Gromacs - Feature #1192
Add support for Verlet scheme with Buckingham

03/16/2013 03:43 AM - Bu Wang

<table>
<thead>
<tr>
<th>Status:</th>
<th>Accepted</th>
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<tr>
<td>Priority:</td>
<td>Normal</td>
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<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
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<td>Category:</td>
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<td>Target version:</td>
<td>5.x</td>
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Description
We are trying to simulate a simple alumina crystal. The forcefield only contains non-bonded interactions defined with our own Buckingham potentials. Everything works fine with the group cutoff scheme. But with the similar settings in Verlet scheme, the simulation would blow up right after step 0 with a segmentation fault error. GDB shows the error happens in pme.c: 415 idxptr[ZZ] = pme->nnz[tiz]. Taking the group scheme .tpr and run mdrun -testverlet fails in the same way.

The step 0 information shows absurdly high buckingham energy and kinetic energy. We tried modifying parameters related to the Verlet scheme, such as verlet-buffer-drift, vdw-modifier and rvdw-switch, but had no luck. We also compared the outputs from group and Verlet schemes but couldn't see anything weird.

I attached the .mdp; changing the cutoff-scheme to group and setting rlist=1.2 will make the simulation run. The .tpr and topology are also attached.

I would greatly appreciate any suggestions. Thanks in advance!

Related issues:
Related to Gromacs - Feature #1347: future of tables

Associated revisions
Revision 81b1cd9b - 05/20/2014 10:31 AM - Rossen Apostolov
Added a note about unsupported Verlet cutoff + Buckingham.
Refs #1192.

Change-Id: I2da3bf8c768de40531e1ffdf6f8c7ec73c9e53314

History
#1 - 03/21/2013 05:03 PM - Berk Hess
- Status changed from New to In Progress
- Assignee set to Berk Hess
- Target version changed from 4.6.1 to 4.6.2
- Affected version - extra info set to 4.6.1

#2 - 05/22/2013 05:03 AM - Mark Abraham
- Target version changed from 4.6.2 to 4.6.3
- Affected version set to 4.6.3

#3 - 06/26/2013 12:39 AM - Mark Abraham
- Target version changed from 4.6.3 to 4.6.x

#4 - 12/18/2013 12:38 AM - Szilárd Páll
This has been marked as "in progress" for quite a long time. Has the issue been identified? Is the status still valid or should we set it to "Accepted"?

11/19/2015 1/2
The issue was that Buckingham or tabulated potentials were not supported by the verlet cutoff scheme. Is there a plan to add the support in a future version?

Gerrit received a related patchset 1 for Issue #1192.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I2da3bf8c768de40531e1f0d618cec73c9e53314
Gerrit URL: https://gerrit.gromacs.org/3440

Status changed from In Progress to Fix uploaded
Tracker changed from Bug to Feature
Subject changed from Segmentation fault switching from group to verlet cutoff scheme to Add support for Verlet scheme with Buckingham
Status changed from Fix uploaded to Accepted
Priority changed from High to Normal

There are plans to support tabulated potentials with the Verlet scheme and GPUs, perhaps in 5.1. Native Buckingham kernels would only be considered after we produce a Verlet kernel generator sometime this year; perhaps it might be straightforward at that time.

But we should put a proper fatal error in 4.6 and 5.0, right?

I think Rossen's patch does an OK job. Could also fatal in grompp.

Files

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<td>11 KB</td>
<td>03/16/2013</td>
<td>Bu Wang</td>
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