GROMACS - Bug #2540

Thread-MPI error in GROMACS-2018

06/01/2018 05:38 PM - Siva Dasetty

Status:	Closed		
Priority:	Normal		
Assignee:	Berk Hess		
Category:	mdrun		
Target version:	2018.2		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018		

Description

Hello,

I have come across an error that causes GROMACS (2018/2018.1) to crash. The message is:

"tMPI error: Receive buffer size too small for transmission (in valid comm)
Aborted"

The error seems to only occur immediately following a LINCS or SETTLE warning. The error is reproducible across different systems. A simple example system is running an energy minimization on a box of 1000 rigid TIP4P/Ice water molecules generated with gmx solvate. When SETTLE is used as the constraint algorithm, there are several SETTLE warnings in the early steps of the energy minimization, and GROMACS will crash with the above error message. If I replace SETTLE with LINCS, GROMACS crashes with the same error message following a LINCS warning. Other systems that have produced this error are -OH terminated self assembled monolayer surfaces (h-bonds constrained by LINCS), and mica surfaces (h-bonds constrained by LINCS). Naturally, reducing -ntmpi to 1 eliminates the error for all cases.

The problem does appear to be hardware dependent. Specifically, the tested node(s) on the cluster contains K20/K40 GPUs with Intel Xeon E5-2680v3 processor (20/24 cores). I used GCC/5.4.0 and CUDA/8.0.44 compilers for installing GROMACS. An installation on my desktop machine with with very similar options does not have the thread MPI error.

Example of procedure that causes error:

1. Node contains 24 cores and 2 K40 GPUs
   gmx solvate -cs tip4p -o box.gro -box 3.2 3.2 3.2 -maxsol 1000
   gmx grompp -f em.mdp -c box.gro -p tip4pice.top -o em
   export OMP_NUM_THREADS=6
   gmx mdrun -v -deffnm em -ntmpi 4 -ntomp 6 -pin on

Attached are the relevant topology (tip4pice.top), mdp (em.mdp), tpr (em.tpr), and log (em.log) files. In addition tip4p.gro and box.gro files are included.

Thanks in advance for any ideas as to what might be causing this problem,
Siva Dasetty

Associated revisions

Revision dce23f77 - 06/07/2018 12:33 AM - Berk Hess

Fix MPI inconsistency in EM after constraint failure

Fixes issue #2540

Change-Id: Id18c17af82f80917388c11fc776b79bf4966a4ac

History

#1 - 06/05/2018 04:01 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2540.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~Id18c17af82f80917388c11fc776b79bf4966a4ac
Gerrit URL: https://gerrit.gromacs.org/7979

#2 - 06/05/2018 04:02 PM - Berk Hess

- Category set to mdrun

- Status changed from New to Fix uploaded

- Assignee set to Berk Hess

- Target version set to 2018.2

#3 - 06/12/2018 01:29 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

#4 - 06/12/2018 03:10 PM - Mark Abraham

- Status changed from Resolved to Closed

Files

tip4p.gro	58.3 KB	06/01/2018	Siva Dasetty
box.gro	176 KB	06/01/2018	Siva Dasetty
em.log	19.7 KB	06/01/2018	Siva Dasetty
tip4pice.top	1.28 KB	06/01/2018	Siva Dasetty
em.mdp	481 Bytes	06/01/2018	Siva Dasetty
em.tpr	96.3 KB	06/01/2018	Siva Dasetty