GROMACS - Bug #2815

gmx msd -mol broken
12/20/2018 08:27 PM - David van der Spoel

| Status:   | Closed   |
| Priority: | Normal   |
| Assignee: | David van der Spoel |
| Category: | analysis tools |
| Target version: | 2020 |
| Affected version - extra info: | Master |
| Affected version: | 2020 |
| Difficulty: | uncategorized |

Description
In a simplification of gmx msd a bug was introduced such that the -mol flag does not work anymore. See https://gerrit.gromacs.org/#/c/8789/

Associated revisions

Revision 52b48193 - 12/22/2018 08:19 PM - David van der Spoel
Revert "Removed t_topology from gmx msd"
This reverts commit b9e0922af7ecbb4b9110dd0ea99cdac0244a27a.
See #2815
Change-Id: le0ae90feb1e170b2c1743ef63b36a567fdabf4

Revision 57b3bfe3 - 01/14/2019 08:08 AM - David van der Spoel
MSD tests for the -mol option.
Had to free some memory as well to make tests pass.
Added basic code for running grompp.
Renamed spc5 files in simulationdatabase that are used in src/programs/mdrun/tests to tip3p5 since they were in fact using tip3p and in this manner a conflict with the gmx_msd tests is avoided.
TODO: re-use the grompp code in moduletest.cpp from src/programs/mdrun/tests
Part of #2815
Change-Id: f5d5d33f431f1d3089ebaf54b6388348d47ce6e2

History

#1 - 12/22/2018 08:21 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2815.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~le0ae90feb1e170b2c1743ef63b36a567fdabf4
Gerrit URL: https://gerrit.gromacs.org/8873

#2 - 12/22/2018 10:35 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2815.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~f5d5d33f431f1d3089ebaf54b6388348d47ce6e2
Gerrit URL: https://gerrit.gromacs.org/8875

#3 - 12/26/2018 11:39 AM - David van der Spoel
Code has been reverted.
Status changed from New to Closed