

## GROMACS - Feature #1030

### adding -tu option to some analysis tools

11/05/2012 04:38 PM - Francesco Oteri

<b>Status:</b>	Fix uploaded	
<b>Priority:</b>	Low	
<b>Assignee:</b>	Rossen Apostolov	
<b>Category:</b>	analysis tools	
<b>Target version:</b>		
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
Good morning, I think it is useful adding the option -tu in g_rmsf. Nowadays people are simulating for several nanoseconds so using yet the picosecond notation is, in my opinion, very annoying. Thank you Francesco		
<b>Related issues:</b>		
Has duplicate GROMACS - Feature #1029: -tu option in g_rmsf		<b>Closed</b> <b>11/05/2012</b>

#### History

##### #1 - 11/05/2012 07:53 PM - David van der Spoel

What do you mean? g\_rmsf gives time averages and no time is printed. Therefore this must be a misunderstanding.

##### #2 - 11/05/2012 08:05 PM - Justin Lemkul

g\_rmsf may not be an appropriate example, but several analysis tools have -tu and others lack it. Perhaps more generally, all analysis tools should include this option (where applicable).

##### #3 - 11/05/2012 08:31 PM - David van der Spoel

I don't see any such program where it is missing.

##### #4 - 11/05/2012 09:00 PM - Francesco Oteri

I mean I cannot use nanoseconds to use -b and -e flags.  
I'd like to use something like:  
g\_rmsf -b 30 -e 50 -tu ns .....

It is not a big problem but, since I am trying to write some script to run analysis. For this lack of uniformity, I've to complicate the scripts.

##### #5 - 11/05/2012 09:03 PM - Justin Lemkul

Francesco Oteri wrote:

I mean I cannot use nanoseconds to use -b and -e flags.  
I'd like to use something like:  
g\_rmsf -b 30 -e 50 -tu ns .....

It is not a big problem but, since I am trying to write some script to run analysis. For this lack of uniformity, I've to complicate the scripts.

All Gromacs trajectories are stored using ps by default. If you want to use ns for everything, you should be able to run trjconv as the first step and reset the units (trjconv -tu ns).

##### #6 - 11/05/2012 09:08 PM - Roland Schulz

Using latest 4.6 the g\_rmsf doesn't have -tu whereas e.g. g\_rms does. The reason is that g\_rmsf doesn't have PCA\_TIME\_UNIT set. It seems to me that PCA\_CAN\_TIME should imply PCA\_TIME\_UNIT.

**#7 - 11/05/2012 09:14 PM - Justin Lemkul**

David van der Spoel wrote:

I don't see any such program where it is missing.

It seems that most analysis tools lack -tu. Those for which it seems like it would make sense to add the -tu option:

g\_analyze (don't really know if this makes sense necessarily)  
g\_angle  
g\_current  
g\_dielectric  
g\_dih  
g\_dipoles  
g\_disre  
g\_dist  
g\_energy  
g\_gyrate  
g\_h2order  
g\_helix  
g\_helixorient  
g\_lie  
g\_rmsdist  
g\_saltbr  
g\_sas  
g\_sgangle  
g\_sorient

The following tools I have never used so I'm not sure if they can use -tu:

g\_rotacf  
g\_spol  
g\_tcaf  
g\_vanhove  
g\_velacc

**#8 - 05/22/2014 07:00 PM - Erik Lindahl**

- *Tracker changed from Bug to Feature*

**#9 - 05/26/2014 11:01 AM - Rossen Apostolov**

- *Has duplicate Feature #1029: -tu option in g\_rmsf added*

**#10 - 06/03/2014 02:16 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#1030](#).

Uploader: Rossen Apostolov ([rossen@kth.se](mailto:rossen@kth.se))

Change-Id: I24140464e0e181c465d0b12d38d0c4d41af5cec7

Gerrit URL: <https://gerrit.gromacs.org/3541>

**#11 - 06/03/2014 02:17 PM - Rossen Apostolov**

- *Status changed from New to Fix uploaded*

- *Target version set to 5.0*

fixed it for 5.0.

**#12 - 06/25/2014 11:01 AM - Rossen Apostolov**

- *Subject changed from g\_rmsf to adding -tu option to some analysis tools*

- *Assignee changed from David van der Spoel to Rossen Apostolov*

**#13 - 06/25/2014 03:16 PM - Rossen Apostolov**

fixed in <https://gerrit.gromacs.org/#/c/3541/>

**#14 - 06/28/2014 08:31 AM - Erik Lindahl**

- *Target version changed from 5.0 to 5.x*

We realized this is a too large fix to commit last-minute since it affects lots of programs.

#15 - 07/11/2016 08:22 PM - Mark Abraham

- Target version deleted (5.x)