

## GROMACS - Bug #1343

### vsiten particles are not integrated

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

<b>Status:</b>	Closed	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	Berk Hess	
<b>Category:</b>	mdrun	
<b>Target version:</b>	5.0	
<b>Affected version - extra info:</b>	master branch	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	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/nonbonded.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**

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vsitebug.zip

68.6 KB

09/27/2013

David van der Spoel