GROMACS - Bug #117

Reading back XTC trajectories yields "wrong" numbers and errors

11/09/2006 12:54 PM - Marc Baaden

Status:	Closed		
Priority:	High		
Assignee:	David van der Spoel		
Category:	mdrun		
Target version:	3.3.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

For analysis I wanted to check XTC files via gmxcheck prior to running other Gromacs tools.

Issue #1) I noticed that I don't always get the same numbers with version 3.3.1 as compared to version 3.2.1. Example:

WITH 3.3.1:
Reading frame 0 time 1.000

1. Atoms 3072
   Precision 0.001 (nm)
   Reading frame 9000 time 9001.000

Item #frames Timestep (ps)
Step 10000 1
Time 10000 1
Lambda 0
Coords 10000 1
Velocities 0
Forces 0
Box 10000 1

WITH 3.2.1:
Reading frame 0 time 1.000

1. Atoms 3072
   Precision 0.001 (nm)
   Last frame 9999 time 10000.000

Item #frames Timestep (ps)
Step 10000 1
Time 10000 1
Lambda 0
Coords 10000 1
Velocities 0
Forces 0
Box 10000 1

Issue #2) For some XTC trajectories I get continuous errors like:
[..]
Warning at frame 2691: coordinates for atom 1741 are large (1.517)
Warning at frame 2691: coordinates for atom 1741 are large (10.574)
Warning at frame 2691: coordinates for atom 1742 are large (-3.856)
[..]
whith 3.3.1 whereas there is no problem with 3.2.1. This is problematic because given the number of warnings that is output it takes an eternity to process the trajectory.

Concerning the first part of the bug, it's hopefully only a difference in the output/printing. But I would want to be sure that XTC reading in 3.3.1 can be trusted before doing all my analysis

with it :)

For the second part - as I couldn't find anything wrong with my trajectory - it would be good to be able to turn those warnings off.

History

#1 - 12/21/2006 11:08 PM - David van der Spoel

Hi Marc,

could you please upload an example? Maybe you can reduce the number of atoms if it's big.

#2 - 04/14/2007 02:55 PM - David van der Spoel

Marc,

can you please upload an example that gives this behavior? We have fixed bugs with xtc io in CVS, but there can also be bugs due to sick compilers, most notably gc 4.1.x

#3 - 04/14/2007 03:16 PM - Marc Baaden

Hi,
sorry for taking so long. The file is a little more than 100 MB. So I put it on a website at

http://www.shaman.ibpc.fr/gmxbug117.xtc

I hope this helps,
Marc

(In reply to comment #2)

> Marc,
>
> can you please upload an example that gives this behavior? We have fixed bugs with xtc io in CVS, but there can also be bugs due to sick compilers, most notably gc 4.1.x

#4 - 04/14/2007 03:28 PM - David van der Spoel

I've reproduced the counting, but this is a feature. Counting is now more or less logarithmic. How about the second problem? Do you have an example for this?

#5 - 04/14/2007 03:37 PM - Marc Baaden

(In reply to comment #4)

> I've reproduced the counting, but this is a feature. Counting is now more or less logarithmic. How about the second problem? Do you have an example for

this?

Ok. The second one is at
http://www.shaman.ibpc.fr/gmxbug117bis.xtc

#6 - 04/14/2007 04:35 PM - David van der Spoel

The message is because your box is zero. Maybe there should be an exemption for that. I've implemented that in CVS now.

Note that some analysis tools assume you have periodic boundary conditions.

#7 - 04/14/2007 05:50 PM - Marc Baaden

This was an implicit solvent simulation, so the absent box makes sense. Is this the expected behavior for "in vacuo" simulations, or should one provide a box even for those? (the trajectory was run with Amber/GB and then converted into Gromacs/XTC)

#8 - 04/14/2007 07:05 PM - David van der Spoel

It's not a problem, and as said I've put in a test for a zero box. You only have to look out for analysis tools that use periodicity. If you find one that gives you a wrong answer then please file a new bugzilla.