GROMACS - Bug #2720

Normal-mode analysis with vsites or shells works for first molecule of each type only

10/31/2018 09:45 AM - David van der Spoel

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:	mdrun		
Target version:			
Affected version - extra info:		**Difficulty:**	simple
Affected version:	2018		

Description

The routine get_atom_index in mtop_util.cpp works for only one molecule at a time. The routine is used for normal mode analysis with vsites or shells and for analysis of the result using gmx nmeig.

Related issues:

Has duplicate GROMACS - Bug #2721: get_atom_index does not work with multiple...	**Closed**

Associated revisions

Revision e9b526ba - 11/01/2018 09:30 PM - David van der Spoel

Updated normal modes output for sw-dimer.

Due to a bug in mtop_util.cpp only the first molecule in the
sw-dimer was used in a normal mode analysis. This is fixed in patch
https://gerrit.gromacs.org/#/c/8631/.

Fixed a bug in gmxtest.pl when comparing two xvg files where the
reference value is zero (it computed the relative difference and
divided by zero). This only showed up in the new output file
normal_modes/sw_dimer/eigenfreq.xvg.

Part of #2720

Change-Id: Iae990bbff2c19c28310618f2cadf1157a62242d0

Revision 4dede5be - 11/09/2018 11:37 AM - David van der Spoel

Change get_atom_index to allow multiple molecules.

Make gromacs take into account atoms in all molecules.
This allows Hessian matrix creation to work over all
molecules in a simulation. An update to the regression
tests has been submitted as well.

During fixing of the problem, another problem surfaced in
the normal mode calculations to do with ordering of atoms
which is fixed here as well.

Fixes #2720

Change-Id: I9fc2dd05cb1c67d46b6d4c3d9139e6b3bed72f17

History

#1 - 10/31/2018 09:47 AM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue #2720.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~release-2019~I153b9a29ba4cd602d77d4ab529ab4e97c68fa264
Gerrit URL: https://gerrit.gromacs.org/8624

#2 - 10/31/2018 11:43 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2720.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)

Change-Id: gromacs~release-2018~I153b9a29ba4cd602d77d4ab529ab4e97c68fa264
Gerrit URL: https://gerrit.gromacs.org/8629

#3 - 10/31/2018 11:52 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2720.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: regressiontests~release-2018~Iae990bbff2c19c28310618f2cadf1157a62242d0
Gerrit URL: https://gerrit.gromacs.org/8630

#4 - 10/31/2018 01:07 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2720.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~release-2018~I9fc2dd05cb1c67d46b6d4c3d9139e6b3bed72f17
Gerrit URL: https://gerrit.gromacs.org/8631

#5 - 10/31/2018 01:31 PM - Mark Abraham

- Has duplicate Bug #2721: get_atom_index does not work with multiple molecules added

#6 - 10/31/2018 01:33 PM - Mark Abraham

- Subject changed from Routine get_atom_index works for one molecule only to Normal-mode analysis with vsites or shells works for one molecule only

#7 - 10/31/2018 02:45 PM - David van der Spoel

- Subject changed from Normal-mode analysis with vsites or shells works for one molecule only to Normal-mode analysis with vsites or shells works for first molecule of each type only

#8 - 11/01/2018 09:36 PM - David van der Spoel

A problem with the normal mode calculations itself surfaced as well unfortunately, related to virtual sites and shells.

#9 - 11/09/2018 12:30 PM - David van der Spoel

- Status changed from New to Resolved

Applied in changeset 4dede5be9361ce05804af3c1493ebd1267f5a3e2.

#10 - 11/28/2018 03:33 PM - Paul Bauer

- Status changed from Resolved to Closed