GROMACS - Bug #1357
genrestr ignores -disre_up2 input
10/12/2013 02:09 AM - Chris Neale

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
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<tr>
<td>Target version:</td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.6.3 and 4.6.1</td>
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<td>Affected version:</td>
<td>4.6.3</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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Description
Regardless of what value I pass to -disre_up2, genrestr always uses a value of 1.0 (gmx version 4.6.1 and 4.6.3).

In src/tools/gmx_genpr.c
line 227 is:

```c
fprintf(out, "%5d %5d %1d %5d %10d %10g %10g %10g %10g",
        ind_grp[i]+1, ind_grp[j]+1, l, k, 1,
        lo, hi, hi+1, 1.0);
```

but I think it should be:

```c
fprintf(out, "%5d %5d %1d %5d %10d %10g %10g %10g %10g",
        ind_grp[i]+1, ind_grp[j]+1, l, k, 1,
        lo, hi, hi+disre_up2, 1.0);
```

Associated revisions
Revision 740ec2f3 - 06/12/2014 11:07 AM - Erik Lindahl
Make sure genrestr uses the disre_up2 parameter
Previously, a constant value of 1.0 was used instead of the margin read from the command line.
Fixes #1357.
Change-Id: I65ef225159e7b6ef818c71d062b619e78fa7ea22

History
#1 - 11/07/2013 08:15 AM - David van der Spoel
- Assignee set to David van der Spoel

#2 - 06/12/2014 01:46 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1357.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: i65ef225159e7b6ef818c71d062b619e78fa7ea22
Gerrit URL: https://gerrit.gromacs.org/3578

#3 - 06/12/2014 01:47 AM - Erik Lindahl
- Status changed from New to Fix uploaded

#4 - 06/12/2014 12:45 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100
#5 - 06/12/2014 02:44 PM - Erik Lindahl

- Status changed from Resolved to Closed