GROMACS - Feature #1598
SIMD acceleration for RB dihedrals
09/18/2014 11:19 AM - Szilárd Páll

Status: Closed
Priority: Normal
Assignee:
Category: core library
Target version: 5.0.2
Difficulty: uncategorized

Description
The RB dihedrals are not SIMD accelerated and can take a substantial amount of runtime. Adding SIMD codepath for these kernels would improve performance not only in exotic cases like the polymer system discussed on gmx-users which has only RB bonded interactions, but also e.g. in membrane systems with Berger lipids.

Associated revisions
Revision ae4be041 - 09/29/2014 05:35 PM - Berk Hess
SIMD acceleration for RB dihedrals
RB dihedrals now use SIMD acceleration analogous to proper dihedrals when no energy and virial is required. This also significantly improves load balancing (issues) for systems with proper+RB dihedrals.
Refs #1598.
Change-Id: I07000125d19db45fc35e1a0c28149c8a19443680

History
#1 - 09/18/2014 05:10 PM - Szilárd Páll
- Description updated

#2 - 09/18/2014 06:50 PM - Mark Abraham
I hope to be able to do this as part of my bonded-stuff upgrade, but people reviewing C++ conversion and https://gerrit.gromacs.org/#/q/status:open+project:gromacs+branch:master+topic:bondeds will speed this up.

#3 - 09/29/2014 12:09 PM - Berk Hess
- Status changed from New to Fix uploaded

#4 - 10/01/2014 05:16 PM - Mark Abraham
- Status changed from Fix uploaded to Closed
- Target version set to 5.0.2