GROMACS - Feature #1498

g_dipoles does not work properly with ionic systems

05/11/2014 05:03 PM - David van der Spoel

Status:	New	
Priority:	Low	
Assignee:	David van der Spoel	
Category:	analysis tools	
Target version:		
Difficulty:	uncategorized	

Description

g_dipoles tries to compensate for charged molecules by subtracting the net charge of each molecule. In (small) periodic systems the dipole is not well defined since it may change rather abruptly if one ion moves to another image.

History

#1 - 06/12/2014 12:43 AM - Erik Lindahl

- Tracker changed from Bug to Feature

David - any suggestions what should be done? If we think of a charge distribution in terms of expansions, I think the dipole should indeed be the first moment around the net charge, so then the subtraction seems correct?

Similarly, as far as I can tell the small system issue is a a problem with system size and PBC, not a problem with how g_dipoles calculates dipoles. It's not obvious to me that it is a problem that can be fixed, and even if it is, that sounds more like a feature. Feel free to change back to "bug" when there is a description of something that can be fixed!

#2 - 07/11/2016 08:11 PM - Mark Abraham

- Target version deleted (5.x)