GROMACS - Bug #1651

System drift with md-vv

12/03/2014 05:27 PM - Kristoffer Johansson

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<td>Difficulty:</td>
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Description

I am trying to simulate a solid molecular crystal but the system builds up translational movement when I use the md-vv integrator with or without pressure coupling. With the leapfrog integrator this never happens.

Without symmetry constraints translation is indeed possible with close to zero friction for a crystallographic (periodic) cell but the center of mass removal should prevent this from happening.

Setting comm-grps to a central part of the system have no effect which may suggest that the center-of-mass removal is broken for md-vv.

Associated revisions

Revision 08b2d506 - 10/12/2015 10:16 PM - Michael Shirts
Fix for lack of COM removal for md-vv

At some point, we seemed to have lost COM removal for md-vv! Currently, putting in into 4.6, will need to be merged forward. Replaces https://gerrit.gromacs.org/#/c/4467/, which was first checked into master, rather than 4.6.

Fixes #1651
Change-Id: I7776f4ad9b5b945f8294171f52b3581a04691250

History

#1 - 12/04/2014 01:55 AM - Mark Abraham
Thanks - can you upload a .tpr that reproduces the problem, please?

For now I would recommend you use leapfrog - the original and ongoing testing of the VV integrator is not as good as we'd like it to be.

#2 - 12/04/2014 09:43 AM - Kristoffer Johansson
- File az_verlet_gaff.tpr added

Yes I am currently using the leapfrog integrator but I would like to use vv for comparison with another software. The drift should be clear after ~10 ps.

Thanks.

#3 - 12/05/2014 04:29 AM - Michael Shirts
Kristoffer Johansson wrote:

Yes I am currently using the leapfrog integrator but I would like to use vv for comparison with another software. The drift should be clear after ~10 ps.

Thanks.

Can you say specifically what you observed? It makes it much easier to find if we have as much information as possible.

#4 - 12/05/2014 08:35 AM - Kristoffer Johansson
Hi Michael,

I'm not sure if you are referring to my research or the problem so I'll try to answer both.

Regarding my research, I am looking for a low temperature solid-state phase transition from monoclinic to triclinic (box angles change). The energy landscape is quite smooth here so it is not a problem for a leapfrog simulation and other methods to find the triclinic structure.

However, as soon as I switch to md-vv I only observe heavy translational drift (as if the box moves in the bulk crystal) which kills the pressure coupling and a phase transition becomes impossible (due to fixed box angles). Center-of-mass removal should prevent this drift but fails to do so with md-vv.

Hope it clear things up. Otherwise, I will be happy to provide more info/files.

Kristoffer

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Hi Mark, Michael and others,

Did you manage to reproduce the drift? If anyone can help I'm still very interested in a solution for this issue.

Kristoffer

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Gerrit received a related patchset '1' for Issue #1651.
Uploader: Michael Shirts (michael.shirts@virginia.edu)
Change-id: i2659fe9422af186c0c6d8de3af0c1b53cd3
Gerrit URL: https://gerrit.gromacs.org/4467

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Kristoffer Johansson wrote:

Hi Mark, Michael and others,

Did you manage to reproduce the drift? If anyone can help I'm still very interested in a solution for this issue.

Kristoffer

OK, found a situation to reproduce the drift. Can you try the commit I put in? Note that this fix is currently in master.

Or perhaps wait until other people have commented to not waste too much time.

If this works, we will include it in bug-fix backports.

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Gerrit received a related patchset '1' for Issue #1651.
Uploader: Michael Shirts (michael.shirts@virginia.edu)
Change-id: i7776f4ad9b5b945f294171f52b3581a04691250
Gerrit URL: https://gerrit.gromacs.org/4649

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- Status changed from New to In Progress

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Gerrit received a related patchset '1' for Issue #1651.
Uploader: Michael Shirts (michael.shirts@virginia.edu)
Change-id: i2659fe9422af186c0c6d8de3af0c1b53cd3
Gerrit URL: https://gerrit.gromacs.org/4467

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- Status changed from New to In Progress

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Applied in changeset 08b2d50643694c22c9ecf5ff08163cfdf86cdc10.

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- Status changed from In Progress to Resolved

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Files

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