

GROMACS - Feature #2283

Force distribution analysis

10/27/2017 11:31 AM - Bernd Doser

Status:	New
Priority:	Normal
Assignee:	Bernd Doser
Category:	analysis tools
Target version:	
Difficulty:	uncategorized
Description	
<p>The force distribution analysis (FDA) is a well-established tool for the calculation of time-resolved pairwise forces and stresses (http://dx.doi.org/10.1186/2046-1682-6-5). Please find a detailed documentation at https://github.com/HITS-MBM/gromacs-fda/blob/master-fda/fda-manual/fda-manual.pdf. At the moment, FDA is maintained in an extra GitHub repository https://github.com/HITS-MBM/gromacs-fda. We would like to integrate FDA into the official GROMACS repository.</p> <p>FDA is using core functions of GROMACS calculating the pairwise forces during a md rerun process. Therefore, an extra binary (mdrun_fda) will be used, which extract the pairwise forces during the rerun process. To obtain a clean separation of FDA and GROMACS, the FDA version will only be built if the cmake flag 'GMX_BUILD_FDA' is switched on. If 'GMX_BUILD_FDA' is switched off, the unchanged GROMACS binaries will be built.</p>	

Associated revisions

Revision c154e321 - 08/26/2019 06:02 AM - Test User

Activation of density fitting and move of module notifications

The densityfitting code is activated by adding it to the MDModules.

Moved the MdModuleNotifications to mdrunutility to break cyclic module dependencies between mdrun and applied_forces via MdModules and DensityFittingModuleInfo.

Observe that this patch changes the default .mdp output. Updated reference data accordingly. Note that the changes in .mdp output lead to "check mdp file differences" warning in the regression tests.

refs #2283

Change-Id: I93c0dd85285cac3f9e94d2dfc7c7fcc434aa81db

History

#1 - 10/27/2017 11:35 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2283](#).

Uploader: Bernd Doser (bernd.doser@h-its.org)

Change-Id: gromacs~master~I3694237be74250220200ee503434b20b921dde01

Gerrit URL: <https://gerrit.gromacs.org/7100>

#2 - 10/27/2017 11:44 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2283](#).

Uploader: Bernd Doser (bernd.doser@h-its.org)

Change-Id: regressiontests~master~I942b638d3d24b5ece7d9bf5553eb07b466d6b1b5

Gerrit URL: <https://gerrit.gromacs.org/7102>