

GROMACS - Bug #580

Code modifications to add -tu option to g_hbond

09/30/2010 03:16 AM - Justin Lemkul

Status: Closed	
Priority: Normal	
Assignee: Justin Lemkul	
Category: analysis tools	
Target version: git master	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	

Description

I made some slight modifications to g_hbond such that it prints a correct x-axis legend (with time unit), and I added the -tu option that many of the analysis tools have. I find it handy to write all of my output in the same units, but g_hbond doesn't seem to have this capability. The relevant git diff is:

```
diff --git a/src/tools/gmx_hbond.c b/src/tools/gmx_hbond.c
index d4769e5..6a3c107 100644
--- a/src/tools/gmx_hbond.c
+++ b/src/tools/gmx_hbond.c
@@ -3262,7 +3262,7 @ int gmx_hbond(int argc, char *argv[])
 npargs = asize(pa);
 ppa = add_acf_pargs(&npargs, pa);

- parse_common_args(&argc, argv, PCA_CAN_TIME | PCA_BE_NICE, NFILE, fnm, npargs,
+ parse_common_args(&argc, argv, PCA_CAN_TIME | PCA_TIME_UNIT | PCA_BE_NICE, NFILE, fnm, npargs,
 ppa, asize(desc), desc, asize(bugs), bugs, &oenv);

/* NN-loop? If so, what estimator to use ?*/
@ -3646,7 +3646,7 @ int gmx_hbond(int argc, char *argv[])
     dump_grid(debug, ngrid, grid);

add_frames(hb, nframes);
-     init_hbframe(hb, nframes, t);
+     init_hbframe(hb, nframes, output_env_conv_time(oenv, t));

if (hb->bDAnr)
     count_da_grid(ngrid, grid, hb->danr[nframes]);
@ -3927,7 +3927,7 @ int gmx_hbond(int argc, char *argv[])
     aver_nhb = 0;
     aver_dist = 0;
     fp = xvgropen(opt2fn("-num", NFILE, fnm), bContact ? "Contacts" :
-     "Hydrogen Bonds", "Time", "Number", oenv);
+     "Hydrogen Bonds", output_env_get_xvgr_tlabel(oenv), "Number", oenv);
     snw(leg, 2);
     snw(leg[0], STRLEN);
     snw(leg[1], STRLEN);
```

Associated revisions

Revision 68fa2250 - 02/16/2011 04:38 PM - Justin Lemkul

Add -tu option to g_hbond.

IssueID #580

Revision 68fa2250 - 02/16/2011 04:38 PM - Justin Lemkul

Add -tu option to g_hbond.

IssueID #580

History

#1 - 11/08/2010 04:50 PM - Rossen Apostolov

Assigning to Erik Marklund

#2 - 11/10/2010 04:42 PM - Justin Lemkul

Created an attachment (id=566)
Modified gmx_hbond.c

#3 - 11/10/2010 04:43 PM - Justin Lemkul

(In reply to comment [#2](#))

Created an attachment (id=566) [details]
Modified gmx_hbond.c

I'm attaching a more thoroughly modified gmx_hbond.c, one that properly implements the time options for all output files. I realized that my earlier proposed modifications only worked for the hbnum.xvg output, not the others. I've done some limited testing, but it all appears to be correct.

#4 - 02/16/2011 10:26 AM - Justin Lemkul

- Status changed from New to In Progress
- Assignee changed from Erik Marklund to Justin Lemkul

#5 - 02/16/2011 12:24 PM - Justin Lemkul

- Status changed from In Progress to Closed

Fixed in commit 68fa2250.

Files

gmx_hbond.c	145 KB	11/10/2010	Justin Lemkul
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