Gromacs - Feature #871
request for trjconv -box to allow modification of only one or two dimensions
01/30/2012 05:16 PM - Chris Neale

Status: Closed
Priority: Low
Assignee:
Category:
Target version:

Description
It would be nice if trjconv -box -1 -1 14 would modify the z-axis to 14 nm but leave the x and y axes as they are. This could be useful in the following way. I have already made my own modified version of trjconv to do this, but other users may be interested.

I desire to center a lipid bilayer along z to make a movie or do analysis (e.g. g_density), but since the simulation used pressure coupling then the center of z actually changes from frame to frame. Thus, I could do this:

trjconv -center -pbc mol -f a.xtc -o b.xtc
trjconv -box -1 -1 20 -f b.xtc -o c.xtc  (note that I selected 20 as larger than the z in any frame)
trjconv -center -pbc none -f c.xtc -o d.xtc

In the second trjconv line above, I used -1 to indicate that I didn't want to change these dimensions.

I can now use d.xtc to make a movie in which the bilayer appears to remain with a constant Center of mass along z. (Note that this would still not really be true unless you have already modified trjconv -center to act on the center of mass instead of (max-min)/2 , but again I already have my own modified version of trjconv to do that.

Thank you,
Chris.

Associated revisions
Revision f99217aa - 05/24/2014 07:33 PM - Rossen Apostolov
Allow trjconv to keep some box dimensions unchanged.
Giving -1 to option box will preserve the original box size for the given dimension.
Fixes #871.
Change-Id: I339aedcf09da8ecb4eb8f32e8057f953a21e0f5f

History
#1 - 08/05/2012 01:00 AM - Roland Schulz
Chris Neale wrote:

I have already made my own modified version of trjconv to do this, but other users may be interested.

Could you upload your patch to gerrit.gromacs.org?
Sorry, I am not sure how to use gerrit.gromacs.org.

I replaced the following code that starts at line 1149 in gmx_trjconv.c from version 4.5.3:

```c
if (bSetBox) {
    /* generate new box */
    clear_mat(fr.box);
    for (m=0; m<DIM; m++)
        fr.box[m][m] = newbox[m];
}
```

with the new code:

```c
if (bSetBox) {
    /* generate new box */
    clear_mat(fr.box);
    for (m=0; m<DIM; m++)
        if(newbox[m]>=0)
            fr.box[m][m] = newbox[m];
}
```

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#3 - 05/23/2014 04:20 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #871.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: Ib761796ebc7a1fa77c894dbd447400ab09677417
Gerrit URL: https://gerrit.gromacs.org/3494

#4 - 05/23/2014 04:30 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #871.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: I339aedcf09da8ecb4eb8f32e8057f953a21e0f5f
Gerrit URL: https://gerrit.gromacs.org/3495

#5 - 05/23/2014 04:32 PM - Rossen Apostolov
applied to 5-0 since it's new feature

#6 - 05/25/2014 01:15 AM - Rossen Apostolov
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset f99217aa26a8d093613c84a607fe5e26000c3261b.

#7 - 06/17/2014 03:11 PM - Rossen Apostolov
- Status changed from Resolved to Closed