GROMACS - Bug #177

position and velocity set to nan

11/16/2007 11:18 PM - Yang Ye

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	3.3.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

it is an customized FF with section

[dihedraltypes]
; i l func q0 cq
;added by Dongsheng
OM OM 0 0.000 1 2
OA OA 0 0.000 1 2
OM OA 0 0.000 1 2

in ffpolymerbon.itp

If there is entries like following in topol.top
[dihedrals]
1 2 3 4 1

It will result in nan in position and velocity and cause error
---
Program mdrun_s, VERSION 3.3.1
Source code file: nsgrid.c, line: 220

Fatal error:
Number of grid cells is zero. Probably the system and box collapsed.

I have verified in bondfree.c that coordinates are the same after calling pdihs.

If there is no dihedral defined in topol.top. The simulation is alright.

Is there any other place which changes the coordinate?

History

#1 - 11/16/2007 11:23 PM - Yang Ye

Created an attachment (id=257)
test case

test file including force field and run files.

type "grompp" and "mdrun" to run the case.

#2 - 11/19/2007 03:04 PM - David van der Spoel

This is because your dihedrals are exactly 0, that is all 4 atoms are co-linear. With more "physical" input this wouldn't happen.

#3 - 11/19/2007 04:39 PM - David van der Spoel

OK, I have made a fix where the dihedral gives zero force if it is completely linear. That means the simulation will not crash but the forces may be discontinuous close to a linear molecule. In addition the linear angles will also give you a discontinuous force close to 180, basically because we disallow 180 degrees angles altogether. This is not a pretty solution but it's the best I can do.

The dihedral angle is defined as the angle between two planes, however we cannot make these planes since the vectors making up the planes are on a line, hence the planes are undefined.

Erik, shall I commit this fix?

#4 - 11/19/2007 05:47 PM - Erik Lindahl

Hi,

That sounds like the only reasonably alternative, so please do!

#5 - 11/19/2007 07:19 PM - David van der Spoel

Created an attachment (id=265)
gmx/include/vec.h

New vec.h

#6 - 11/19/2007 07:19 PM - David van der Spoel

Created an attachment (id=266)
gmx/src/gmxlib/bondfree.c

#7 - 11/19/2007 07:20 PM - David van der Spoel

With the two file attached the problem is solved, but please keep in mind my previous comments.

#8 - 11/19/2007 07:56 PM - Yang Ye

Thanks. I am aware for the effects of the fix.

Files

temp2.tar.gz	24.1 KB	11/16/2007	Yang Ye
vec.h	19.7 KB	11/19/2007	David van der Spoel
bondfree.c	47.1 KB	11/19/2007	David van der Spoel