GROMACS - Bug #348

Hanging / Segfaulting Gromacs

09/24/2009 05:27 PM - schrader empty

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

Description

Created an attachment (id=391)
two topol.tpr files

I'm using the very latest gromacs version.

Using two quite similar configurations (one without and one with very few water molecules) gromacs ends up in either hanging at step 600 oder segfault after step 400.

History

#1 - 09/25/2009 11:23 AM - Berk Hess

You system seems to be simply instable.
mdrun -pforce 10000
will tell you that large forces start appearing at some point.

These kind of problems can not be detected easily in an
automated fashion. With constraint you would have probably
gotten constraint warnings before the hang/crash.

Your systems seems very unequilibrated.
Also I don't understand why you are running without constraints
and a timestep of 1 fs, you should probably use 0.5 fs.
But why not use bond constraints?

Berk

#2 - 09/25/2009 02:39 PM - schrader empty

I'm beginner, but will try with constraints / different timestep.
Thanks a lot for your answer!

Files

Archive.tar.gz	545 KB	09/24/2009	schrader empty