

## GROMACS - Bug #1462

### Constraining v or f in parallel can give incorrect results

03/17/2014 04:52 PM - Berk Hess

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> Berk Hess	
<b>Category:</b> mdrun	
<b>Target version:</b> 4.6.6	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 4.0	

#### Description

With 3 or more decomposition domains in at least one dimension, the constraint code would always apply periodic shifts to the constraint quantity vector, even if it was not a coordinate. This means that velocities and forces sent over to other domains could be incorrectly modified by the box length. Note that intra charge-group constraints are not affected by this bug.

This bug affects:

- The velocity Verlet integrator (4.6). Since the box is large compared to  $v$ , this will make most simulations completely unstable (no silent errors).
- Multiple time stepping with twin-range cut-off's (4.5). Forces are large compared to the box size, so this might not be easy to notice. But multiple time stepping is rarely used in Gromacs, since the typical Gromos setup became unstable with the Trotter decomposition multiple time stepping.
- Energy minimization with constraints (4.0). The force will not converge to an error below the box size. In most cases forces with constraints are much larger during energy minimization, and errors don't accumulate, so this bug will have little effect.

#### Associated revisions

##### Revision b58afa7e - 03/23/2014 11:58 AM - Berk Hess

Fixed bug in parallel v/f constraining

Constraining v or f with 3 or more decomposition domains in one or more dimensions could lead to modification of communicated v and f components by the box size for inter charge-group constraints. Fixes #1462

Change-Id: Idece9d2d0d8f48e65a654d5c2892f8e1ff836ba0

#### History

##### #1 - 03/17/2014 04:55 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1462](#).

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

Change-Id: Idece9d2d0d8f48e65a654d5c2892f8e1ff836ba0

Gerrit URL: <https://gerrit.gromacs.org/3274>

##### #2 - 03/23/2014 12:00 PM - Berk Hess

- Status changed from New to Resolved

- % Done changed from 0 to 100

Applied in changeset [b58afa7e304477f48ce48dfc11b9e9afd2987bc3](#).

##### #3 - 03/29/2014 06:17 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1462](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: Idece9d2d0d8f48e65a654d5c2892f8e1ff836ba0

Gerrit URL: <https://gerrit.gromacs.org/3303>

##### #4 - 04/03/2014 07:33 PM - Roland Schulz

- Status changed from Resolved to Closed