

## GROMACS - Bug #579

### nstcalcenergy = -1 leads to wrong pressure

09/29/2010 09:58 PM - David van der Spoel

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> mdrun	
<b>Target version:</b> 4.5.1	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

I have confirmed this as a bug.

In 4.0.5 (which I had handy) the density is constant

Density (SI) 999.554 3.82377 3.80651 0.0628345 1.25694

In 4.5.1 with 4.0.5 tpr file it is as you say:

Density 995.277 1.3 4.32625 -1.24517 (kg/m3)

In 4.5.1 with 4.5.1 tpr file I get

Density 709.919 66 137.824 -467.285 (kg/m3)

Now the differences in the tpr files are revealing:

```
[anfin: test-volume-drift] % gmxcheck s1-topol405.tpr s2-topol.tpr
```

<snip>

Note: tpr file version 58, software version 73

Reading file topol.tpr, VERSION 4.5.1%ci-21e8a32 (single precision)

comparing inputrec

inputrec->nstcalcenergy (1 - 10)

inputrec->rgbradii (2.000000e+00 - 1.000000e+00)

inputrec->sa\_surface\_tension (2.092000e+00 - 2.050160e+00)

inputrec->sc\_sigma\_min (0.000000e+00 - 3.000000e-01)

inputrec->nstdhdl (1 - 10)

inputrec->separate\_dhdl\_file (0 - 10)

<snip>

After setting nstcalcenergy = 1 I get

Density 996.894 1.2 3.85083 1.86718 (kg/m3)

In other words the bug can be circumvented by setting this variable to 1. I will file a bugzilla.

#### History

##### #1 - 09/29/2010 09:59 PM - David van der Spoel

Created an attachment (id=544)

Files to reproduce the problem

Run with gromacs 4.0.7

```
grompp -v
```

```
mdrun -v
```

```
echo Dens | g_energy -w
```

Then run the same with gromacs 4.5.1 and see the difference.

##### #2 - 09/29/2010 10:01 PM - David van der Spoel

I guess the nstlist = -1 does not play nice with nstcalcenergy = 10 (default)

##### #3 - 10/05/2010 12:43 PM - Berk Hess

This was not due to nstcalcenergy being -1, but rather due to nstlist being -1.

Fixed it:  
commit de946652ba14e3bb9953f2154f7b1653e09448a2

Berk

## Files

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test-volume-drift.tar	190 KB	09/29/2010	David van der Spoel
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