Task # 1793 (New): cleanup of integration loop

implement force calculation via ForceProviders containing collections of IForceProvider

04/26/2018 02:28 PM - Mark Abraham

Status: New
Priority: Normal
Assignee: Mark Abraham
Category: core library
Target version: future
Difficulty: uncategorized

Description
In order to simplify high-level code (#1793), implement hardware- and locality-aware task parallelism, and expose functionality to APIs (gmxapi, #2229) we need a more flexible framework for code that calculates forces. That is likely to include all such code implementing the IForceProvider interface, and for ForceProviders to arrange for them to be called. For now, that will also still involve t_forcerec. In future, it is hoped the collaboration between the ForceProviders, the available hardware, the state of any auto-tuners, user input, and the integration schedule (#1137) will be able to implement a highly flexible, modular, yet optimizeable, run-time framework to replace the hard-coded execution schedules in e.g. do_md() and do_force() (and sub-functions).

This will take a while and the exact endpoint is rather unclear!

Related issues:
Related to GROMACS - Task #2623: Allow extensible MDModules and forceProviders. Closed
Related to GROMACS - Task #3040: Refactor Restraint module New

Associated revisions
Revision 26ba7a31 - 05/24/2018 06:29 PM - Mark Abraham
Move responsibility for bonded threading decomposition

This is an aspect of force calculation, not of the topology needed for that force calculation.

Removed use of assert no longer needed now that the responsibility has been moved.

Also updated some use of struct keyword.

Refs #2492
Change-Id: lf9d356dc9c4de49b84f23e9c432baa84a8335731

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: lbb16d1453003213a49622810ed8bad4ed4b06e2d

History
#1 - 05/04/2018 12:26 AM - Gerrit Code Review Bot
Gerrit received a related patchset `1` for Issue #2492.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
There will need to be a lot other cleanup as we progress to this point, e.g. that data structures for bonded threading move from t_idef to t_forcerec.

Perhaps some wrapper around do_force and the relax_shell_flexcon will be helpful too.