GROMACS - Bug #1385
segfault with multi-node runs and GPU sharing
11/19/2013 02:37 AM - Szilárd Páll

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Szilárd Páll</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.5</td>
</tr>
<tr>
<td>Affected version:</td>
<td>4.6.4</td>
</tr>
<tr>
<td>Difficulty:</td>
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**Description**

When running on more than one physical nodes with GPU, under certain circumstances (but quite often), a segmentation fault occurs; e.g. on a Cray XK7 with 8 ranks per node and two nodes:

```
OMP_NUM_THREADS=2 aprun -cc none -n 16 -N 8 -d 2 mdrun_mpi -npme 0 -pin on -nb gpu -gpu_id 0000000 0
```

**Associated revisions**

Revision 904d4645 - 11/19/2013 04:18 PM - Szilárd Páll
Fix DD load balancing bug with GPU sharing

The recent DD load balancing fix which solved the issue of incorrect imbalance measure with GPU sharing (ba8232e9) addressed GPUs with incorrect indexing. This caused out of bounds indexing in the GPU ID query function. The query function also had a bug in the error checking which allowed the incorrect indexing. Now also mdrun -nb cpu -gpu_id ... is allowed, which before would give a fatal error.

This commit addresses both issues; fixes #1385

Change-Id: i2800f610b873da92afe78bbd869258f378ba2d7

**History**

- #1 - 11/19/2013 02:53 AM - Szilárd Páll
  - Status changed from New to In Progress
  - Assignee changed from Berk Hess to Szilárd Páll

The bug is triggered by incorrect GPU ID indexing with Nranks > 2 and GPU sharing among ranks: [link](http://redmine.gromacs.org/projects/gromacs/repository/revisions/ba8232e965652669cc0b558a273f81a4d9733d25/entry/src/mdlib/domdec.c#L5700)

A fix will be uploaded shortly.

- #2 - 11/19/2013 04:20 PM - Szilárd Páll
  - Status changed from In Progress to Resolved
  - % Done changed from 0 to 100

Applied in changeset 904d4645ca712bd58a0a22fcdebead6291ec19d3.

- #3 - 11/28/2013 07:52 PM - Mark Abraham
  - Status changed from Resolved to Closed

03/20/2020