GROMACS - Feature #2018

Pulling along a line between given points

07/27/2016 09:59 AM - Semen Yesylevskyy

Status:	New	
Priority:	Normal	
Assignee:		
Category:		
Target version:		
Difficulty:	uncategorized	

Description

Pulling the molecule strictly along the line connecting points A and B (which are either absolute coordinates or centers of masses of two groups) is needed sometimes. This means not along the vector AB but exactly along the connecting line. Current pull options do not allow this because one can only define the distances from A and B but can't ensure that the molecule will always reside in a straight line between these two points. Such pulling is essentially "direction-relative" plus a constraint, which keeps the moving group at a connecting line.
It is possible to emulate such pulling roughly with two "distance" pull coordinates if A and B are absolute coordinates, but if A and B are centers of two groups it's impossible to do now.