GROMACS - Bug #2290
Genion fails to neutralize a box
11/08/2017 03:48 PM - Michal H. Kolar

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: build system
Target version: 2016.5
Affected version - extra info: 
Affected version: 2016.5

Difficulty: uncategorized

Description

genion -neutral gives a wrong number of positive ions. The resulting box has a charge of -3.0.

Used as:
gmx genion -s ion.tpr -o -p -pname KJ -neutral
TPR attached.

Associated revisions

Revision c7d68ac5 - 11/10/2017 10:16 AM - Berk Hess
Fix genion charge summation accuracy

genion accumulated the charge is a float, which could cause underestimation of the net charge for highly charged systems.

Fixes #2290
Change-Id: I22db5284e492f58dcdba99785cd904042d7aab7f

History

#1 - 11/10/2017 10:19 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2290.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2016~I22db5284e492f58dcdba99785cd904042d7aab7f
Gerrit URL: https://gerrit.gromacs.org/7169

#2 - 11/10/2017 10:20 AM - Berk Hess
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Target version set to 2016.5

Ha, that's a stupid rounding issue. Your net charge is so high that the accumulation into a float results in too much error. Thanks for reporting this.

#3 - 11/10/2017 01:46 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset c7d688ac54b1e22f6072a2d34c68c49ec011d88fc.

#4 - 12/11/2017 12:14 PM - Erik Lindahl
- Status changed from Resolved to Closed

Files
ion.tpr 20.6 MB 11/08/2017 Michal H. Kolar