Energy minimisation exits with floating point exception in ctests / silently moves over division by zero in normal runs.

01/30/2016 04:13 PM - Christian Blau

Description

Energy minimisation (steep and cg) with cutoff-scheme=verlet trigger division by zero in

calc_verletbuf.cpp:683

c_exp = std::exp(-rsh*rsh/(2*s2))/std::sqrt(2*M_PI);

...because s2=0, since temperature is not defined in energy minimisation thus the energy drift due to using the verlet cutoff scheme in energy minimization itself is not defined.

A suggested solution would be to never reset the rlist value in prepare_verlet_scheme in runner.cpp. However it is unclear what a reasonable generic rlist value would be. Enormous movement in the initial steps of energy minimisation would require large rlist values, but would waste lots of computer time in later stages with only minimal atom movement.

A code snippet that triggers the division by zero behaviour:

```
#include "gmxpre.h"
#include "config.h"
#include <gtest/gtest.h>
#include "gromacs/utility/stringutil.h"
#include "moduletest.h"

class EnminTest : public gmx::test::MdrunTestFixture,
                     public ::testing::WithParamInterface<const char *>
{
    public:
        void runTest(){
            std::string theMdpFile = gmx::formatString("integrator = steep
cutoff-scheme=verlet

");
            runner_.useStringAsMdpFile(theMdpFile);
            runner_.useTopGroAndNdxFromDatabase("argon12");
            runner_.callGrompp();
            runner_.callMdrun();
        }
};

TEST_F(EnminTest, Runs)
{
    runTest();
}
```
Using cutoff-scheme=group above yields no errors.

Associated revisions

Revision d0799464 - 02/03/2016 01:42 PM - Berk Hess
Fix mdrun removing Verlet buffer with EM

With energy minimization, grompp by default adds a Verlet buffer of 5% to rlist, but mdrun erroneously removed this. Added checks to prevent future misuse of calc_verlet_buffer_size.

Fixes #1896.

Change-Id: I4d16d48857494ebc6240842ed04571562de771b6

History

#1 - 02/01/2016 07:57 AM - Mark Abraham
- Description updated

#2 - 02/01/2016 08:10 AM - Mark Abraham
Yeah, there's some TODOs in src/programs/mdrun/tests/[grompp,moduletest].cpp that note that empty-ish .mdp files don't work in an acceptable way. That's because the responsibility the assumptions about when neighbour searching takes place are implemented in multiple places, and incompletely. EM looks like it does (DD and) NS every step if nstlist > 0, so buffer size should be zero when nstlist != 0, and given by rlist when nstlist == 0.

A better design would be that for the concept of an "integrator" that we had an abstract base type with methods to call for enforcing appropriate grompp-time and mdrun-time checks, another for coordinating management of buffer size, and another to call from the MD loop to manage the logic of when to re-partition and/or search.

#3 - 02/01/2016 10:55 AM - Berk Hess
When does this happen exactly?
I thought I properly took care of this. grompp adds 5% buffer to rlist without dynamics and mdrun should not increase nstlist, so we should never end up in the buffer estimation code. So I don't understand where this can go wrong.
We should add a GMX_RELEASE_ASSERT on EI_DYNAMICS(ir) in calc_verlet_buffer_size.

#4 - 02/01/2016 12:57 PM - Mark Abraham
Berk Hess wrote:

When does this happen exactly?

runner calls calc_verlet_buffer_size with -1 for reference_temperature, which leads to zero being used when ir->opts.ngtc is zero (or ref_t[0] is 0).

I thought I properly took care of this. grompp adds 5% buffer to rlist without dynamics and mdrun should not increase nstlist, so we should never end up in the buffer estimation code. So I don't understand where this can go wrong.
We should add a GMX_RELEASE_ASSERT on EI_DYNAMICS(ir) in calc_verlet_buffer_size.

#5 - 02/01/2016 01:42 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1896.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I4d16d48857494ebc6240842ed04571562de771b6
Gerrit URL: https://gerrit.gromacs.org/5602

#6 - 02/01/2016 01:43 PM - Berk Hess
- Status changed from New to Fix uploaded
- Assignee changed from Mark Abraham to Berk Hess
- Affected version - extra info set to 5.0, 5.1

The temperature is not the issue, calc_verlet_buffer_size should not be called.
I pushed a fix to 5.1, but we might want this in 5.0

#7 - 02/03/2016 01:45 PM - Berk Hess
- Status changed from Fix uploaded to Resolved
#8 - 04/03/2016 08:31 PM - Erik Lindahl
- Status changed from Resolved to Closed