GROMACS - Bug #1981

dd121 regressiontest fails with >=4 MPI ranks + OpenMP

05/31/2016 10:40 PM - Roland Schulz

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 2016
Affected version - extra info:
Affected version: 2016

Difficulty: Uncategorized

Description
E.g. with 4 MPI and 2 OpenMP I get:
checkpot.out (3 errors), checkforce.out (2 errors)

| Improper Dih. | step 20: 5.84165, step 20: 5.98111 |

I get the error both the GCC (4.9.3) and ICC (16).

Associated revisions

Revision 0e31b39c - 06/26/2016 08:14 PM - Berk Hess
Fix vsite bug with MPI+OpenMP

The recent commit b7e4f30d caused non-local virtual sites not be treated when using OpenMP. This means their coordinates lagged one step behind and their forces are not spread to the atoms, leading to small errors in the forces. Note that non-local virtual sites are only used when local virtual sites use them as a constructing atom; the most common case is a C/N in a CH3/NH3 group with vsite H's. Also added a check on the vsite count for debug builds.

Fixes #1981.

Change-Id: Ibe13b75b8ae9841937ad4abc007dba5ad78a30cd

History

#1 - 06/01/2016 09:34 AM - Berk Hess
- Subject changed from dd121 regressiontest fails with >=4 MPI ranks to dd121 regressiontest fails with >=4 MPI ranks + OpenMP
- Category changed from testing to mdrun
- Status changed from New to In Progress
- Assignee set to Berk Hess
- Priority changed from Normal to High
- Target version set to 2016

This is an OpenMP in the vsite code rather than an MPI issue.

#2 - 06/01/2016 11:46 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1981.
Uploader: Berk Hess (hess@kth.se)
Change-Id: lbe13b75b8ae9841937ad4abc007dba5ad78a30cd
Gerrit URL: https://gerrit.gromacs.org/5920

#3 - 06/01/2016 11:53 AM - Berk Hess
- Status changed from In Progress to Fix uploaded
Good that you caught this (before the 2016 release).
This was a subtle bug that only affect non-local vsites, which don't occur often. And even then, the errors in the force are rather small.

#4 - 06/27/2016 11:01 AM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 0e31b39cff097be192272615abee0344336eef2.

#5 - 06/27/2016 07:28 PM - Mark Abraham
- Status changed from Resolved to Closed