GROMACS - Feature #3429
Feature # 3417 (New): Make modular simulator feature-complete

Implement graph for modular simulator
03/11/2020 12:28 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>
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<tr>
<td>Difficulty:</td>
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Description
Cases requiring the graph struct, namely

- simulations with Ewald surface correction,
- simulations using orientation restraints, and
- any simulation using the GMX_USE_GRAPH environment variable,

are currently disabled in modular simulator.

Related issues:
Related to GROMACS - Feature #3430: Implement NMR restraints for modular simu... New

History
#1 - 03/11/2020 12:29 AM - Pascal Merz
- Related to Feature #3430: Implement NMR restraints for modular simulator added

#2 - 03/11/2020 11:29 AM - Berk Hess
I am removing the graph from md.cpp and do_force(), so I think this would not be necessary.