GROMACS - Task #2391

re-enable TPI test

01/23/2018 10:50 AM - Aleksei Iupinov

<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>Berk Hess</td>
</tr>
<tr>
<td>Category</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version</td>
<td>2020</td>
</tr>
<tr>
<td>Difficulty</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

While trying to refactor away some annoying atom count parameter in the PME code, I ran into TPI logic again, and realized it's not covered by tests.

While trying to throw together a test, I ran into "TPI does not work (yet) with the Verlet cut-off scheme" message. Without at least a basic TPI sanity test, I doubt this feature will survive much longer...

**Subtasks:**

- Bug # 2416: TPI producing invalid results with nsteps too small (Closed)

**Related issues:**

- Related to GROMACS - Task #1971: Removing buggy features vs. keeping workflows (New)

**Associated revisions**

- Revision 9a1268fa - 03/16/2018 02:27 PM - Aleksei Iupinov
  
  Add a basic TPI sanity test
  
  The floating point exceptions are for now toggled off in the test body instead of mdrun itself.
  
  Refs #2391
  
  Change-Id: l41b584f4753b9b0e126256a94c1304f0a870aa73

- Revision 289868da - 01/14/2019 01:46 PM - Mark Abraham
  
  Migrate TPI testing to Verlet scheme
  
  For now, this also disables TPI testing, since TPI does not yet support the Verlet scheme. If that gets fixed before this change gets incorporated, the test should not be disabled.
  
  Refs #2391
  
  Change-Id: l83483bd23a03e9175571f2194dae0df96960e6c7

**History**

#1 - 01/23/2018 10:51 AM - Aleksei Iupinov

- Related to Task #1971: Removing buggy features vs. keeping workflows added

#2 - 01/23/2018 12:04 PM - Berk Hess

- Status changed from New to Accepted

Indeed.

Do you already have a test set up? We can add it with the group scheme and later convert it to Verlet. I should fix up the nbnxn pair search for TPI, that's actually easier than the group scheme code.

#3 - 01/23/2018 12:08 PM - Aleksei Iupinov

No, I don't. I've only tried adding some more mdp parameters to the PmeTest. Maybe you could provide the mdrun input/arguments?

#4 - 02/19/2018 03:59 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2391.
Uploader: Aleksei lupinov (a.yupinov@gmail.com)
Change-Id: gromacs~master~I41b584f4753b9b0e126256a94c1304f0a870aa73
Gerrit URL: https://gerrit.gromacs.org/7596

#5 - 02/19/2018 04:02 PM - Aleksei lupinov
Here's one test with files provided by Berk.

There's more to test here - tpic, PME..

#6 - 09/19/2018 03:14 PM - Mark Abraham
- Subject changed from TPI status to improve TPI testing coverage
- Category set to mdrun
- Target version changed from 2019 to 2020

#7 - 01/09/2019 05:08 PM - Mark Abraham
- Subject changed from improve TPI testing coverage to re-enable TPI test

Once TPI works with the Verlet scheme, we can re-enable the test.

#8 - 01/09/2019 05:17 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2391.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I83483bd23a03e9175571f12194dae0df96960e6c7
Gerrit URL: https://gerrit.gromacs.org/8946

#9 - 12/20/2019 12:13 PM - Paul Bauer
- Status changed from Accepted to Resolved

TPI is being tested again

#10 - 12/20/2019 12:13 PM - Paul Bauer
- Status changed from Resolved to Closed