder called "terptest" in your home directory, then cd into that directory and create another folder called "n1". After you cd into "n1", place into it the 9 files: freqinHP, job, prog1stpoint, prog2ndpoint, proganal, progdynf.conf, progdynb, progdynstarterHP, proggenHP. These test files are created to run a simple dynamics trajectory that start at the pinyl cation minimum, proceed through the bornyl cation TS, and on to the camphyl cation product.

The file, freqinHP, is the output of a Gaussian frequency calculation with the keyword: freq=hpmodes. All that is required to generate this file is the keyword specified and the optimized geometry of the transition state you would like to run dynamics on.

Now get back into the folder where you placed the 9 files by typing "cd terptest/n1". The progdynstarterHP file also needs to be executable. So "chmod 755 progdynstarterHP" to do that. Now you are ready to submit the dynamics calculation. Typing "qsub job" while in the terptest/n1 directory does this. A message will show up that your job was submitted successfully. You can view the status of your job by typing "qstat –u username" where username is replaced with your unique username.

Once a trajectory has finished, it will be assigned a number (i.e., traj3). The file type for this is an xyz file. This file can be viewed in Molden, and you can watch the movie of the trajectory. Babel can also be used to convert this file into a file type of your preference.

A script has also been written to accomplish this task, yielding a new .xyz and .mol2 file, and is also located on strider.ucdavis.edu (Dynamics/Scripts). This script also allows you to watch the movie of the trajectory as a reactant to product transformation, instead of TS to reactant and TS to product since this is the format of the traj file. The script is called "work". To run it, place both the "work" and "invert_traj" file into

a folder on redline (it must be run on redline because of the way Babel is used in the script) with the traj file (like traj3). Type “chmod 755 work”, and then “chmod 755 invert_traj” to make these two files executable. Then type “./work traj3 traj3.mol2” to convert your traj file into a xyz and mol2 movie file.

Modifying files to fit your system. Once you have completed the test to verify that all the settings are correct for your Comet/Bridges account, you will be able to start modifying files to fit your system. The instructions in part 1 are a good guide to setting up the trajectory for your system, and the things that will need to modified are listed below:

A. Setting up a new directory – In your home directory, make a new directory for your dynamics trajectory calculation. Within that new directory, make a directory called “n1”

B. freqinHP – This file contains the geometry of the transition state you wish to perform dynamics on. This file will need to be created each time you are running a new TS. It is a simple file to create. Just run a Gaussian09 frequency calculation (no checkpoint needed) on the optimized TS geometry by using “freq=hpmodes” in the route card. Also include the same level of theory used for the optimization, and perhaps geom=connectivity if needed, and that’s it! Rename the output file from the frequency calculation as “freqinHP” (note: there is not an extension), and place the new freqinHP file into the new “n1” subdirectory of the new directory.

C. Copy files that begin with “p” into your new “n1” directory (there are 7 of them). Also, copy the job file into the “n1” directory as well. Now we will begin to modify them. Including the freqinHP file, there should be a total of 9 files in the “n1” directory before you submit the trajectory.

D. progdyn.conf – This file will need to be modified. It contains information like level of theory, charge, multiplicity, classical vs. quasiclassical, etc. There are detailed instruction on how to change it for your system within the script file. Open it in vi editor or nano to make the necessary changes.

E. job – This is the script that starts the calculation. The folders must all be correct. The progdynstarterHP folder must be correctly cited, along with the scratch directory.

F. progdynstarterHP – This file is the workhorse. It is doing most of the work linking the scripts to Gaussian09 and Comet/Bridges. Only 2 lines will need to be changed. They should be lines 37 & 38, which contain the main directory of your specific TS, and point to the correct freqinHP file. The keywords on these lines are “proggramdir” and “freqfile”.

G. proganal – This file is the one file that can be time consuming to setup. The purpose of this file is to develop stopping criteria for your trajectory. Good luck!!

H. All the other prog files will never need to be changed, but do need to be in the n1 folder. These files are: prog1stpoint, prog2ndpoint, progdynb, and proggenHP.

Creating multiple trajectories. Once you have generated the first trajectory for your system, there two ways you can obtain multiple trajectories. First, any trajectory can be resubmitted (after the first 48hrs have

passed) by typing “qsub job” again, it will pick up where it left off. This is one way to have multiple trajectories, but by using this method, only one trajectory can be generated at a time.

To have multiple trajectories running at the same time, you can create another subdirectory called “n2”. In this directory, you will only need two files: job and progdyn.conf. You will not (usually) need to change the progdyn.conf file. The job file will need to be changed. The working directory line should also be changed to “n2”. Note: do not change the location of the freqinHP file, it is still in folder “n1”.

Additional questions – send an email to Stephanie (share@ucdavis.edu) or Ryan (ryanppemberton@gmail.com)