GROMACS - Bug #404

energy increase in nvt and nve simiulations

04/06/2010 02:43 PM - srinivasa rao

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	4.0_rc1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Hi

When i am trying to run NVT and NVE simulations, i found that energy is continuously blowing up. I have two temperature coupling groups in my system. This observation is made only when i freeze portion of my system, on the other hand if i repeat the simulations with out freezing options energy is fine.

Herewith i am attaching the tpr and gromacs files that i have used to run the simulation.

Thanks very much
Srinivas.

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History

#1 - 04/06/2010 02:45 PM - srinivasa rao

Created an attachment (id=444)
tar file contains the tpr, md.mdp and .gro files that i have used for the simulations

#2 - 04/21/2010 04:18 PM - Berk Hess

Your setup is internally inconsistent.
You can not accelerate one group, free the rest
and fix the center of mass.
It does not surprise me that the system blows up.

Berk

Files

prepare.tar	4.99 MB	04/06/2010	srinivasa rao