Gromacs - Bug #1357

genrestr ignores -disre_up2 input
10/12/2013 02:09 AM - Chris Neale

Status: Closed
Priority: Low
Assignee: David van der Spoel
Category:
Target version:
Affected version -
extra info: 4.6.3 and 4.6.1

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:

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

but I think it should be:

```
fprintf(out, "%5d %5d %1d %5d %10d %10g %10g %10g %10g
",
ind_grp[i]+1, ind_grp[j]+1, 1, 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)
#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

Applied in changeset 740ec2f3ba8de3d7cd16104c8f664259a7faed53.

#5 - 06/12/2014 02:44 PM - Erik Lindahl
- Status changed from Resolved to Closed