pull-code constant-force direction gives unexpected error about distance larger than box size

I am trying to use the pull code to add a constant force in a particular direction. I am getting an error that the initial distance is greater than 1/2 the box size. (error in 4.5.5, 4.6.1, 4.6.3)

I checked the online .mdp options:
http://manual.gromacs.org/online/mdp_opt.html#pull

which read as if there is no concept of "distance" in this case, just an applied force along the specified vector.

My .mdp options are:

```
pull                    = constant-force
pull_geometry           = direction
pull_dim                = Y Y Y
pull NSTxout            = 500
pull NSTfout            = 500
pull ngroups            = 1
pull group1             = r_1_&_CA
pull pbcatom1           = 0
pull k1                 = 30
pull vec1               = -0.848 -0.179 0.497
```

And when I run:
grompp -p ../this.top -c ../start.gro -n ../index.ndx -f this.mdp

The error message is:

```
Pull group 1 'r_1_&_CA' has 1 atoms
Number of degrees of freedom in T-Coupling group System is 113574.00
```

WARNING 1 [file this.mdp]:
You are using an absolute reference for pulling, but the rest of the system does not have an absolute reference. This will lead to artifacts.

```
Largest charge group radii for Van der Waals: 0.040, 0.040 nm
Largest charge group radii for Coulomb: 0.079, 0.079 nm
Calculating fourier grid dimensions for X Y Z
Using a fourier grid of 64x64x96, spacing 0.117 0.117 0.110
Pull group natoms pbc atom distance at start reference at t=0
0 0 0
1 1 0
```

Program grompp, VERSION 4.6.3
Source code file: /project/p/pomes/cneale/GPC/exe/intel/gromacs-4.6.3/source/src/mdlib/pull.c, line: 331

Fatal error:
Distance of pull group 1 (4.706043 nm) is larger than 0.49 times the box size (3.738000)
For more information and tips for troubleshooting, please check the GROMACS website at http://www.gromacs.org/Documentation/Errors
initial position of r.1 & CA: 5.466 3.477 2.453
pull_vec1: -0.848 -0.179 0.497
box:  7.47600  7.47600 10.55300
shortest distance from initial position of r.1 & CA to (0,0,0): 2.01 3.477 2.453 = 4.706

But why does it matter what the distance from (0,0,0) to the initial position is?

Moreover, adding pull_start = yes does not change the error, nor does setting pull_init1 = 5.466 3.477 2.453
(I didn't expect pull_init1 to have any effect, but I tried it just in case).

Finally, If I do use direction-periodic, I don't get an error with grompp, but I get the following output,
which is hard for me to align with my current understanding of what the pull code should be doing:

Pull group  natoms  pbc atom  distance at start     reference at t=0
0         0         0
1         1         0   2.301                 0.000

(why is there a "distance at start" and why is the reference at t=0 affected if I set:
pull_init1 = 5.466 3.477 2.453)

Pull group  natoms  pbc atom  distance at start     reference at t=0
0         0         0
1         1         0   2.301                5.466

when pull_init1 is supposed to be ignored for constant-force pulling?

This may be related to: http://gromacs.5086.x6.nabble.com/constant-force-pulling-td5010180.html

I originally posted this at: http://lists.gromacs.org/pipermail/gmx-users/2013-October/084598.html

Commenting out the gmx_fatal() call in src/mdlib/pull.c, line: 331 and recompiling grompp and mdrun
allows the run to proceed. Everything is stable for 250 ps. I will report if it fails.

Proposed solution is to:
(a) wrap the gmx_fatal call at line 331 of src/mdlib/pull.c like this:

```c
if (max_dist2 >= 0 && dr2 > 0.98*0.98*max_dist2 && !(pull->eGeom == epullgDIR && ePull == epullCONST_F))
{
    gmx_fatal(FARGS, "Distance of pull group %d (%f nm) is larger than 0.49 times the box size (%f)", g, sqrt(dr2),
    sqrt(max_dist2));
}
```
// requires sending the value of ePull to get_pullgrps_dr() in src/mdlib/pull.c calling functions do_constraint() get_pullgrp_dr()
pull_constraint() get_pullgrp_distance() and in src/mdlib/constr.c constrain() and perhaps other functions that I have missed (or why
not redefine ePull as a boolean flag and have all of the relevant information (including the enumerated ePull in the pull type?).

(b) Modify the output to the log file in the src/kernel/readpull.c function set_pull_init() so that it doesn't output an intital distance when
pull->eGeom == epullgDIR for the output that comes after:

```c
fprintf(stderr, "Pull group natoms pbc atom distance at start reference at t=0\n");
```

Thank you,
Chris.

Associated revisions
Revision d72236eb - 05/20/2014 10:33 AM - Rossen Apostolov
Added a note about using direction-periodic pulling.
Files attached can be run through grompp and mdrun successfully only after commenting out the gmx_fatal() call at line 331 in pull.c

#2 10/06/2013 07:20 PM - Chris Neale
I am currently running 500 simulations, all of which are still running stably after 5 ns of simulation each (total of 2.5 us) using the binary in which I have commented out the above mentioned gmx_fatal() call. Furthermore, the force vector seems to be acting as I intended.

#3 10/09/2013 03:40 PM - Berk Hess
I think this is one of the cases where direction-periodic is useful: it circumvents the check (and does some other magic which, I hope, should not affect your results).

#4 10/22/2013 04:26 PM - Berk Hess
Status changed from New to Feedback wanted

#5 01/10/2014 11:30 PM - Rossen Apostolov
Bump: Berk, shall we e.g. modify the log output as Chris suggests or not just leave it the way it is?

#6 04/17/2014 02:57 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1352.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: If7793ad08cfb975a6893ba9f54ebabc64cbd0fb0
Gerrit URL: https://gerrit.gromacs.org/3376

#7 04/17/2014 02:58 PM - Rossen Apostolov
I added a note about it in 5.0. Let me know what you think.

#8 04/17/2014 03:00 PM - Rossen Apostolov
Status changed from Feedback wanted to Fix uploaded

#9 05/06/2014 03:28 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1352.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: If7793ad08cfb975a6893ba9f54ebabc64cbd0fb0
Gerrit URL: https://gerrit.gromacs.org/3410

#10 05/06/2014 03:30 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1352.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I867fe1372b82063bb221880e8021089f9ded14e7
Gerrit URL: https://gerrit.gromacs.org/3411
#11 - 05/13/2014 01:59 PM - Rossen Apostolov
- Assignee set to Rossen Apostolov
- Target version set to 4.6.x

#12 - 06/19/2014 12:09 PM - Rossen Apostolov
- Status changed from Fix uploaded to Closed

Files

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<td>10/05/2013</td>
<td>Chris Neale</td>
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