GROMACS - Bug #332

Can not invert matrix, determinant =

05/28/2009 09:55 AM - Igor Leontyev

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

The error appears each time when I am trying to minimize structure
protein+internal+external solvent). The initial structure is far away
from the minimum (there are some large forces), but it should not be a
problem, isn't it? I am able to do minimization of the same system by
gmx3.3.1 version but gmx4.0.4 fails in both domain and particle decomposition mode. Below is the error message for particle decomposition mode (-pd) :

```
Reading file CcO_4hcav_3Dch_E242side_OH-_O2-_PM.tpr, VERSION 4.0.4
(single
precision)
Steepest Descents:
Tolerance (Fmax)   =  1.00000e+01
Number of steps    =        1000

--------------------------------------------------------
Program mdrun, VERSION 4.0.4
Source code file: ../../include/vec.h, line: 706

Fatal error:
Can not invert matrix, determinant =
```

Related issues:

Has duplicate GROMACS - Bug #331: Minimization error "Can not invert matrix, ...	**Closed**	**05/28/2009**

History

#1 - 05/28/2009 09:59 AM - Igor Leontyev

Created an attachment (id=378)
output and tpr-file

#2 - 05/28/2009 11:11 AM - Berk Hess

The problem was caused by frozen water molecules,
for which I set the inverse mass to 1e-30.
This is only a problem with energy minimization.
I have fixed it for 4.0.6 and 4.1.
I will attach the corrected csettle.c.

Berk

#3 - 05/28/2009 11:11 AM - Berk Hess

Created an attachment (id=379)
fixed src/mdlib/csettle.c

#5 - 05/29/2009 03:41 AM - Igor Leontyev

Guys, the minimization with corrected "csettle.c" seems to be running now, but output configuration as well as all intermediate configurations are the

same as the initial configuration. The goal of the minimization is the final structure, isn't it?

#6 - 05/29/2009 08:36 AM - Erik Lindahl

"invalid" means the bug report would be incorrect, so I've reopened it for you until Berk has a chance to comment. However, of you have frozen water molecules it seems quite reasonable that they shouldn't move ;-)

#7 - 05/29/2009 09:39 AM - Berk Hess

You froze the whole system, except for 166 atoms.
So only those 166 atoms will move, and these will move
very little, since they still interact with the rest
of the system which is completely frozen.

Berk

#8 - 05/29/2009 11:08 AM - Igor Leontyev

The system is quite complex and its dynamics depends on the quilaity of the minimized structure due to long relaxation time. The minimization should be done in few steps. On the first minimization step there are only few residues allowed to optimize positions. This step, however, results to a significant energy change. The output obtained with corrected "csettle.c" is given bellow. The energy change in -8e+07 Kj/mol should lead to a shift of the released atoms at least 1A. However, all atoms of the initial and final structures as well as all intermediate steps are identical.

```
Step           Time         Lambda
               0        0.00000        0.00000

Step           Time         Lambda
               1        1.00000        0.00000

Energies (kJ/mol)
           Bond           Angle    Proper Dih. Ryckaert-Bell.          LJ-14
    1.35230e+04    1.86168e+04    2.17942e+02    2.76666e+04    1.61981e+04
     Coulomb-14        LJ (SR)   Coulomb (SR) Position Rest.      Potential
    1.45153e+05    7.91281e+07   -6.45074e+05    7.98086e+00    7.87044e+07
 Pressure (bar)  Cons. rmsd ()
    5.88856e+33    1.89108e-06
```

#//-//-//-//-//-//

Steepest Descents converged to machine precision in 32 steps,
but did not reach the requested Fmax < 10.
Potential Energy = -2.8848306e+05
Maximum force = 4.2317715e+03 on atom 1035
Norm of force = 3.2447533e+01

#9 - 05/29/2009 12:21 PM - Berk Hess

I ran your simulation.
The energy indeed changes by 10^7.
But the input and output coordinates are NOT indentical.
Most of them are, since they are frozen.
But the few residues you leave free do move a bit.

Only one atom that lies on top of another can give an energy
change of 10^7 when it moves by even less than an Angstrom.

Berk

#10 - 05/29/2009 12:46 PM - Igor Leontyev

In my simulation the initial and final configurations are identical for all atoms with a machine precision. Could be the reason for this contradiction between your and mine results that my binary was created recompiling just the "csettle.c" object file with untouched other object files?

#11 - 05/29/2009 01:07 PM - Berk Hess

Ah, you are using 4.0.4.

I fixed a bug with energy minimization in serial (not parallel),
where are trajectory frames, except the last one would be identical
to the first one. I forgot to add this to the release notes.
You should upgrade to 4.0.5.

But the last frame and confout.gro should have the modified coordinates.

Berk

#12 - 05/29/2009 01:19 PM - Igor Leontyev

I used gmx 4.0.5 (parallel on 4 cpu) for this calculation.

#13 - 05/29/2009 02:38 PM - Berk Hess

Ah, I introduced a new bug in 4.0.5, which makes all energy minimization
output coordinates zero with particles decomposition.
I assume you use particle decomposition, since your system crashes
with domain decomposition.
Not running in parallel should work fine.
Or use my attached minimize.c.

Berk

#14 - 05/29/2009 02:40 PM - Berk Hess

Created an attachment (id=380)
fixed src/mdlib/minimize.c

Files

minimization.zip	987 KB	05/28/2009	Igor Leontyev
csettle.c	15.3 KB	05/28/2009	Berk Hess
minimize.c	82.9 KB	05/29/2009	Berk Hess