GROMACS - Feature #2307

Implement MiMiC-based QM/MM functionality in GROMACS

11/28/2017 12:53 PM - Viacheslav Bolnykh

Status:	Closed
Priority:	Normal
Assignee:	Viacheslav Bolnykh
Category:	
Target version:	2019
Difficulty:	hard

Description

Within BioExcel project we are tasked to develop a new QM/MM interface between GROMACS and CPMD. The new interface is done using Multiple-Program Multiple-Data approach. Within this strategy both CPMD and GROMACS are running in parallel independently. GROMACS is used as an MM force provider in this framework. In the beginning of a timestep GROMACS receives the set of coordinates, computes forces and potential energy and sends them to CPMD. CPMD is handling the QM forces as well as the integration and thermostats.

In order to achieve that a number of things has to be done:

1. Zero charges in the QM region of GROMACS (to avoid double-counting of electrostatics)
2. Remove LJ interactions between QM atoms (modification of exclusion lists)

This would require the modification of the GROMACS preprocessor to zero charges and modify intra-molecular exclusion lists. Moreover, additional changes in core GROMACS are required. First, we need to implement inter-molecular exclusions of non-bonded interactions of QM atoms with QM atoms. Then, additional work is needed to implement the MiMiC protocol (see attached pdf document)

Subtasks:

Feature # 2308: Implement QM/MM updates in GROMACS preprocessor	**Closed**
Feature # 2309: Implement MiMiC QM/MM workflow in the GROMACS core	**Closed**
Task # 2690: relax new dependency cycle	**Closed**
Feature # 2691: MiMiC needs reference documentation	**Closed**

History

#1 - 11/28/2017 01:10 PM - Viacheslav Bolnykh

For some reason I cannot set the relations between issues but this is the parent issue to issues #2308 and #2309

#2 - 11/28/2017 05:56 PM - Mark Abraham

- Target version changed from 2018 to 2019

#3 - 10/08/2018 06:53 PM - Mark Abraham

- Status changed from New to In Progress

#4 - 11/27/2018 03:39 PM - Mark Abraham

- Subject changed from Implememnt the QM/MM functionality in GROMACS to Implement MiMiC-based QM/MM functionality in GROMACS

#5 - 11/29/2018 10:55 AM - Mark Abraham

- Status changed from In Progress to Fix uploaded

#6 - 12/03/2018 03:54 PM - Paul Bauer

- Status changed from Fix uploaded to Closed

Files

protocol_doc.pdf	227 KB	11/28/2017	Viacheslav Bolnykh