## Gromacs - Bug #1393

**genbox segfaults with after verlet scheme become default**

12/05/2013 07:47 AM - Alexey Shvetsov

<table>
<thead>
<tr>
<th>Status</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority</td>
<td>High</td>
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<tr>
<td>Assignee</td>
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<td>Category</td>
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<td>Target version</td>
<td>5.0</td>
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<tr>
<td>Affected version - extra info</td>
<td>git master</td>
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### Description

Program received signal SIGSEGV, Segmentation fault.

init_nb_verlet (nbpu_opt=0x0, cr=0x8a5bf0, fr=0x8a54d0, ir=0x681b60, nb_verlet=0x8a56d0, fp=0x7ffff54532a0)

<__I0_2_1__stdout_>) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:1976

pick_nbxn_resources(cr, fr->hwininfo, (gdb) bt

#0 init_nb_verlet (nbpu_opt=0x0, cr=0x8a5bf0, fr=0x8a54d0, ir=0x681b60, nb_verlet=0x8a56d0, fp=0x7ffff54532a0)

<__I0_2_1__stdout_>) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:1976

#1 init_forcerec (fp=0x7ffff54532a0 <__I0_2_1__stdout_>, oenv=oenv@entry=0x674eb0, fr=<optimized out>, fcd=fcd@entry=0x0, ir=ir@entry=0x681b60, mtop=mtop@entry=0x681070, cr=cr@entry=0x8a5bf0, box=box@entry=0x7fffff90f0, tabfn=tabfn@entry=0x0, tabafn=tabafn@entry=0x0, tabbfn=tabbfn@entry=0x0, nbpu_opt=nbpu_opt@entry=0x0, bNoSolvOpt=bNoSolvOpt@entry=0x0, print_force=print_force@entry=0x0) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:2986

#2 0x00007fffff65982f in do_nsgrid (fp=0x7fffff54532a0 <__I0_2_1__stdout_>, bVerbose=bVerbose@entry=1, box=box@entry=0x7fffff90f0, x=x@entry=0x7fffff90f0, rlong=rlong@entry=0x307799995, oenv=oenv@entry=0x674eb0) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/addconf.c:297

#3 0x00007fffff7980ef in add_conf (atoms=0x7fffffffffa50, x=0x7fffffffff970, v=0x0, r=0x7fffffffff968, bSrenew=1, ePBC=1, box=0x7fffff90f0, at taxes_=0x677c80, x Solvl0=0x7fffff805010, v solv=0x682e0, bVerbose=1, rshell=0, max sol=0, oenv=0x674eb0) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/addconf.c:411

#4 0x00007fffff706dfdf in add_sol (oenv=0x674eb0, max sol=0, rshell=0, residues added=synthetic pointer, atoms added=synthetic pointer at taxes_=0.569999999, r scale=0.104999997, at taxes_=0.676340, box=0x7fffffffff90f0, ePBC=1, x=0x7fffffffff970, oenv=0x7fffffffff968, at taxes_=0.569999999, syn optimized out) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/gmx_genbox.cpp:632

#5 gmx_genbox (argc=1, argv=optimized out) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/gmx_genbox.cpp:1047

#6 0x00007fffff642e5 in gmx:CommandLineModuleManager::run () at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/gmx_genbox.cpp:1047

#7 0x000000000041153c in main (argc=8, argv=0x7fffffd040, arg=8, argv=0x7fffffd158) at /home/alexxy/Develop/gromacs/src/programs/gmx/gmx.cpp:58 (gdb)

### steps to reproduce

get attached file
prepare system
pdx2gmx -f speptide.pdb -o speptide.pdb -f speptide -f amber99sb-ildn -water tip3p
edtconf -f speptide.gro -o speptide.boxed -d 2 -princ -c

and run genbox

### Related issues:

- Related to Gromacs - Bug #1499: Memory bug in solvate - Closed 05/11/2014

### Associated revisions

11/25/2015
Revision 96fb3956 - 02/03/2014 05:47 AM - Mark Abraham

Add hack to fix genbox

Using a lighter-weight neighbour search is a better idea, but this bug needs fixing right now.

Add integration tests for major functionality of genbox. These pass only with the fix in this patch. These are not the most glorious tests, but as demonstrated by this bug, "does not segfault in routine workflows" is useful.

Fixes #1393

Change-Id: i5628f52cd91dcbe64d6e690b2e611e524f450972

History

#1 - 12/06/2013 08:16 AM - David van der Spoel
This might be worked around by using the neighborsearching that is in the analysis framework. Since that is much easier to use it will prevent errors due to incomplete initialization of the gromacs core.

#2 - 02/01/2014 10:46 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1393.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: i5628f52cd91dcbe64d6e690b2e611e524f450972
Gerrit URL: https://gerrit.gromacs.org/3060

#3 - 02/06/2014 12:58 PM - Mark Abraham
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset 96fb3956baa3b8c1956a0079f7c78152f581639.

#4 - 02/06/2014 10:27 PM - Rossen Apostolov
- Status changed from Resolved to Closed

#5 - 05/12/2014 11:31 AM - Mark Abraham
- Related to Bug #1499: Memory bug in solvate added

Files
speptide.pdb  11.6 KB  12/05/2013  Alexey Shvetsov