

GROMACS - Feature #3424

Feature # 3417 (New): Make modular simulator feature-complete

Implement stochastic dynamics / langevin integrator in modular simulator

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

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|---|----------------------------|------------|
| 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 , also discussed in 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 ne... | | New |
| Related to GROMACS - Feature #3428: Implement SIMD version of modular simulat... | | New |

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