

## GROMACS - Bug #2223

### Orientation restraints broken with OpenMP

08/02/2017 07:14 PM - Mark Abraham

<b>Status:</b>	Closed	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	David van der Spoel	
<b>Category:</b>	core library	
<b>Target version:</b>	2016.4	
<b>Affected version - extra info:</b>	probably all since GROMACS 4.6	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	git master	

#### Description

I'm hazy on the details of why the issue occurs, or the form of the proper fix, but for posterity, the implementation of orientation restraints was buggy when run with OpenMP (so group scheme is fine, as is single-thread-per-MPI-rank with Verlet scheme).

For now, David has hacked that we go single threaded for orientation restraints during the bonded kernels. This will let us get the new test case merged and some other fixes testable.

#### Associated revisions

##### Revision 0be497b7 - 08/02/2017 07:14 PM - David van der Spoel

Worked around missing OpenMP implementation in orires.

The orientation restraint code is not aware of OpenMP threads and uses some global information. By only running it on the master node results are now independent of number of threads used.

Fixes #2223

Change-Id: le86f4bd4e645fa71a58114950f6a297b5788e022

##### Revision 71a17da6 - 08/15/2017 04:55 PM - David van der Spoel

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#### History

##### #1 - 08/02/2017 07:14 PM - Mark Abraham

- Status changed from New to Accepted

##### #2 - 08/02/2017 07:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#2223](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~master~le86f4bd4e645fa71a58114950f6a297b5788e022

Gerrit URL: <https://gerrit.gromacs.org/6814>

##### #3 - 08/02/2017 09:36 PM - David van der Spoel

- Status changed from Accepted to Resolved

Applied in changeset [0be497b7a9ea605dad3780c479c3018f3c93bc41](#).

**#4 - 08/03/2017 03:06 PM - Mark Abraham**

- Status changed from Resolved to Closed

**#5 - 08/15/2017 04:55 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2223](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~release-2016~1e86f4bd4e645fa71a58114950f6a297b5788e022

Gerrit URL: <https://gerrit.gromacs.org/6847>