Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: analysis tools
Target version:
Affected version:
extra info: release-4-5-localpressure
Affected version: N/A

Description
I have been trying to reproduce the lateral pressure profile results recently published in

"Probing microscopic material properties inside simulated membranes through spatially resolved three-dimensional local pressure fields and surface tensions"
Peter M. Kasson, Berk Hess and Erik Lindahl
Chemistry and Physics of Lipids Volume 169, April 2013, Pages 106–112
http://dx.doi.org/10.1016/j.chemphyslip.2013.01.001

by using the release-4-5-localpressure from:
http://repo.or.cz/w/gromacs.git/shortlog/refs/heads/release-4-5-localpressure

As a test system I used a POPC bilayer simulated with the berger force field, as used in the publication as well.

The lateral pressure profile results from this version are attached in the file 2Dlpp45version.dat.
The result is quite different compared to the one in the publication.

For comparison, I have also attached the results calculated with the version downloaded from here (2Dlpp402version.dat):
ftp://ftp.gromacs.org/pub/tmp/gromacs-4.0.2_localpressure.tar.gz

I guess that there is some bug developed during the transformation of the code into the 4.5 version?

The analysis was done over 10ns simulation with both codes. The files to reproduce the simulation data (pr1ns.mdp) and the local pressure calculation (localpressure.mdp) are attached.

History
#1 - 09/03/2013 11:36 AM - Erik Lindahl
- Status changed from New to Fix uploaded

Fixed in commit 1e433fc7cf7a2f2c5b1cb1baab89b976eaa1e0e of the localpressure branch. There is also a new tarball of
gromacs-4.5.2-localpressure in /pub/tmp on ftp.gromacs.org now.

This was due to a change in the graph shift code that we had missed between 4.0 and 4.5.2. It should not have affected any published results, since those were done with an internal version, but we might not have tested this part of the code on large-enough molecules when moving to 4.5.

Samuli: For now I've only been testing on a single frame, but there I get identical results. Please check, and see if you get the versions to match even for longer trajectories now.

#2 - 09/04/2013 11:14 AM - Samuli Ollila
- File 2DlppAV.dat added

Thanks.

The single frame works fine. However, for the average over 10ns I get the attached result. Also the average over 100 frames is weird. Maybe there is still a bug in the averaging over the frames part?

#3 - 10/20/2013 03:21 PM - Erik Lindahl
(Mostly) fixed averaging in git and a new tarball. Note that averages might not be perfect, since we always redo neighboursearching during reruns.

#4 - 10/22/2013 01:00 PM - Samuli Ollila
- File lppAV.png added

Now I get the same results as with the 4.0.2 version (ftp://ftp.gromacs.org/pub/tmp/gromacs-4.0.2_localpressure.tar.gz). The result with the current version is shown in the attached figure. I understood from your paper (Chem. Phys. Lipids 169, 106–112 (2013)) that you have fixed the nonconstant normal component issue. However, the normal component in the attached result is similar as with 4.0.2 version which is clearly not constant. Did I understood the paper wrong or is there still something to fix in the code?

#5 - 05/13/2014 02:04 PM - Rossen Apostolov
- Priority changed from Normal to Low

#6 - 06/11/2014 11:23 PM - Erik Lindahl
- Status changed from Fix uploaded to Closed

Moving this out of the central tracking system. I should still have a look at this, but the localpressure extensions are intentionally kept out of the repository since they are unsupported. Thus, the rest of the developers should not have to worry about features/bugs there.

Files

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