GROMACS - Bug #1506

Selecting groups does not work as expected

05/21/2014 11:26 PM - Justin Lemkul

Description

Interactive selection of groups for analysis is somewhat confusing. For instance:

```gmx gangle -f lastframe.xtc -s md_200_300.tpr -n angle_topleaflet.ndx -oav test.xvg -g1 vector -g2 z```

gives the following:

Available static index groups:

- Group 1 "same_residue_as_name_P8_and_(z>3.5)_0.000" (3328 atoms)
- Group 2 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C17" (64 atoms)
- Group 3 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C36_same_residue_as_name_P8_and_(z>3.5)_0.000&_C17" (128 atoms)
- Group 4 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C50" (64 atoms)
- Group 5 "same_residue_as_name_P8_and_(z>3.5)_0.000&_CA2" (64 atoms)
- Group 6 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C36" (64 atoms)
- Group 7 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C50_same_residue_as_name_P8_and_(z>3.5)_0.000&_C36" (128 atoms)
- Group 8 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C17_same_residue_as_name_P8_and_(z>3.5)_0.000&_CA2" (128 atoms)
- Group 9 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C36_same_residue_as_name_P8_and_(z>3.5)_0.000&_C50" (64 atoms)
- Group 10 "same_residue_as_name_P8_and_(z>3.5)_0.000&_C17_same_residue_as_name_P8_and_(z>3.5)_0.000&_C36" (128 atoms)

Specify any number of selections for option 'group1'
(First analysis/vector selection):
(one per line, <enter> for status/groups, 'help' for help, Ctrl-D to end)
> 11

Cannot match 'group 11', because no such index group can be found.
invalid selection '11'

So it seems that the program expects zero-indexed selections, while the printed options are numbered from 1. This can be very problematic, because if the user supplies '1' as the selection, it actually analyzes group 2 (as indicated in the legend printed in the .xvg file.

Problem is reproducible in 5.0-rc1 and current master. I can provide example input files, if needed.

Associated revisions

Revision 1b890257 - 05/22/2014 09:15 AM - Teemu Murtola

Fix static group list indices in selection prompt

In 4.6, the list was zero-based, and this is what the selection parser uses when resolving numeric group references, so it should still be. Also the list shown by various functions in index.c is zero-based.

The printing code had been inadvertently changed to one-based in cleanup of the handling of group names within the selection code.

Fixes #1506
Some cleanup of the code appears to have shifted the indices in the printed list.

#2 - 05/22/2014 05:23 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1506.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: i9a573b921802d2276e3bdb653359a961c90ff29a
Gerrit URL: https://gerrit.gromacs.org/3478

#3 - 05/22/2014 05:24 AM - Teemu Murtola
- Status changed from New to Fix uploaded

#4 - 05/22/2014 09:30 AM - Teemu Murtola
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 1b89025717a6227f5bf62f472ba92f4c2c8c81f7.

#5 - 05/22/2014 04:38 PM - Erik Lindahl
- Status changed from Resolved to Closed