

GROMACS - Bug #2871

grompp segfault when using annealing

02/26/2019 07:14 PM - Daniel Fragiadakis

Status:	Closed	
Priority:	Normal	
Assignee:	Paul Bauer	
Category:	preprocessing (pdb2gmx,grompp)	
Target version:	2019.2	
Affected version - extra info:		Difficulty: uncategorized
Affected version:	2019.2	

Description

grompp crashes with a SIGSEGV when reading an input file with the annealing-* commands making annealing unusable.

The culprit is src/gromacs/gmxpreprocess/readir.cpp

In revision fe1788de the way in which these commands are read were changed introducing an error in reading the floating point values for anneal-time and anneal-temp into opts.anneal_{time,temp}, they are being put in memory location 0. I think the problem is still there in all subsequent versions.

The following patch fixes the problem (I was not able to attach a file to this bug report)

```
diff --git a/src/gromacs/gmxpreprocess/readir.cpp b/src/gromacs/gmxpreprocess/readir.cpp
index f9b1f27e2..85e0393df 100644
--- a/src/gromacs/gmxpreprocess/readir.cpp
+++ b/src/gromacs/gmxpreprocess/readir.cpp
@@ -3396,8 +3396,18 @@ void do_index(const char* mdparin, const char *ndx,
                    simulatedAnnealingTemperatures.size(), k);
     }

-    convertReals(wi, simulatedAnnealingTimes, "anneal-time", ir->opts.anneal_time[i])
;
-    convertReals(wi, simulatedAnnealingTemperatures, "anneal-temp", ir->opts.anneal_t
emp[i]);
+    for (i = 0, k = 0; i < nr; i++)
+    {
+        std::vector<std::string> temps(simulatedAnnealingTemperatures.begin(),
+                                     simulatedAnnealingTemperatures.begin() + ir->o
pts.anneal_npoints[i]);
+        std::vector<std::string> times(simulatedAnnealingTimes.begin(),
+                                     simulatedAnnealingTimes.begin() + ir->opts.ann
eal_npoints[i]);
+        convertReals(wi, times, "anneal-time", ir->opts.anneal_time[i]);
+        convertReals(wi, temps, "anneal-temp", ir->opts.anneal_temp[i]);
+        k += ir->opts.anneal_npoints[i];
+    }

+    for (i = 0, k = 0; i < nr; i++)
+    {
+        for (j = 0; j < ir->opts.anneal_npoints[i]; j++)
```

Associated revisions

Revision 2404693f - 04/02/2019 03:18 PM - Paul Bauer

Fix simulated annealing and add test

Refs #2871

Change-Id: Ibde5226a664d3d4d5558477fdf9b81e1219a5295

Revision 9453ea8c - 04/04/2019 05:04 PM - Paul Bauer

Fix segmentation fault with simulated annealing

Fix contributed by Daniel Fragiadakis.

Fixes #2871

Change-Id: I237d49f9996eb2ae869d59e4c39a6c2d33c9ece7

History

#1 - 02/28/2019 10:33 AM - Paul Bauer

Hello, can you upload a minimal test case for this (you should be able to attach files here as well). I'm going to upload your patch, but we also need to be able to test it.

#2 - 02/28/2019 10:42 AM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#2871](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~release-2019~I237d49f9996eb2ae869d59e4c39a6c2d33c9ece7

Gerrit URL: <https://gerrit.gromacs.org/9247>

#3 - 03/19/2019 10:46 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2871](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~master~Ibde5226a664d3d4d5558477fd9b81e1219a5295

Gerrit URL: <https://gerrit.gromacs.org/9332>

#4 - 04/01/2019 12:06 PM - Mark Abraham

- Description updated

- Assignee changed from Daniel Fragiadakis to Paul Bauer

#5 - 04/01/2019 12:07 PM - Mark Abraham

- Status changed from New to Fix uploaded

#6 - 04/04/2019 05:15 PM - Paul Bauer

- Status changed from Fix uploaded to Resolved

Applied in changeset [9453ea8cfa76d999a3bb9659a4916519f012](#).

#7 - 04/05/2019 04:47 PM - Paul Bauer

- Status changed from Resolved to Closed