GROMACS - Bug #2549

Inconsistent graph PBC results with monomers connected by restraints

06/07/2018 10:22 AM - Berk Hess

Status:	Closed			
Priority:	Normal			
Assignee:	Berk Hess			
Category:	core library			
Target version:				
Affected version - extra info:	all GROMACS versions	**Difficulty:**	uncategorized	
Affected version:	2018			

Description

The graph code implicitly assumes that the bonded interactions connecting atoms in a moleculetype a short-ranged compared to the box size. But this is not necessarily the case when multiple monomers in a single moleculetype are connected by restraints. Such restraints can work over more than half the box length. In the current code this can lead to monomers being broken over PBC.
The least we should do is add a check for this, but this might be computationally expensive and/or complicated. The solution for the user would then be to increase the box size.
Ideally we would want a solution, but that can only be done through allowing the user to specify how the monomers should be connected.

Associated revisions

Revision 0ef40b73 - 06/12/2018 10:13 AM - Berk Hess

Add fatal error for inconsistent graph

In case a moleculetype consists of multiple monomers connected
by restraints, an inconsistent graph could be generated.
Now a fatal error with explanation is generated for such cases.
Also a fatal error is generated with an inconsistent graph with long
bonds in general.

Fixes #2549

Change-Id: I6fa11fb7cefd74ed077c1fb523a2147c91e0d0fd

History

#1 - 06/07/2018 01:23 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2549.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I6fa11fb7cefd74ed077c1fb523a2147c91e0d0fd
Gerrit URL: https://gerrit.gromacs.org/7981

#2 - 06/07/2018 01:25 PM - Berk Hess

- Status changed from Accepted to Fix uploaded

Resolved this by issuing a descriptive fatal error instead of only printing "inconsistent shifts" without terminating.

#3 - 06/12/2018 12:00 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 0ef40b73132cefee07bb7eca443208bb1d1b4c7c.

#4 - 09/04/2018 03:40 PM - Paul Bauer

- Status changed from Resolved to Closed