GROMACS - Feature #1627

DPD integrator

10/17/2014 04:51 PM - Berk Hess

Status:	In Progress	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:		
Difficulty:	uncategorized	

Description

The MD group in Groningen has developed a DPD integrator with nice properties, which we would like to include in the Gromacs distribution.

There is a basic version, but some work needs to be done to make it work with MPI, (OpenMP) threads, the Verlet cut-off scheme and constraints.
I am not up to date on the details of the integrator. Nicu, could you post a link to the manuscript describing the integrator?

I assume the integrator should randomly pick a fraction of the pairs to act on. Then we need an mdp parameter to set this and then loop over the complete nbnxn pairlist (multi-threaded) and select pairs using a random number generator. All our other stochastic integrators now produce reproducible dynamics, even when running on different numbers of ranks and/or threads. It is going to be hard to achieve that for DPD. The only easy way I can see to achieve this is to use a random number for each particle pair, which is going to be very expensive when the probability of taking a pair is set low.

Related issues:

Related to GROMACS - Feature #1885: DPD Thermostat	**New**

History

#1 - 10/17/2014 05:11 PM - Nicolae goga

- File proof.pdf added

Thanks Berk,

Here is the link to the article:

http://gbb.eldoc.ub.rug.nl/FILES/root/2012/JChemThCompGoga/2012JChemTheoryComputGoga.pdf

Constraints had a problem. Therefore a second article was written and published quite recentely. Attached here as a file.

Keep in touch
Nicu

#2 - 04/09/2015 11:26 AM - Mark Abraham

- Target version changed from 5.1 to 5.x

#3 - 07/11/2016 08:08 PM - Mark Abraham

- Target version deleted (5.x)

#4 - 01/07/2019 01:59 AM - Mark Abraham

- Related to Feature #1885: DPD Thermostat added

Files

proof.pdf	645 KB	10/17/2014	Nicolae goga