GROMACS - Bug #1596

mdrun crashes in specific free energy runs

09/16/2014 12:04 AM - Oleg Titov

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:	mdrun		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	5.0.1		

Description

mdrun crashes with segfault for a particular kind of systems.

I have PhBr molecule solvated by water. I'm trying to calculate free energy difference between PhBr molecule and PhBr molecule with atomic charges from PhF using thermodynamic integration. mdrun terminates with segfault after a couple of seconds after initialization finishes.

The same system without water (and without periodic boundaries) runs fine.

Input files attached.

Associated revisions

Revision 77356f36 - 12/08/2014 10:11 PM - Mark Abraham

Fix group-scheme bug with changing LJ parameters in FE

We don't optimize for the case when we have only changed one of charge or type, so the other vector must always be valid even when it is not changing. The logic of calling ewald_LRcorrection didn't do this correctly, perhaps because the construction logic in md2atoms was unclear.

Changed name, origin and logic for bFreeEnergy to bHaveChargeOrTypePerturbed to better reflect the correct usage and meaning. Avoided testing any pointers for NULL - we should use explicit control-flow constructs.

Fixes #1596

Change-Id: I61172681048075d3022bd6c4b781c6c9153eeadd

History

#1 - 09/24/2014 12:02 PM - Oleg Titov

I ran it with debugger and localized the bug.

For version 5.0.1
In file src/gromacs/mdlib/force.c
lines 540-557

```
ewald_LRcorrection(fr->excl_load[t], fr->excl_load[t+1],
                   cr, t, fr,
                   md->chargeA,
                   md->nChargePerturbed ? md->chargeB : NULL,
                   md->sqrt_c6A,
                   md->nTypePerturbed ? md->sqrt_c6B : NULL,
                   md->sigmaA,
                   md->nTypePerturbed ? md->sigmaB : NULL,
                   md->sigma3A,
                   md->nTypePerturbed ? md->sigma3B : NULL,
                   ir->cutoff_scheme != ecutsVERLET,
                   excl, x, bSB ? boxs : box, mu_tot,
```

```
                    ir->ewald_geometry,
                    ir->epsilon_surface,
                    fnv, *vir_q, *vir_lj,
                    Vcorrt_q, Vcorrt_lj,
                    lambda[efptCOUL], lambda[efptVDW],
                    dvdlt_q, dvdlt_lj);
```

There are two checks for free energy parameter presence in this function call: for El and for VdW.

At the same time in this function
In file src/gromacs/gmxlib/ewald_util.c
in function ewald_LRcorrection()
line 159

```
    gmx_bool    bFreeEnergy  = (chargeB != NULL);
```

The presence of free energy calculation is determined only by presence of valid pointer for charges of B and presence of VdW data for system B is never checked.
The crash happens in the same function at line 400, where VdW parameters for system B are requested (but null-pointer was passed during call, since VdW does not change in this system).

```
c6Bi = C6B[i];
```

#2 - 10/13/2014 12:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1596.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I61172681048075d3022bd6c4b781c6c9153eeadd
Gerrit URL: https://gerrit.gromacs.org/4148

#3 - 10/14/2014 02:12 PM - Mark Abraham

I've uploaded a fix, Oleg. It would be great if you could follow the link to Gerrit, download the latest patch and verify that it produces the correct answers. Then we can likely have it in 5.0.3

#4 - 10/17/2014 10:42 AM - Berk Hess

I have two, somewhat unrelated questions:

You are using the group cut-off scheme, maybe because you were also running vacuum calculations before. This bug does not affect the Verlet cut-off scheme. Don't you want to use the Verlet cut-off scheme?

The mdp file you attached does not use temperature coupling, but does use pressure coupling. Is this an error in preparing the files for redmine, or are you really running with these settings, which will not give reasonable results?

#5 - 10/22/2014 11:13 AM - Oleg Titov

Berk Hess wrote:

> I have two, somewhat unrelated questions:
>
> You are using the group cut-off scheme, maybe because you were also running vacuum calculations before. This bug does not affect the Verlet cut-off scheme. Don't you want to use the Verlet cut-off scheme?

I was using group cut-off scheme because manual for version 4.6.x stated that free energy perturbed non-bondeds were not implemented for Verlet. I didn't notice that this was changed in 5.0 release. Anyway, Verlet was tested while investigating issue #1442
http://redmine.gromacs.org/issues/1442#note-36 .

Berk Hess wrote:

> The mdp file you attached does not use temperature coupling, but does use pressure coupling. Is this an error in preparing the files for redmine, or are you really running with these settings, which will not give reasonable results?

I'm using sd integrator with ref-t=300 and tau-t=0.2, which should result in Langevein thermostat, so the results should be reasonable. Am I correct?

#6 - 10/23/2014 12:27 PM - Oleg Titov

Mark Abraham wrote:

> I've uploaded a fix, Oleg. It would be great if you could follow the link to Gerrit, download the latest patch and verify that it produces the correct answers. Then we can likely have it in 5.0.3

The answers look correct.

#7 - 06/16/2015 11:03 PM - Erik Lindahl

- Status changed from New to Resolved

#8 - 06/16/2015 11:03 PM - Erik Lindahl

- Status changed from Resolved to Closed

Files

phbr-phf.segfault.top	10.7 KB	09/15/2014	Oleg Titov
phbr.equil.segfault.gro	111 KB	09/15/2014	Oleg Titov
prod.0.5.segfault.mdp	1.41 KB	09/15/2014	Oleg Titov