

GROMACS - Bug #2257

Vsites not constructed for initial decomposition with threads

09/25/2017 10:43 PM - Berk Hess

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|---------------------------------------|-----------------------------------|--------------------|---------------|
| Status: | Closed | Difficulty: | uncategorized |
| Priority: | Normal | | |
| Assignee: | Berk Hess | | |
| Category: | mdrun | | |
| Target version: | 2018 | | |
| Affected version - extra info: | any version with OpenMP threading | | |
| Affected version: | 2016 | | |
| Description | | | |

Associated revisions

Revision ccf60bde - 10/15/2017 09:56 PM - Berk Hess

Improve vsite parallel checking

The vsite struct now stores internally whether it has been configured with domain decomposition. This allows for internal checks on valid commrec, which have now been added.

The vsite constructor now initializes to atom range to invalid values, so we can check that the thread splitting has been called before constructing. This would have caught bug #2257.

Removed the vsite struct from the global construct function argument list, which simplifies the vsite code in several places and fixes #2257.

Also some general clean-up: removed some snews, added some camelCasing and doxygen documentation.

More renaming would be beneficial, but should be a separate commit.

Change-Id: I467ec8b8ebfa0da090d4ac0a1d096ad9fab87eb5

History

#1 - 09/25/2017 10:46 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2257](#).

Uploader: Berk Hess (hess@kth.se)

Change-Id: gromacs~master~I467ec8b8ebfa0da090d4ac0a1d096ad9fab87eb5

Gerrit URL: <https://gerrit.gromacs.org/6965>

#2 - 09/26/2017 09:05 AM - Berk Hess

- Subject changed from Vsites not constructed for initial coordinates with periodic molecules and threads to Vsites not constructed for initial decomposition with threads

- Status changed from In Progress to Fix uploaded

At the start of a, non-continuation, simulation the virtual sites are not constructed before the first domain decomposition partitioning when using OpenMP threading. This is because the thread work data structures have a zero work range. There is a second partitioning which occurs after a second, correct virtual site construction, so likely this bug has not lead to any incorrect results.

#3 - 09/26/2017 03:35 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2257](#).

Uploader: Berk Hess (hess@kth.se)

Change-Id: gromacs~master~I26d0422ac2d95f21dcb6aef297110938acc991d7

Gerrit URL: <https://gerrit.gromacs.org/6967>

#4 - 09/27/2017 01:06 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2257](#).

Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~master~l60d28af78b26db2d64c77834ca21772b7ec9b825
Gerrit URL: <https://gerrit.gromacs.org/6969>

#5 - 10/16/2017 10:22 AM - Berk Hess

- Status changed from *Fix uploaded* to *Resolved*

Applied in changeset [ccf60bde3a741b1ee64b40c93c59f6fe9ce38c17](#).

#6 - 11/28/2017 05:59 PM - Mark Abraham

- Status changed from *Resolved* to *Closed*