GROMACS - Bug #1660

pbc=xy with 2 walls segvs with the Verlet scheme

12/15/2014 08:31 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 5.0.5

Description
Since this case is bounded, it is allowed to run, and should be able to run, with the Verlet cut-off scheme, even though general pbc=xy is not yet supported.

Associated revisions
Revision 30782acb - 12/22/2014 02:33 AM - Berk Hess
Fixed pbc=xy + 2 walls + Verlet scheme
Fixes #1660.
Change-Id: Id28f5d164c24d9bc6cb80faa8f4cba5e95262995

History
#1 - 12/15/2014 08:32 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1660.
Uploader: Berk Hess (hess@kth.se)
Change-Id: ld28f5d164c24d9bc6cb80faa8f4cba5e95262995
Gerrit URL: https://gerrit.gromacs.org/4316

#2 - 12/15/2014 09:24 PM - Berk Hess
- Status changed from In Progress to Fix uploaded
- Target version changed from 5.0.4 to 5.0.5

#3 - 01/08/2015 05:43 PM - Mark Abraham
- Status changed from Fix uploaded to Closed