GROMACS - Bug #190

rerun interaction energy components error

04/02/2008 11:28 PM - Willis Martin

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	3.3		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Hello-
I am attempting to analyze the energy components of a biomolecular system in water. The original simulation ran fine, and the total energy looks reasonable. I am encountering a problem when attempting to use the -rerun option to compute interactions between specific energy groups. In this case, all interactions involving the solvent component report and LJ-SR energy of 10^32 kJ/mol, while other energy components appear normal. On the other hand, in the original simulation, the total LJ-SR (including the biomolecules and solvent) was roasonable at 6*10^4 kJ/mol. When doing the rerun I am using the same parameters as in the original simulation (simply specifying the solvent and ions as one energy group, and the biomolecules as seperate energy groups). I am using gromacs version 3.3.0, is there a bug or am I doing something wrong?

-Willis Martin

History

#1 - 04/22/2008 11:45 AM - Berk Hess

Could you attach the original tpr, the rerun tpr
and a trajectory with a single frame that you used for the rerun
and that gives the strange energy?

#2 - 06/29/2008 02:09 PM - David van der Spoel

Can we close this bug report?

#3 - 07/03/2008 05:45 PM - Berk Hess

This sounds like a real bug, but without a tpr we can't check it.

#4 - 10/08/2008 04:20 AM - Erik Lindahl

I'm closing this since we haven't gotten any feedback/testcase. Feel free to reopen once we have an example!