GROMACS - Bug #1709

gmx_rmsdist.c: calc_rms argument order error
03/19/2015 09:41 PM - Alan Manning

Description

Symptoms

With gmx rmsdist:

- -scl behaves like -mean should
- -mean behaves like -rms should
- -rms behaves like -scl should

I haven't tested all these cases, but I have manually calculated the atom-atom distances in a one-frame two-water pdb file. Only gmx rmsdist -f em.trr -em.gro -nosumh -nopbc -nlevels 1000 -scl produces a matrix that closely this, but I think the -mean option should.

Cause?

In /gmxana/gmx_rmsdist.c, the function calc_rms is define as

```c
static void calc_rms(int nind, int nframes,
                real **dtot, real **dtot2,
                real **rmsmat, real *rmsmax,
                real **rmscmat, real *rmscmax,
                real **meanmat, real *meanmax)
```

However, it is called as

```c
calc_rms(isize, teller, dtot, dtot2, mean, &meanmax, rms, &rmsmax, rmsc, &rmscmax)
```

The arguments are out of order, I believe it should be

```c
calc_rms(isize, teller, dtot, dtot2, rms, &rmsmax, rmsc, &rmscmax, mean, &meanmax)
```

Associated revisions

Revision d8930b37 - 06/22/2015 11:48 AM - Erik Lindahl
Fix argument order error for g_rmsdist
Incorrect argument order to calc_rms() caused command options to be permuted.
Fixes #1709.
Change-Id: I82042dac463c8bb305ab3d3bc2a122b5409c55ef

History

#1 - 06/17/2015 12:19 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1709.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: I82042dac463c8bb305ab3d3bc2a122b5409c55ef
Gerrit URL: https://gerrit.gromacs.org/4725
#2 - 06/17/2015 12:19 AM - Erik Lindahl
- Status changed from New to Fix uploaded

#3 - 06/22/2015 11:49 AM - Mark Abraham
- Category set to analysis tools
- Status changed from Fix uploaded to Closed
- Assignee set to Erik Lindahl
- Target version set to 5.0.6