### GROMACS - Bug #3241

**Bonded GPU kernel launched in the wrong stream with 1 PP + 1 PME rank**

**12/14/2019 11:12 PM - Szilárd Páll**

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Szilárd Páll</td>
</tr>
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<td>Category:</td>
<td>mdrun</td>
</tr>
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<td>Target version:</td>
<td>2019.5</td>
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<td>Affected version - extra info:</td>
<td>2019.4</td>
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**Description**

Due to a confusion od the DOMAINDECOMP(cr) check, when there is only 1 PP and 1 PME rank (and the check evaluates to true), the bonded module gets initialized with a null stream and therefore ends up blocking the overlap of other operations when it gets launched.

**Related issues:**

Related to GROMACS - Task #2395: break up commrec

**Associated revisions**

**Revision e8ea4480** - 12/16/2019 05:56 PM - Szilárd Páll

Fix the GPU bonded stream with 1 PP + 1 PME rank

With 1 PP + 1 PME rank the GpuBonded constructor gets passed the non-local nonbonded stream which is nullptr and as a result the bonded kernel launch happens in the default stream blocking concurrent kernel execution.

This change makes sure that only when there is PP domain decomposition is the GpuBonded constructor passed the nonlocal stream.

Fixes #3241

Change-Id: I858401b78c620adc3bea176e40e6fa179e583483

**History**

**#1 - 12/15/2019 03:29 AM - Szilárd Páll**
- Status changed from New to In Progress

**#2 - 12/15/2019 11:51 AM - Mark Abraham**
- Related to Task #2395: break up commrec added

**#3 - 12/16/2019 06:00 PM - Szilárd Páll**
- Status changed from In Progress to Resolved

Applied in changeset e8ea448085d91a26b82da0eada215306c35e7e9e.

**#4 - 12/20/2019 11:25 AM - Paul Bauer**
- Status changed from Resolved to Closed