GROMACS - Feature #760

Implement rigid body groups

06/03/2011 05:19 PM - Adam Herbst

Status:	New	
Priority:	Low	
Assignee:	Berk Hess	
Category:	mdrun	
Target version:	future	
Difficulty:	uncategorized	

Description

It should be possible to treat a group of atoms from the index file as a rigid body in one or more dimensions. The "freezedim" parameter of the .mdp file could be modified so that "Y" means frozen, "N" means free, and "R" means all atoms of the group must have the same velocity in this dimension. Hurdles that must be overcome include:

-potential unstable oscillations of the rigid body group unless damping is included
-efficient parallel summation of the forces on the group at each timestep, when running a parallel simulation
-rotation of the rigid body when 2 or more dimensions are specified as "R"

I posted a fork on the Git repository called "rigidbody-4-5" that implements a rudimentary version of this, with no rotation and a hard-coded damping coefficient. Also, I am not sure whether I calculate the mass of the rigid body group correctly.

History

#1 - 08/22/2011 05:36 PM - Berk Hess

- Priority changed from Normal to Low

#2 - 12/30/2012 06:04 AM - Teemu Murtola

- Target version set to future