### 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>
</tr>
</thead>
<tbody>
<tr>
<td>Priority</td>
<td>Normal</td>
</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>
</tr>
<tr>
<td>Affected version</td>
<td>4.5.1</td>
</tr>
</tbody>
</table>

**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: l64947405c138f601db7daa4f9628a04cff9fa8bb

**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: l64947405c138f601db7daa4f9628a04cff9fa8bb
Gerrit URL: https://gerrit.gromacs.org/4359

**#2 - 04/09/2015 10:52 AM - Mark Abraham**

- Status changed from New to Closed