

GROMACS - Bug #1343

vsiten particles are not integrated

09/27/2013 10:24 PM - David van der Spoel

Status:	Closed	
Priority:	Normal	
Assignee:	Berk Hess	
Category:	mdrun	
Target version:	5.0	
Affected version - extra info:	master branch	Difficulty: uncategorized
Affected version:	5.0	

Description

Sometime in 2013 during the master branch development a bug was introduced that makes that the coordinates of vsiten particles are not integrated, that is they remain at the same position. In the attached example one has to change the particle type of the MW particle in amber99sb-ild.ff/ffnonbonded.itp to V (or D) to make it work, then

```
grompp -maxwarn 20
mdrun
```

```
gmx gmxdump -f traj.xtc | grep ' 1100\]'
x[ 1100]={ 5.35100e+00, 6.43100e+00, 5.72700e+00}
x[ 1100]={ 5.35100e+00, 6.43100e+00, 5.72700e+00}
x[ 1100]={ 5.35100e+00, 6.43100e+00, 5.72700e+00}
x[ 1100]={ 5.35100e+00, 6.43100e+00, 5.72700e+00}
x[ 1100]={ 5.35100e+00, 6.43100e+00, 5.72700e+00}
```

As you see the coordinates of this vsiten particle is exactly constant!

It works fine in 4.6 and earlier, as well as in older master branches. I tried git bisect but could not find the right position :(.

Associated revisions

Revision cd41feab - 09/29/2013 09:59 AM - David van der Spoel

Fixes bug in processing virtual_sitesn in grompp.

Fixes #1343

Change-Id: Ia1d39199a12292ef86d086a6c1bb5f1a0bdb5d35

History

#1 - 09/27/2013 10:25 PM - David van der Spoel

Didn't mean to assign it to Berk just added him as a watcher. Will try more tomorrow :(.

#2 - 09/28/2013 01:54 PM - David van der Spoel

- Status changed from New to Fix uploaded

Gerrit <https://gerrit.gromacs.org/#/c/2648/>

#3 - 09/29/2013 10:00 AM - David van der Spoel

- Status changed from Fix uploaded to Resolved

- % Done changed from 0 to 100

Applied in changeset [cd41feabe8eafc90dd9c4e3d4f509ce988fc7949](#).

#4 - 09/29/2013 03:53 PM - David van der Spoel

- Status changed from Resolved to Closed

Files

vsitebug.zip

68.6 KB

09/27/2013

David van der Spoel