### GROMACS - Bug #2497

**SIMD update is never activated**

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

**Status:** Closed  
**Priority:** Normal  
**Assignee:** Berk Hess  
**Category:** mdrun  
**Target version:** 2018.2  
**Affected version - extra info:**  
**Affected version:** 2018  
**Difficulty:** uncategorized

**Description**
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)  
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 db33bb790d03a97604764514f996bcde025530db.

#4 - 05/04/2018 12:24 AM - Mark Abraham
- Status changed from Resolved to Closed