

GROMACS - Bug #12

Forces between frozen particles contribute to pressure.

09/12/2005 05:49 PM - Ramon Garcia

Status: Closed	
Priority: Low	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 3.2.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
If two particles are frozen, their force should not contribute to pressure. It does currently in Gromacs.	

History

#1 - 09/12/2005 05:57 PM - Erik Lindahl

Frozen means a particle is not moved in the update algorithm, but all interactions are still calculated for it (and it should thus contribute to pressure - imagine the case where just one particle is frozen). To avoid interactions and pressure, use exclusions or exclusion groups.

#2 - 09/12/2005 09:25 PM - Ramon Garcia

This is the opposite of what the user expects. Furthermore, it produces broken results with a barostat. As those interactions may create high pressure, the barostat makes the system expand, but the frozen particles do not move. This causes the system to explode.

#3 - 09/12/2005 09:47 PM - Erik Lindahl

Again, this is not a bug - the code behaves as intended and documented. The proper way to deal with the problem described is exclusions. You could argue that it would be nice if grompp created this exclusion automatically, but that's a discussion for the mailing list, not the bugtracker.

#4 - 09/12/2005 11:41 PM - Ramon Garcia

OK.

I will try to implement this feature if I have time.