**GROMACS - Feature #1095**

Fix all-vs-all kernels

12/28/2012 10:02 AM - Erik Lindahl

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>Erik Lindahl</td>
</tr>
<tr>
<td>Category:</td>
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<td>Target version:</td>
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<td>Difficulty:</td>
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**Description**

They were temporarily disabled during testing of the normal kernels, but should be straightforward to turn on again.

**Related issues:**

- Related to GROMACS - Bug #1249: no-PBC no-cutoff is broken with SIMD group ke... Closed 05/14/2013
- Related to GROMACS - Bug #1134: gromacs 4.6 GB/SA problem and poor performance Closed 01/27/2013
- Related to GROMACS - Task #1971: Removing buggy features vs. keeping workflows New

**Associated revisions**

**Revision 6a8acbaa** - 05/30/2013 10:16 AM - Mark Abraham

Work around for correct treatment of all-vs-all

Neither C or accelerated all-vs-all kernels work in 4.6. The group SIMD kernels do not work either. The non-accelerated kernel is OK, though.

Fixes #1249 (for certain values of "fixes"), refs #1095

Change-Id: ld52c0ba110aa915e77859585c2cbfd4d529fe3ca

**Revision 8d3da2fb** - 01/07/2019 02:26 AM - Mark Abraham

Finish removing group-scheme all-vs-all support

These kernels haven't been callable since before GROMACS 4.6

No release notes entry as no functionality is actually changed with this commit.

Fixes #1095

Change-Id: l3de3b9bbabaaafa70fee4e9845880c973e9dc352

**History**

#1 - 01/07/2013 01:54 AM - Erik Lindahl

- Status changed from New to In Progress

#2 - 01/07/2013 01:55 AM - Erik Lindahl

- Assignee set to Erik Lindahl

#3 - 01/18/2013 03:29 PM - Erik Lindahl

- Target version changed from 4.6 to 4.6.1

#4 - 04/29/2013 08:02 PM - Mark Abraham

- Target version deleted (4.6.1)

- Affected version set to 4.6

#5 - 05/24/2013 04:57 PM - Mark Abraham

Hack in gerrit to stop this code path being triggered [https://gerrit.gromacs.org/#/c/2399/](https://gerrit.gromacs.org/#/c/2399/)
we can close this one also

I don't think the underlying issue is resolved. My patch just stopped wrong results being generated. Resolution ought to be removing or fixing the broken code. This might be trickier now with PD (and perhaps simple search?) removed.

Changing to a feature; we should still improve this for post 5.0 to improve performance, but Mark's fix means we no longer produce any incorrect results.

Actually I think the gmx_incons I put into do_nonbonded() back then has meant that this code path hasn't worked at all since 4.6.x.

While we plan to add back some all-vs-all support to the Verlet scheme, it seems like the group-scheme implementation may as well be removed ASAP.

Removing last vestiges of this functionality.

Applied in changeset 8d3da2b965d6bed25458175fb9434a0f91a29644.

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