GROMACS - Bug #1578

PME incorrect with MPI+OpenMP and multiple MPI communication pulses

08/15/2014 05:47 PM - Berk Hess

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.7
Affected version - extra info:
Affected version: 4.6.7

Description
Change 272736bc fixed a related issue with additionally multiple OpenMP thread domains along a PME domain decomposition dimension. But his fix broke a more common case without this specific thread division.

Now the PME energies and forces are incorrect with MPI+OpenMP when multiple MPI communication pulses are used, that is when:
fftgrid_size[d]/#PME_ranks[d] < pme_order && fftgrid_size[d]/#PME_ranks[d] != pme_order-1

Note that without OpenMP threads there are no issues.

Related issues:
Related to GROMACS - Bug #1572: Incorrect PME energies and forces with high n...
Closed 08/02/2014

Associated revisions
Revision 6ba80a26 - 08/28/2014 04:08 PM - Berk Hess
Fixed two PME issues with MPI+OpenMP

Change 272736bc partially fixed #1388, but broke the more general case of multiple MPI communication pulses in PME. Change 272736bc incorrectly changed tx1 and ty1. This change has been reverted.

Change 27189bba fixed the incorrect PME grid reduction with multiple thread grid overlap in y. But it broke the, much more common, case where the y-size of the PME grid is not divisible by the domains in y. This change, incorrectly, changed buf_my.

Now buf_my is set to the correct value, which solves both issues.

Fixes #1578.
Refs #1388 and #1572.
Change-id: ld2d7d013a3b8cc04eda1f026567088a38ec81f

History
#1 - 08/18/2014 03:05 AM - Gerrit Code Review Bot
Gerrit received a related DRAFT patchset '1' for Issue #1578.
Uploader: Szilárd Páll (pall.szilard@gmail.com)
Change-id: l3649294a143bb744a2e26f1d9dfb87de421ca
Gerrit URL: https://gerrit.gromacs.org/3905

#2 - 09/05/2014 01:47 PM - Berk Hess
- Status changed from In Progress to Closed

#3 - 12/06/2014 01:21 AM - Roland Schulz
- Related to Bug #1572: Incorrect PME energies and forces with high numbers of OpenMP threads added