GROMACS - Feature #1102

Detect incompletely written itp files

01/03/2013 03:55 AM - Roland Schulz

Status:	New	
Priority:	Normal	
Assignee:		
Category:	preprocessing (pdb2gmx,grompp)	
Target version:		
Difficulty:	uncategorized	

Description

Most gromacs topology files have some internal consistency checks (e.g. number of atoms and names between gro and top) when running grompp. This is currently not true for itp files for anything after the [atoms] section. If the writing of the itp for some reason gets interrupted, after the atoms section is complete, and later sections are missing or are incomplete no checks catch that. The itp files should have some kind of internal check (e.g. end of file marker, or chechsum, or warning for unnatural low number of dihedrals/angles/pairs/bonds).

History

#1 - 01/03/2013 11:29 AM - Berk Hess

I think this is not generally possible with the current format. Any number of interactions is allowed. For proteins one could come up with a check, but this will require some work. It would be much better to change the format such that we have delimiters. This also avoids the issue of people adding restraints in topol.top which usually end up in the water and not in the protein. We are working on new file formats, so I don't know if it's worth the effort to write a check for itp.

#2 - 01/03/2013 05:55 PM - Roland Schulz

Yes if we have a new format for 5.0, then we shouldn't do anything for itp and just make sure that we don't have the problem with the new format.

#3 - 06/19/2014 03:23 PM - Rossen Apostolov

- Target version deleted (5.0)

Removing 5.0 target

#4 - 06/19/2014 03:23 PM - Rossen Apostolov

- Assignee deleted (Berk Hess)