GROMACS - Task #2367

construct pbc_simd less often

12/26/2017 01:53 PM - Mark Abraham

Status: New
Priority: Normal
Assignee: core library
Category: core library
Target version: future
Difficulty: uncategorized

Description

We now use SIMD forms of the pbc data structures in multiple places per MD step. It would be slightly more efficient to construct that once per step (e.g. when we know the box has been updated), and would mean we don't have to make temporary SIMD data structures on the stack, for which there is no fully portable implementation in the C++11 standard (support for extended alignment e.g. for SIMD operations is at the discretion of the implementation, which we didn't realise when we used the standard alignas to implement GMX_ALIGNED(), and maybe GMX_ALIGNED() was broken before that, too).

Related issues:
Related to GROMACS - Bug #2365: UtilityUnitTests is broken on ppc64le, aarch6... Closed

History

#1 - 12/26/2017 01:53 PM - Mark Abraham
- Related to Bug #2365: UtilityUnitTests is broken on ppc64le, aarch64, ppc64, s390x and armv7hl added

#2 - 09/24/2018 11:02 PM - Mark Abraham
- Target version changed from 2019 to future

I presume this is a necessary task at some point, but nobody has a plan to do it now