GROMACS - Bug #1669

Issue with VV integrator and domain decomposition of small systems

01/12/2015 03:22 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>mdrun</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.5</td>
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<td>Affected version - extra info:</td>
<td></td>
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<td>Affected version:</td>
<td>4.5.1</td>
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Difficulty: uncategorized

Description

At the first MD step the virial computation for the VV integrator requires a backup of the velocities. The backup array was allocated using the global instead of the local atom count. For small systems the local atom count, including communicated and constraint atoms, can be larger than the global atom count. This can cause crashes due to a buffer out of range.

Associated revisions

Revision 78ae40d4 - 01/15/2015 11:04 AM - Berk Hess
Fix allocation issue with VV integrator
Allocation of temp buffers for VV and VVAK now uses state->natoms instead of top_global->natoms. Fixes #1669.
Change-Id: I64947405c138f601db7daa4f9628a04c0f9fa8bb

History

#1 - 01/12/2015 03:25 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1669.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I64947405c138f601db7daa4f9628a04c0f9fa8bb
Gerrit URL: https://gerrit.gromacs.org/4359

#2 - 04/09/2015 10:52 AM - Mark Abraham
- Status changed from New to Closed