

GROMACS - Feature #1095

Fix all-vs-all kernels

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

Status:	Closed	
Priority:	Normal	
Assignee:	Erik Lindahl	
Category:		
Target version:		
Difficulty:	uncategorized	
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: Id52c0ba110aa915e77859585c2cbfd4d529fe3ca

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: I3de3b9bbabaafae70fee4e9845880c973e8dc352

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/>

#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.

#10 - 07/11/2016 09:11 PM - Mark Abraham

- Related to Task #1971: *Removing buggy features vs. keeping workflows added*

#11 - 03/06/2018 11:19 PM - Mark Abraham

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.

#12 - 01/07/2019 02:28 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1095](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: `gromacs~master~I3de3b9bbabaafae70fee4e9845880c973e8dc352`

Gerrit URL: <https://gerrit.gromacs.org/8930>

#13 - 01/07/2019 02:29 AM - Mark Abraham

- Status changed from *In Progress* to *Fix uploaded*

Removing last vestiges of this functionality.

#14 - 01/07/2019 11:30 AM - Mark Abraham

- Status changed from *Fix uploaded* to *Resolved*

Applied in changeset [8d3da2fb965dbed25458175fb9434a0f91a29644](#).

#15 - 01/08/2019 05:26 PM - Paul Bauer

- Status changed from *Resolved* to *Closed*