

GROMACS - Bug #1354

Constant acceleration NEMD is broken.

10/08/2013 08:32 AM - David van der Spoel

Status: New	
Priority: Normal	
Assignee: David van der Spoel	
Category: mdrun	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 4.6	
Description	
Constant acceleration NEMD has probably been broken for over four years since a6ee084bcf removed the only call to update_ekindata().	
Related issues:	
Related to GROMACS - Task #1971: Removing buggy features vs. keeping workflows	New
Related to GROMACS - Feature #3426: Support acceleration in modular simulator	New

History

#1 - 10/08/2013 11:38 AM - Mark Abraham

Also does not get anything checkpointed, but not sure that is relevant.

#2 - 10/08/2013 09:43 PM - Mark Abraham

Also, it gets turned on by

```
(opts->ngacc > 1 || norm(opts->acc[0]) > 0)
```

i.e. that there is more than one acceleration group or that the first acceleration group has a non-zero acceleration. This does not deal with the silly case of multiple zero-norm acceleration groups.

#3 - 10/09/2013 06:58 PM - Michael Shirts

Can you be more specific about what is broken? We're actually trying to use it to compute contact angles. The drop is indeed accelerating until it hits a terminal velocity --- but now I'm not sure how to interpret that!

#4 - 10/09/2013 07:01 PM - David van der Spoel

Haven't looked into it yet, but I opened this redmine in order not to forget about it.

#5 - 12/23/2013 01:37 AM - Mark Abraham

Michael Shirts wrote:

Can you be more specific about what is broken? We're actually trying to use it to compute contact angles. The drop is indeed accelerating until it hits a terminal velocity --- but now I'm not sure how to interpret that!

e.g. search git show a6ee084bcf3ac87d9dd493702b1c737d86506bdc for update_ekindata. That function used to be called from update(...) to compute some kind of group-based KE things. Now that function is never called, so who knows what junk is being computed!

#6 - 02/11/2014 01:24 PM - Rossen Apostolov

Michael: do you have a working version or shall we remove the functionality completely?

#7 - 06/12/2014 01:37 AM - Erik Lindahl

David/Michael - unless somebody volunteers to look into it, we'll remove the feature before 5.0.

#8 - 06/24/2015 10:46 PM - Berk Hess

It shouldn't be hard to fix this, but if nobody uses it, it's better to remove it. We shouldn't forget to also remove ekind->grpstat[g].u.

#9 - 07/11/2016 08:14 PM - Mark Abraham

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

#10 - 07/11/2016 08:14 PM - Mark Abraham

- Target version deleted (5.x)

#11 - 01/07/2019 03:34 AM - Mark Abraham

I'll remove this. Ten years is long enough for something to sit broken and unfixed. Simplifying the update code would be very useful right now.

#12 - 01/09/2019 04:42 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1354](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: gromacs~master~I3d8b3c89ec0a65655aca30a35a722f4010a9f782

Gerrit URL: <https://gerrit.gromacs.org/8944>

#13 - 03/11/2020 12:06 AM - Pascal Merz

- Related to Feature #3426: Support acceleration in modular simulator added