Installation on Unix/Linux

Getting the code

Ensure that your g77 fortran compiler is up-to-date. (If you insist on using another compiler, there should not be much problem with the Brenner code. However, with the tools, you will have to remove the "2" executables from the chiral and coordmod makefiles. Also, congnu[w].f will have to be replaced by congen.f and argsun.f by argsgen.f)

First make a folder for the code. Then, depending on what you want, select files from the following list and put them in that folder.

- The source code with my bug fixes. Save the link to your code directory, unzip and it will create a folder "md" with many subfolders. (If you want just this code, you will need to compile by copying all relevant files from all the subdirectories together in a single folder, and compile main.f with your fortran compiler. If you want my basic improvements, do *not* copy the files together, but go to the next item.)
- The actual program directory with my mods. If you unzip this, it will create a folder "mdexe" in addition to folder md.
- My tools. To use my tools, you will also need ranlib from netlib. For your convenience, I have a copy of that one too here. Unzip both archives, it will create several folders. (You do not need the previous two items to get my tools.)

Now you need to create the actual programs using g77. This should be done from a command or xterm window.

To create the Brenner program, cd to the mdexe folder and compile main.f with your g77 fortran compiler. For example, "g77 -I . -o main main.f" will create program "main." (The" -I ." is not needed with various other compilers.) (Note the point behind -I.)

To create my tools, cd to the ranlib folder and execute "make" to make ranlib.a. Then cd to folder util and run "make" to make util.a. Then cd to folder coordmod and run "make" to make all my tools except the chiral program. Cd to folder chiral and run "make" to make the chiral program.

Note that there are two versions of every tool. For example, there is both "chiral" and "chiral2". They are equivalent, except the "2" versions must be run through con_shell and then allow you to correct your input lines in an easier way. For example, the more user-friendly way to run the chiral tool is to use "../lib/con_shell chiral2".

There is a program custom.f that you can customize yourself to do things my tools will not. To compile after you customized it, use "make custom" or "make custom2."

Running the code

To run the program

- Create a coord.d file using the separate program chiral found in the chiral folder (if you downloaded the tools), maketube, or other. Put coord.d in the mdexe folder. (There is a diamond.d file in md, but that one crashes for some reason.)
- Edit input.d in the mdexe folder to set the run parameters.
- Run "main" in the mdexe folder.
- Examine output.d (and other files) for the results.

Making changes

If you need to make changes in the Brenner code (increasing storage, changing parameters, ...), you will need to rebuild the main executable by repeating the g77 command.

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