GROMACS - Bug #1743

Selections like "x 1 to 1.5 2 to 2.5" select unwanted atoms

05/20/2015 08:21 PM - Teemu Murtola

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
</tr>
<tr>
<td>Category:</td>
<td>selections</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.6</td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.5.<em>, 4.6.</em>, 5.0-5.0.5</td>
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<td>Difficulty:</td>
<td>uncategorized</td>
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<td>Affected version:</td>
<td>5.1-beta1</td>
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Description

If a selection fulfills the following conditions, it is incorrectly evaluated:

* it uses a real-valued keyword (like x or charge),
* it uses multiple A to B parts in the same expression (like in the title), and
* the difference between the closer endpoints of two to ranges is less than one.

In such a case, the selection incorrectly selects also values between the two to ranges. For example, in the case in the title, also positions with x between 1.5 and 2 are incorrectly selected.

Will upload a fix shortly; the issue is a copy-paste bug between integer and real to implementations.

Associated revisions

Revision 4124756a - 05/20/2015 09:35 PM - Teemu Murtola
Fix handling of real-valued 'to' selection ranges

Two adjacent ranges were incorrectly merged to a single range if the difference between their nearest endpoints was less than one (the extra +1 in the code is incorrectly copy-pasted from the integer case).

Add tests for handling overlapping and near-overlapping ranges.

Fixes #1743.

Change-Id: I3ac79c55dc3817e6325e43e27e0ccbcfe360e609

History

#1 - 05/20/2015 08:25 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1743.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: I3ac79c55dc3817e6325e43e27e0ccbcfe360e609
Gerrit URL: https://gerrit.gromacs.org/4637

#2 - 05/21/2015 02:17 PM - Teemu Murtola
- Status changed from Fix uploaded to Closed