GROMACS - Feature #3426

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

Support acceleration in modular simulator

03/11/2020 12:06 AM - Pascal Merz

<table>
<thead>
<tr>
<th>Status:</th>
<th>New</th>
</tr>
</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>
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<td>Difficulty:</td>
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Description
Decide which acceleration schemes should be supported (cf. #1354). Implement supported acceleration in modular simulator propagators.

Related issues:
- Related to GROMACS - Bug #1354: Constant acceleration NEMD is broken. New
- Related to GROMACS - Feature #3428: Implement SIMD version of modular simulator propagators New

History

#1 - 03/11/2020 12:06 AM - Pascal Merz
- Related to Bug #1354: Constant acceleration NEMD is broken. added

#2 - 03/11/2020 12:13 AM - Pascal Merz
- Related to Feature #3428: Implement SIMD version of modular simulator propagators added

#3 - 03/11/2020 04:09 PM - Pascal Merz
Mark has a patch on gerrit to remove constant acceleration: https://gerrit.gromacs.org/c/gromacs+/8944