

GROMACS - Bug #384

tabulated potentials derivative not interpolated correctly in some cases

01/08/2010 08:31 PM - M. Sandal

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	

Description

Created an attachment (id=411)
.mdp of the run

There is a relevant thread on the gmx-users mailing list:

<http://www.mail-archive.com/gmx-users@gromacs.org/msg27392.html>

David van der Spoel asked me there to report a bug here.

In trying to use a tabulated potential with GROMACS 4.0.5, I noticed mdrun warnings about deviations of my table from the estimated numerical derivative, of this kind:

```
"WARNING: For the 268 non-zero entries for table 2 in
table_10_70_0.4_1_C-alpha_C-alpha.xvg the forces deviate on average
120138% from minus the numerical derivative of the potential"
```

The command line is (as launched from a python script I use):

```
/home/ms872/software/bin/mdrun -v -s
$STARTDIR/"'+top_name+'_fullmd_'+jobname+"'.tpr -o
$STARTDIR/"'+top_name+'_'+jobname+"'.trr -x
$STARTDIR/"'+top_name+'_'+jobname+"'.xtc -c
$STARTDIR/"'+top_name+'_final_'+jobname+"'.gro -e
$STARTDIR/"'+top_name+'_minbox_'+jobname+"'.edr -table "'+table+'
-tablep "'+tablep+' " 2>&1 > $STARTDIR/output_"'+jobname+"'.txt -debug 1
```

The input table is like this:

as you can see, the derivative values of the repulsion are monotonically negative.

```
...
0.324 0 0 0 0 19.057170805 -4903.66757218
0.325 0 0 0 0 14.5544681537 -4122.12982071
0.326 0 0 0 0 10.7761004826 -3452.22019522
0.327 0 0 0 0 7.61823859882 -2878.71133959
0.328 0 0 0 0 4.99123976902 -2388.40876887
0.329 0 0 0 0 2.81775232212 -1969.88234765
0.33 0 0 0 0 1.03107071308 -1613.23304761
...
```

And the rtab.xvg outputted by mdrun is like this: signs are oscillating every few values:

```
...
3.2873699069e-01 3.0300402641e+00 -2.9821022949e+03
3.2893705368e-01 2.7424881458e+00 4.5555401611e+02
3.2913714647e-01 2.9011108875e+00 -6.1965881348e+02
3.2933723927e-01 2.5153810978e+00 -2.9490820312e+03
3.2953730226e-01 1.8357653618e+00 -3.5592436523e+03
3.2973739505e-01 1.2058072090e+00 -2.4505161133e+03
3.2993748784e-01 9.6973133087e-01 3.7754727173e+02
3.3013758063e-01 1.1429694891e+00 8.3080635071e+01
```

```
3.3033764362e-01 9.9677509069e-01 -1.3973664551e+03
3.3053773642e-01 6.4262789488e-01 -1.9951014404e+03
3.3073782921e-01 2.5727045536e-01 -1.7099414062e+03
3.3093789220e-01 1.7271757126e-02 -5.4204510498e+02
```

...

Now, the table I used **was wrong** indeed (see attachment for full tables, good and wrong), but in the **attractive** part (it had the wrong sign). When I correct the table, the sign oscillation in the **repulsive** part go away.

There is also a small positive part in the derivative part of the rtab14.xvg, which is, in my system, the **default LJ** (table.xvg):

rtab14.xvg excerpt:

...

```
3.7760000676e-02 0.0000000000e+00 0.0000000000e+00
3.8079999387e-02 3.3338824642e+14 8.2109411802e+18 <-positive
3.8400001824e-02 7.3433434198e+15 3.3617108423e+19
3.8720004261e-02 2.0579002939e+16 4.7121167299e+19
3.9040002972e-02 3.6231459346e+16 4.8723151343e+19
3.9360001683e-02 5.0492120863e+16 3.8423506956e+19
3.9680000395e-02 5.9552762396e+16 1.6221962559e+19
3.9999999106e-02 5.9604645601e+16 -1.7881392787e+19 <-here begin the negatives
4.0320001543e-02 5.4162767418e+16 -1.6154702134e+19
4.0640003979e-02 4.9250029206e+16 -1.4573871595e+19
4.0960002691e-02 4.4819873519e+16 -1.3138938552e+19
```

...

This remains, no matter what I do to the custom table.

History

#1 - 01/08/2010 08:32 PM - M. Sandal

Created an attachment (id=412)
rtab14 , coming from table6-12.xvg

#2 - 01/08/2010 08:33 PM - M. Sandal

Created an attachment (id=413)
rtab as coming from correct table

#3 - 01/08/2010 08:33 PM - M. Sandal

Created an attachment (id=414)
rtab as coming from incorrect table

#4 - 01/08/2010 08:33 PM - M. Sandal

Created an attachment (id=415)
correct table

#5 - 01/08/2010 08:34 PM - M. Sandal

Created an attachment (id=416)
incorrect table

#6 - 01/19/2010 11:04 AM - Berk Hess

I don't understand your problem.
The input file marked WRONG has the wrong sign and gives
an oscillating force.
The input file marked GOOD is correct and rtab_GOOD.xvg
has no oscillations.
So I don't see any problem.
Or does rtab_WRONG.xvg come out of the run with input file GOOD?

Berk

#7 - 02/09/2010 10:28 AM - Berk Hess

Could you please answer if there is a problem in Gromacs or not?
So we can fix or close this bug?

Thanks,

Berk

#8 - 02/24/2010 03:31 PM - Berk Hess

No answer for more than a month and I can not reproduce the bug,
I will close it.

Berk

Files

fullmd.mdp	1.9 KB	01/08/2010	M. Sandal
rtab14.xvg	394 KB	01/08/2010	M. Sandal
rtab_GOOD.xvg	580 KB	01/08/2010	M. Sandal
rtab_WRONG.xvg	579 KB	01/08/2010	M. Sandal
table_C-alpha_C-alpha_GOOD.xvg	116 KB	01/08/2010	M. Sandal
table_C-alpha_C-alpha_WRONG.xvg	117 KB	01/08/2010	M. Sandal