Gromacs - Bug #785
Entropy calculation using g_anaeig
07/27/2011 12:23 AM - Justin Lemkul

Status: Closed
Priority: Normal
Assignee: David van der Spoel
Category: analysis tools
Target version: 4.5.6

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

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

Revision 80a3b80e - 03/05/2012 12:18 PM - Berk Hess
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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 eigenvales, whereas g_covar can produce two (length^2 and mass*length^2). 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:98333af8