GROMACS - Feature #2667

Suggested steps for calculating entropy in solution and binding

10/04/2018 09:02 AM - Magnus Lundborg

Status:	New	
Priority:	Normal	
Assignee:	David van der Spoel	
Category:	documentation	
Target version:	2020.2	
Difficulty:	simple	

Description

I think it would be good to include in the manual (or in the gmx anaeig/covar tools) a brief guide to how to calculate the entropy of a molecule/ligand in solution and while binding to e.g. a protein. Previously it was suggested to do a gmx trjconv -pbc nojump -ur compact. Is that still needed now that gmx covar can apply corrections for pbc? When running gmx covar what groups make sense to fit - should any groups be avoided?

There seems to be a fair amount of interest in calculating entropy, and some questions are asked how to do it or why the results seem wrong, but there is often no conclusion reached. It would be good to list best-practice.

History

#1 - 10/04/2018 09:41 AM - David van der Spoel

I would say there is little physics behind it and therefore this must be discouraged. The best way is to a potential of mean force or otherwise free energy calculation at multiple temperatures.
I can propose some text for the latex manual, or where should it go?

#2 - 10/04/2018 09:44 AM - Magnus Lundborg

If it should be discouraged that would indeed be good to note. I think giving a brief list how to do it best in the LaTeX manual would be appreciated by many.

#3 - 10/30/2018 12:10 PM - Mark Abraham

Seems too late for 2019 now?

#4 - 10/30/2018 12:28 PM - Magnus Lundborg

- Target version changed from 2019 to 2020

#5 - 10/30/2018 01:57 PM - David van der Spoel

The code has been restored in https://gerrit.gromacs.org/#/c/8482/
A description how to do it is in https://pubs.acs.org/doi/abs/10.1021/ct400404q
I could still try to add it to the manual.

#6 - 10/30/2018 02:06 PM - Magnus Lundborg

This feature request is not about the restored code (that was a separate issue). At least a reference to that publication would be good, but a brief instruction in the manual would be helpful.

#7 - 12/27/2019 03:54 PM - Paul Bauer

- Target version changed from 2020 to 2020.1

documentation targeted on first 2020 patch release

#8 - 02/27/2020 11:08 AM - Paul Bauer

- Target version changed from 2020.1 to 2020.2

bump, Magnus is this planned for 2020 patches or in master?

#9 - 03/01/2020 01:35 PM - Magnus Lundborg

I don't know. I just requested this feature since I don't know the proper process and people wonder on different mailing lists.