00README

Thomas M Griffiths

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If you've run a MD simulation on a machine of opposite endianness (e.g. on the VLSCI BlueGene machine AVOCA (big endian)) you'll need to flip the binary data of your trajectories before you can perform analysis with CHARMM on the local machine (hpc.its.uow.edu.au (little endian)).

There are two methods of doing this, either you can use the flipdcd utility supplied as a separate executable with VMD or the catdcd utility (`www.ks.uiuc.edu/Development/MDTools/catdcd/`) to flip the endianness of your binary data. Unfortunately, when using flipdcd any unit cell information from a PBC calculation is lost in the flipping process. Hindering any attempts at re-centering a constant pressure simulation and severely impeding a constant volume simulation if you don't know the initial setup conditions.

Catdcd will take an input of any endianness, and output a trajectory with the local endianness. During this process, unfortunately, header information is lost regarding the previous dynamics steps, number of steps, and the frequency of saving. This will present a problem later on if you're trying to combine or manipulate the trajectories with the MERGe commands in CHARMM, and any subsequent analyses. This header information however is easier to fix than a unit cell for every set of coordinates. There are two very nice packages written by Jim Phillips at UIUC to just this, dumpdcd and loaddcd. The former dumps out the DCD header, and the latter reloads it.

In this directory are the uncompiled `dumpdcd.c` and `loaddcd.c` files. along with the require library, `largefiles.h`. To compile dumpdcd and loaddcd on your system run these commands:

```
gcc dumpdcd.c -o dumpdcd
```

```
gcc loaddcd.c -o loaddcd
```

This should make the binary executable for both, which you can now use to change up the header details of your trajectory files as you see fit. Ensure that the full contents of the directory are present when you compile the two binaries, in particular `largefiles.h`.

The output plain text file from dumpdcd will contain the header information (see the format below).

Usage: `./dumpdcd <filename> > <data>`

Once you've changed the details on the text file it can be inserted back into the trajectory file with loaddcd.

Usage: `./loaddcd <filename> < <data>`

There is a c-shell script (`big-little-and-headfix.csh`) included in the directory as an example of a full conversion process.

1. Taking the big endian trajectories and flipping them with catdcd.
2. Printing out the header information with dumpdcd.
3. Changing the header info. with sed.
4. Reloading the header information with loaddcd.

Header Field Details (Line# Field)

1. Number of frames in this file
2. Number of previous integration steps
3. Frequency (integration steps) for saving of frames
4. Number of integration steps in the run that created this file
5. Frequency of coordinate saving (if this is a velocity trajectory??)
6. Number of degrees of freedom during the run
7. Number of fixed atoms
8. Timestep in AKMA-units. Bit-copy from the 32-bit real number
9. 1 if crystal lattice information is present in the frames
10. 1 if this is a 4D trajectory
11. 1 if fluctuating charges are present

20 1 if trajectory is the result of merge without consistency checks 20 CHARMM version number

Lines 11 – 14 are either a 0 or 1 value indicating that the property doesn't exist (0) or does (1).