Gromacs - Task #1290

OpenMPI 1.4.3 in Ubuntu 12.04 can produce simulation crashes with any version of GROMACS

06/25/2013 06:46 PM - Mark Abraham

Status: Closed
Priority: Low
Assignee:
Category:
Target version:

Description
While testing #1254, we observed that the default OpenMPI 1.4.3(-2.1ubuntu) in Ubuntu 12.04 LTS (precise) sometimes crashes with GROMACS versions from the whole 4.x series. We believe this is a memory corruption issue in that version of OpenMPI, perhaps in communicator splitting, but we have not been able to identify from the OpenMPI 1.4 branch commit logs a patch that fixes it. The OpenMPI 1.5.4-ubuntu1 package seems to work OK, and we recommend people use it when compiling GROMACS from source. We also recommend people generally avoid the OpenMPI 1.4.x branch (which is years old and will make no new releases).

The gromacs-openmpi package (4.5.5-1) in precise depends on the buggy version of OpenMPI, as does a lot of other packages (including octave, parpack). A proper solution for it would either involve

- identifying the OpenMPI fix and backporting it to the 1.4.3 package, or
- bumping the required libopenmpi version to 1.5 (if it is possible to have both libopenmpi versions installed on the same system).

This information is provided as a "public safety" message for people searching for the reason for such an irreproducible crash. We're not planning to try to identify the bug in a years-old version of MPI. If someone wishes to attempt to solve the issue, to (often) reproduce the crash, use

mpirun -np 24 mdrun_mpi -npme 6 -s waterbox-sim.tpr

with the attached version 4.5.5 .tpr.

From the point of view of GROMACS, there is no issue to solve, so the status is "resolved" in our bug tracker.

Related Issues:
Related to Gromacs - Bug #1254: a likely mdrun memory corruption/race condition Closed 05/17/2013

History
#1 - 06/25/2013 06:48 PM - Mark Abraham
- Description updated

#2 - 12/03/2013 04:19 PM - Rossen Apostolov
- Status changed from Resolved to Closed

Files
waterbox-sim.tpr 412 KB 06/25/2013 Mark Abraham