Dear all,

there are several issues with g_dos and g_velacc.

1. they both do not accept "-n" as they should;
2. g_dos does not accept "--normalize";
3. The output of g_velacc, i.e. -o vel.xvg -os spec1.xvg do not match that of g_dos, i.e. -vacf vel.xvg -dos spec.xvg, respectively;
4. The g_dos .log file has some errors.

Associated revisions
Revision d51fdb5b - 06/29/2015 10:24 PM - Erik Lindahl
Fix bugs in gmx dos

- Velocity autocorrelations were not normalized by default, so they did not agree with gmx velacc.
- The normalize option had no effect on the VACs.
- The index group option was available, but no index groups were processed.
- Since the DoS is calculated from the mass-weighted VAC and by default only from the real part, it was not clear why these results would differ from data obtained with gmx velacc. There is at least a note about this now, and more docs will be added in the future.
- The hidden option to dump some plots has been removed since it was not documented what these contained (beyond a paper reference), and the contents was not based on any data from the trajectory, but rather plotting a custom function.

Fixes #1608.

History
#1 - 09/29/2014 03:40 PM - Yao x
I use a 2 fs integration step for a typical protein-water binary system.

#2 - 06/24/2015 10:00 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1608.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: lcfca060f94efb34bd7871bd90245ab0ddbbe91c1
Gerrit URL: https://gerrit.gromacs.org/4781
The density-of-states tool appears to have been largely abandoned, and since it also produces velocity autocorrelations that do not agree with those of gmx velacc we should remove it until somebody wants to look into the tool and provide documentation and fixes.

The -n option does not make sense for gmx dos. I will look into the difference between gmx dos and gmx velacc, but much is probably implemented in patch https://gerrit.gromacs.org/#/c/3175/ already.

Files

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