GROMACS - Bug #2385

PME mixed mode produces incorrect results with box scaling

01/16/2018 05:58 PM - Aleksei Iupinov

Status: Closed
Priority: Normal
Assignee: Aleksei Iupinov
Category: mdrun
Target version: 2018.1
Affected version - extra info:
Affected version: 2018

Difficulty: simple

Description
I've made a simple test which exposed the issue. Will submit the test to master later. As mixed mode PME is opt-in, I think it's fine to only submit the fix itself for release-2018.

Related issues:
Related to GROMACS - Task #2379: check leftover FIXMEs in r2018

Associated revisions
Revision fbbd3df6 - 01/17/2018 03:13 PM - Aleksei Iupinov
Fix box scaling in PME mixed mode
A TODO is left to test and handle this better in master.
Fixes #2385
Change-id: l34d01d3ea6802f624888a1fd85eef72711a82f2f

Revision dd6a868c - 01/23/2018 04:45 PM - Aleksei Iupinov
Test the mixed mode PME with walls and box scaling
Refs #2385
Change-id: l42281dd6b3da30c777a0819d97c1d85e69049674

History
#1 - 01/16/2018 05:58 PM - Aleksei Iupinov
- Related to Task #2379: check leftover FIXMEs in r2018 added

#2 - 01/16/2018 06:10 PM - Aleksei Iupinov
- Subject changed from PME mixed mode broken with box scaling to PME mixed mode produces incorrect results with box scaling

#3 - 01/16/2018 06:17 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2385.
Uploader: Aleksei Iupinov (a.yupinov@gmail.com)
Change-id: gromacs~release-2018~l34d01d3ea6802f624888a1fd85eef72711a82f2f
Gerrit URL: https://gerrit.gromacs.org/7474

#4 - 01/17/2018 01:55 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2385.
Uploader: Aleksei Iupinov (a.yupinov@gmail.com)
Change-id: gromacs~master~l42281dd6b3da30c777a0819d97c1d85e69049674
Gerrit URL: https://gerrit.gromacs.org/7463

#5 - 01/17/2018 09:18 PM - Aleksei Iupinov
- Status changed from In Progress to Resolved
Applied in changeset fbbd3df6b5ff5c1b8591838a143ef85d95ac32cf.

#6 - 01/31/2018 02:14 PM - Aleksei Iupinov

- Status changed from Resolved to Closed