Gromacs - Bug #850

Some types of selections don't work correctly when compiled in double precision

12/01/2011 04:59 PM - 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

Affected version: 4.5.5

Description
There is a bug in handling integer to floating-point parameters for selection methods, which causes some types of selections to behave erratically if Gromacs is compiled in double precision. Or more accurately, if sizeof(real) != sizeof(int).

This only affects g_select, and possible user code written using the new trajectory analysis framework.

Associated revisions

Revision f35e2ca8 - 12/01/2011 05:00 PM - Teemu Murtola
Fix selection parsing in double precision.
Fixes #850.
Change-Id: lfd0bf1f5401ca4d62571c8c2fc39e67cac537ecf

Revision f35e2ca8 - 12/01/2011 05:00 PM - Teemu Murtola
Fix selection parsing in double precision.
Fixes #850.
Change-Id: lfd0bf1f5401ca4d62571c8c2fc39e67cac537ecf

History

#1 - 12/09/2011 07:10 PM - Teemu Murtola
- Status changed from New to Closed

Fix has been reviewed in Gerrit and merged into release-4-5-patches.

#2 - 07/17/2013 07:13 AM - Teemu Murtola
- Category changed from analysis tools to selections
- Affected version set to 4.5.5