GROMACS - Bug #2614

mdrun can exit with atom moved to far in DD or PME due to too small domains

08/16/2018 01:48 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status</th>
<th>Closed</th>
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<tr>
<td>Priority</td>
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</tr>
<tr>
<td>Assignee</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category</td>
<td>mdrun</td>
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<td>Target version</td>
<td>2018.3</td>
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<tr>
<td>Affected version</td>
<td>2018</td>
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<tr>
<td>Difficulty</td>
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Description
Because of the large nstlist values that are used now, often by default with GPUs, atom displacements are far larger than they use to be. This can lead to mdrun stopping with a fatal error due to particle moving too far in DD repartitioning or PME. Possible solutions are limiting the minimum domain size and/or maximum nstlist appropriately for the system.

Associated revisions

Revision 2cb82175 - 08/21/2018 01:49 AM - Berk Hess
Refactor calc_verlet_buffer_size()
Splitted parts, which will be reused, from calc_verlet_buffer_size(). This change is only code motion.
Refs #2614
Change-Id: l9cf68a2661ee10eb991240d2768c077df9f9c0c5

Revision cd41b0fe - 08/21/2018 03:10 PM - Berk Hess
Ensure domains are large enough for atom motion
The introduction of the dual pair list has led to larger nstlist values, which leads to larger atom displacements between domain decomposition steps. This has made it much more likely that "atom moved to far" errors appeared at DD and PME redistribution. Now minimum DD cell size setting correctly takes into account atom displacement (when there is a reference temperature).

Note that this can significantly increase the minimum DD cell size for solvent systems and slightly for systems with large molecules.
Fixes #2614
Change-Id: le41131e9eed3ef828928516a6b8e8bfb9b5ba2bdb

History

#1 - 08/17/2018 10:40 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2614.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~l9cf68a2661ee10eb991240d2768c077df9f9c0c5
Gerrit URL: https://gerrit.gromacs.org/8197

#2 - 08/17/2018 10:40 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2614.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~le41131e9eed3ef828928516a6b8e8bfb9b5ba2bdb
Gerrit URL: https://gerrit.gromacs.org/8198

#3 - 08/17/2018 10:43 AM - Berk Hess
- Status changed from In Progress to Fix uploaded

02/23/2020
I uploaded a fix for systems with a reference temperature. Note that for systems without T-coupling or T=0 will should think of a better solution than using the pairlist buffer size.

#4 - 08/17/2018 05:18 PM - Szilárd Páll

Berk Hess wrote:

Note that for systems without T-coupling or T=0 will should think of a better solution than using the pairlist buffer size.

Should we have a separate issue for that given that the current fix is partial -- asking because of the "Fix uploaded" status?

#5 - 08/21/2018 03:15 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset cd41b0f6b5a682c6fd05ebeaa7c139d45206d7.

#6 - 08/22/2018 11:21 AM - Paul Bauer

- Status changed from Resolved to Closed