The Parrinello-Rahman barostat using modular simulator does not allow restarts from checkpoint file.

Fatal error:
Cannot change a simulation algorithm during a checkpoint restart. Perhaps you should make a new .tpr with grompp [...] 

This error is thrown by the checkpoint loading routine. While the legacy implementation of the P-R barostat required the pressure at the previous step to be checkpointed, the modular implementation does not require this. load_checkpoint is, however, expecting this field to be present and throws an error.

While resolving this, another error was found. When initializing the modular simulator, the Parrinello-Rahman scaling might have happened one step too late under specific circumstances. Specifically, this could happen if the checkpoint was taken exactly on the scaling step, and later restarted from there. As checkpoint reading was not working, this is certain to never have happened, but needs to be fixed as well.

The steps to resolve this problem are as follows:

1. Move the decision on whether to use modular simulator before checkpoint reading. This change will be likely be useful very soon anyways, as checkpointing reading is planned to be modularized.
2. Fix the initialization of the scaling.
3. Fix the reading of checkpoints using Parrinello-Rahman.
4. Finally, this bug could only go unnoticed due to a lack of tests for the continuation using Parrinello-Rahman and md-vv (which was previously not implemented), so these need to be added.

Associated revisions

Revision 2078fd06 - 02/13/2020 03:45 AM - Pascal Merz
Expose vsite counting
This allows to check whether vsites are present before the respective object is created.
Refs #3377 (prepares point 1)
Change-Id: I8273daf38d46e2f052573f48323b5b6137965e9f

Revision 42ba62e1 - 02/14/2020 03:08 AM - Pascal Merz
Move modular simulator decision before checkpoint loading
Currently, the decision on whether to use modular simulator is done relatively late during the runner stage. This makes it impossible to allow for different behavior at checkpoint loading time. The current change therefore moves this decision before checkpoint loading time.
To achieve this, some adaptations were needed:

- Use gmx_mtop_interaction_count to determine whether virtual sites will be used before the respective object is created.
- The membrane embedding check via pointer is replaced by a boolean set earlier during the runner phase.
The essential dynamics check was split to catch command line inputs during the runner phase, and mismatching checkpointing data during the simulator phase (mirroring legacy behavior in do_md()).

Replace the ensemble restraint check by a low-level alternative for the early runner call (mimicking the distance restraint initialization), while keeping the current check for the simulator-level call. Note that as multi sims are disabled, this low-level test will effectively never fail, but the additional clarity is helpful in further development. The later test ensures that changes to the init_disres() don't make this check invalid - if they would ever get out of sync, the simulations would exit with a fatal error.

Refs #3377 (fixes point 1)

Revision 009ed957 - 02/14/2020 03:10 AM - Pascal Merz

Fix Parrinello-Rahman scaling on initial step (modular simulator)

If Parrinello-Rahman scaling was requested on the first step, it was not properly initialized. The setup routine would have correctly (although non-obviously so) calculated the scaling matrix, but have requested the propagator to use the scaling one step too late.

For new simulations, this never happens (since scaling happens on the second step, not the first). It could, however, lead to slight errors if restarting from a checkpoint occurred exactly on a scaling step. As restarting from Parrinello-Rahman simulations using modular simulator was broken anyway, we can be sure that this has never happened in practice.

This change fixes the bug, adds explanations of what happens on the initial step, and makes the function calls more explicit (at the cost of a very small amount of code duplication).

Refs #3377 (fixes point 2)

Revision ca89e41 - 02/14/2020 03:14 AM - Pascal Merz

Fix reading of checkpoints with Parrinello-Rahman (modular simulator)

Using modular simulator, simulations using Parrinello-Rahman barostat could not be read from checkpoint, throwing an error in the checkpoint loading routine. While the legacy implementation of the P-R barostat required the pressure at the previous step to be checkpointed, the modular implementation does not require this. load_checkpoint is, however, expecting this field to be present and throws an error.

This change fixes this by setting the globalState flags in dependence of whether the modular simulator will be used, avoiding read_checkpoint to expect this entry.

Note that tests ensuring this bug not to reappear are introduced in the child change I9bcd0729.

Refs #3377 (fixes point 3)

Revision 3d9ea0b8 - 02/14/2020 05:26 AM - Pascal Merz

Expand test coverage of exact continuation tests

The exact continuation tests were not covering the new Parrinello-Rahman functionality of modular simulator, nor the berendsen-berendsen NPT case using md-vv. This change fixes this.

Fixes #3377 (fixes point 4, last task on the list)

Revision 3d9ea0b8
#1 - 02/14/2020 08:45 PM - Anonymous
- Status changed from Fix uploaded to Resolved

Applied in changeset 3d9ea0b8bb29c313b047e24f3736e608744a7689.

#2 - 02/21/2020 08:14 AM - Paul Bauer
- Status changed from Resolved to Closed