Gromacs - Bug #1579
virtual sites type N does not work with OpenMP
08/19/2014 10:04 AM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.8
Affected version: 4.6.7

Description
With OpenMP the use of virtual sites type N results in a segv or completely incorrect vsite coordinates.

Associated revisions
Revision f86bed5e - 08/25/2014 01:42 PM - Berk Hess
Fixed bugs in vsiteN with OpenMP

Fixes #1579.
Change-Id: l42d234f4ad6a94e8f7b6b8236ea119860dd9f7ab

Revision 0336ab2d - 08/30/2014 04:17 PM - David van der Spoel
Fixes issue with vsiten and verlet buffers.

A loop counter for a loop over vsiten did not take into account that multiple entries make up one vsiten particle. Part of #1579.

Change-Id: lc9a79e89ea9ef8f529c9d4a6c5cf0565e9c7d

Revision f2007baa - 10/07/2014 07:23 PM - Berk Hess
Fixes issue with vsiten and Verlet buffers

Commit 0336ab2d only fixed part of the vsiten issue in the Verlet buffer calculation code. Parameters were read from incorrect memory locations, which could lead to a segmentation fault or incorrect masses for vsiten particles. It unlikely that this affected results. Part of #1579.

Change-Id: l76cdb94e34194d2f6d49d98a49486ce1d76d91a

History

11/25/2015
Gerrit received a related patchset '1' for Issue #1579.  
Uploader: Berk Hess (hess@kth.se)
Change-Id: I42d234f4ad6a94e8f76b8236ea119860dd9f7ab
Gerrit URL: https://gerrit.gromacs.org/3912

File vsiten.tgz added

The attached file reproduces the problem: the confout.gro shows that the vsiten particles have coordinates corresponding to 0 0 0 modulo a box length.

To reproduce:
grompp
mdrun

Gerrit received a related patchset '1' for Issue #1579.  
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: lcf9a79e89e9a9e8f9f529c9d4a8c5c05f65e9c7d
Gerrit URL: https://gerrit.gromacs.org/3964

Status changed from In Progress to Closed

Gerrit received a related patchset '1' for Issue #1579.  
Uploader: Berk Hess (hess@kth.se)
Change-Id: I76cdb94e34194d2f6d98a49486ce1d76d91a
Gerrit URL: https://gerrit.gromacs.org/4123

Status changed from Closed to Fix uploaded  
Target version changed from 4.6.7 to 4.6.8  
Affected version changed from 4.6.6 to 4.6.7

https://gerrit.gromacs.org/4123 only fixed part of the grompp issue.  
Due to incorrect parameter indexing, grompp could produce a segv, or nonsense parameters and thus vsite masses could be used for the buffer calculation. Since vsiten locations are usually heavy and/or used as interaction sites only, these have little or no effect on the buffer drift, so incorrect results are unlikely.

Berk Hess wrote:

https://gerrit.gromacs.org/4123 only fixed part of the grompp issue.
I don't understand - does 4123 complete the fix of 3912? If so, are we done here?

Due to incorrect parameter indexing, grompp could produce a segv, or nonsense parameters and thus vsite masses could be used for the buffer calculation. Since vsiten locations are usually heavy and/or used as interaction sites only, these have little or no effect on the buffer drift, so incorrect results are unlikely.

#8 - 04/20/2015 03:04 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

My last update contained the wrong gerrit number. It should have said:
https://gerrit.gromacs.org/#/c/3912/ only fixed part of the grompp issue.
https://gerrit.gromacs.org/4123 fixed the rest.
So this issue has been fully resolved.

#9 - 04/20/2015 03:05 PM - Berk Hess
- Status changed from Resolved to Closed

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
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<tbody>
<tr>
<td>vsiten.tgz</td>
<td>178 KB</td>
<td>08/19/2014</td>
<td>David van der Spoel</td>
</tr>
</tbody>
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