GROMACS - Bug #1917

Bug in calculation of Distance Restraints energy by gmx energy

03/10/2016 01:47 PM - Vojtech Kuban

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:	analysis tools		
Target version:	2018		
Affected version - extra info:	And some older versions too.	**Difficulty:**	uncategorized
Affected version:	5.1.1		

Description

Hi there,

I have noticed different values of DistRest energy given by gmx energy (on multiple machines). So I tested it on notebook and found that it depends on numbers of MPI, openMP (even with single MPI). More testing with only 2 dist. rest. showed me that some of dist rest were counted for multiple times. Similar problem has a D.R. viol. calculation.

I am using Gromacs 5.1.1., however I tested it with versions 5.0.5 (GPU, MPI) and 4.6.1 and observed different dist. rest. energies. OS Fedora, Debian.

Hope, it will help!

Related issues:

Related to GROMACS - Bug #1316: distance restraints with multiple pairs segv ...	**Closed**	**08/07/2013**

History

#1 - 03/30/2016 06:37 PM - Mark Abraham

Thanks for the report. The implementation of some kinds of distance restraints needs work. I'll look into it soon.

#2 - 05/06/2016 09:38 PM - Mark Abraham

- Related to Bug #1316: distance restraints with multiple pairs segv with OpenMP added

#3 - 05/06/2016 09:43 PM - Mark Abraham

- Status changed from New to Accepted

The measurement of total distance restraint violation does not work reliably with multiple OpenMP threads, because there is a race condition on fcd.disres.sumviol, where each thread writes from ta_disres.

#4 - 01/02/2018 04:26 PM - Mark Abraham

Possibly fixed by c1364cf4e4b14d3726ed7bcb7caa5c17affbecf7?

#5 - 01/02/2018 04:26 PM - Mark Abraham

- Target version set to 2018

#6 - 01/03/2018 01:20 AM - Erik Lindahl

- Status changed from Accepted to Resolved

Yes, this now works. For MPI runs we exit and explain that we cannot output pair info with MPI, and with OpenMP I get the same result no matter the number of threads used.

#7 - 01/03/2018 01:21 AM - Erik Lindahl

- Status changed from Resolved to Closed

Files