GROMACS - Bug #1116

incorrect volume with MTTK + particle decompostion

01/11/2013 04:46 PM - Berk Hess

Status:	Closed			
Priority:	High			
Assignee:	Michael Shirts			
Category:				
Target version:	4.5.7			
Affected version - extra info:	4.5	**Difficulty:**	uncategorized	
Affected version:	4.5.6			

Description

In version 4.5 running MTTK pressure coupling with particle decomposition give a too large volume. The error seems to roughly scale with the number of nodes. With domain decomposition it is correct.
In 4.6 I can't reproduce this, so it seems to be fixed.
We should find and backport this fix to 4.5, or disable MTTK with particle decomposition.

Associated revisions

Revision b77fa706 - 04/19/2013 06:55 AM - Michael Shirts

Some changes for md-vv extracted from 4.6

a. Fixes for the pressure in MTTK with constraints + dispersion + rerun

- Dispersion is correctly added in rerun
- COM motion is removed only on the second half of the timestep.
- Now can do md-vv + rerun with multiple threads.
- Now gives exact kinetic energy reruns for everything except MTTK, where the iterative algorithm makes exact kinetic energy impossible when nstpcouple == 1.

b. md-vv works with v-rescale and berendsen

c. Fixes a bug when pressure control in md-vv when nstcalcenergy is not a multiple of nstpcouple or nsttcouple. This bug results in boxes slowly expanding to unphysical sizes because the virial is neglected in the second half of the md-vv calculation.

Also discovered that as part of the bug, global energies were being communicated where they did not need to be when nstpcouple and nsttcouple are > 1 in the case of md-vv, so redid some of the iteration counting and global communication to fix this all together. In the process, this simplified some of the iteration counting.

Should fix bugs #1116, #1012, #1000, #1129 in redmine.

Change-Id: I1b628d03ab588c29fef2b8789e61254da49c2b6f

History

#1 - 01/11/2013 04:50 PM - Berk Hess

Forgot to add that this was noticed for a system with SHAKE (H-only) constraints.
The constraint/virial coupling is a likely source of error here.

#2 - 01/11/2013 11:38 PM - Michael Shirts

- *Target version set to 4.5.6*

I'm tracking down the last 4.6 bugs over the next 1-2 days but I will go back afterwards and identify where to backport them.

#3 - 01/15/2013 12:42 AM - Mark Abraham

OK. In practice, there will be a window after 4.6 and before 4.5.6 because I'm taking a long weekend. This could go in at that time. Otherwise I'll bump the target version to 4.5.7.

#4 - 01/15/2013 07:53 PM - Mark Abraham

- Status changed from New to In Progress

#5 - 02/09/2013 06:18 PM - Mark Abraham

- Target version changed from 4.5.6 to 4.5.7

Draft https://gerrit.gromacs.org/#/c/2101/ should solve this

#6 - 02/09/2013 07:23 PM - Roland Schulz

Drafts are not visible to anyone but reviewers. Never mind if that was the intention, just saying in case you didn't know.

#7 - 02/14/2013 06:12 AM - Michael Shirts

Roland Schulz wrote:

> Drafts are not visible to anyone but reviewers. Never mind if that was the intention, just saying in case you didn't know.

Yes. It's now been moved to the main page.

#8 - 04/19/2013 06:30 PM - Mark Abraham

- Status changed from In Progress to Resolved

- Affected version set to 4.5.6

#9 - 12/16/2013 05:38 PM - Rossen Apostolov

- Status changed from Resolved to Closed