

## GROMACS - Bug #2974

### position-restraints regressiontest fails on intel GPU with OpenCL

06/11/2019 12:09 AM - Szilárd Páll

<b>Status:</b> New	
<b>Priority:</b> Normal	
<b>Assignee:</b>	
<b>Category:</b> mdrun	
<b>Target version:</b> 2020.2	
<b>Affected version - extra info:</b> master	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2019.2	
<b>Description</b> Tested on i7-8550U + UHD 620 and i7-8559U + Iris Plus 655. Only reproduces without DD and nonbonded offloaded. The forces seem to be just slightly off.  Attached log and checkforce output.	
<b>Related issues:</b> Related to GROMACS - Bug #3405: intermitted OpenCL regressiontest failures <b>Accepted</b>	

#### History

##### #1 - 06/11/2019 12:10 AM - Szilárd Páll

Target tentative, unless we have a quick solution bump to next release.

##### #2 - 06/12/2019 10:42 AM - Mark Abraham

- Target version changed from 2019.3 to 2019.4

I reproduced on my i7-7500U (neo), but without leads, we'll have to bump this for now

##### #3 - 06/12/2019 01:24 PM - Szilárd Páll

Mark Abraham wrote:

I reproduced on my i7-7500U (neo), but without leads, we'll have to bump this for now

Sure, I agree.

##### #4 - 09/23/2019 06:43 PM - Szilárd Páll

Still failing on both 2019 and master. I have no leads, but it can't be a PME issue as this test does not use PME.

##### #5 - 09/24/2019 08:32 AM - Mark Abraham

The logic about whether and how position restraints get run is pretty convoluted, so I could well believe that force contributions could be missed

##### #6 - 09/24/2019 08:47 AM - Berk Hess

The differences are very small though, so I wouldn't exclude a too tight tolerance either.

##### #7 - 10/01/2019 11:12 AM - Paul Bauer

- Target version changed from 2019.4 to 2019.5

no fix in sight, bumped

##### #8 - 12/04/2019 12:40 AM - Szilárd Páll

Something changed that seems to make the same test on the same hardware on the current 2020 branch whereas on 2019 it still fails.

##### #9 - 12/04/2019 10:05 AM - Paul Bauer

should I move this to 2020 instead? to indicate it is fixed there?

**#10 - 12/04/2019 10:49 AM - Szilárd Páll**

It would be good to know what has changed, even if we don't fix it in 2019, so I'd prefer to not close this yet.

**#11 - 12/04/2019 06:18 PM - Szilárd Páll**

- *Subject changed from position-restraints regressiontest fails on intel GPU to position-restraints regressiontest fails on intel GPU with OpenCL*

**#12 - 12/20/2019 11:28 AM - Paul Bauer**

- *Target version changed from 2019.5 to 2020*

ok, changed to 2020 target

**#13 - 12/27/2019 04:38 PM - Paul Bauer**

- *Target version changed from 2020 to 2020.1*

I would prefer closing this instead

**#14 - 02/25/2020 03:52 PM - Paul Bauer**

- *Target version changed from 2020.1 to 2020.2*

still not sure what happens here

**#15 - 02/28/2020 07:59 PM - Szilárd Páll**

- *Related to Bug #3405: intermitted OpenCL regressiontest failures added*

**Files**

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md.log	20.3 KB	06/10/2019	Szilárd Páll
checkforce.out	39.4 KB	06/10/2019	Szilárd Páll