g_msd entering infinite loop when analyzing systems with xy periodicity.

When g_msd is applied to a system with xy periodicity, it stalls, as it continually tries to subtract a zero box vector.

I've added some files to reproduce the error (note that this is a 4.5.5 tpr), with command gmx_msd -s md3.tpr -f md3.xtc. Any group selection will lead to the error.

A proposed change (in 4.6 code) is as follows:

```c
for(m=DIM-1; m>=0; m--)
{
+    if (hbox[m] == 0)
+    {
+        continue;
+    }

    while(xcur[ind][m]-xprev[ind][m] <= hbox[m])
        rvec_inc(xcur[ind],box[m]);
    while(xcur[ind][m]-xprev[ind][m] > hbox[m])
        rvec_dec(xcur[ind],box[m]);
}
```

Associated revisions

Revision 9770ca5f - 04/02/2012 11:47 PM - Michael Shirts

Fixes problems with g_msd and g_energy

- Fixes a problem where g_msd will stall on reading a file with xy periodic boxes.
- Fixes a problem with gmxs_energy ignoring the -skip option.
  Was correct in 4.0.7, but was wrong by 4.5.5. Redmine issue #910

Change-Id: I4247a4bd1cf1ab15ea6157646c97452216a887aa

History

#1 - 03/29/2012 10:22 PM - Michael Shirts
   - Affected version - extra info set to all

#2 - 03/30/2012 02:57 PM - David van der Spoel
   I would suggest rather the following, seems that a - sign has gone missing.
for(m=DIM-1; m>=0; m--) {
  while(xcur[ind][m]-xprev[ind][m] <= -hbox[m])
    rvec_inc(xcur[ind],box[m]);
  while(xcur[ind][m]-xprev[ind][m] > hbox[m])
    rvec_dec(xcur[ind],box[m]);
}

#3 - 03/30/2012 08:09 PM - Michael Shirts
Yeah, that didn't show up well with formatting.  See proposed gerrit change for something more clear.

#4 - 04/12/2012 11:21 AM - Rossen Apostolov
Is that the patch?  https://gerrit.gromacs.org/#/c/643/
If so we can close this bug.

#5 - 04/12/2012 04:36 PM - Michael Shirts
Rossen Apostolov wrote:

  Is that the patch?  https://gerrit.gromacs.org/#/c/643/
  If so we can close this bug.

Yes, this is the patch.

#6 - 04/12/2012 04:37 PM - Michael Shirts
- Status changed from New to Closed

Files

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