

GROMACS - Feature #2308

Feature # 2307 (Closed): Implement MiMiC-based QM/MM functionality in GROMACS

Implement QM/MM updates in GROMACS preprocessor

11/28/2017 01:05 PM - Viacheslav Bolnykh

Status:	Closed
Priority:	Normal
Assignee:	Viacheslav Bolnykh
Category:	preprocessing (pdb2gmx,grompp)
Target version:	2019
Difficulty:	hard
Description	
In order to support the new QM/MM workflow developed within BioExcel (working name MiMiC) we need to implement new features in the preprocessor.	
<ol style="list-style-type: none">1. Additional group to define QM/MM atoms (to avoid overlap with an old QM/MM code)2. New input file section mimic-grps of type string - to define the QM group3. Modifications of options in QMMM section: no (no QM/MM), yes (original QM/MM implementation), mimic (MiMiC QM/MM interface)4. Zeroing charges of QM atoms5. Update the intra-molecular exclusion lists6. Replace bonds between QM atoms with CONNBOND7. Add tests for the new functionality	

Associated revisions

Revision 61e7a6a1 - 10/09/2018 01:50 PM - Viacheslav Bolnykh

Implemented changes to preprocessor to work with MiMiC QM/MM

Added new integrator "mimic" and updated usage of QMMM-grps to be used with MiMiC QM/MM. Updated code zeros charges within QM region and changes bonds to CONNBOND and updates exclusion lists to exclude non-bonded interactions between quantum atoms

Refs #2308

Change-Id: I34e798ae0c54457dad8f9a8f220482468db34708

History

#1 - 11/28/2017 02:16 PM - Aleksei lupinov

- Parent task set to #2307

#2 - 11/28/2017 05:58 PM - Mark Abraham

- Target version changed from 2018 to 2019

#3 - 01/05/2018 06:19 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2308](#).

Uploader: Viacheslav Bolnykh (bolnykh@gmail.com)

Change-Id: gromacs~master~I34e798ae0c54457dad8f9a8f220482468db34708

Gerrit URL: <https://gerrit.gromacs.org/7434>

#4 - 10/08/2018 06:53 PM - Mark Abraham

- Status changed from New to Fix uploaded

#5 - 10/12/2018 02:36 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

#6 - 10/12/2018 02:36 PM - Mark Abraham

- Status changed from Resolved to Closed