GROMACS - Bug #620

Total dipole in energy files is incorrect

12/09/2010 12:30 PM - David van der Spoel

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:	mdrun		
Target version:	4.6		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Due to the fact that gromacs internally breaks molecules during a simulation the total dipole is incorrect. If this total dipole is stored in the energy file it can be used for computing the dielectric constant in g_dipoles, resulting in values that are way too large. I have put a fatal error in g_dipoles whenever someone tries to use the energy file for computing the dielectric constant. This is unfortunate since that would be much quicker.

We can choose to either
- fix the computation of the dipole in mdrun
- not store the total dipole in the energy file anymore

History

#1 - 08/29/2011 05:40 PM - Rossen Apostolov

- Description updated

- Assignee deleted (Erik Lindahl)

- Target version deleted (4.5.1)

#2 - 08/29/2011 05:56 PM - David van der Spoel

Let's go for the option not to store the dipole anymore.

#3 - 09/13/2011 10:05 PM - David van der Spoel

- Status changed from New to 3

git commit -m "Augmented redmin issue 620, by not writing the total dipole anymore to the energy file, since it is incorrect. The total dipole is still computed though, and some overhead may be reduced if that computation is removed from the code as well." -a
[release-4-5-patches 6a25aa5] Augmented redmin issue 620, by not writing the total dipole anymore to the energy file, since it is incorrect. The total dipole is still computed though, and some overhead may be reduced if that computation is removed from the code as well.

#4 - 09/21/2011 11:08 AM - Rossen Apostolov

- Status changed from 3 to Closed

#5 - 09/21/2011 11:13 AM - David van der Spoel

- Status changed from Closed to New

- Target version set to 4.6

The change was abandoned in gerrit and postponed to 4.6 because it would create incompatible energy files. Therefore the issue needs to remain open until later.

#6 - 03/05/2012 10:50 AM - Berk Hess

- Status changed from New to In Progress

The dipole can not (easily) be calculated correctly with broken molecules.
Thus I have removed it from the energy file, unless it is used for Ewald
surface correction or dipole correction for 2D geometry (which you should
anyhow only use for system where molecules do not move across periodic

boundaries).
This fix is currently in the nbnxn_hybrid_acc branch and will be merged into 4.6.

#7 - 12/28/2012 08:15 PM - Erik Lindahl

- Status changed from In Progress to Closed

Now merged in release-4.6.