

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

Status:	Closed	
Priority:	Normal	
Assignee:	Teemu Murtola	
Category:	selections	
Target version:	5.0.6	
Affected version - extra info:	4.5.*, 4.6.*, 5.0-5.0.5	Difficulty: uncategorized
Affected version:	5.1-beta1	

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: I3ac79c55dc3817e6325e43e27e0ccb4fe360e609

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: I3ac79c55dc3817e6325e43e27e0ccb4fe360e609

Gerrit URL: <https://gerrit.gromacs.org/4637>

#2 - 05/21/2015 02:17 PM - Teemu Murtola

- Status changed from Fix uploaded to Closed