GROMACS - Feature #3423

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

Implement additional temperature and pressure control algorithms for modular simulator

03/10/2020 11:22 PM - Pascal Merz

<table>
<thead>
<tr>
<th>Status</th>
<th>New</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority</td>
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</tr>
<tr>
<td>Assignee</td>
<td>Pascal Merz</td>
</tr>
<tr>
<td>Category</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version</td>
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<td>Difficulty</td>
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Description

Currently, the modular simulator implements

- v-rescale
- Parrinello-Rahman (both md and md-vv)

Legacy simulator implements

- Berendsen T-coupling
- Nose-Hoover, Nose-Hoover chains
- v-rescale
- Berendsen P-coupling
- Parrinello-Rahman (md only)
- MTTK (md-vv, Parrinello-Rahman equivalent with Nose-Hoover, no constraints)

To be able to call modular simulator feature-complete, we need to either implement all algorithms in the second list into modular simulator, or officially deprecate them.

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 11:30 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