Value of AWH coordinate not set for certain numbers of MPI ranks

I have a simulation with AWH that runs fine for a smaller number of ranks, e.g.: aprun -n 32 -N 32 $gmx mdrun -npme 0 -ntomp 1
but when instead using -n 64 I get:

Simulation instability detected:
Function: void gmx::CoordState::setCoordValue(const gmx::Grid&, const double*)
Coordinate 1 of an AWH bias has a value 0.000000 which is more than 10 sigma
MPI rank: 32 (out of 64)
out of the AWH range of [0.250000, 0.600000]. You seem to have an unstable
reaction coordinate setup or an unequilibrated system.

Related issues:
Related to GROMACS - Task #2488: use MPI non-blocking collectives to overlap ...

Associated revisions
Revision 97240d25 - 03/14/2018 11:54 AM - Berk Hess
Fix COM pulling with external potential with #ranks>32
With more than 32 PP-ranks, the pull code could use only a subset
of the PP-ranks. This change forces all ranks to do pulling when
external potentials are present (currently only used by AWH).
Fixes #2441
Change-Id: I8501024b7961600ec79f3707e239dd25525aa79

History
#1 - 03/11/2018 10:49 PM - Szilárd Páll
- Status changed from New to Accepted

Reproduced. My first thought was it may be due to the switch from 2D to 3D decomposition, but I've just tried and I observe:
- 32 ranks npme 0, 8x4x1 DD working
- 40 ranks npme 0, 8x5x1 DD not working
- 64 ranks npme 16 (same as default), 4x4x3 DD not working
- 64 ranks npme 16 (same as default), 12x4x1 DD not working

#2 - 03/12/2018 04:20 PM - Berk Hess
- Category set to mdrun
- Assignee set to Berk Hess

This is because with #PP-ranks > 32, the pull code is only active on a subset of the ranks to minimize communication.
It is rather complex to also make the AWH code only work on subranks, so I think I will implement the simple solution of turning off the pull sub
communicator when we use external pull potentials.

#3 - 03/12/2018 04:56 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2441.
Berk Hess wrote:

This is because with #PP-ranks > 32, the pull code is only active on a subset of the ranks to minimize communication. It is rather complex to also make the AWH code only work on subranks, so I think I will implement the simple solution of turning off the pull sub communicator when we use external pull potentials.

Sounds like a gap to close in integration testing. >32 ranks even when combined with pull / AWH should ideally be covered by weekly tests rather than tested when first used in production.

Berk Hess wrote:

- Status changed from Fix uploaded to Resolved

Applied in changeset 97240d25461968932102b5a7b077f3070188fe.

Mark Abraham wrote:

- Status changed from Resolved to Closed

Szilárd Páll wrote:

- Related to Task #2488: use MPI non-blocking collectives to overlap pull comm added

Files

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