Gromacs - Feature #1095
Fix all-vs-all kernels
12/28/2012 10:02 AM - Erik Lindahl

<table>
<thead>
<tr>
<th>Status:</th>
<th>In Progress</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<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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**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 key
  - Closed 05/14/2013
- Related to Gromacs - Bug #1134: gromacs 4.6 GB/SA problem and poor performance
  - Closed 01/27/2013

**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: Id52c0ba110aa915e77859585c2cbfd4d529fe3ca

**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/)

#6 - 05/14/2014 10:55 AM - Rossen Apostolov
- Status changed from In Progress to Resolved
we can close this one also

#7 - 05/15/2014 10:37 PM - Mark Abraham
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.

#8 - 05/16/2014 08:55 AM - Rossen Apostolov
- Status changed from Resolved to In Progress

#9 - 06/09/2014 09:12 PM - Erik Lindahl
- Tracker changed from Bug to Feature

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.