

GROMACS - Bug #1476

Odd behavior with verlet-buffer-drift

04/09/2014 08:15 AM - Roland Schulz

Status: New	
Priority: Low	
Assignee:	
Category: mdrun	
Target version: future	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 4.6.6	

Description

After change [a586b4168d35](#) the nbxn_vsite test failed with nstlist 25 (default for GPU). This was fixed for 4.6 by regressiontest change [92d615e56929](#). Two things are odd about this. When running the Gromacs version with the change but without the fix in the tests:

- The output in md.log is "The maximum allowed number of cells is: X 3 Y 3 Z 2". But then "There is no domain decomposition for 2 nodes". So something is wrong about the log output.
- It seems odd that we automatically change nstlist to a value which then causes an error. It seems it would make sense that we change nstlist at maximum as much, so that the requested number of nodes give a valid domain decomposition.

History

#1 - 04/09/2014 08:17 AM - Roland Schulz

- Description updated

#2 - 05/20/2014 05:02 PM - Szilárd Páll

Roland Schulz wrote:

- It seems odd that we automatically change nstlist to a value which then causes an error. It seems it would make sense that we change nstlist at maximum as much, so that the requested number of nodes give a valid domain decomposition.

Indeed, this can happen, IIRC I've seen it too.

it should be possible to the the effect of nstlist on DD and avoid failures (unlike avoiding slowdown which does happen too) - although it may require some complex logic (as the nstlist override happens before the DD initialization).

#3 - 05/20/2014 05:02 PM - Szilárd Páll

- Category set to mdrun

#4 - 06/09/2014 04:49 PM - Berk Hess

This message is not contradictory. It prints the maximum number of cells. In triclinic boxes with relatively large cut-offs, 2 domains in x or y might not work, whereas 1 or 3 will work. This is a bit counterintuitive, but unfortunately this is the case.

It would be nice to prevent the nstlist increase in such cases, but since that is done before the DD is initialized, this is hard. A better practical solution for this issue would be to allow one domain to utilize multiple GPUs. We are working on this.

#5 - 06/09/2014 04:49 PM - Berk Hess

- Priority changed from Normal to Low

- Target version set to future

#6 - 05/25/2016 01:45 AM - Erik Lindahl

I would agree with roland that the message itself is highly inconsistent, even though the code might not be. If we haven't done any work on this, could we at least update the error message to be more explicit and convey the message that even 2 nodes might not work in some cases?