GROMACS - Bug #592

Long-range LJ correction for test particle insertion

10/10/2010 07:58 PM - Kevin Daly

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	git master		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

When inserting a molecule with multiple atoms, Gromacs does not appear to compute <C6> properly for the long-range correction. Instead, it computes <C6> for only one of the atoms in the inserted molecule. For instance, if I insert a TIP4P/2005 water molecule, which has one site with nonzero LJ parameters and three others with zero-valued LJ parameters, the <C6> value is nonetheless calculated to be zero. In the tpi.xvg output file, U_{dispcorr} is also reported to be zero.

History

#1 - 10/10/2010 07:59 PM - Kevin Daly

Created an attachment (id=552)
Input files

#2 - 10/12/2010 09:39 AM - Berk Hess

I think I fixed it with commit c99629bef0e89518ddef7b740e0081bd027fd29a
Could you test the attached fix?

Thanks,

Berk

#3 - 10/12/2010 09:39 AM - Berk Hess

Created an attachment (id=553)
fix

#4 - 10/22/2010 11:26 AM - Berk Hess

Could you please confirm that I fixed this issue?
Then we can close the bug.

Berk

#5 - 10/22/2010 03:21 PM - Kevin Daly

(In reply to comment #4)

> Could you please confirm that I fixed this issue?
> Then we can close the bug.
>
> Berk

Thank you for fixing the bug. I have confirmed that it works by comparing it to a "brute-force" calculation involving the difference in the LJ correction between a configuration with N+1 water molecules and one with N water molecules.

-Kevin

Files

input_files.tar.gz	277 KB	10/10/2010	Kevin Daly
forcerec.c	56.8 KB	10/12/2010	Berk Hess