GROMACS - Feature #1962

smarter box-size checking with the pull code

05/16/2016 10:18 PM - Chris Neale

Status: Closed
Priority: Low
Assignee: Berk Hess
Category: mdrun
Target version: 2016
Difficulty: uncategorized

Description

src/gromacs/pulling/pull.c on line 520 in gromacs v5.1.2 has a check that the distance between pull groups not get larger than 0.49 times the box size. It would be nice if this check were a little smarter given the mdp options. For example, if pulling is only along z, then a system with large z but relatively small x and y might fail this test when there is no good reason for the run to be stopped. The change would be in the max_pull_distance2() function also in pull.c

Associated revisions

Revision 3dfdadb8 - 07/07/2016 12:04 PM - Berk Hess
Relax pull PBC check

The check in the pull code for COM distances close to half the box was to strict for directional pulling. Now dimensions orthogonal to the pull vector are no longer checked. The check was actually not strict enough for directional pulling along x or y in triclinic units cells, but that is a corner case. Furthermore, the direction-periodic hint is now only printed with geometry direction.

Added tests for the maximum pull distance calcuation.

Fixes #1962.

Change-Id: I8e389ba3f0490ca67586fd10bdc9d71d9957ab45

History

#1 - 05/18/2016 01:40 PM - Semen Yesylevskyy
I was just about submitting the same one! We have a long and thin system and it fails due to smallest dimension over Y while pulling is along Z only.

#2 - 05/18/2016 05:10 PM - Chris Neale
Dear Semen:

my solution was to simply comment out the entire if statement near line 520 in pull.c so that this error never arises. Obviously not safe for general usage, but I convinced myself that for this particular run it would behave properly. It's an OK workaround until smarter checking is developed.

#3 - 05/18/2016 05:57 PM - Roland Schulz
Do you have a specific suggestion for how to make the smarter check? Of course we love most, direct code submission to gerrit ;). 

#4 - 05/18/2016 07:57 PM - Chris Neale
Let me take some more time to diagnose this. Looking again at max_pull_distance2(), it does seem to do what one would want (i.e., it excludes dimensions that are turned off from the test for distances that are too long). Furthermore, I made a test system with box dimensions 3x3x90 nm and two atoms separated by 30 nm along z with a pull only in z and the simulation did not complain. Unfortunately, I have deleted my system that gave the error message upon exit. It seems likely that I actually just did something wrong. Semen, what is your usage for the pull code .mdp parameters that gives this issue and how quickly do you get the message? I recall that I got it in less than a minute, but I'm having trouble reproducing it now.

#5 - 05/18/2016 08:58 PM - Chris Neale
After further review, I withdraw the request. I must have made some other error. I think that the checking is actually pretty smart. It doesn't work when pull-coord1-vec = 0 0 1 and pull-coord1-dim = Y Y Y, but it does work when pull-coord1-dim = N N Y, so the user already has a workaround. Thank you, Chris.

#6 - 05/19/2016 02:33 PM - Semen Yesylevskyy
I can't check if this workaround works for me now, but if it is this have to be clearly written in the manual since such fails due to the box size are usual and rather annoying.

#7 - 05/19/2016 04:48 PM - Semen Yesylevskyy
Chris Neale wrote:
Semen, what is your usage for the pull code .mdp parameters that gives this issue and how quickly do you get the message? I recall that I got it in less than a minute, but I'm having trouble reproducing it now.

I can't reproduce it as well but for me it was complaining immediately.

#8 - 06/13/2016 04:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1962.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I9e99c2b1b3f259a758e110c6d858c5704671b703
Gerrit URL: https://gerrit.gromacs.org/5954

#9 - 06/17/2016 02:36 PM - Mark Abraham
- Assignee set to Berk Hess
- Target version changed from future to 2016

#10 - 06/21/2016 10:47 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1962.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I8e389ba3f0490ca67586fd10bdcd9d71d9957ab45
Gerrit URL: https://gerrit.gromacs.org/5971

#11 - 06/21/2016 10:53 AM - Berk Hess
I just realized the extra, unused dims are not an issue at all. I think that before I thought that we would not always get the closest periodic image distance in dr, but we actually do.
I uploaded a proper fix at:
https://gerrit.gromacs.org/#/c/5971/

#12 - 06/22/2016 05:42 PM - Mark Abraham
- Status changed from New to Fix uploaded

#13 - 07/07/2016 05:54 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 3dfdadbd8b7d632e4602d9348a4ff1c7f56115472.

#14 - 07/08/2016 01:48 AM - Erik Lindahl
- Status changed from Resolved to Closed