### Gromacs - Bug #850

**Some types of selections don't work correctly when compiled in double precision**

12/01/2011 04:59 PM - Teemu Murtola

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
</tr>
<tr>
<td>Category:</td>
<td>selections</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.5.6</td>
</tr>
<tr>
<td>Affected version -</td>
<td>4.5-4.5.5</td>
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<td>extra info:</td>
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| Affected version: 4.5.5 |

**Description**

There is a bug in handling integer to floating-point parameters for selection methods, which causes some types of selections to behave erratically if Gromacs is compiled in double precision. Or more accurately, if sizeof(real) != sizeof(int).

This only affects g_select, and possible user code written using the new trajectory analysis framework.

**Associated revisions**

**Revision f35e2ca8 - 12/01/2011 05:00 PM - Teemu Murtola**

Fix selection parsing in double precision.

Fixes #850.

Change-Id: ffd0bf1f5401ca4d6257c8c2fc39e67cac537ecf

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Fixes #850.

Change-Id: ffd0bf1f5401ca4d6257c8c2fc39e67cac537ecf

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**History**

**#1 - 12/09/2011 07:10 PM - Teemu Murtola**

- Status changed from New to Closed

Fix has been reviewed in Gerrit and merged into release-4-5-patches.

**#2 - 07/17/2013 07:13 AM - Teemu Murtola**

- Category changed from analysis tools to selections
- Affected version set to 4.5.5