GROMACS - Bug #2433
Error in MPI_Allreduce when applying AWH biasing and for multiple sharing biases

03/01/2018 05:12 PM - Viveca Lindahl

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</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>2018.1</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2018</td>
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</tbody>
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Difficulty: uncategorized

Description
When running e.g. mpirun -np 4 $gmx_mpi mdrun -v -multidir walker-1 walker-2 there is an error from MPI_Allreduce:

```
*** An error occurred in MPI_Allreduce
*** on communicator MPI_COMM_WORLD
*** MPI_ERR_COMM: invalid communicator
```
on my machine, or when running on the cluster

```
Rank 8 [Thu Mar  1 16:03:40 2018] [c1-0c0s8n3] Fatal error in MPI_Allreduce: Invalid communicator, error stack:
MPI_Allreduce(1007): MPI_Allreduce(sbuf=MPI_IN_PLACE, rbuf=0x22e08f0, count=337, MPI_INT, MPI_SUM, MPI_COMM_NULL) failed
MPI_Allreduce(926).: Null communicator
```

A tpr for this is attached. This is similar to [https://redmine.gromacs.org/issues/2403](https://redmine.gromacs.org/issues/2403) in that there is no error when there only one rank per directory multidir argument. I.e. mpirun -np 2 $gmx_mpi mdrun -v -multidir walker-1 walker-2 runs error-free. I have all related fixes up until now applied.

Associated revisions
Revision cb1947ec - 03/02/2018 10:14 AM - Berk Hess
Fix AWH bias-sharing with parallel simulation

Sharing the AWH bias over multiple simulations only worked when each simulation was running on a single MPI rank. Now parallel simulations also work.

Fixes #2433.

Change-Id: i71f9069a31b033151c772aac84c9912d91b213a1

History
#1 - 03/01/2018 10:04 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2433.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018-171f9069a31b033151c772aac84c9912d91b213a1
Gerrit URL: https://gerrit.gromacs.org/7637

#2 - 03/01/2018 10:15 PM - Berk Hess
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Target version set to 2018.1

#3 - 03/02/2018 03:53 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

02/19/2020
Status changed from Resolved to Closed

Files

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<th>Name</th>
<th>Size</th>
<th>Date</th>
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<td>awh-share-on.tpr</td>
<td>365 KB</td>
<td>03/01/2018</td>
<td>Viveca Lindahl</td>
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