

GROMACS - Bug #1006

Incorrect selections with numeric or position variables that are used multiple times

09/18/2012 06:58 AM - Teemu Murtola

Status:	Closed	
Priority:	Normal	
Assignee:	Teemu Murtola	
Category:	selections	
Target version:	4.5.6	
Affected version - extra info:	4.5-4.5.5	Difficulty: uncategorized
Affected version:	4.5.5	

Description

If selections use variables with a numeric value (e.g., an arithmetic expression), and those variables are referenced more than once, and the variable needs to be evaluated for different set of atoms in different contexts, this in some cases results in an out-of-bounds memory access and/or wrong selection.

As a separate issue, variables with a position value that are referenced more than once cause seg faults.

Found in tests added in <https://gerrit.gromacs.org/#/c/1436> and fixed in the same commit for 5.0. The fix should be backported to 4.5.

Associated revisions

Revision caf863c4 - 09/18/2012 08:37 PM - Teemu Murtola

Fixes for numeric and position selection variables.

Fixed handling of numeric and position selection variables in cases where they were referenced multiple times.

Backported from lffb585ca.

Fixes #1006.

Change-Id: leaa479b4b870e044dc269339be57f6b33533c46e

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History

#1 - 09/18/2012 01:50 PM - Teemu Murtola

- Status changed from New to Feedback wanted

#2 - 09/24/2012 05:28 PM - Teemu Murtola

- Status changed from Feedback wanted to Closed

#3 - 07/17/2013 07:09 AM - Teemu Murtola

- Category changed from analysis tools to selections

- Affected version set to 4.5.5