GROMACS - Bug #2399

group scheme always uses generic non-bonded kernel

02/05/2018 04:05 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.1
Affected version - extra info:
Affected version: 2018
Difficulty: uncategorized

Description
The cutoff-modifiers were not copied from interaction_const_t to forcerc_t, which is only used by the group scheme. This causes the generic kernel to be chosen instead of SIMD or the plain-C kernel. It seems this only affects performance and not correctness.

Associated revisions
Revision c54cf431 - 02/05/2018 04:05 PM - Berk Hess
Set cutoff modifiers in forcerc

The cutoff modifiers were not copied from interaction_const_t to forcerc_t which meant only the generic kernels was used with the group scheme.

Fixes #2399

Change-Id: l2890cbd556e48e434ad3817edc4e5fe4c5697162

History
#1 - 02/05/2018 04:06 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2399.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I2890cbd55e648e434ad3817edc4e5fe4c5697162
Gerrit URL: https://gerrit.gromacs.org/7543

#2 - 02/05/2018 04:13 PM - Berk Hess
- Status changed from In Progress to Fix uploaded

#3 - 02/06/2018 10:30 AM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset c54cf431c2420b4142f8743924dcco736754880d2.

#4 - 02/06/2018 04:33 PM - Mark Abraham
- Status changed from Resolved to Closed