GROMACS - Feature #3428

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

Implement SIMD version of modular simulator propagators

03/11/2020 12:12 AM - Pascal Merz

<table>
<thead>
<tr>
<th>Status:</th>
<th>New</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Pascal Merz</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2021-infrastructure-stable</td>
</tr>
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<td>Difficulty:</td>
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Description
Currently, SIMD versions of the modular simulator propagators are missing. Note that it might be worth to wait for #3423, #3424, #3426 and #3427 as they might extend the functionality in the propagators.

Related Issues:
- Related to GROMACS - Feature #3423: Implement additional temperature and pressure control algorithms for modular simulator added
- Related to GROMACS - Feature #3424: Implement stochastic dynamics / langevin integrator in modular simulator added
- Related to GROMACS - Feature #3426: Support acceleration in modular simulator added
- Related to GROMACS - Feature #3427: Support freeze groups in modular simulator added

History
#1 - 03/11/2020 12:12 AM - Pascal Merz
- Related to Feature #3423: Implement additional temperature and pressure control algorithms for modular simulator added

#2 - 03/11/2020 12:12 AM - Pascal Merz
- Related to Feature #3424: Implement stochastic dynamics / langevin integrator in modular simulator added

#3 - 03/11/2020 12:13 AM - Pascal Merz
- Related to Feature #3426: Support acceleration in modular simulator added

#4 - 03/11/2020 12:13 AM - Pascal Merz
- Related to Feature #3427: Support freeze groups in modular simulator added