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

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

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.1
Affected version -
extra info:
GROMACS version: 2018.1-dev-20180301-6358ce7
Affected version: 2018

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 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~I71f9069a31b033151c772aac84c9912d91b213a1
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
<table>
<thead>
<tr>
<th>Files</th>
<th>Size</th>
<th>Date</th>
<th>Contributor</th>
</tr>
</thead>
<tbody>
<tr>
<td>awh-share-on.tpr</td>
<td>365 KB</td>
<td>03/01/2018</td>
<td>Viveca Lindahl</td>
</tr>
</tbody>
</table>

- Status changed from Resolved to Closed