

## GROMACS - Bug #155

### Inconsistent averages usign g\_analyze\_d --v3.3.1

06/25/2007 06:28 PM - Anonymous

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Berk Hess	
<b>Category:</b> analysis tools	
<b>Target version:</b> 3.3.1	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

this is in relation to the <http://www.gromacs.org/pipermail/gmx-users/2007-June/028214.html> gmx-users thread. David van der Spoel recommended the creation of a bugzilla entry.

g\_analyze\_d as compiled here sometimes gives erroneous averages as exemplified by considering block averages.

Using the attached .xvg file (dg/dl during a 4ns run with dt=0.002ps), and using options -b and -e for g\_analyze\_d gives the following

```
from 0 to 1000ps ->g_analyze_d average is 1.634425e+03
from 1000 to 2000ps -> g_analyze_d average is 1.634059e+03
from 0 to 2000ps -> g_analyze_d average is 1.637816e+03 ---> a difference
of ~ 3kJ/mol compared with the 1ns blocks
from 2000 to 4000 ps > g_analyze_d average is 1.637791e+03
from 0 to 4000ps -> g_analyze_d average is 1.620341e+03 --> a difference of
~ 17kJ/mol compared with the 2ns blocks
```

The expected average for the full data set is ~ 1634 kJ/mol, not ~ 1620 kJ/mol.

Let me know if other details are needed.

Thanks,  
Philippe

#### History

##### #1 - 06/25/2007 06:43 PM - Anonymous

Created an attachment (id=214)  
dg/dl data file

##### #2 - 06/25/2007 06:54 PM - Anonymous

Created an attachment (id=215)  
perl script to generate data file for bug 155

to use the script:

```
-make script executable (modify first line of script, if need be)
-redirect output to data file. Resulting data file can be used with g_analyze_d to reproduce bug.
```

##### #3 - 06/25/2007 07:50 PM - Anonymous

Just to clarify a little bit...

The dg/dl data file being relatively large and possibly difficult to download, i created this little perl script to generate ~ 2million repeats of the 1634.00 value in the format of a typical .xvg file to mimic a 4ns,dt=0.002 data file. Clearly, the average value should be 1634.00 but g\_analyze\_d wrongly gives

Read 1 sets of 2000001 points, dt = 0.002

```
std. dev.      relative deviation of
set           average      standard deviation      sqrt(n-1)      cumulants from those of
                                                    a Gaussian distribution
                                                    cum. 3      cum. 4
```

SS1 1.613756e+03 2.008756e+01 1.420405e-02 0.635 -0.660

Philippe

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

Created an attachment (id=215) [details]  
perl script to generate data file for bug 155  
to use the script:  
-make script executable (modify first line of script, if need be)  
-redirect output to data file. Resulting data file can be used with g\_analyze\_d  
to reproduce bug.

#### #4 - 07/05/2007 12:49 PM - Berk Hess

Does the single precision g\_analyze have the same problem?

I tried the perl script output in the single precision version  
and that gives exactly the correct output.

I have tried g\_analyze\_d of the 3.3 branch with a few fixes  
(but none that I recall have any effect on this)  
and that also works fine.

Berk.

#### #5 - 07/05/2007 02:02 PM - Berk Hess

I have now compiled a proper 3.3.1 distribution double precision g\_analyze.  
It gives the correct results, both for your dgdl file as well as  
the perl script output.

So I can not reproduce you problem.  
I am running on an AMD64 under linux, with gcc version 3.3.5.

What are you running?

Berk.

#### #6 - 08/02/2007 04:48 PM - Berk Hess

There has been no answer since a month.  
Since I can not reproduce the problem,  
I close this bug.

### Files

---

first4ns.xvg.gz	9.65 MB	06/25/2007	Anonymous
makedata4bug155.pl	102 Bytes	06/25/2007	Anonymous