

GROMACS - Feature #3417

Make modular simulator feature-complete

03/10/2020 08:55 PM - Pascal Merz

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|---|----------------------------|---------------|
| Status: | New | |
| Priority: | Normal | |
| Assignee: | Pascal Merz | |
| Category: | mdrun | |
| Target version: | 2021-infrastructure-stable | |
| Difficulty: | hard | |
| Description | | |
| <p>In GROMACS 2020, the modular simulator is implemented for specific cases only. It allows to</p> <ul style="list-style-type: none">• run simulations using almost all parallelization and optimization schemes, with the notable exceptions of<ul style="list-style-type: none">- state propagation on the GPU, and- SIMD acceleration of the leap-frog simulator,• use the leap-frog (md) and velocity-verlet (md-vv) integration schemes,• use all constraining schemes,• couple the system to a temperature bath using the v-rescale thermostat,• couple the system to a pressure bath using the Parrinello-Rahman barostat,• use all free energy perturbation schemes with the exception of expanded ensemble. <p>The modular simulator code path is chosen by default for all compatible simulation types using the velocity-verlet integration scheme. Users can request the use of either the modular simulator code path or the legacy code path for all compatible simulation types using the environment variables <code>GMX_USE_MODULAR_SIMULATOR</code> and <code>GMX_DISABLE_MODULAR_SIMULATOR</code>, respectively.</p> <p>For GROMACS 2021, we are aiming at making the modular simulator code path feature-complete, i.e. have all GROMACS functionality compatible with modular simulator. This will allow to reduce code duplication between modular and legacy simulator code paths.</p> <p>This feature will serve as an umbrella issue for the multiple sub-tasks.</p> | | |
| Subtasks: | | |
| Feature # 3423: Implement additional temperature and pressure control algorithms for mo... | | New |
| Feature # 3424: Implement stochastic dynamics / langevin integrator in modular simulator | | New |
| Feature # 3425: Implement rerun for the modular simulator | | New |
| Feature # 3426: Support acceleration in modular simulator | | New |
| Feature # 3427: Support freeze groups in modular simulator | | New |
| Feature # 3428: Implement SIMD version of modular simulator propagators | | New |
| Feature # 3429: Implement graph for modular simulator | | Closed |
| Feature # 3430: Implement NMR restraints for modular simulator | | New |
| Feature # 3431: Implement virtual sites for modular simulator | | New |
| Feature # 3432: Implement essential dynamics for modular simulator | | New |
| Feature # 3433: Decide how to handle multisim with modular simulator | | New |
| Feature # 3434: Support box deformation in modular simulator | | New |
| Feature # 3435: Implement pull for modular simulator | | New |
| Feature # 3436: Implement AWH for modular simulator | | New |
| Related issues: | | |
| Related to GROMACS - Task #3418: Infrastructure improvements for modular simu... | New | |
| Related to GROMACS - Feature #1137: Proposal for integrator framework (do_md)... | New | |

History

#1 - 03/10/2020 09:21 PM - Pascal Merz

- Related to Task #3418: Infrastructure improvements for modular simulator added

#2 - 03/10/2020 09:21 PM - Pascal Merz

- Related to Feature #1137: Proposal for integrator framework (do_md) in future GROMACS added

#3 - 03/10/2020 11:35 PM - Pascal Merz

- Private changed from Yes to No

#4 - 03/11/2020 06:36 AM - Pascal Merz

Additional functionality that might need to be added to the to do list:

- simulated tempering
- simulated annealing
- expanded ensemble
- ion / water swapping
- interactive MD
- membrane embedding

Some of these have been at least discussed as being potentially deprecated, some others might be targets for algorithms to be supported through an API rather than at the simulator level. Leaving them here for now, further discussion needed.