

GROMACS - Bug #1473

gmx energy -driftcorr broken.

04/03/2014 03:45 PM - David van der Spoel

Status: Closed	
Priority: Normal	
Assignee: David van der Spoel	
Category: analysis tools	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.0	

Description

The gmx energy -driftcorr -fluctprops now produces ridiculous results (1e16). It was fine in 4.6.x

History

#1 - 05/22/2014 04:49 PM - Erik Lindahl

Problem exists in 4.6 branch too.

#2 - 05/22/2014 05:17 PM - David van der Spoel

This is why I am rewriting and refactoring this code here <https://gerrit.gromacs.org/#/c/3471/>.

#3 - 05/22/2014 07:03 PM - Erik Lindahl

- Status changed from New to In Progress

- Target version changed from 5.0 to 5.x

Ah, changing it for a future version then (since the patch is against master).

#4 - 06/16/2015 11:45 PM - Erik Lindahl

- Status changed from In Progress to Closed

Assuming this was fixed by David's rewrite.

#5 - 07/11/2016 07:48 PM - Mark Abraham

- Target version deleted (5.x)