Implement stochastic dynamics / langevin integrator in modular simulator

03/10/2020 11:48 PM - Pascal Merz

Status: New
Priority: Normal
Assignee: Pascal Merz
Category: mdrun
Target version: 2021-infrastructure-stable
Difficulty: uncategorized

Description

Unlike GROMACS 2020, GROMACS 2021 should have the sd integrator available in modular simulator.

From #2944:

We are planning on implementing the framework presented by Leimkuhler et al. ([https://aip.scitation.org/doi/10.1063/1.4802990](https://aip.scitation.org/doi/10.1063/1.4802990), also discussed in [https://pubs.acs.org/doi/abs/10.1021/jp411770f](https://pubs.acs.org/doi/abs/10.1021/jp411770f)). Note that this would not just be a SINGLE Langevin integrator, but the framework to swap around orders of the different steps (velocity/position/Ornstein-Uhlenbeck process), so that a number of different algorithms could be implemented easily.

So part of this task is to understand whether we need a new integrator flag, and which scheme the current integrator = sd flag should call.

Related issues:

- Related to GROMACS - Feature #2944: Roadmap for thermostats / barostats in new propagation/integration scheme added
- Related to GROMACS - Feature #3428: Implement SIMD version of modular simulator propagators added

History

#1 - 03/10/2020 11:48 PM - Pascal Merz
- Related to Feature #2944: Roadmap for thermostats / barostats in new propagation/integration scheme added

#2 - 03/11/2020 12:12 AM - Pascal Merz
- Related to Feature #3428: Implement SIMD version of modular simulator propagators added