GROMACS - Feature #2339

sum of two largest charge group is enormous and bigger than rlist

12/07/2017 06:55 PM - Mark Abraham

| Status:    | Closed      |
| Priority:  | Low         |
| Assignee:  |             |
| Category:  | preprocessing (pdb2gmx,grompp) |
| Target version: | 2018-beta3 |
| Difficulty: | uncategorized |

Description

grompp warns if a charge group is larger than rlist, but if it's crazy large then that might because of a PBC split, particularly if the group has few particles. If so, then a better warning would suggest that the solution is to make molecules whole. In fact, grompp could probably just do the latter routinely after building the topology, which might help for other things.

But if the warning can only happen with the group scheme, then let's not bother.

Associated revisions

Revision 930725b2 - 12/14/2017 09:38 AM - Paul Bauer

Remove PBC before generating TPR with group scheme

Ensure that all molecules have been made whole before generating the run input file when using the group scheme, to avoid error messages for large charge groups when molecules are broken over PBC boundaries.

Fixes #2339

Change-Id: Iecba013826cbe46e7f70bd674935f9946806ee2e

History

#1 - 12/09/2017 12:50 PM - Berk Hess
- Status changed from New to Closed

There are no charge groups with the Verlet scheme or you can view it a single atom charge groups, so this can't happen there. So will not fix.

#2 - 12/11/2017 12:55 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue #2339.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~Iecba013826cbe46e7f70bd674935f9946806ee2e
Gerrit URL: https://gerrit.gromacs.org/7324

#3 - 12/12/2017 08:05 PM - Mark Abraham
- Status changed from Closed to Fix uploaded
- Target version set to 2018-beta3

#4 - 12/14/2017 10:12 AM - Paul Bauer
- Status changed from Fix uploaded to Resolved

Applied in changeset 930725b2cf4bd9634ce411383086a8b9e4790b3e.

#5 - 12/15/2017 11:40 AM - Paul Bauer
- Status changed from Resolved to Closed