Gromacs - Bug #1153
inconsistency error triggered in GPU neighbor search
02/20/2013 04:13 AM - Szilárd Páll

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</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>4.6.1</td>
</tr>
<tr>
<td>Affected version</td>
<td>4.6.1-dev</td>
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</tbody>
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**Affected version:** 4.6.1

**Description**

A recent commit ([8d6cc14](#)) introduced a bug which can trigger a software inconsistency error in certain cases.

The bug is consistently reproducible using [8d6cc14](#) with the attached tpr when running with domain-decomposition (two or more MPI ranks) and GPU mode, including emulation.

Program mdrun, VERSION 4.6.1-dev-20130218-8d6cc14
Source code file: /home/pszilard/projects/gromacs/gromacs-gpu/src/mdlib/nbnxn_search.c, line: 688

Software inconsistency error:
Lost particles while sorting

**Associated revisions**

**Revision bdcca19a - 03/05/2013 08:18 PM - Berk Hess**

fixed recent bug with sorting atoms for GPUs

The sort buffer in the nbnxn gridding for GPUs was made too small in 8d6cc146. This led to inconsistency errors (not incorrect output). This is fixed and the sort_atoms call is now made simpler and multiple consistency checks are now always on in debug builds.
Fixes #1153

Change-Id: Ifcdf45bb4de88e7584628d3ed2699e2fd469d5c6

**Revision 9b399648 - 06/13/2013 09:45 AM - Berk Hess**

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Fixes #1153

Change-Id: Ifcdf45bb4de88e7584628d3ed2699e2fd469d5c6
#1 - 02/20/2013 10:51 AM - Berk Hess
- Status changed from New to In Progress

Patch uploaded: https://gerrit.gromacs.org/#/c/2187

#2 - 04/29/2013 03:51 PM - Szilárd Páll
- Affected version set to 4.6.1

The fix has been merged and this open bug contributes to the slightly bizarre 78% "not done" state of 4.6.1. Can this be closed?

#3 - 04/29/2013 07:48 PM - Mark Abraham
- Status changed from In Progress to Resolved

#4 - 06/13/2013 09:55 AM - Berk Hess
- % Done changed from 0 to 100

Applied in changeset 9b3996483c517b8ca7ee34705fe6d65defbb2c0e.

#5 - 09/18/2013 06:00 PM - Szilárd Páll
- Status changed from Resolved to Closed

Files

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<tr>
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