

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 - extra info:	Difficulty: uncategorized
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: I42d234f4ad6a94e8f7b6b8236ea119860dd9f7ab

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: Ic9a79e89ea9ef8f9f529c9d4a6c5cf05f65e9c7d

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: I76cdb94e34194d2f6d49d98a49486ce1df76d91a

History

#1 - 08/19/2014 10:05 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1579](#).

Uploader: Berk Hess (hess@kth.se)

Change-Id: I42d234f4ad6a94e8f7b6b8236ea119860dd9f7ab

Gerrit URL: <https://gerrit.gromacs.org/3912>

#2 - 08/19/2014 10:26 AM - David van der Spoel

- 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

#3 - 08/30/2014 04:19 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1579](#).
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: Ic9a79e89ea9ef8f9f529c9d4a6c5cf05f65e9c7d
Gerrit URL: <https://gerrit.gromacs.org/3964>

#4 - 09/05/2014 01:48 PM - Berk Hess

- Status changed from In Progress to Closed

#5 - 10/03/2014 03:25 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1579](#).
Uploader: Berk Hess (hess@kth.se)
Change-Id: I76cdb94e34194d2f6d49d98a49486ce1df76d91a
Gerrit URL: <https://gerrit.gromacs.org/4123>

#6 - 10/03/2014 03:28 PM - Berk Hess

- 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.

#7 - 04/09/2015 11:00 AM - Mark Abraham

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

vsiten.tgz	178 KB	08/19/2014	David van der Spoel
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