Gromacs - Bug #1608

g_velacc g_dos do not match

09/29/2014 03:33 PM - Yao x

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td></td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.6</td>
</tr>
<tr>
<td>Affected version</td>
<td>4.6.5</td>
</tr>
</tbody>
</table>

Description
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.

Change-Id: lcfca060f94efb34bd7871bd90245ab0ddbbe91c1
I use a 2 fs integration step for a typical protein-water binary system.

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.

Applied in changeset d51fdb5bf505682196ff7bb290377c581ead208.

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>gdos_spec.xvg</td>
<td>35 KB</td>
<td>09/29/2014</td>
<td>Yao x</td>
</tr>
<tr>
<td>gdos_vacf.xvg</td>
<td>35.9 KB</td>
<td>09/29/2014</td>
<td>Yao x</td>
</tr>
<tr>
<td>gvelacc_spec.xvg</td>
<td>17.2 KB</td>
<td>09/29/2014</td>
<td>Yao x</td>
</tr>
<tr>
<td>gvelacc_vacf.xvg</td>
<td>34.1 KB</td>
<td>09/29/2014</td>
<td>Yao x</td>
</tr>
</tbody>
</table>