Dear Gromacs Developers,

one of our users ran into problems with -multidir and having messages like:
Rank 19 [Fri Feb 16 13:51:22 2018] [c0-0c0s2n2] Fatal error in PMPI_Barrier: Invalid communicator, error stack:
PMPI_Barrier(434): MPI_Barrier(MPI_COMM_NULL) failed
PMPI_Barrier(395): Null communicator

The reason for this behaviour is an erroneous use of MPI_Comm_create together with MPI_Barrier. The fix to this problem is to modify gromacs-2018/src/programs/mdrun/runner.cpp in a following way:

```c
#if GMX_MPI
if (PAR)     {
    MPI_Barrier(cr->mpi_comm_mysim);
}
if (MULTISIM)     {
    if(MPI_COMM_NULL != cr->ms->mpi_comm_masters)   /* this is the only new line */
        MPI_Barrier(cr->ms->mpi_comm_masters);
}
#endif
```

Kind regards,
Maciej Cytowski

Related issues:
Is duplicate of GROMACS - Bug #2403: Multidir sim with #mpiranks = 2*#sim fails

History
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#1 - 02/16/2018 10:57 AM - Berk Hess
- Status changed from New to Fix uploaded

Duplicate of #2403

#2 - 02/16/2018 03:27 PM - Mark Abraham
- Is duplicate of Bug #2403: Multidir sim with #mpiranks = 2*#sim fails added

#3 - 02/16/2018 03:27 PM - Mark Abraham
- Status changed from Fix uploaded to Closed

Is fixed for 2018.1, out next week