The issue sounds related to Bug #1660.

With

```plaintext
pbc = xy
nwall = 2
```

and cutoff-scheme = group everything runs fine.

When I switch to cutoff-scheme = verlet the simulation crashes with a floating exception.

History

#1 - 10/26/2015 02:37 PM - Berk Hess
- Status changed from New to In Progress

Your simulation crashes because an H atom is beyond the top wall. This can happen because your tabulated potential is far too weak to keep the water oxygens away from the wall: at distance zero the potential is 0.77*C6 (C6=0.0025, if I'm not mistaken), which is much smaller than 1. You should increase the potential by several orders of magnitude.

Still the crash here could happen in valid circumstances, e.g. when the user sets r-linpot. But there is not an easy solution to this without affecting performance for common run setups. I'll think a bit more...

#2 - 05/08/2016 11:56 AM - Erik Lindahl

Berk: Can we add a check for this?

Gromacs should never ever just crash, so there is something wrong with code that produces a floating-point exception. If the price for that is lower performance, so be it, IMHO.

#3 - 05/26/2016 12:02 AM - Erik Lindahl
- Assignee set to Berk Hess
- Target version set to 2016

#4 - 09/07/2016 03:24 PM - Mark Abraham
- Description updated

#5 - 09/07/2016 03:24 PM - Mark Abraham
- Target version changed from 2016 to 2016.1

#6 - 10/31/2016 11:35 AM - Mark Abraham
- Target version deleted (2016.1)

Files

- group.tar.gz 10.6 MB 10/15/2015 Joerg Sauter