

GROMACS - Bug #785

Entropy calculation using g_anaeig

07/27/2011 12:23 AM - Justin Lemkul

Status:	Closed	Difficulty:	uncategorized
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	4.5.6		
Affected version - extra info:			
Affected version:			

Description

There appear to be some issues with the code used to calculate entropy in g_anaeig, as reported to the list this morning:

<http://lists.gromacs.org/pipermail/gmx-users/2011-July/063247.html>

Associated revisions

Revision 80a3b80e - 03/05/2012 12:18 PM - Berk Hess

added check for mass-weighting with g_anaeig -entropy, fixes #785

Change-Id: I7a1623ba7a7c7987078901876fb4717d8c0a7261

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History

#1 - 07/27/2011 12:23 AM - Justin Lemkul

- Assignee deleted (David van der Spoel)

#2 - 08/22/2011 05:03 PM - Berk Hess

- Assignee set to David van der Spoel

The g_anaeig entropy calculation code seems to assume one unit for the eigenvalues, whereas g_covar can produce two (length² and mass*length²). This gives unit errors, but also only one of the two would give correct entropies, I assume the masses should not come into play here. Furthermore, the original report complained about possible incorrect use of g_nmeig eigenvalues.

#3 - 09/22/2011 03:49 PM - Rossen Apostolov

- Target version changed from 4.5.5 to 4.5.6

#4 - 03/05/2012 11:57 AM - Rossen Apostolov

- Status changed from New to Closed

Berk fixed it in commit:98333afb