GROMACS - Bug #3375
Oories consistency check too strict
02/12/2020 02:53 PM - David van der Spoel

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2019.6</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Probably earlier versions affected too.</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2019.3</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**
The orientation restraint code checks whether there were molecules with more than one copy and bail out if so, even if there were no orientation restraints in that molecule (e.g. water).

**To reproduce:**
gmx mdrun -s md1.tpr

**Associated revisions**

**Revision c9a55080** - 02/20/2020 08:45 AM - David van der Spoel
Fixed bug in orires code that was checking too strict.
Added one test to see that input is accepted.

Fixes #3375
Change-Id: I0f64b386477b9a72f18c95fd977ac8cf5dbeeccd

**Revision d4ef04** - 02/20/2020 10:07 AM - David van der Spoel
Fixed bug in orires code that was checking too strict.

Fixes #3375
Change-Id: I0f64b386477b9a72f18c95fd977ac8cf5dbeeccd

**History**

#1 - 02/20/2020 10:00 PM - David van der Spoel
- Status changed from New to Resolved

Applied in changeset c9a55080a79dfe508962e2f6515611982f9559.

#2 - 02/21/2020 08:14 AM - Paul Bauer
- Status changed from Resolved to Closed

**Files**
md1.tpr 267 KB 02/12/2020 David van der Spoel