GROMACS - Bug #2257
Vsites not constructed for inital decomposition with threads
09/25/2017 10:43 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>any version with OpenMP threading</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2016</td>
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**Description**

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.

**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~I467ec8b8e6bfa0da090d4ac0a1d096ad9faba87eb5
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~I60d28af78bb26db2d64c77834ca21772b7ec9b825
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