GROMACS - Task #3089

Task # 3370 (New): Further improvements to GPU Buffer Ops and Comms
Feature # 2890 (In Progress): GPU Halo Exchange

relax dlb scaling limit when that would suit GPU halo exchange

09/15/2019 08:21 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2020-beta2</td>
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<td>Difficulty:</td>
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**Description**

The new GPU halo exchange is limited to 1D decompositions that need only one pulse.

We should consider automatically relaxing the DLB scale limit to allow GPU DD halo communication.

**Associated revisions**

Revision 3f1e9ce0 - 09/16/2019 10:42 AM - Berk Hess
Add option request 1D DD with 1 pulse

The option is currently controlled by an (undocumented) environment variable GMX_DD_1D_1PULSE, but is intended to be used when requesting GPU DD halo communication.

Note that requesting 1D DD and 1 pulse increases the lower limit on the system size. We should consider automatically relaxing the DLB scale limit to allow GPU DD halo communication.

Refs #3089
Change-Id: i6152c8590726c803fb99ca45ace15ae10dcfba

**History**

#1 - 10/11/2019 05:31 PM - Szilárd Páll
- Tracker changed from Feature to Task

Do we have plans to complete this by beta2? Do we need testing before updating the heuristics?

#2 - 10/12/2019 09:39 PM - Mark Abraham
- Status changed from New to Resolved

I think this is already fixed, as Berk's change made it possible to adapt

#3 - 10/14/2019 01:32 PM - Paul Bauer
- Status changed from Resolved to Closed