Gromacs - Bug #1742

Unexpected behavior and seg. fault for gmx select

05/20/2015 04:03 PM - Viveca Lindahl

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<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
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<td>Category:</td>
<td>selections</td>
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<td>Target version:</td>
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<td>Affected version - extra info:</td>
<td>4.5.<em>, 4.6.</em>, 5.0-5.0.5</td>
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**Affected version:** 5.0

**Description**

1) gmx select -select '(resname SOL and atomnr 1)' -on

produces the error

'Error in user input:
Selection '(resname SOL and atomnr 1)' never matches any atoms.'

if atom 1 is not a SOL. In turn,

gmx select -select '(same residue as (resname SOL and atomnr 1))' -on

produces a segmentation fault which makes it difficult to spot the original problem.

2) Another surprise:

Assuming the first SOL has atomnr 52345,

gmx select -select '(resname SOL and atomnr 1 to 52345)' -on

yields an index file of 1 atom as expected, while

gmx select -select '(resname SOL and atomnr 52346 to 52345)' -on

does not yield an error (but an index file with atoms 52345, 52346) although there is probably something wrong.

**Associated revisions**

**Revision fe649c41 - 05/22/2015 05:02 AM - Teemu Murtola**

Add note about atom order in selections

Clarity the behavior of selections in that they always select atoms in increasing order. In the same context, mention the mechanisms in place to work around this. Use an example that shows the equivalence of 'a to b' and 'b to a' in the selection syntax.

Also clean up the formatting of the selection limitations help topic, now that bullet lists are properly supported.

Related to #1742

**Change-Id:** I3daa17521767b3eaadcb1d8c0c6fc986fa0ae3e3

11/19/2015 1/3
Avoid crash with empty reference for 'same as' selection

Make 'same ... as none' selections not segfault. If there were no atoms in the reference group, the code that sorted the values and removed duplicates incorrectly set the number of values as one, resulting in incorrect memory access later.

Fixes #1742 (segfault part).

Change-Id: i9d14c30404121356ee3abf1a5575fb0baa82fb7b

History

#1 - 05/20/2015 05:00 PM - Teemu Murtola
- Category set to selections
- Status changed from New to Accepted
- Assignee set to Teemu Murtola

The segfault is easily reproducible; I'll try to fix it.

It is intentional that "a to b" is interpreted the same as "b to a", no matter what a and b are. What would you expect to happen in the latter case? What would be a reasonable logic to detect that error that would not prevent reasonable input?

#2 - 05/20/2015 06:47 PM - Viveca Lindahl
I wouldn't expect "a to b" to be symmetric but I would expect a < b. Perhaps this is my misunderstanding and not actually incorrect behavior.

#3 - 05/20/2015 09:27 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1742.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: i9d14c30404121356ee3abf1a5575fb0baa82fb7b
Gerrit URL: https://gerrit.gromacs.org/4638

#4 - 05/20/2015 09:30 PM - Teemu Murtola
- Status changed from Accepted to Fix uploaded
- Target version set to 5.0.6

Fix for the segfault is in Gerrit.

For the behavior of a to b, I guess that a case can be made for both behaviors, but I still think that it is reasonable to expect that, e.g., charge [-0.7 to -1] to be a valid selection. At minimum, I'll add a note about this to the documentation (possibly only for 5.1 onwards), but other suggestions are also welcome.

#5 - 05/21/2015 05:56 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1742
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: I3daa17521767b3eaadcb1d8c0c6fc986fa0ae63
Gerrit URL: https://gerrit.gromacs.org/4640

#6 - 05/21/2015 05:57 AM - Teemu Murtola
The second change updates the selection documentation to be clearer on the atom order and the behavior of a to b, partially prompted by this issue.

#7 - 05/21/2015 05:58 AM - Teemu Murtola
- Affected version - extra info set to 4.5.*, 4.6.*, 5.0-5.0.5

#8 - 05/22/2015 02:04 PM - Teemu Murtola
- Status changed from Fix uploaded to Resolved

#9 - 05/27/2015 05:33 AM - Teemu Murtola
- Status changed from Resolved to Closed