

GROMACS - Bug #1685

mdrun reports incorrect thread count use

02/10/2015 08:29 PM - Szilárd Páll

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: core library	
Target version: 5.1	
Affected version - extra info: 5.1-dev-20150207-fc0c893	Difficulty: uncategorized
Affected version: git master	
Description mdrun has been reporting Using 0 OpenMP thread per tMPI thread for PME When it should in fact be reporting a >1 PP thread count. Some logic got obviously messed up.	
Related issues: Is duplicate of GROMACS - Bug #1681: use of incorrect initial value of variable Closed 02/06/2015	

Associated revisions

Revision 6cb0f92a - 02/24/2015 11:31 PM - Berk Hess

Fixed parallel distribution and thread count reporting

The domain decomposition no longer prints the atom count for all ranks (which gets far too long at high parallelization), but rather av, stddev, min and max.

Corrected the OpenMP thread count print, which often printed 0 thread for (non-existent) PME ranks.

Fixes #1681, #1685.

Change-Id: Ia0e01c1c458e464ba2469d45c94d9e8c6b85d128

History

#1 - 02/11/2015 12:04 AM - Mark Abraham

- Is duplicate of Bug #1681: use of incorrect initial value of variable added

#2 - 02/24/2015 09:26 PM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue [#1685](#).

Uploader: Berk Hess (hess@kth.se)

Change-Id: Ia0e01c1c458e464ba2469d45c94d9e8c6b85d128

Gerrit URL: <https://gerrit.gromacs.org/4472>

#3 - 03/10/2015 10:22 PM - Szilárd Páll

- Category set to core library

- Status changed from New to Resolved

- Assignee set to Berk Hess

- Target version set to 5.1

#4 - 04/09/2015 11:07 AM - Mark Abraham

- Status changed from Resolved to Closed