Gromacs - Bug #1709

gmx_rmsdist.c: calc_rms argument order error

03/19/2015 09:41 PM - Alan Manning

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Erik Lindahl</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
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<td>Target version:</td>
<td>5.0.6</td>
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<td>Affected version - extra info:</td>
<td>Current version in repository seems to have same issue</td>
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**Affected version:** 5.0.4

**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, rsmc, &rmscmax)
```

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

```c
calc_rms(isize, teller, dtot, dtot2, rms, &rmsmax, rsmc, &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