GROMACS - Feature #2229

Full Object Oriented Modularization of GROMACS MDRUN Codebase

08/10/2017 05:13 PM - Prashanth Kanduri

Status:	New
Priority:	High
Assignee:	Mark Abraham
Category:	mdrun
Target version:	future
Difficulty:	hard

Description

At CSCS, we aim to create a library out of GROMACS for the compute intensive non-bonded force computations. We envision an API consisting of a non-bonded computation back-end which developers could plug into their own custom MD simulation codes.

En route to accomplishing this, we would like to turn GROMACS's MDRUN program into a modular software where new and potentially exascale-friendly methods like FMM or Multigrid could be added by developers with little overhead. These would become new features for the GROMACS software package itself complementing the already efficient PME based methods.

This refactor would certainly beneficial for the GROMACS Development, but the library and API would allow developers/advanced users to write more complex programs consisting of ensembles, replica exchange, etc on their own MD code.

As a first step, we want to create a (global) Domain Decomposition Manager which amounts to aggregating the various functions that operate on the `gmx_domdec_t` struct and the struct itself into a single class object. Renaming functionalities with intuitive names would also be helpful. A flowchart providing a schematic of the planned refactor with the GROMACS workflow is attached for reference.

We are fully open for discussions and would look forward to your inputs.

Related issues:

Related to GROMACS - Feature #2585: Infrastructure supporting external API	**Resolved**
Related to GROMACS - Feature #2605: Library access to MD runner	**Closed**
Related to GROMACS - Task #2623: Allow extensible MDModules and forceProviders.	**Closed**

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 - 08/11/2017 04:49 PM - Vedran Miletic

Prashanth Kanduri wrote:

> At CSCS, we aim to create a library out of GROMACS for the compute intensive non-bonded force computations. We envision an API consisting of a non-bonded computation back-end which developers could plug into their own custom MD simulation codes.
>
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Are you aware of the modularization effort already in progress?

> This refactor would certainly beneficial for the GROMACS Development, but the library and API would allow developers/advanced users to write more complex programs consisting of ensembles, replica exchange, etc on their own MD code.
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> We are fully open for discussions and would look forward to your inputs.

#2 - 07/30/2018 05:47 PM - Eric Irrgang

- Related to Feature #2585: Infrastructure supporting external API added

#3 - 08/09/2018 02:32 PM - Eric Irrgang

- Related to Feature #2605: Library access to MD runner added

#4 - 08/21/2018 08:01 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2229.
Uploader: M. Eric Irrgang (ericirrgang@gmail.com)
Change-Id: gromacs~master~I1db1d34b07ec0f8ba5f246ab763c74ad9eafe8f3
Gerrit URL: https://gerrit.gromacs.org/8213

#5 - 08/22/2018 05:03 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2229.
Uploader: M. Eric Irrgang (ericirrgang@gmail.com)
Change-Id: gromacs~master~Ibb16d1453003213a49622810ed8bad4ed4b06e2d
Gerrit URL: https://gerrit.gromacs.org/8219

#6 - 08/22/2018 05:03 PM - Eric Irrgang

- Related to Task #2623: Allow extensible MDModules and forceProviders. added

Files

gromacs-workflow-diagram.png	65 KB	08/10/2017	Prashanth Kanduri