Hi users,

I was experimenting with using a hexagonal unit cell for a lipid membrane system by building a box with vectors A A C (i.e. two equivalent vectors in the xy plane and distinct z vector) and angles 90 90 60, which is correctly represented as hexagonal after converting with trjconv. I equilibrated this box and a system with the same number of lipids and water molecules but in a rectangular box. I confirmed that after equilibration the area per lipid for each system is the same, and after visualization confirmed that the hexagonal system and rectangular system occupied about the same area (of course subject to fluctuations).

For a hexagon and square of equivalent area, the minimum distance between periodic images should be 1/sqrt( sin 60 degrees) = ~1.075 times larger for the hexagon than in the square case if I worked out the geometry correctly. To test to make sure I had the correct new minimum distance, I ran g_mindist -pi with both a single atom and a single water molecule from the simulation box after resizing the Z axis to a large value, restricting the minimum distance between periodic images to only the xy plane. Surprisingly, the result came out as smaller than the equivalent minimum distance in the rectangular box, and was equal to the box vector B. Since in GMX box vectors are stored in the .gro file in a 3x3 matrix, the box[YY][YY] vector for an ab angle of 60 degrees was (correctly) equal to sin 60 * the A vector. However, the correct periodic distance should have been the A vector, which again was correctly ~1.075 * the box vector in the rectangular box by comparing the .gro files.

I believe that this is a small bug in g_mindist, and found the source: on lines 71 and 92 of gmx_mindist.c (version 4.6), the initial minimum distance is set based on the minimum of the box[XX][XX], box[YY][YY], and box[ZZ][ZZ] vectors. I think this is fine for rectangular boxes, but fails for triclinic boxes with box angles differing from 90 degrees. In my particular case of a hexagonal xy plane, the box[YY][YY] vector is shorter than the box[XX][XX] vector by a factor of sin 60, but this is not actual the shortest distance. Explicitly printing out the distances calculated between periodic images in the current version of the code for both a single atom and a water molecule confirms that the minimum distance is the box[XX][XX] vector.

A fix for this was substituting norm(box^0), norm(box^1), and norm(box^2) for the box[XX][XX] etc. vectors in line 71, as then the minimum was properly set.

I realize this is a bug that is unlikely to affect many users, but given the prevalence of non-rectangular boxes and the observation of previous complaints about mindist in the user list, I thought it would be good to report.
Associated revisions
Revision 90abdcf9 - 03/07/2013 07:26 PM - David van der Spoel
Fixes #1183 PBC bug in g_mindist
Fixes minimum size of the box if triclinic when checking the periodic image distance.
Change-id: f54cb593c42f791b6540147233c345069f84e2f33

History
#1 - 03/07/2013 07:16 PM - David van der Spoel
- Target version changed from 4.5.7 to 4.6.2

#2 - 03/07/2013 07:28 PM - David van der Spoel
- Target version changed from 4.6.2 to 4.5.7

Fixed in https://gerrit.gromacs.org/#/c/2221/

#3 - 04/29/2013 06:42 PM - Mark Abraham
- Status changed from New to Accepted
- Affected version set to 4.5.5

#4 - 04/29/2013 06:42 PM - Mark Abraham
- Status changed from Accepted to In Progress

#5 - 04/29/2013 06:42 PM - Mark Abraham
- Status changed from In Progress to Resolved

#6 - 12/16/2013 05:40 PM - Rossen Apostolov
- Status changed from Resolved to Closed