GROMACS - Bug #2668

gmx anaeig entropy output are not consistent between runs

10/04/2018 09:10 AM - Magnus Lundborg

Status:	Closed		
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	2020		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018		

Description

The entropy results I'm getting from anaeig are not consistent.

In this case I'm have a molecule/ligand in solution. When running gmx covar I'm fitting the ligand and using it for covariance analysis.

gmx covar -f ../../equil/equil.xtc -s topol_no_restr_0.tpr -b 1000

That might be right or wrong. However, the results from anaeig is confusing. I'm running:

~/install/gromacs_debug/bin/gmx anaeig -v eigenvec.trr -s topol_no_restr_0.tpr -entropy

If I run it repeatedly with the same input I get:
The Entropy due to the Schlitter formula is 1848.75 J/mol K
The Entropy due to the Schlitter formula is nan J/mol K
The Entropy due to the Schlitter formula is nan J/mol K
The Entropy due to the Schlitter formula is 3156.24 J/mol K
The Entropy due to the Schlitter formula is 1848.75 J/mol K

Associated revisions

Revision 1538aaba - 11/11/2018 03:08 AM - David van der Spoel

Fix entropy calculation in gmx anaeig

gmx anaeig reads eigenvectors produced by gmx covar and
can compute entropy according to Schlitter's formula or
based on the quasiharmonic method. If the number of
eigenvectors is not consistent with the number of atoms
the entropy calculation could use uninitialized variables.
Added a warning when this happens.

Fixes #2668

Change-Id: I4f265212ce0a7bf82e25e1aa6f9cbb544c45db3f

History

#1 - 10/04/2018 09:32 AM - David van der Spoel

Can you please upload an example?

#2 - 10/04/2018 09:40 AM - Magnus Lundborg

- File covar.log added

- File eigenvec.trr added

- File eigenval.xvg added

- File topol_no_restr_0.tpr added

I'm not uploading the .xtc file. I could do that if needed.

#3 - 10/30/2018 02:07 PM - Magnus Lundborg

- Target version changed from 2019 to 2020

#4 - 11/09/2018 08:39 PM - David van der Spoel

The tpr file is from master so I can not use it with 2018.

#5 - 11/09/2018 08:42 PM - David van der Spoel

In addition the tpr files is for 15230 atoms while the eigenvec.trr is for 49 atoms.

#6 - 11/10/2018 07:11 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2668.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~release-2018~I4f265212ce0a7bf82e25e1aa6f9cbb544c45db3f
Gerrit URL: https://gerrit.gromacs.org/8680

#7 - 11/10/2018 07:12 AM - David van der Spoel

- Status changed from New to Fix uploaded

Ok the tpr is not needed, however there still is something fishy:

gmx_mpi_d anaeig -f eigenvec.trr -entropy

Read non mass weighted reference structure with 49 atoms from eigenvec.trr
Read non mass weighted average/minimum structure with 49 atoms from eigenvec.trr
Read 90 eigenvectors (for 49 atoms)

The code assumes there should be 3 x 49 = 147 eigenvectors, but there are only 90.

#8 - 11/11/2018 02:30 PM - David van der Spoel

- Status changed from Fix uploaded to Resolved

Applied in changeset 1538aaba79e66e76f4b8af4d273882ddc0d9ad39.

#9 - 11/11/2018 04:08 PM - David van der Spoel

- Status changed from Resolved to Closed

Files

eigenvec.trr	63.6 KB	10/04/2018	Magnus Lundborg
covar.log	791 Bytes	10/04/2018	Magnus Lundborg
eigenval.xvg	2.66 KB	10/04/2018	Magnus Lundborg
topol_no_restr_0.tpr	420 KB	10/04/2018	Magnus Lundborg