

GROMACS - Feature #1192

Add support for Verlet scheme with Buckingham

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

Status:	Accepted	
Priority:	Normal	
Assignee:	Berk Hess	
Category:		
Target version:		
Difficulty:	uncategorized	
Description		
<p>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->nanz[tiz]. Taking the group scheme .tpr and run mdrun -testverlet fails in the same way.</p> <p>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.</p> <p>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.</p> <p>I would greatly appreciate any suggestions. Thanks in advance!</p>		
Related issues:		
Related to GROMACS - Feature #1347: future of tables		New

Associated revisions

Revision 81b1cd9b - 05/20/2014 10:31 AM - Rossen Apostolov

Added a note about unsupported Verlet cutoff + Buckingham.

Refs #1192.

Change-Id: I2da3bf8c768de40531e1ffdf6f8cec73c9e53314

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"?

#5 - 12/18/2013 02:51 AM - Bu Wang

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?

#6 - 05/14/2014 12:12 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1192](#).
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I2da3bf8c768de40531e1ffdf6f8cec73c9e53314
Gerrit URL: <https://gerrit.gromacs.org/3440>

#7 - 05/14/2014 12:12 PM - Rossen Apostolov

- Status changed from In Progress to Fix uploaded

#8 - 05/14/2014 12:33 PM - Rossen Apostolov

- 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

Changed the report to a "feature"

#9 - 05/15/2014 10:33 PM - Mark Abraham

- Target version changed from 4.6.x to 5.x

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.

#10 - 05/15/2014 10:36 PM - Berk Hess

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

#11 - 05/16/2014 12:08 PM - Mark Abraham

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

#12 - 10/14/2015 06:14 PM - Mark Abraham

- Related to Feature #1347: future of tables added

#13 - 07/11/2016 08:19 PM - Mark Abraham

- Target version deleted (5.x)

Files

6x7x1.mdp	11 KB	03/16/2013	Bu Wang
6x7x1.tpr	175 KB	03/16/2013	Bu Wang
6x7x1.top	1.6 KB	03/16/2013	Bu Wang