

GROMACS - Bug #2247

PME forces with SIMD 2xNN tabulated kernels are incorrect

09/14/2017 04:18 PM - Berk Hess

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|--|----------------------------------|
| Status: Closed | |
| Priority: High | |
| Assignee: Berk Hess | |
| Category: mdrun | |
| Target version: 2016.4 | |
| Affected version - extra info: | Difficulty: uncategorized |
| Affected version: 2016 | |
| Description | |
| This likely did not affect any production runs, since no architecture used this combination by default, it could only be chosen by environment variables. But AVX512 will use this by default from release-2016.4 onward. | |

Associated revisions

Revision 12e9ea41 - 09/14/2017 04:34 PM - Berk Hess

Fix nbnxxn SIMD 2xNN PME tabulated kernel

This kernel produced completely incorrect forces and slightly incorrect energies.
This kernel was not (yet) selected by default in a 2016 release.

Fixes #2247

Change-Id: I297ad257932eaabe6cf84b17f34ad555921f48b0

History

#1 - 09/14/2017 04:37 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2247](#).
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2016~I297ad257932eaabe6cf84b17f34ad555921f48b0
Gerrit URL: <https://gerrit.gromacs.org/6930>

#2 - 09/14/2017 04:41 PM - Aleksei lupinov

So how did you test it, for posterity? :-)

#3 - 09/14/2017 04:59 PM - Berk Hess

- Status changed from *In Progress* to *Fix uploaded*

Roland found this.
I tested it using the env.vars. GMX_NBNXXN_SIMD_2XNN=1 GMX_NBNXXN_EWALD_TABLE=1

#4 - 09/15/2017 01:40 PM - Berk Hess

- Status changed from *Fix uploaded* to *Resolved*

Applied in changeset [12e9ea41a9cee3fe2ea844044d1d47bb30759b97](#).

#5 - 09/15/2017 05:14 PM - Mark Abraham

- Status changed from *Resolved* to *Closed*