While debugging [http://redmine.gromacs.org/issues/1343](http://redmine.gromacs.org/issues/1343) I stumbled over the following code in grompp (from 4.5 and still present):

```c
plist, the force field parameters etc. is initiated as an array:

```new(plist,F_NRE);

- `init_plist(plist);

```snip

/* If we are using CMAP, setup the pre-interpolation grid */
if(plist->ncmap>0)
{
    init_cmap_grid(&sys->ffparams.cmap_grid, plist->nc, plist->grid_spacing);
    setup_cmap(plist->grid_spacing, plist->nc, plist->cmap,&sys->ffparams.cmap_grid);
}
```n

In other words, this if statement is checking the first entry in the plist array, which is F_LJ, and hence I assume the if statement always evaluates to false.

It could of course be that the if statement is irrelevant.

Associated revisions

Revision c1547047 - 06/24/2014 02:11 PM - Erik Lindahl

Clean up CMAP placement in parameter list

Some of the CMAP variables were always placed into and read from the first entry of the parameter list. While this did not result in any errors, this patch now places them correctly in the F_CMAP position.

Fixes #1345.

Change-Id: lc6e09e46c352976dcecf157f903c082b4ec43df8

History

#1 - 06/12/2014 10:08 AM - David van der Spoel
- Assignee changed from David van der Spoel to Erik Lindahl

#2 - 06/15/2014 05:19 AM - Roland Schulz
- Status changed from New to Feedback wanted

push_cmaptype uses "bt->ncmap" and bt is plist. Thus plist is used for all CMAP access. This is really confusing code but it does seem consistent and not a bug. Do I you agree?

#3 - 06/15/2014 09:59 AM - David van der Spoel
- Tracker changed from Bug to Feature
- Priority changed from Normal to Low
- Target version set to 5.x
It is not a bug in the sense that the code probably works. In grompp.h we have:

```c
typedef struct {
    int nr;        /* The number of bonds in this record */
    int maxnr;    /* The amount of elements in the array */
    t_param *param; /* Array of parameters (dim: nr) */

    /* CMAP tmp data, there are probably better places for this */
    int grid_spacing;       /* Cmap grid spacing */
    int nc;              /* Number of cmap angles */
    real cmap;               /* Temporary storage of the raw cmap grid data */
    int ncmmap;          /* Number of allocated elements in cmap grid*/

    int cmap_types;        /* Store the five atomtypes followed by a number that identifies the type */
    int nct;              /* Number of allocated elements in cmap_types */
} t_params;
```

Note the comment by the author, presumably Erik's old student. Simultaneously, there is F_CMAP entry in the list of energies which I presume is used for storing the energy. Thus plist[F_CMAP] should be used for storing the grompp data as well.

All in all, this is the kind of code that will come back to haunt us, but it not being a bug in practice, I will reduce the severity to low, and change it to a feature request - for cleanup.

#4 - 06/15/2014 10:34 AM - Roland Schulz
- Status changed from Feedback wanted to Accepted

#5 - 06/23/2014 02:09 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1345.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: Ic6e09e46c352976cfc1f57ff903c082b4ec43df8
Gerrit URL: https://gerrit.gromacs.org/3662

#6 - 06/23/2014 02:09 PM - Erik Lindahl
- Status changed from Accepted to Fix uploaded

#7 - 06/24/2014 08:29 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#8 - 06/24/2014 08:29 PM - Erik Lindahl
- Status changed from Resolved to Closed

#9 - 07/15/2014 06:42 AM - Teemu Murtola
- Tracker changed from Feature to Task
- Target version changed from 5.x to 5.0