**Gromacs - Feature #1598**

**SIMD acceleration for RB dihedrals**

09/18/2014 11:19 AM - Szilárd Páll

<table>
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<th>Status:</th>
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<td>Assignee:</td>
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<td>Target version:</td>
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**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:bonedds 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