GROMACS - Bug #10

mdrun - exploding system with FEP turned on

09/10/2005 08:31 PM - David Bostick

Status:	Closed		
Priority:	High		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	CVS		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Files to reproduce this bug can be downloaded from

http://www.scripps.edu/~dbostick/temp/fep_bug.tgz

the naming of the files are explanatory. See the README file for explicit instructions. I was able to reproduce the bug on Mac OS X (G5 machine), and on a linux cluster (x86-64).

I found a problem when trying to do a FEP run transforming a

blocked GLUH

--> GLU in water. Here is what I observed:

1) When free_energy = no: a test run goes to completion

2) When doing the equivalent run with free_energy = yes as follows:

;Free Energy Perturbation

free_energy = yes

init_lambda = 0.0

delta_lambda = 0.0

the exact same run crashes on the first step. step-1.pdb shows the

initial configuration and step0.pdb shows an apparently exploded

History

#1 - 09/10/2005 08:35 PM - David Bostick

Created an attachment (id=2)

files to reproduce (1) crashed fep run and (2) successful non-fep run

see README file

#2 - 09/12/2005 03:43 PM - Erik Lindahl

This error seems to be caused by a bug in the free energy version of switch VdW interactions.

#3 - 09/12/2005 06:03 PM - Erik Lindahl

We always use the combined Coulomb+VdW table for all free energy interactions (including 1,4) now.

Files

fep_bug.tgz	581 KB	09/10/2005	David Bostick