Selectively activate MdModules during simulation instead of instantiating all of them

GROMACS - Task #3076

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

Status: New
Priority: Normal
Assignee: Christian Blau
Category: core library
Target version: 2021-infrastructure-stable
Difficulty: uncategorized

Description
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

if (module.active())

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

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