

GROMACS - Task #2623

Feature # 2585 (Resolved): Infrastructure supporting external API

Allow extensible MDModules and forceProviders.

08/22/2018 05:01 PM - Eric Irrgang

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Difficulty: uncategorized	
Description	
gmxapi milestone 6 as described in #2585	
Provide for runtime extension of MDModules and the initialization of force providers.	
This task supports gmxapi milestones 7, 8, and 9, but the accompanying Gerrit change is small and has no dependencies, so it is submitted separately. This change also does not migrate the current lone IForceProvider because the binding protocols can be treated as separate issues. Alternatively, progress in other abstractions currently being developed could remove the need to bundle MDModules together like this, but for the moment it seems like the appropriate container.	
Related issues:	
Related to GROMACS - Feature #1972: external potential modules for refinement...	New
Related to GROMACS - Feature #2229: Full Object Oriented Modularization of GR...	New
Related to GROMACS - Task #2492: implement force calculation via ForceProvide...	New
Related to GROMACS - Feature #2574: iForceSchedule Abstraction	New
Related to GROMACS - Task #2590: Essential Dynamics as module providing forces	New
Related to GROMACS - Task #3040: Refactor Restraint module	New

Associated revisions

Revision 9864b201 - 08/29/2018 02:32 PM - Eric Irrgang

Allow extensible MDModules and forceProviders.

supports gmxapi milestone 6, described at #2585.

MDModules::Impl gets a std::vector for (shared) ownership of objects providing the IMDModule interface. An add() method is added to the MDModules public member functions, but the binding protocols are separated into separate issues to allow minimal changes and varying dependencies on other pending changes.

Relates to #1972, #2229, #2492, #2574, #2590.

Refs #2623

Change-Id: Ibb16d1453003213a49622810ed8bad4ed4b06e2d

History

#1 - 08/22/2018 05:03 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2623](#).

Uploader: M. Eric Irrgang (ericirrgang@gmail.com)

Change-Id: gromacs~master~Ibb16d1453003213a49622810ed8bad4ed4b06e2d

Gerrit URL: <https://gerrit.gromacs.org/8219>

#2 - 08/22/2018 05:03 PM - Eric Irrgang

- Related to Feature #1972: external potential modules for refinement against experimental data added

#3 - 08/22/2018 05:03 PM - Eric Irrgang

- Related to Feature #2229: Full Object Oriented Modularization of GROMACS MDRUN Codebase added

#4 - 08/22/2018 05:03 PM - Eric Irrgang

- Related to Task #2492: implement force calculation via ForceProviders containing collections of IForceProvider added

#5 - 08/22/2018 05:04 PM - Eric Irrgang

- Related to Feature #2574: iForceSchedule Abstraction added

#6 - 08/22/2018 05:04 PM - Eric Irrgang

- Related to Task #2590: Essential Dynamics as module providing forces added

#7 - 08/22/2018 05:05 PM - Eric Irrgang

- Description updated

#8 - 10/15/2018 03:44 PM - Eric Irrgang

- Status changed from New to Resolved

The gmx::MDModules object created during launch of Mdrunner now owns a list of MDModule objects through their IMDModule handle. Modules in the list may provide an IForceProvider.

In future work, the other IMDModule interfaces should be handled, and we should do whatever we need to to accommodate the initialization requirements such that built-in modules (electric field) can be handled the same way as externally provided modules. This is deferred to a separate issue for GROMACS 2020.

#9 - 07/18/2019 04:33 PM - Eric Irrgang

- Related to Task #3040: Refactor Restraint module added

#10 - 12/11/2019 12:39 PM - Eric Irrgang

- Status changed from Resolved to Closed