**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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
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<td>Target version</td>
<td>4.5.6</td>
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<td>Affected version</td>
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**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\n",
                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: le4bbc3cbbaf33fc0386d12c2e142a9c076c2e946

Revision dcb9b355 - 01/31/2012 06:20 AM - Mark Abraham

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**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