GROMACS - Bug #1631

Triclinic 1xNx1 domain decomposition with Verlet scheme gives incorrect results

10/24/2014 03:41 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.8</td>
</tr>
<tr>
<td>Affected version</td>
<td>5.0</td>
</tr>
<tr>
<td>Affected version</td>
<td>4.6</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

With the Verlet scheme and triclinic boxes, a 1D decomposition over y, i.e. 1xNx1, produces incorrect bounding boxes for the non-bonded grid, which results in missing non-bonded interactions. Unless box angles are very close to 90 degrees, many interactions will be missing and the system will crash after a few steps. This was never noticed before, because the default 1D domain decomposition is Nx1x1, unless the box is longer in y than in x. Because the high number of missing interactions makes the system crash quickly, this will not lead to silent errors.

**Associated revisions**

Revision c8d919a3 - 11/26/2014 11:22 AM - Berk Hess

Fixed triclinic 1xNx1 domain decomposition

With the Verlet scheme, 1D triclinic domain decomposition along dimension y produces incorrect bounding boxes for the non-bonded grid. This led to a lot of missing non-bonded interactions, which quickly crashes any simulation affected by this. Fixes #1631.

Change-Id: l9bd1fc9d983be839e0c9a8e62d47f6cf17684a03

Revision 29b6eedc - 12/09/2014 04:59 PM - Berk Hess

Fix recent bug with trilinic 1D DD

A recent bug-fix (c8d919a3) for triclinic 1D domain decompostion introduced a bug for boxes with box[YY][XX]!=0. Fixes #1656. Refs #1631.

Change-Id: l06b9376212390b73e90a3ce9704dee2bad9693fb

Revision 61f49916 - 12/15/2014 04:17 PM - Berk Hess

Add test cases to show bugs are fixed

- octahedron adds a fully trilinic test case
- dd121 adds a test case that will default to more ranks in a direction other than X (here, Y)

The reference data is generated with a "last known good" patch from release-5-0 from before the fix for #1631 was introduced, not that it really matters. The reference build is unaffected by any of the bugs, because it runs single-core.

Refs #1631, #1656

Change-Id: l46c63a91aaae19a37bbe39e0c973cb9888019591

**History**

#1 - 10/24/2014 03:44 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1631.
Uploader: Berk Hess (hess@kth.se)
#2 - 12/08/2014 10:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1631.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I06b9376212390b73e90a3ce9704dee2bad9693fb
Gerrit URL: https://gerrit.gromacs.org/4276

#3 - 02/05/2015 08:41 PM - Berk Hess
- Status changed from In Progress to Closed