Gromacs - Bug #872

Precedence error in gmx_mindist.c leads to omitted output in atm-pair (-o) file for g_mindist

01/30/2012 11:06 PM - Matthew Zwier

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: analysis tools
Target version: 4.5.6

Description
Line 390 of gmx_mindist.c is responsible for only printing out atom pairs of minimum/maximum distance when a valid distance has been found:

```c
if ( bMin?min1:max1 != -1 )
if (atm)
    fprintf(atm,"%12e  %12d  %12d
", output_env_conv_time(oenv,t),1+(bMin ? min1 : max1),
```

but the "!=" operator binds more tightly than the ternary conditional "?:", so the resulting test evaluates as:

```c
if ( bMin?(min1):(max1 != -1) )
```

which fails whenever the atom from the first group of minimum/maximum distance to the second group is the first atom in the topology (with index 0). Explicit parentheses around the bMin conditional correct this problem:

```c
if ( (bMin?min1:max1) != -1 )
```

A (tested) patch against the latest gromacs-release-4.5-patches is attached.

Associated revisions

Revision dcb9b355 - 01/31/2012 06:20 AM - Mark Abraham
Corrected use of ?: in conditional
Patch contributed by Matthew Zwier to fix the incorrect use of precedence of ?: and != operators.
Fixes #872
Change-id: le4bbc3cbdafa33fc0386d12c2e142a9c076c2e946
precedence of ?: and != operators.

Fixes #872

Change-Id: i:e4bb3cbda3f33fc0386d12c2e142a9c076c2e946

History

#1 - 01/31/2012 06:23 AM - Mark Abraham

#2 - 02/01/2012 02:41 PM - Mark Abraham
- Status changed from New to Closed
- Assignee changed from David van der Spoel to Mark Abraham

Files

| gmx_mindist_ternary_prec.patch | 482 Bytes | 01/30/2012 | Matthew Zwier |