

## GROMACS - Bug #2497

### SIMD update is never activated

05/02/2018 04:33 PM - Berk Hess

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Berk Hess	
<b>Category:</b> mdrun	
<b>Target version:</b> 2018.2	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018	
<b>Description</b>	
Due to a bug mdatoms->havePartiallyFrozenAtoms always ended up as true, which deactivated the SIMD version of the update (when this was possible).	

#### Associated revisions

##### Revision db33bb79 - 05/03/2018 02:33 PM - Berk Hess

Enable SIMD version of update

A bug in setting mdatoms->havePartiallyFrozenAtoms caused the SIMD version of the leap-frog update to always be deactivated.

Fixes #2497

Change-Id: I670549c95c983cac5033ea6bb71b77561e063223

#### History

##### #1 - 05/02/2018 04:37 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2497](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: gromacs~release-2018~I670549c95c983cac5033ea6bb71b77561e063223

Gerrit URL: <https://gerrit.gromacs.org/7819>

##### #2 - 05/02/2018 04:39 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

##### #3 - 05/04/2018 12:15 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset [db33bb790d03a97604764514f396bcde025530db](#).

##### #4 - 05/04/2018 12:24 AM - Mark Abraham

- Status changed from Resolved to Closed