GROMACS - Bug #343

g_sas crash on x86_64

08/05/2009 11:46 AM - Edoardo Morandi

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Hi!
I'm running two Debian linux system, one i386 and one x86_64, both with the same version. I installed gromacs 4.0.5-3 (it's basically the 4.0.5). I have to do some solvent accessibility analysis, and I've got a big problem when trying to run one simulation on the x86_64 machine. In fact on the i386 one it goes perfectly, but in the other case g_sas crashes. I tried to compile it with -g flag, and I saw that there's a problem in nsc.c, at line 681. It seems this error is caused by an integer overflow at line 629, because we have:

d = xmax-xmin; nxbox = (int) max(ceil(d/ra2max), 1.);

From gdb I see that:
d = 2.9035636e+32
ra2max = 0.25
d/ra2max = 1.16142544e+33
...but nxbox = -2147483648

Same problem for nybox and nzbox. I don't know how this code works, but the problem should be around here. During the loop that starts at 670 I can see i changing from 0 to -2147483648 when setting to min(i,nxbox-1).

I hope I can help.
Bye and have a good work.

History

#1 - 08/05/2009 02:25 PM - Edoardo Morandi

Oh, I noticed one thing: I used a trajectory file modified by trjconv, in which I kept only the protein. If I use the original files the x86_64 machine goes too.

#2 - 08/13/2009 10:06 PM - Berk Hess

I think I fixed this bug for the git master branch.
I just put the fix in the 4.0 release branch for 4.0.6.

To check that this is what I think:
I assume you have a trilinic box, probably a rhombic dodecahedron?
Does g_sas not crash when you use -nopbc?

If both answers are yes, I fixed the bug and we can close it.

Berk

#3 - 08/21/2009 07:06 PM - Edoardo Morandi

I tried the cvs version, and g_sas doesn't crash anymore. The bug can be closed.
Thanks for your support and good work!