

## GROMACS - Bug #970

### segfault in tip4pflex test case

07/13/2012 09:58 PM - Christoph Junghans

<b>Status:</b>	Closed	
<b>Priority:</b>	High	
<b>Assignee:</b>	Berk Hess	
<b>Category:</b>	mdrun	
<b>Target version:</b>	4.6	
<b>Affected version - extra info:</b>	51f2f97d29cb6e57851a4b7ff037068c355e8b72	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>		

#### Description

This happens in 50% of the cases for the tip4p{,flex} examples on my x86 laptop (Intel Core 2 Duo, T7100, gcc with gcc (Gentoo 4.6.3 p1.0, pie-0.5.1) 4.6.3).

```
Program received signal SIGSEGV, Segmentation fault.
sse_mask_init (order=4, work=0xb5313ce8) at
/home/christoph/votca/src/gromacs/src/mdlib/pme.c:2881
2881     work->mask_SSE0[of] = _mm_loadu_ps(tmp);
(gdb) bt
#0  sse_mask_init (order=4, work=0xb5313ce8) at
/home/christoph/votca/src/gromacs/src/mdlib/pme.c:2881
#1  gmw_pme_init (pmedata=0xb530676c, cr=0xb5303ab8, nnodes_major=1,
nnodes_minor=2, ir=0x807e9b8,
homenr=3072, bFreeEnergy=0, bReproducible=0, nthread=1)
at /home/christoph/votca/src/gromacs/src/mdlib/pme.c:3164
#2  0x08054732 in mdrunner (nthreads_requested=0, fplog=0x807e378,
cr=0xb5303ab8, nfile=36, fnm=0xbfffe1a8,
oenv=0x807e2d8, bVerbose=0, bCompact=1, nstglobalcomm=-1,
ddxyz=0xbfffe7e4, dd_node_order=1, rdd=0,
rconstr=0, dddlb_opt=0x807238d "auto", dlb_scale=0.800000012,
ddcsx=0x0, ddcsy=0x0, ddcsz=0x0,
nstepout=100, resetstep=-1, nmultisim=0, repl_ex_nst=0,
repl_ex_nex=0, repl_ex_seed=-1, pforce=-1,
cpt_period=15, max_hours=-1, deviceOptions=0x80704ba "", Flags=7168)
at /home/christoph/votca/src/gromacs/src/kernel/runner.c:841
#3  0x0804e581 in main (argc=1, argv=0xbfffe9f4) at
/home/christoph/votca/src/gromacs/src/kernel/mdrun.c:685
```

Roland's 1st clue was that the segfault on SSE intrinsic mean that the data isn't aligned sufficiently, so:  
(gdb) print &tmp  
\$1 = (float (\*)[8]) 0xbfffc50  
but it not the case.

#### Associated revisions

##### Revision 3ee63ecf - 07/17/2012 06:50 PM - Berk Hess

fix a segfault in sse\_mask\_init

- work array was unaligned in some cases
- fixes #970

Change-Id: I1b474019bf93e6ef6f7cc935aa3f73f2597a91a8

##### Revision 3ee63ecf - 07/17/2012 06:50 PM - Berk Hess

fix a segfault in sse\_mask\_init

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## History

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### #1 - 07/16/2012 05:37 PM - Berk Hess

What are the tip4p{,flex} examples exactly?  
Have you run valgrind on this?

### #2 - 07/16/2012 05:43 PM - Berk Hess

I think this is an alignment issue.  
tmp doesn't need to be aligned, we are using loadu.  
But mask\_SSE0 should be aligned and I think putting an SSE register in a struct does not guarantee this.

### #3 - 07/16/2012 05:55 PM - Berk Hess

- File pme.c added

Please try the patched version of pme.c attached.

### #4 - 07/16/2012 05:56 PM - Christoph Junghans

Berk Hess wrote:

What are the tip4p{,flex} examples exactly?

These are two "complex" tests for the regressionstests repository.

Have you run valgrind on this?

No, just gdb, but if you tell me, what exactly you need I can provide it.

### #5 - 07/16/2012 05:58 PM - Christoph Junghans

Berk Hess wrote:

Please try the patched version of pme.c attached.

It happens on my machine at home, I will test and come back.

### #6 - 07/26/2012 01:31 AM - Roland Schulz

- Status changed from New to Closed

## Files

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pme.c	130 KB	07/16/2012	Berk Hess
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