

## GROMACS - Task #2492

Task # 1793 (New): cleanup of integration loop

### implement force calculation via ForceProviders containing collections of IForceProvider

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

<b>Status:</b>	New	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	Mark Abraham	
<b>Category:</b>	core library	
<b>Target version:</b>	future	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
<p>In order to simplify high-level code (<a href="#">#1793</a>), implement hardware- and locality-aware task parallelism, and expose functionality to APIs (gmxapi, <a href="#">#2229</a>) 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 <code>t_forcerec</code>. 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 (<a href="#">#1137</a>) will be able to implement a highly flexible, modular, yet optimizable, run-time framework to replace the hard-coded execution schedules in e.g. <code>do_md()</code> and <code>do_force()</code> (and sub-functions).</p> <p>This will take a while and the exact endpoint is rather unclear!</p>		
<b>Related issues:</b>		
Related to GROMACS - Task #2623: Allow extensible MDModules and forceProviders.		<b>Closed</b>
Related to GROMACS - Task #3040: Refactor Restraint module		<b>New</b>

#### 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: `If9d356dc9c4de49b84f23e9c432baa84a8335731`

##### 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](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~master~lf9d356dc9c4de49b84f23e9c432baa84a8335731  
Gerrit URL: <https://gerrit.gromacs.org/7828>

**#2 - 05/24/2018 09:29 AM - Mark Abraham**

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.

**#3 - 06/04/2018 10:57 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2492](#).  
Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))  
Change-Id: gromacs~master~l3c75d75b13c93d3159dea9a364bfa3258484bd68  
Gerrit URL: <https://gerrit.gromacs.org/7971>

**#4 - 08/22/2018 05:03 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2492](#).  
Uploader: M. Eric Irrgang ([ericirrgang@gmail.com](mailto:ericirrgang@gmail.com))  
Change-Id: gromacs~master~lbb16d1453003213a49622810ed8bad4ed4b06e2d  
Gerrit URL: <https://gerrit.gromacs.org/8219>

**#5 - 08/22/2018 05:03 PM - Eric Irrgang**

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

**#6 - 09/19/2018 03:13 PM - Mark Abraham**

- *Target version changed from 2019 to future*

**#7 - 07/18/2019 04:32 PM - Eric Irrgang**

- *Related to Task #3040: Refactor Restraint module added*