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>
<td></td>
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<tr>
<td>Category:</td>
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<tr>
<td>Target version:</td>
<td>5.0</td>
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<td>Affected version:</td>
<td>git master</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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</tbody>
</table>

**Description**

genbox segfaults since verlet scheme became default one

Program received signal SIGSEGV, Segmentation fault.

```
init_nb_verlet (nbpu_opt=0x0, cr=0x8a5bf0, fr=0x8a54d0, ir=0x681b60, nb_verlet=0x8a56d0, fp=0x7ffff54532a0
<_IO_2_1_stdout_>) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:1976
1976        pick_nbxn_resources(cr, fr->hwinfo, (gdb) bt
#0  init_nb_verlet (nbpu_opt=0x0, cr=0x8a5bf0, fr=0x8a54d0, ir=0x681b60, nb_verlet=0x8a56d0, fp=0x7ffff54532a0
<_IO_2_1_stdout_>) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:1976
#1  init_forcerec (fp=0x7ffff54532a0 <_IO_2_1_stdio_>, oenv=oenv@entry=0x674eb0, fr=<optimized out>, fcd=fcd@entry=0x0, ir=ir@entry=0x681b60, box=box@entry=0x7fffffa9c0, tabfn=tabfn@entry=0x0, tabafn=tabafn@entry=0x0, tabbfn=tabbfn@entry=0x0, tabbfn=tabbfn@entry=0x0, nbpu_opt=nbpu_opt@entry=0x0, bNoSolvOpt=bNoSolvOpt@entry=1, print_force=print_force@entry=-1) at /home/alexxy/Develop/gromacs/src/gromacs/mdlib/forcerec.c:2986
#2  0x00007fffff88eef9 in do_nsgrid (fp=0x7ffff54532a0 <_IO_2_1_stdio_>, bVerbose=bVerbose@entry=1, box=box@entry=0x7fffffa9c0, x=x@entry=0x7fffff48e2010, atoms=atoms@entry=0x677cd0, rlong=rlong@entry=0.307799995, oenv=oenv@entry=0x674eb0) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/addconf.c:297
#3  0x00007fffff8f6ec in add_conf (atoms=0x7fffffffaa50, x=0x7fffffffa970, v=0x0, r=0x7fffffa968, bSnewew=1, ePBC=-1, box=0x7fffffa9c0, binsert=0, atoms_solvt=0x677c80, x_solvt=0x7fffff7e05010, v_solvt=0x0, r_solvt=0x682e0, bVerbose=1, rshell=0, max_sol=0, oenv=0x674eb0) at /home/alexxy/Develop/gromacs/src/gromacs/gmxana/addconf.c:411
#4  0x00007fffff70649df in add_solv (oenv=0x674eb0, max_sol=0, rshell=0, residues_added=<synthetic pointer>, atoms_added=<synthetic pointer>, r_scale=0.569999993, r_distance=0.104999997, aps=0x676340, box=0x7fffffa9c0, ePBC=-1, r=0x7fffffa968, v=0x0, x=0x7fffffffa970, atoms=0x7fffffa50, fn=<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  0x00007ffffe42e5 in gmx::CommandLineModuleManager::run (this=0x7fffff0d40, argc=8, argv=0x7fffff1d58) at /home/alexxy/Develop/gromacs/src/gromacs/commandline/cmdlinemodulemanager.cpp:1327
#7  0x0000000000041153c in main (argc=8, argv=0x7fffff1d58) at /home/alexxy/Develop/gromacs/src/programs/gmx/gmx.cpp:58 (gdb)
```

steps to reproduce

1. get attached file
2. prepare system
3. pdb2gmx -f speptide.pdb -o speptide.pdb -p speptide -ff amber99sb-ildn -water tip3p
4. editconf -f speptide.gro -o speptide.boxed -d 2 -princ -c
5. and run genbox
6. genbox -cp speptide.boxed.gro -cs -o speptide.solvated -p speptide.top

**Related issues:**

- Related to GROMACS - Bug #1499: Memory bug in solvate

Closed 05/11/2014

03/20/2020
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: I5628f52cd91dcbe64de6e690b2e611e524f450972

History

#1 - 12/06/2013 08:16 AM - David van der Spoel
This might be worked around by using the neighboursearching 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: i5628f52cd91dcbe64de6e690b2e611e524f450972
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 96fb3956baa3b8c1956ae079fd7c78152f581639.

#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