

GROMACS - Feature #2691

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

MiMiC needs reference documentation

10/12/2018 08:28 AM - Mark Abraham

Status:	Closed	
Priority:	Normal	
Assignee:		
Category:	core library	
Target version:	2019	
Difficulty:	uncategorized	
Description		
The reference manual needs a description of what the functionality computes, how it interacts with MiMiC. User guide might need what needs to go in the .tpr, how that matches with CPMD, etc.		
Related issues:		
Has duplicate GROMACS - Feature #2780: Add documentation for MiMiC QM/MM inte...		Closed

Associated revisions

Revision c01282f3 - 11/29/2018 09:01 PM - Viacheslav Bolnykh

Added reference-manual entry for MiMiC

Added the documentation entry describing the way to set up and run the QM/MM simulation with MiMiC, plus cross references to install guide and mdp options documentation.

Fixes #2691

Change-Id: Id600c621d24bb41f99b02ddb8bacb175a6bac520

History

#1 - 10/30/2018 12:01 PM - Mark Abraham

Documentation about what is implemented and how to use it are still needed, Slava

#2 - 11/27/2018 03:38 PM - Mark Abraham

I have reminded Slava and Emiliano again

#3 - 11/28/2018 12:18 PM - Viacheslav Bolnykh

Mark Abraham wrote:

I have reminded Slava and Emiliano again

Sorry, I have not seen notifications about this issue and created another one by accident

#4 - 11/28/2018 12:19 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2691](#).

Uploader: Viacheslav Bolnykh (bolnykh@gmail.com)

Change-Id: gromacs~release-2019~Id600c621d24bb41f99b02ddb8bacb175a6bac520

Gerrit URL: <https://gerrit.gromacs.org/8754>

#5 - 11/29/2018 10:42 AM - Mark Abraham

- Has duplicate Feature #2780: Add documentation for MiMiC QM/MM interface added

#6 - 11/29/2018 10:45 AM - Mark Abraham

- Status changed from New to Fix uploaded

#7 - 11/29/2018 09:15 PM - Viacheslav Bolnykh

- Status changed from Fix uploaded to Resolved

Applied in changeset [c01282f3e2a587f131dca0bda867111ab42817e7](#).

#8 - 12/03/2018 12:06 PM - Paul Bauer

- Status changed from Resolved to Closed