GROMACS - Bug #181

Pressure scaling distorts dodecahedron boxes

12/15/2007 10:12 PM - David van der Spoel

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

Description

When doing long simulations of dodecahedron (and most likely truncated octahedron boxes) combined with isotropic pressure scaling the box looses its shape a little bit due to the fact that all the components of the box vectors are scaled with the same number. A solution would be to keep the angles constant and only scale the box axes.

History

#1 - 12/18/2007 11:00 AM - Berk Hess

I assume this is only a very little bit, due to rounding errors,
right?

All easy fixes I can think of would destroy the binary reproducability.

Berk.

#2 - 12/18/2007 11:20 AM - Erik Lindahl

Hi,

Unfortunately not. David and I chatted about this on the flight back, and we've had hexagonal boxes where the angle between the vectors change several degrees during ~100ns.

#3 - 12/18/2007 04:38 PM - Berk Hess

I now see that I also have 3 degrees deviation after 800 ns.

I have been thinking about a solution.
One option would be to check if the box angles or relative
box vector components are close to "nice" values and then
fix the relative value by only scaling the length or the box
diagonal and then determining the other components "exactly".
This would still result in reproducable runs.
The only disadvantage is that one would need to check for
several "nice" values which would affect the performance somewhat,
although probably negligibly for most systems.

Berk.

#4 - 02/13/2008 02:41 PM - Berk Hess

I fixed this issue by storing and using box components
relative to box[XX][XX] when using (semi)isotropic pressure coupling.
Components that are affected by the deform option are not relative.

Berk.