

## GROMACS - Task #3076

### Selectively activate MdModules during simulation instead of instantiating all of them

09/05/2019 11:36 AM - Christian Blau

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	Christian Blau
<b>Category:</b>	core library
<b>Target version:</b>	2021-infrastructure-stable
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
Change the interface to MdModules that allows the MdModules to subscribe to callbacks only after they know if they are active or not so that we avoid the	
<pre>if (module.active())</pre>	
within the modules that may be to easily overlooked.	

#### Associated revisions

##### Revision 6dc7d1ec - 02/18/2020 11:44 AM - Test User

Split MdModuleNotifications into topics

Use different notifiers to distinguish MdModule callbacks to

```
- preprocessing
- simulation setup
- checkpointing
```

refs #3076

Change-Id: I08b2ff7e90e42fce44043d7c0f2a9304d404445c

##### Revision 5c8a0229 - 03/05/2020 11:00 AM - Test User

Add function calls to MdModules to sign up for notifications

Allow MdModules to sign up to notifications after they know their own options. This makes it possible that modules only get called back when they need to and not by default and skips the if(active) logic in functions that are called back in favour of not subscribing to the notifications to begin with.

refs #3076

Change-Id: Ib95c1f734f919805c661ac6f6451af5da8187eec

#### History

##### #1 - 01/17/2020 02:40 PM - Christian Blau

Selective activation of the modules is easier when MdModules don't have to be constructed with the notifications early on, but can be handed the notification handles later.

Currently all notifications are subscribed to during module construction, but some notifications will only be needed during pre-processing at grompp-time, while others are only needed during md run setup, thus

```
- split notifications into pre-processing notifications, notifications during simulations, and checkpointing notifications
- hand over notification handle for pre-processing callbacks and simulation callbacks separately instead of all of them at construction time
- callback notifications only if modules are active
```