GROMACS - Bug #22

simulation box increase abnormally with emty space formation

10/19/2005 05:00 PM - Dai Liang

Status:	Closed		
Priority:	High		
Assignee:	David van der Spoel		
Category:	mdrun		
Target version:	3.2.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

when I simulated a DNA counter-ion system in a parallelogram box (bottom line of GRO file 3.90480 3.38166 7.20000 0.0000 0.0000 1.95240 0.0000 -0.0000 -0.0000), I found a strange phenomenon. During the simulation, the box size increased fast but there was a lot of empty space in the box (not filled by any atom)when I view by ngmx. Before viewing, I used trjconv -pbc inbox to make sure every atom in the box. Now I fix the simulation box size and it still happens, i.e. some empty space in the corner of box. Before it, I simulated in rectangle box many times and this strange phenomenon never happened. So I am wondering is it caused by the parallelogram box used?

Thanks very much

History

#1 - 11/28/2005 02:38 PM - David van der Spoel

Have you tried equilibrating with constant volume?