GROMACS - Feature #3410

Random Acceleration Molecular Dynamics (RAMD)

03/05/2020 03:22 PM - Bernd Doser

Status:	New
Priority:	Normal
Assignee:	Bernd Doser
Category:	mdrun
Target version:	2021
Difficulty:	uncategorized

Description

The RAMD method was developed in the group of Rebecca Wade (MCM) at HITS (https://www.h-its.org/research/mcm/). It is a method to carry out molecular dynamics simulations with an additional randomly oriented force applied to a molecule in the system. Please find more details about the method at https://projects.h-its.org/mcm/software/ramd/.

Based on an implementation in NAMD, the RAMD method is now implemented in GROMACS. The code is already public available as https://github.com/HITS-MCM/gromacs-ramd. Now, we would like to integrate the new feature to the official GROMACS repository.

I, as a permanent software developer at HITS, will be responsible for the integration process and the future maintenance. Stefan Richter and Daria Kokh (MCM group) will be responsible for methodical questions.

The GROMACS-RAMD implementation is using the PULL code. The corresponding pull mdp options will be set during the preprocessor depending on the RAMD mdp options.