### Gromacs - Bug #1219

Selections that use a dynamically evaluated variable in different context may be evaluated incorrectly

04/10/2013 05:58 AM - 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>5.0</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>4.5-4.5.6, 4.6-4.6.1</td>
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**Description**

Selections are not evaluated correctly if they have a variable with a dynamic value (i.e., needs to be evaluated for each frame) and use that variable both

1. in a boolean expression such that its evaluation group was not known in advance, and
2. in a context where it was always evaluated for all atoms (either as a selection, or as a parameter to a selection method),

and additionally the latter context appear later in the selection set.

Example of an affected selection is

```
var = atomnr 1 to 8 and x < 10;
atomnr 1 to 5 and y < 10 and var;
var;
```

Typical result is an internal error (out of pooled memory) in the selection engine, but it may be possible that incorrect results also occur.

**Related issues:**

- Related to Gromacs - Bug #1216: Selections that contain “same ... as” in a co... Closed 04/05/2013

**Associated revisions**

Revision c049a1ce - 04/10/2013 05:59 AM - Teemu Murtola

Fix another bug in selection subexpression handling.

In this case, it did not work correctly if a variable with a dynamic value was used both

1. in a boolean expression such that its evaluation group was not known in advance, and
2. in a context where it was always evaluated for all atoms (either as a selection, or as a parameter to a selection method),

and additionally the latter context appeared later in the selection set.

The initialization of the SEL_CDATA_STATICEVAL flag has a dependency on SEL_CDATA_FULLEVAL flag, and they were not initialized in the correct sequence in the above case.

Fixes #1219.

Change-Id: lc95d37a424c82c796806b3a5b39678e206c467a1
Fix another bug in selection subexpression handling.

In this case, it did not work correctly if a variable with a dynamic value was used both 1. in a boolean expression such that its evaluation group was not known in advance, and 2. in a context where it was always evaluated for all atoms (either as a selection, or as a parameter to a selection method), and additionally the latter context appeared later in the selection set. The initialization of the SEL_CDATA_STATIC_EVAL flag has a dependency on SEL_CDATA_FULL_EVAL flag, and they were not initialized in the correct sequence in the above case.

Fixes #1219.

Backported from master with the same Change-Id.

Change-Id: lc95d37a424c82c7968086b3a5b39678e206c467a1

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Revision fd6f7645 - 06/13/2013 09:45 AM - Teemu Murtola

Fix another bug in selection subexpression handling.

In this case, it did not work correctly if a variable with a dynamic value was used both 1. in a boolean expression such that its evaluation group was not known in advance, and 2. in a context where it was always evaluated for all atoms (either as a selection, or as a parameter to a selection method), and additionally the latter context appeared later in the selection set. The initialization of the SEL_CDATA_STATIC_EVAL flag has a dependency on SEL_CDATA_FULL_EVAL flag, and they were not initialized in the correct sequence in the above case.

Fixes #1219.

Change-Id: lc95d37a424c82c7968086b3a5b39678e206c467a1

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History
Fix and a backport of it are in gerrit.

#2 - 04/19/2013 06:19 PM - Mark Abraham
- Status changed from In Progress to Resolved
- Affected version set to 4.5.6

#3 - 04/24/2013 08:26 PM - Teemu Murtola
This is not yet fully resolved, since https://gerrit.gromacs.org/#/c/2316/ (which fixes this for master, and also adds unit tests) is not yet merged. However, it is not possible to change the status back...

#4 - 04/24/2013 10:55 PM - Mark Abraham
- Status changed from Resolved to Feedback wanted

#5 - 04/24/2013 10:56 PM - Mark Abraham
- Status changed from Feedback wanted to In Progress

#6 - 04/26/2013 05:43 AM - Teemu Murtola
- Status changed from In Progress to Fix uploaded

#7 - 04/29/2013 06:33 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

#8 - 04/29/2013 10:06 PM - Mark Abraham
- Status changed from Resolved to Feedback wanted

#9 - 04/29/2013 10:06 PM - Mark Abraham
- Status changed from Feedback wanted to In Progress

#10 - 04/29/2013 10:16 PM - Mark Abraham
- Target version changed from 4.5.7 to 5.0

#11 - 04/30/2013 05:40 AM - Teemu Murtola
- Status changed from In Progress to Resolved

#12 - 04/30/2013 05:40 AM - Teemu Murtola
- Status changed from Resolved to Closed

#13 - 07/17/2013 07:16 AM - Teemu Murtola
- Category changed from analysis tools to selections